Community Project for Accelerator Science and Simulation

Field Work Proposal
Cover Page

Particle accelerators are critical to scientific discovery both nationally and worldwide. The development and optimization of accelerators are essential for advancing our understanding of the fundamental properties of matter, energy, space and time. In the past ten years, the SciDAC program has produced accelerator modeling tools using high-performance computing (HPC), and these have been employed to tackle some of the most difficult accelerator science problems. These codes obtain good scalability and parallel performance efficiency to several tens of thousands of processors.
In the next decade, the high energy physics (HEP) community will explore the intensity frontier of particle physics by designing high intensity proton sources for neutrino physics and rare process searches, as well as high intensity muon sources for neutrino physics. It will also be exploring the energy frontier of particle physics by operating the Large Hadron Collider, developing novel concepts and technologies necessary for the design of the next lepton collider, and undertaking R&D for new acceleration technologies. The proposed project will develop the HPC tools and applications necessary to design Project X, the proposed proton driver at Fermilab, the next lepton collider, with either electron or muon beams, and with either conventional or advanced (plasma, dielectric structure) acceleration technology, and perform R&D at FACET and BELLA. It will build on the successful HPC accelerator modeling tools developed under SciDAC1 and SciDAC2 and augment and evolve them so they can drive and support the accelerator science required for the above applications.

Victoria White Associate Director for Computing & CIO	Date

U. S. DEPARTMENT OF ENERGY
WORK PROPOSAL

1. Work Proposal Number: **FNAL-11-xxxx**	2. Revision Number: **1.0**	3. Date Prepared: **January-3-2012**

4. Work Proposal Title: **Community Project for Accelerator Science and Simulation - HEP**	5. Budget and Reporting Code: KA140103
6. Work Proposal Term: **3 Years**	
7. Name (Last, First, MI) and Phone Number of the Headquarters Program Manager: **Dr. Lali Chatterjee, 301-903-0435**	Headquarters Organization: **Office of Science - SC**
9. DOE Field Organization Work Proposal Reviewer:	10. DOE Field Organization: **Fermi Site Office (FSO)**
11. Contractor Work Proposal Manager: **Panagiotis Spentzouris, 630-840-3266**	12. Contractor Name: **Fermi National Accelerator Laboratory Pier J. Oddone, Director F. R. A. : Contract Number DE-AC02-07CH11359**

13.

Particle accelerators are critical to scientific discovery both nationally and worldwide. The development and optimization of accelerators are essential for advancing our understanding of the fundamental properties of matter, energy, space and time. In the past ten years, the SciDAC program has produced accelerator modeling tools using high-performance computing (HPC), and these have been employed to tackle some of the most difficult accelerator science problems. These codes obtain good scalability and parallel performance efficiency to several tens of thousands of processors.
In the next decade, the high energy physics (HEP) community will explore the intensity frontier of particle physics by designing high intensity proton sources for neutrino physics and rare process searches, as well as high intensity muon sources for neutrino physics. It will also be exploring the energy frontier of particle physics by operating the Large Hadron Collider, developing novel concepts and technologies necessary for the design of the next lepton collider, and undertaking R&D for new acceleration technologies. The proposed project will develop the HPC tools and applications necessary to design Project X, the proposed proton driver at Fermilab, the next lepton collider, with either electron or muon beams, and with either conventional or advanced (plasma, dielectric structure) acceleration technology, and perform R&D at FACET and BELLA. It will build on the successful HPC accelerator modeling tools developed under SciDAC1 and SciDAC2 and augment and evolve them so they can drive and support the accelerator science required for the above applications.

14.	15. DOE Field Organization Official:
(Signature) *Pier J. Oddone* *(Date)*	*(Signature)* *(Date)*

16. Detail Attachments (See Specific Attachments)

- [ ] a. Facility Requirements
- [ ] b. Publications
- [ ] c. Purpose (mandatory)
- [ ] d. Background
- [ ] e. Approach
- [ ] f. Technical Progress
- [ ] g. Future Accomplishments
- [ ] h. Relationship to Other Projects
- [ ] i. NEPA Requirements
- [ ] j. Milestones
- [ ] k. Deliverables
- [ ] l. Performance Measures/ Expectations
- [ ] m. ES&H Considerations
- [ ] n. Human/Animal Subjects
- [ ] o. Security Requirements
- [ ] p. Other (specify)

WORK PROPOSAL REQUIREMENTS FOR OPERATING/EQUIPMENT OBLIGATIONS AND COSTS

CONTRACTOR NAME	WORK PROPOSAL NO.	REV. NO.:	DATE PREPARED
Fermilab	FNAL-11-xxxx	1.0	January-3-2012

	Prior Years	BY-1	Budget Year (BY)		BY+1	BY+2	Total to Complete
17. Staffing (staff years)			Request	Authorized			
a. Scientific			0.46		0.3	0.3	
b. Other Direct			0.64		0.8	0.8	
c. Total Direct			1.10		1.1	1.1	
18. Operating Expense							
a. Total Obligations							
b. Total Costs							
19. Equipment							
a. Equipment Obligations							
b. Equipment Costs							

20. Milestone Schedule Proposed Authorized

The milestone schedule is detailed in the Fermilab statement of work, in Appendix B of the proposal.

21. Reporting Requirements (Description)

Reporting for the project is detailed in the management section of the proposal. The Program Director (PD) serves as the principal contact with the DOE. Each institution receiving funds under this grant has a co-PI. The co-PIs assume responsibility for the work carried out at their institutions and submit quarterly reports to the PD. The Executivr Board (EB) holds regular (bi-weekly) meetings, chaired by the PD to discuss, monitor, and coordinate project activities. The PD will submit progress reports to DOE semi-annually and is responsible for tracking the overall grant budget. The EB will organize full collaboration meetings prior to the submission of project reports.

U. S. DEPARTMENT OF ENERGY
WORK PROPOSAL

1. Work Proposal Number: **FNAL-11-xxxx**	2. Revision Number: 1.0	3. Date Prepared: **January-3-2012**

4. Work Proposal Title: **Community Project for Accelerator Science and Simulation - ASCR**	5. Budget and Reporting Code KA140103
6. Work Proposal Term: 3 years	
7. Name (Last, First, MI) and Phone Number of the Headquarters Program Manager **Dr. Randall Laviolette, 301-903-5195**	Headquarters Organization **Office of Science - SC**
9. DOE Field Organization Work Proposal Reviewer:	10. DOE Field Organization: **Fermi Site Office (FSO)**
11. Contractor Work Proposal Manager: **Panagiotis Spentzouris, 630-840-3266**	12. Contractor Name: **Fermi National Accelerator Laboratory** **Pier J. Oddone, Director** **F. R. A. : Contract Number DE-AC02-07CH11359**

13.

Particle accelerators are critical to scientific discovery both nationally and worldwide. The development and optimization of accelerators are essential for advancing our understanding of the fundamental properties of matter, energy, space and time. In the past ten years, the SciDAC program has produced accelerator modeling tools using high-performance computing (HPC), and these have been employed to tackle some of the most difficult accelerator science problems. These codes obtain good scalability and parallel performance efficiency to several tens of thousands of processors.
In the next decade, the high energy physics (HEP) community will explore the intensity frontier of particle physics by designing high intensity proton sources for neutrino physics and rare process searches, as well as high intensity muon sources for neutrino physics. It will also be exploring the energy frontier of particle physics by operating the Large Hadron Collider, developing novel concepts and technologies necessary for the design of the next lepton collider, and undertaking R&D for new acceleration technologies. The proposed project will develop the HPC tools and applications necessary to design Project X, the proposed proton driver at Fermilab, the next lepton collider, with either electron or muon beams, and with either conventional or advanced (plasma, dielectric structure) acceleration technology, and perform R&D at FACET and BELLA. It will build on the successful HPC accelerator modeling tools developed under SciDAC1 and SciDAC2 and augment and evolve them so they can drive and support the accelerator science required for the above applications.

14.	15. DOE Field Organization Official:
(Signature) *Pier J. Oddone* *(Date)*	*(Signature)* *(Date)*

16. Detail Attachments (See Specific Attachments)

☐ a. Facility Requirements	☐ g. Future Accomplishments	☐ m. ES&H Considerations
☐ b. Publications	☐ h. Relationship to Other Projects	☐ n. Human/Animal Subjects
☐ c. Purpose (mandatory)	☐ i. NEPA Requirements	☐ o. Security Requirements
☐ d. Background	☐ j. Milestones	☐ p. Other (specify)
☐ e. Approach	☐ k. Deliverables	
☐ f. Technical Progress	☐ l. Performance Measures/ Expectations	

WORK PROPOSAL REQUIREMENTS FOR OPERATING/EQUIPMENT OBLIGATIONS AND COSTS

CONTRACTOR NAME	WORK PROPOSAL NO.	REV. NO.:	DATE PREPARED
Fermilab	FNAL-11-xxxx	1.0	January-3-2012

	Prior Years	BY-1	Budget Year (BY)		BY+1	BY+2	Total to Complete
17. Staffing (staff years)			Request	Authorized			
					0.15	0.15	
a. Scientific			0.15		0.60	0.60	
b. Other Direct			0.60		0.75	0.75	
c. Total Direct			0.75				
18. Operating Expense							
a. Total Obligations							
b. Total Costs							
19. Equipment							
a. Equipment Obligations							
b. Equipment Costs							

20. Milestone Schedule Proposec Authorized

```
The milestone schedule is detailed in the Fermilab
statement of work, in Appendix B of the proposal.
```

21. Reporting Requirements (Description)

Reporting for the project is detailed in the management section of the proposal. The Program Director (PD) serves as the principal contact with the DOE. Each institution receiving funds under this grant has a co-PI. The co-PIs assume responsibility for the work carried out at their institutions and submit quarterly reports to the PD. The Executivr Board (EB) holds regular (bi-weekly) meetings, chaired by the PD to discuss, monitor, and coordinate project activities. The PD will submit progress reports to DOE semi-annually and is responsible for tracking the overall grant budget. The EB will organize full collaboration meetings prior to the submission of project reports.

Cover Page

Title of Proposed Project:

Community Project for Accelerator Science and Simulation

Office of Science Announcement Title/#:

FNAL 11-580 – Office of Science

Principal Investigator(s):

Panagiotis Spentzouris
P.O. Box 500, MS203
Batavia, IL 60510-5011
spentz@fnal.gov 630-840-3266

Official signing for Fermi National Accelerator Laboratory:

Dr. Piermaria J. Oddone, Laboratory Director
pjoddone@fnal.gov
630-840-3211 (phone), 630-840-2900 (fax)
Fermi National Accelerator Laboratory

Requested funding for Project; KA14103

Partnership	Year 1 (HEP/ASCR)	Year 2 (HEP/ASCR)	Year 3 (HEP/ASCR)	Total (HEP/ASCR)
FNAL - Panagiotis Spentzouris	325/115	332/117.3	341.4/120.8	998.4/353.1
ANL - Boyana R. Norris	0/145	0/147.9	0/152.3	0/445.2
LBNL - Jean-Luc Vay/Esmond Ng	220/425	225/434	231/447	676/1,306
SLAC - Dr. Cho Ng	255/174.8	260.9/178.9	270/185.1	786/538.8
Tech-X - John R. Cary	270/145	275.3/147.9	283.5/152.3	828.8/445.3
UCLA - Warren Mori	225/145	229.5/147.9	236.4/152.3	690.9/445.2
UT-Austin - Ernesto Prudencio	0/119.6	0/120	0/123	0/362.7
Total	1,295/1,269.4	1,332.8/1,294	1,362.4/1,333	3,980.2/3,896.5

Duration of Entire Project Period: 3 Years

Use of human subjects in proposed project: No
Use of vertebrate animals in proposed project: No

Signature of PI, Date of Signature:

____

Signature of Official, Date of Signature:

____

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

Year 1 Funding Proposal

ORGANIZATION: FERMILAB Computing Division — **Budget Page No:** 1

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR: Panagiotis Spentzouris — Requested Duration: 12 (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Panagiotis Spentzouris, Scientist	3.60			$35,850	
2. Chong-Shik Park, Research Associate	1.60			$15,933	
3. James Amundson, Computational Physics Developer	0.40			$3,983	
4. Alex Macridin, Computational Physics Developer	1.60			$15,933	
5. Paul Lebrun, Scientist	2.00			$19,917	
6. Eric Stern, Computational Physics Developer	2.80			$27,883	
7. (6) TOTAL SENIOR PERSONNEL (1-6)	12.00			$119,500	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. (1) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)	1.00			$4,296	
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$123,796	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$70,861	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$194,657	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					
H. TOTAL DIRECT COSTS (A THROUGH G)				$194,657	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 11.6% on Travel expense and 18.03% on all other M&S expense; 66.96% on SWF					
TOTAL INDIRECT COSTS				$130,342	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$325,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$325,000	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

Year 2 Funding Proposal

ORGANIZATION FERMILAB Computing Division				**Budget Page No:**	2
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Panagiotis Spentzouris				Requested Duration:	12 (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Panagiotis Spentzouris, Scientist	1.20			$12,428	
2. Chong-Shik Park, Research Associate	1.60			$16,571	
3. James Amundson, Computational Physics Developer	2.60			$26,927	
4. Alex Macridin, Computational Physics Developer	1.60			$16,571	
5. Paul Lebrun, Scientist	2.00			$20,713	
6. Eric Stern, Computational Physics Developer	2.80			$28,999	
7. (6) TOTAL SENIOR PERSONNEL (1-6)	11.80			$122,209	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES				$0	
2. (1) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)	1.00			$4,254	
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$126,463	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$72,387	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$198,850	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$0	
2. FOREIGN					
TOTAL TRAVEL				$0	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS (0) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$0	
H. TOTAL DIRECT COSTS (A THROUGH G)				$198,850	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 11.6% on Travel expense and 18.03% on all other M&S expense; 66.96% on SWF					
TOTAL INDIRECT COSTS				$133,150	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$332,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$332,000	

DOE F 4620.1 (04-93) All Other Editions Are Obsolete	U.S. Department of Energy **Budget Page** (See reverse for Instructions)	OMB Control No. 1910-1400 OMB Burden Disclosure Statement on Reverse

Year 3 Funding Proposal

ORGANIZATION FERMILAB Computing Division				**Budget Page No:** 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Panagiotis Spentzouris				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applpicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. Panagiotis Spentzouris, Scientist	1.20			$12,860	
2. Chong-Shik Park, Research Associate	1.60			$17,147	
3. James Amundson, Computational Physics Developer	2.60			$27,864	
4. Alex Macridin, Computational Physics Developer	1.60			$17,147	
5. Paul Lebrun, Scientist	2.00			$21,434	
6. Eric Stern, Computational Physics Developer	2.80			$30,007	
				$0	
7. (6) TOTAL SENIOR PERSONNEL (1-6)	11.80			$126,459	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES Graduate Student				$0	
2. (1) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)	1.00			$3,585	
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$130,043	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$74,437	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$204,480	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$0	
2. FOREIGN					
TOTAL TRAVEL				$0	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS (0) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$0	
H. TOTAL DIRECT COSTS (A THROUGH G)				$204,480	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 11.6% on Travel expense and 18.03% on all other M&S expense; 66.96% on SWF					
TOTAL INDIRECT COSTS				$136,920	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$341,400	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$341,400	

DOE F 4620.1	**U.S. Department of Energy**	OMB Control No.
(04-93)	**Budget Page**	1910-1400
All Other Editions Are Obsolete	(See reverse for Instructions)	OMB Burden Disclosure Statement on Reverse

TOTAL of 3 Year Funding Proposal

ORGANIZATION				**Budget Page No:**	4
FERMILAB Computing Division					
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR				Requested Duration:	36 (Months)
Panagiotis Spentzouris					

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Panagiotis Spentzouris, Scientist	6.00			$61,138	
2. Chong-Shik Park, Research Associate	4.80			$49,651	
3. James Amundson, Computational Physics Developer	5.60			$58,774	
4. Alex Macridin, Computational Physics Developer	4.80			$49,651	
5. Paul Lebrun, Scientist	6.00			$62,064	
6. Eric Stern, Computational Physics Developer	8.40			$86,889	
7. (6) TOTAL SENIOR PERSONNEL (1-6)	35.60			$368,168	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES	0.00			$0	
2. (1) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)	3.00			$12,135	
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$380,302	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$217,685	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$597,988	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$0	
2. FOREIGN				$0	
TOTAL TRAVEL				$0	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$0	
H. TOTAL DIRECT COSTS (A THROUGH G)				$597,988	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 11.6% on Travel expense and 18.03% on all other M&S expense; 66.96% on SWF					
TOTAL INDIRECT COSTS				$400,412	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$998,400	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$998,400	

Community Project for Accelerator Science and Simulation

BUDGET JUSTIFICATION

Fermi Research Alliance, LLC (FRA) / Fermi National Accelerator Laboratory

Fermi Research Alliance, LLC (FRA) / Fermilab will be providing approximately 1.1 FTE of effort towards accelerator physics applications for Intensity Frontier (Fermilab Proton Improvement Plan, Project X) and Energy Frontier (beam-driven plasma acceleration). Under the SciDAC program, Fermilab has developed state-of-the-art beam dynamics capabilities in Synergia. Synergia is a multi-language, extensible, parallel PIC framework, which utilizes state-of-the-art numerical libraries, solvers, and physics models. Because this framework supports complex simulation scenarios, we will take advantage of the scaling and optimization work on solvers by performing multi-physics, multibunch simulations. In addition, we have established close collaboration with accelerator designers and machine physicists, which ensure that the applications will be tailored to the needs of the above projects. The compensation is consistent with similar work both within and outside of Fermilab.
Personnel Cost amounts in Years 2-3 are estimated based upon a uniform escalation of 3%. This proposed budget covers all effort requested from the OHEP.

A. SENIOR PERSONNEL.

Panagiotis Spentzouris (28% year 1, 10% years 2 and 3), to lead and coordinate the project and work on Muon Collider to Project X interface applications
James Amundson (5% year 1, 22% years 2 and 3), to work on Muon Collider to Project X applications and capability development
Paul Lebrun (17%) for Project X applications and capability development
Alex Macridin (13%) for Proton Improvement Plan application and capability development
C.S. Park (13%) for proton-driven plasma acceleration capability and application development
Eric Stern (24%) for Project X applications and capabilty development

B. OTHER PERSONNEL.

ComPASS funds at Fermilab will also support 8% of a project support specialist for outreach and web interface design

C. FRINGE BENEFITS
Benefits are requested at the rate of 56.16% of professional salaries. This includes vacation accrual rate (10.5%), OPTO (7.8%), and Fringe Benefits rate (32%)

D. PERMANENT EQUIPMENT
None

E. TRAVEL AND SUBSISTENCE.
None

G. OTHER DIRECT COSTS
None

I. TOTAL INDIRECT COSTS
Fermi Research Alliance, LLC (FRA) / Fermilab FY2012 provisional indirect cost rate is currently 66.96% (Salaries), 11.6% (Travel), and 18.03% (Other M&S) of MTDC, in accordance with Fermilab's contract with the Fermi Research Alliance, LLC (FRA) and the Department of Energy.

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

Year 1 Funding Proposal

ORGANIZATION FERMILAB Computing Division				**Budget Page No:** 1	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Panagiotis Spentzouris				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applpicant	by DOE
1. James Amundson, Computational Physics Developer	3.60			$17,522	
2. Qiming Lu, Computational Physics Developer	3.60			$17,522	
3. Mark Fischler, Scientist	1.80			$8,761	
4.					
5.					
6.					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	9.00			$43,805	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$43,805	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$25,074	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$68,879	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL					
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS					
H. TOTAL DIRECT COSTS (A THROUGH G)				$68,879	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 11.6% on Travel expense and 18.03% on all other M&S expense; 66.96% on SWF					
TOTAL INDIRECT COSTS				$46,121	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$115,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$115,000	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

Year 2 Funding Proposal

ORGANIZATION FERMILAB Computing Division				**Budget Page No:** 2	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Panagiotis Spentzouris				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applpicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. James Amundson, Computational Physics Developer	3.60			$17,872	
2. Qiming Lu, Computational Physics Developer	3.60			$17,872	
3. Mark Fischler, Scientist	1.80			$8,936	
4.				$0	
5.				$0	
6.				$0	
7. (3) TOTAL SENIOR PERSONNEL (1-6)	9.00			$44,681	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES				$0	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				$0	
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$44,681	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$25,575	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$70,256	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$0	
2. FOREIGN					
TOTAL TRAVEL				$0	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS (0) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$0	
H. TOTAL DIRECT COSTS (A THROUGH G)				$70,256	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 11.6% on Travel expense and 18.03% on all other M&S expense; 66.96% on SWF					
TOTAL INDIRECT COSTS				$47,044	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$117,300	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$117,300	

DOE F 4620.1	**U.S. Department of Energy**	OMB Control No.
(04-93)	**Budget Page**	1910-1400
All Other Editions Are Obsolete	(See reverse for Instructions)	OMB Burden Disclosure Statement on Reverse

Year 3 Funding Proposal

ORGANIZATION FERMILAB Computing Division				**Budget Page No:** 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Panagiotis Spentzouris				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. James Amundson, Computational Physics Developer	3.60			$18,409	
2. Qiming Lu, Computational Physics Developer	3.60			$18,409	
3. Mark Fischler, Scientist	1.80			$9,204	
4.				$0	
5.				$0	
6.				$0	
7. (3) TOTAL SENIOR PERSONNEL (1-6)	9.00			$46,021	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES Graduate Student				$0	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)				$0	
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$46,021	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$26,343	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$72,364	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$0	
2. FOREIGN					
TOTAL TRAVEL				$0	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS (0) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$0	
H. TOTAL DIRECT COSTS (A THROUGH G)				$72,364	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 11.6% on Travel expense and 18.03% on all other M&S expense; 66.96% on SWF					
TOTAL INDIRECT COSTS				$48,455	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$120,819	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$120,819	

DOE F 4620.1 (04-93) All Other Editions Are Obsolete	**U.S. Department of Energy** **Budget Page** (See reverse for Instructions)	OMB Control No. 1910-1400 OMB Burden Disclosure Statement on Reverse

TOTAL of 3 Year Funding Proposal

ORGANIZATION FERMILAB Computing Division				**Budget Page No:**	4
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Panagiotis Spentzouris				Requested Duration:	36 (Months)
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. James Amundson, Computational Physics Developer	10.80			$53,803	
2. Qiming Lu, Computational Physics Developer	10.80			$53,803	
3. Mark Fischler, Scientist	5.40			$26,901	
4.					
5.					
6.					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	27.00			$134,507	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES	0.00			$0	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)	0.00			$0	
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$134,507	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$76,992	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$211,499	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$0	
2. FOREIGN				$0	
TOTAL TRAVEL				$0	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$0	
H. TOTAL DIRECT COSTS (A THROUGH G)				$211,499	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 11.6% on Travel expense and 18.03% on all other M&S expense; 66.96% on SWF					
TOTAL INDIRECT COSTS				$141,620	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$353,120	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$353,120	

Community Project for Accelerator Science and Simulation
ASCR

BUDGET JUSTIFICATION

Fermi Research Alliance, LLC (FRA) / Fermi National Accelerator Laboratory

Fermi Research Alliance, LLC (FRA) / Fermilab will be providing approximately 0.75 FTE of effort towards scalable solvers and Particle In Cell (PIC) algorithms, exploring new techniques and technologies, and providing domain expertise to the development of data, visualization and parameter optimization capabilities. Under SciDAC2, Fermilab has developed significant expertise in PIC and solver development, including hybrid and GPU environments. In addition to contributing to the development of general-purpose libraries developed by the collaboration, the new capabilities will be incorporated to the Synergia framework and utilized in the accelerator physics applications described in the HEP part of our budget. The compensation is consistent with similar work both within and outside of Fermilab.
Personnel Cost amounts in Years 2-3 are estimated based upon a uniform escalation of 3%. This proposed budget covers all effort to be requested from OASCR.

A. SENIOR PERSONNEL.

James Amundson (30%), to work on data, visualization, and parameter optimization capability development
Mark Fischler (15%) for PIC algorithm development
Qiming Lu (30%) for PIC algorithm development

B. OTHER PERSONNEL.

C. FRINGE BENEFITS
Benefits are requested at the rate of 56.16% of professional salaries. This includes vacation accrual rate (10.5%), OPTO (7.8%), and Fringe Benefits rate (32%)

D. PERMANENT EQUIPMENT
None

E. TRAVEL AND SUBSISTENCE.
None

G. OTHER DIRECT COSTS
None

I. TOTAL INDIRECT COSTS
Fermi Research Alliance, LLC (FRA) / Fermilab FY2012 provisional indirect cost rate is currently 66.96% (Salaries), 11.6% (Travel), and 18.03% (Other M&S) of MTDC, in accordance with Fermilab's contract with the Fermi Research Alliance, LLC (FRA) and the Department of Energy.

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION UChicago Argonne, LLC, Operator of Argonne National Laboratory				**Budget Page No:** pg 1 of 4 Yr 1 of 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Boyana R. Norris, PI				Requested Duration: 12 (Months) FWP #50363	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Boyana R. Norris, Computer Scientist	1.20			$24,511	
2. Todd S. Munson, Computational Scientist	0.60			$12,256	
3. Stefan M. Wild, Asst. Computational Mathematician	0.60			$9,187	
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	2.40			$45,954	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	6.10			$46,043	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$91,997	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$91,997	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$4,800	
2. FOREIGN					
TOTAL TRAVEL				$4,800	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$3,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$3,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				$99,797	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Section H. Direct cost X Aggregate rate of: 45.295%					
TOTAL INDIRECT COSTS				$45,203	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$145,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$145,000	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION UChicago Argonne, LLC, Operator of Argonne National Laboratory				**Budget Page No:** 2 of 4 Yr. 2 of 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Boyana R. Norris, PI				Requested Duration: 12 (Months) FWP #50363	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Boyana R. Norris, Computer Scientist	1.20			$25,557	
2. Todd S. Munson, Computational Scientist	0.60			$12,779	
3. Stefan M. Wild, Asst. Computational Mathematician	0.60			$9,572	
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	2.40			$47,908	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	6.00			$47,562	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$95,470	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$95,470	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$4,800	
2. FOREIGN					
TOTAL TRAVEL				$4,800	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$1,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$1,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				$101,270	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Section H. Direct cost X Aggregate rate of: 46.044%					
TOTAL INDIRECT COSTS				$46,629	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$147,899	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$147,899	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION
UChicago Argonne, LLC, Operator of Argonne National Laboratory

Budget Page No: 3 of 4
Yr 3 of 3

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR
Boyana R. Norris, PI

Requested Duration: 12 (Months)
FWP #50363

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Boyana R. Norris, Computer Scientist	1.20			$26,649	
2. Todd S. Munson, Computational Scientist	0.60			$13,324	
3. Stefan M. Wild, Asst. Computational Mathematician	0.60			$9,973	
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	2.40			$49,946	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	5.80			$48,520	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$98,466	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$98,466	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$4,800	
2. FOREIGN					
TOTAL TRAVEL				$4,800	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$1,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$1,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				$104,266	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Section H. Direct cost X Aggregate rate of: 46.104%					
TOTAL INDIRECT COSTS				$48,071	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$152,337	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$152,337	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION UChicago Argonne, LLC, Operator of Argonne National Laboratory				**Budget Page No:** 4 of 4 3 Yr. ANL Total Project	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Boyana R. Norris, PI				Requested Duration: 36 (Months) FWP #50363	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Boyana R. Norris, Computer Scientist	3.60			$76,717	
2. Todd S. Munson, Computational Scientist	1.80			$38,359	
3. Stefan M. Wild, Asst. Computational Mathematician	1.80			$28,732	
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	7.20			$143,808	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	17.90			$142,125	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$285,933	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$285,933	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$14,400	
2. FOREIGN					
TOTAL TRAVEL				$14,400	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$5,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				$5,000	
H. TOTAL DIRECT COSTS (A THROUGH G)				$305,333	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$139,903	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$445,236	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$445,236	

Community Project for Accelerator
Science and Simulation
Boyana R. Norris, PI
FWP #50363

Budget Explanation

A-C. Salaries and Fringe Benefits

Argonne National Laboratory is a government-owned facility operated by the UChicago Argonne, LLC. As a contractor for the Department of Energy, Argonne National Laboratory must comply with DOE general policies and procedures on budgeting and accounting. The Laboratory's costing procedures are based on the assumption that all costs incurred will be recovered. The costing procedures use Laboratory-wide pay bands for base effort cost on a consistent basis and are uniformly applied to all work supported by the Department of Energy and other federal agencies.

Pay band rates are established at the beginning of the fiscal year for the Laboratory, and are monitored and revised as necessary. All effort costs are distributed as Laboratory-wide pay band rates which are developed by the Laboratory's Budget Office for each major payroll classification. The pay bands are based on salary ranges, fringe benefits (31.0% for a regular staff and clerical, 16.0% for postdoctoral and 11.0% for Special/Term appointees), plus a factor for divisional overhead and for paid absences. Graduate and undergraduate student costs include housing allowance and fringe benefits (7.65%). The fringe benefit costs include payroll-related items such as annuities, social security, and hospital and medical payments. Effort is escalated each year by a rate (~ 4.5% for regular staff and postdoctoral appointees) provided by the Argonne Budget Department.

The principal investigator for this proposal is:	Boyana R. Norris, Computer Scientist	
The PI's effort charged per year to this proposal is :		1.20 man-months
Senior Personnel includes:	Todd S. Munson, Computational Scientist	0.60 man-months
	Stefan M. Wild, Asst. Computational Mathematician	0.60 man-months
Post doctoral appointees' effort charged per year to this proposal is :		5.97 man-months

E. Travel

Domestic: $1.0 K per trip
Projecting 1-2 trips per staff member per year to present results/status to collaborative institutions and conferences.

G. Other Direct Costs

1. Materials and Supplies:
Hardware/software maintenance, software, low-end computers (<$3k), computer and misc. supplies.
2. Publication Costs: N/A
3. Consultant Services: N/A
4. Computer (ADPE) Services: N/A
5. Subcontracts: N/A
6. Other: N/A

I. Indirect Costs

Standard rates are developed for Laboratory General and Administrative (G&A) expense. The procedures for distributing Laboratory G&A and program expense is applied on the basis of the total cost of the work performed. The following indirect rates are provisional and have been estimated for each fiscal year budget period:
Computing and Life Sciences Program Expense @ 3.8%
Laboratory G&A:
Common Support @ 25.5%
Laboratory Directed Research & Development @ 8.3%
Materials, Equipment & Subcontracts @ 4.5%
IGPP @ 6.6%
General & Administrative Burden @ 3.9%

These rates are subject to change after review and approval by the Laboratory management. Argonne's indirect rates are continuously reviewed and audited by Cognizant Federal Agency:
James R. Gotchie, Financial Analyst — Department of Energy-Chicago Operations Office
Phone: (630) 252-2278

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Ernest O. Lawrence Berkeley National Laboratory				Budget Page No:	1
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Jean-Luc Vay				Requested Duration: 12 (Months) July 1, 2012 - June 30, 2013	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applpicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. Vay, Jean-Luc	2.46			$26,309	
2. Geddes, Cameron	1.74			$19,468	
3. Qiang, Ji	0.77			$8,878	
4. Furman, Miguel	0.90			$11,906	
5.					
6.					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	5.87			$66,560	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES				$7,716	
2. ( ) OTHER PROFESSIONAL (SCIENTIST, TECHNICIAN. PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER - BUDGET ANALYST					
TOTAL SALARIES AND WAGES (A+B)				$74,277	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$40,602	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$114,879	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$5,000	
Travel Recharge				$700	
TOTAL TRAVEL				$5,700	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PROCUEMENT RECHARGE ON M&S					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER - Telephone Recharges					
TOTAL OTHER DIRECT COSTS					
H. TOTAL DIRECT COSTS (A THROUGH G)				$120,579	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
Org Burden 18%; Base - Total Salaries & Fringe Benefits		20,678			
G&A 51%; Base - Total Salaries & FB, Org Burden and Recharges		69,491			
LDRD & IGPP; 6.55% on Total Direct Costs and Org Burden		9,252			
TOTAL INDIRECT COSTS				$99,421	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$220,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$220,000	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION: Ernest O. Lawrence Berkeley National Laboratory

Budget Page No: 2

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR: Jean-Luc Vay

Requested Duration: 12 (Months)
July 1, 2013 - June 30, 2014

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Vay, Jean-Luc	2.40			$26,213	
2. Geddes, Cameron	1.69			$19,296	
3. Qiang, Ji	0.74			$8,784	
4. Furman, Miguel	0.90			$12,159	
5.					
6.					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	5.73			$66,452	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES				$7,881	
2. ( ) OTHER PROFESSIONAL (SCIENTIST, TECHNICIAN. PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER - BUDGET ANALYST					
TOTAL SALARIES AND WAGES (A+B)				$74,333	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$43,235	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$117,568	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$5,000	
Travel Recharge				$700	
TOTAL TRAVEL				$5,700	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PROCUEMENT RECHARGE ON M&S					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER - Telephone Recharges					
TOTAL OTHER DIRECT COSTS					
H. TOTAL DIRECT COSTS (A THROUGH G)				$123,268	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
Org Burden 18%; Base - Total Salaries & Fringe Benefits		21,162			
G&A 51%; Base - Total Salaries & FB, Org Burden and Recharges		71,110			
LDRD & IGPP; 6.55% on Total Direct Costs and Org Burden		9,460			
TOTAL INDIRECT COSTS				$101,732	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$225,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$225,000	

DOE F 4620.1	**U.S. Department of Energy**	OMB Control No.
(04-93)	**Budget Page**	1910-1400
All Other Editions Are Obsolete	(See reverse for Instructions)	OMB Burden Disclosure Statement on Reverse

ORGANIZATION Ernest O. Lawrence Berkeley National Laboratory				Budget Page No: 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Jean-Luc Vay				Requested Duration: 12 (Months) July 1, 2014 - June 30, 2015	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applpicant	by DOE
1. Vay, Jean-Luc	2.40			$26,869	
2. Geddes, Cameron	1.68			$19,676	
3. Qiang, Ji	0.72			$8,713	
4. Furman, Miguel	0.84			$11,672	
5.					
6.					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	5.64			$66,930	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES				$8,078	
2. ( ) OTHER PROFESSIONAL (SCIENTIST, TECHNICIAN. PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER - BUDGET ANALYST					
TOTAL SALARIES AND WAGES (A+B)				$75,008	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$45,788	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$120,796	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$5,000	
Travel Recharge				$700	
TOTAL TRAVEL				$5,700	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PROCUEMENT RECHARGE ON M&S					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER - Telephone Recharges					
TOTAL OTHER DIRECT COSTS					
H. TOTAL DIRECT COSTS (A THROUGH G)				$126,496	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
Org Burden 18%; Base - Total Salaries & Fringe Benefits	21,743				
G&A 51%; Base - Total Salaries & FB, Org Burden and Recharges	73,052				
LDRD & IGPP; 6.55% on Total Direct Costs and Org Burden	9,710				
TOTAL INDIRECT COSTS				$104,505	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$231,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$231,000	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION
Ernest O. Lawrence Berkeley National Laboratory

Budget Page No: 4

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR
Jean-Luc Vay

Requested Duration: 36 (Months)
July 1, 2012 - June 30, 2015

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. Vay, Jean-Luc	7.26			79,391	
2. Geddes, Cameron	5.11			58,440	
3. Qiang, Ji	2.23			26,375	
4. Furman, Miguel	2.64			35,737	
5.					
6.					
7. (4) TOTAL SENIOR PERSONNEL (1-6)	17.24			199,942	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES				23,675	
2. ( ) OTHER PROFESSIONAL (SCIENTIST, TECHNICIAN. PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER - BUDGET ANALYST					
TOTAL SALARIES AND WAGES (A+B)				$223,617	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				129,625	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				353,242	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				15,000	
Travel Recharge				2,100	
TOTAL TRAVEL				$17,100	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PROCUEMENT RECHARGE ON M&S					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER - Telephone Recharges					
TOTAL OTHER DIRECT COSTS					
H. TOTAL DIRECT COSTS (A THROUGH G)				370,342	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
Org Burden 18%; Base - Total Salaries & Fringe Benefits 63,584					
G&A 51%; Base - Total Salaries & FB, Org Burden and Recharges 213,652					
LDRD & IGPP; 6.55% on Total Direct Costs and Org Burden 28,422					
TOTAL INDIRECT COSTS				305,658	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				676,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				676,000	

LBNL (Accelerator and Fusion Research Division)
Budget Rate Cost Basis Explanation

DIRECT COSTS

Senior Personnel
The salary figure listed for Senior Personnel is an estimate based on the current actual salary for an employee in her/his division plus 1% inflation for Fiscal Year 2012 and 2013, 2.5% inflation for Fiscal Years 2014 and 2015.

Fringe Benefits
Fringe Benefits for LBNL employees are estimated to be the following percent calculated on labor costs:
Career Employees –Year 1: 57.5%, Year 2: 61.3%, Year 3: 64.5%
Postdoctoral Fellows –Year 1: 30.6%, Year 2: 31.7%, Year 3: 32.8%

Travel
The senior staff members plan to attend domestic technical conferences/workshops in the areas of research covered by this proposal. Total cost includes plane fare, housing, meals and other allowable costs under government per diem rules.

INDIRECT COSTS

Organizational Burden
Use of organizational burden pools in LBNL Accelerator Fusion Research Division (AFRD) Organization is the approved method for collection and distribution of indirect costs associated with personnel. These pools are established to collect costs associated with personnel engaged in a single operation or several closely related operations. The objective is to establish uniformity and compatibility in recording, distributing, and reporting organizational burden. The types of costs that can be charged to these pools are labor and labor- related costs of secretaries, division administration and general materials/service costs such as environmental, safety, and health, finance and budget provided for the general benefit of a division. The Accelerator Fusion Research Division (AFRD) is part of the General Sciences Organization and has an estimated LBNL organizational burden rate of 18%, which is calculated on all AFRD research salaries.

Other LBNL on-site indirect estimated costs are as follows:
Travel – 14.0% calculated on all travel
General & Administrative – 57.55% calculated on all direct and indirect costs. This rate includes a General Rate of 51.0%, LDRD Rate of 5.4% and an IGPP Rate of 1.15%

SENIOR PERSONNEL

Jean-Luc Vay: work on electron cloud simulation code and simulations of laser plasma acceleration in a boosted frame.

Miguel Furman: work on electron cloud simulation code development and data analysis.

Cameron Geddes: work on simulations of laser plasma acceleration.

Ji Qiang: work on non-linear parameter optimization.

Serge Rykovalanov (Postdoc): work on simulations of laser plasma acceleration.

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Lawrence Berkeley National Laboratory				**Budget Page No:**	1
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Ng, Esmond				Requested Duration:	12 (Months)
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. Ng, Esmond G	0.60			$8,844	
2. Li, Xiaoye Sherry	1.20			$12,323	
3. Yang, Chao	1.20			$12,190	
4. Graves, Daniel T	3.43			$34,157	
5. Schwartz, Peter O	2.73			$25,609	
6. Van Straalen, Brian	2.29			$25,633	
7.					
8.					
9. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
10. (6) TOTAL SENIOR PERSONNEL (1-6)	11.45			$118,757	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	4.74			$28,915	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$147,672	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$147,672	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL — 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$5,000	
2. FOREIGN					
TOTAL TRAVEL				$5,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER - recharges (telephone, space, etc.)				$1,816	
TOTAL OTHER DIRECT COSTS				$1,816	
H. TOTAL DIRECT COSTS (A THROUGH G)				$154,488	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$270,512	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$425,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$425,000	

DOE F 4620.1 (04-93) All Other Editions Are Obsolete	**U.S. Department of Energy** **Budget Page** (See reverse for Instructions)	OMB Control No. 1910-1400 OMB Burden Disclosure Statement on Reverse

ORGANIZATION Lawrence Berkeley National Laboratory				**Budget Page No:**	2
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Ng, Esmond				Requested Duration:	12 (Months)
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Ng, Esmond G	0.60			$9,029	
2. Li, Xiaoye Sherry	1.20			$12,580	
3. Yang, Chao	1.20			$12,444	
4. Graves, Daniel T	3.43			$34,870	
5. Schwartz, Peter O	2.73			$26,144	
6. Van Straalen, Brian	2.29			$26,168	
7.					
8.					
9. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
10. (6) TOTAL SENIOR PERSONNEL (1-6)	11.45			$121,236	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	4.74			$25,778	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$147,013	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$147,013	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL — 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$5,100	
2. FOREIGN					
TOTAL TRAVEL				$5,100	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER - recharges (telephone, space, etc.)				$1,818	
TOTAL OTHER DIRECT COSTS				$1,818	
H. TOTAL DIRECT COSTS (A THROUGH G)				$153,931	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$280,069	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$434,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$434,000	

DOE F 4620.1 *(04-93)* *All Other Editions Are Obsolete*	**U.S. Department of Energy** **Budget Page** (See reverse for Instructions)	OMB Control No. 1910-1400 OMB Burden Disclosure Statement on Reverse

ORGANIZATION Lawrence Berkeley National Laboratory				**Budget Page No:**	3
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Ng, Esmond				Requested Duration:	12 (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Ng, Esmond G	0.59			$9,083	
2. Li, Xiaoye Sherry	1.18			$12,655	
3. Yang, Chao	1.18			$12,519	
4. Graves, Daniel T	3.37			$35,080	
5. Schwartz, Peter O	2.68			$26,301	
6. Van Straalen, Brian	2.25			$26,618	
7.					
8.					
9. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
10. (6) TOTAL SENIOR PERSONNEL (1-6)	11.24			$122,257	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	4.74			$26,422	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$148,679	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$148,679	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$5,202	
2. FOREIGN					
TOTAL TRAVEL				$5,202	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER - recharges (telephone, space, etc.)				$1,819	
TOTAL OTHER DIRECT COSTS				$1,819	
H. TOTAL DIRECT COSTS (A THROUGH G)				$155,700	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$291,300	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$447,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$447,000	

DOE F 4620.1	**U.S. Department of Energy**	OMB Control No.
(04-93)	**Budget Page**	1910-1400
All Other Editions Are Obsolete	(See reverse for Instructions)	OMB Burden Disclosure Statement on Reverse

ORGANIZATION Lawrence Berkeley National Laboratory				**Budget Page No:**	4
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Ng, Esmond				Requested Duration:	36 (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Ng, Esmond G	1.79			$26,956	
2. Li, Xiaoye Sherry	3.58			$37,558	
3. Yang, Chao	3.58			$37,154	
4. Graves, Daniel T	10.23			$104,108	
5. Schwartz, Peter O	8.15			$78,054	
6. Van Straalen, Brian	6.83			$78,420	
7.					
8.					
9. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
10. (6) TOTAL SENIOR PERSONNEL (1-6)	34.15			$362,250	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	23.69			$81,115	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$443,365	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$443,365	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$15,302	
2. FOREIGN					
TOTAL TRAVEL				$15,302	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER - recharges (telephone, space, etc.)				$5,452	
TOTAL OTHER DIRECT COSTS				$5,452	
H. TOTAL DIRECT COSTS (A THROUGH G)				$464,119	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS				$841,881	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$1,306,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$1,306,000	

LBNL (Computational Research Division)
Budget Rate Cost Basis Explanation

DIRECT COSTS

Senior Personnel
The salary figure listed for Senior Personnel is an estimate based on the current actual salary for an employee in her/his division plus 3.0% per fiscal year for inflation.

Fringe Benefits
Fringe Benefits for LBNL employees are estimated to be the following percent calculated on labor costs:
Career Employees –FY12 33.3%; FY13 37.3%; FY14 40.4% FY15 43.0% FY16 45.4%
Postdoctoral Fellows –FY12 17.9%; FY13 18.9%; FY14 19.9% FY15 20.9% FY16 22.0%
GSRAs – FY12 through FY16 0.7%
Students/Other – FY12 through FY15 2.6%

Travel
The senior staff members plan to attend domestic and/or foreign technical conferences/workshops in the areas of research covered by this proposal. Total cost includes plane fare, housing, meals and other allowable costs under government per diem rules.

Other Direct Costs
The estimated cost of telephone, space, computer usage, etc., calculated on person-months directly associated with the project.

INDIRECT COSTS

Organizational Burden
Use of organizational burden pools in LBNL Computing Sciences (CS) Organization is the approved method for collection and distribution of indirect costs associated with personnel. These pools are established to collect costs associated with personnel engaged in a single operation or several closely related operations. The objective is to establish uniformity and compatibility in recording, distributing, and reporting organizational burden. The types of costs that can be charged to these pools are labor and labor- related costs of secretaries, division administration and general materials/service costs such as environmental, safety, and health, finance and budget provided for the general benefit of a division. The Computational Research Division (CRD) is part of the CS Organization and has an estimated LBNL organizational burden rate of 18.6%, which is calculated on all CRD research salaries.

Other LBNL on-site indirect estimated costs are as follows:
Procurement Burden – 9.7% calculated on general procurements purchased through the Procurement Department; 5.1% on R&D subcontracts; 5.4% on Intra-University Transfers
Travel – 14.0% calculated on all travel
General & Administrative – 57.55% calculated on all direct and indirect costs, electricity excluded. This rate includes a General Rate of 51.0%, LDRD Rate of 5.4% and an IGPP Rate of 1.15%

SENIOR PERSONNEL

Daniel T. Graves – Work on improving performance and scalability of Poisson solvers.

Xiaoye Sherry Li – Work on sparse linear solvers.

Esmond G. Ng – Work on sparse matrix computation and is the Computation Director in ComPASS. Also serve as liaison to the FASTMath Institute.

Peter O. Schwartz – Work high-order map and finite-volume schemes in support of hydrodynamics simulations.

Brian Van Straalen – Work on high performance computing implementation of Poisson and hydrodynamics codes.

Chao Yang – Work on sparse eigenvalue problems.

DOE F 4620.1	**U.S. Department of Energy**	OMB Control No.
(04-93)	**Budget Page**	1910-1400
All Other Editions Are Obsolete	(See reverse for Instructions)	OMB Burden Disclosure Statement on Reverse

ORGANIZATION AD 2012-2015				**Budget Page No:** 1		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Cho Ng				Requested Duration: 36 (Months)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted	
	CAL	ACAD	SUMR	by Applicant	by DOE	
1. Dr. Cho Ng	9.00			$107,221		
2. Dr. Greg Schussman	5.40			$53,925		
3. Dr. Zenghai Li	9.00			$99,614		
4. Dr. Liling Xiao	9.00			$90,199		
5. 0	0.00			$0		
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.00			$0		
7. (4) TOTAL SENIOR PERSONNEL (1-6)	32.40			$350,959		
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. () POST DOCTORAL ASSOCIATES	0.00			$0		
2. () OTHER PROFESSIONAL (Computer Cluster Manager)	0.00			$0		
3. () GRADUATE STUDENTS	0.00			$0		
4. () UNDERGRADUATE STUDENTS	0.00			$0		
5. () SECRETARIAL - CLERICAL	0.00			$0		
6. (1) OTHER	0.00			$0		
7. () OTHERS (LIST INDIVIDUALLY ON OTHER PERSONNEL PAGE)	0.00			$0		
TOTAL SALARIES AND WAGES (A+B)				$350,959		
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$109,850		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$460,810		
PROGRAM SUPPORT				$46,081		
TOTAL LABOR, including PROGRAM SUPPORT				$506,891		
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.) See Budget Justification						
TOTAL PERMANENT EQUIPMENT				$0		
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$9,227		
incl. visitor program 2. FOREIGN				$0		
TOTAL TRAVEL				$9,227		
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)				$0		
2. TUITION & FEES				$0		
3. TRAINEE TRAVEL				$0		
4. WORKSHOPS AND SUMMER SCHOOL				$0		
TOTAL PARTICIPANTS () TOTAL COST				$0		
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES				$0		
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$1,384		
3. CONSULTANT SERVICES				$0		
4. SCIENTIFIC COMPUTING SERVICES				$0		
5. SUBCONTRACTS				$0		
6. OTHER Tuition				$0		
TOTAL OTHER DIRECT COSTS				$1,384		
H. TOTAL DIRECT COSTS (A THROUGH G)				$517,502		
I. INDIRECT COSTS (SPECIFY RATE AND BASE) PS @ 10.0%; Labor and Travel @ 52.0%						
TOTAL INDIRECT COSTS All Other @ 9.42%				$268,512		
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$786,013		
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0		
L. TOTAL COST OF PROJECT (J+K)				$786,013		

DOE F 4620.1 (04-93) All Other Editions Are Obsolete	**U.S. Department of Energy** **Budget Page** (See reverse for Instructions)	OMB Control No. 1910-1400 OMB Burden Disclosure Statement on Reverse

ORGANIZATION AD 2012				**Budget Page No:** 2	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Cho Ng				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Dr. Cho Ng	3.00			$34,785	
2. Dr. Greg Schussman	1.80			$17,494	
3. Dr. Zenghai Li	3.00			$32,317	
4. Dr. Liling Xiao	3.00			$29,262	
5. 0	0.00			$0	
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.00			$0	
7. (4) TOTAL SENIOR PERSONNEL (1-6)	10.80			$113,859	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. () POST DOCTORAL ASSOCIATES	0.0			$0	
2. () OTHER PROFESSIONAL (Computer Cluster Manager)	0.00			$0	
3. () GRADUATE STUDENTS	0.0			$0	
4. () UNDERGRADUATE STUDENTS	0.0			$0	
5. () SECRETARIAL - CLERICAL	0.0			$0	
6. (1) OTHER	0.0			$0	
7. () OTHERS (LIST INDIVIDUALLY ON OTHER PERSONNEL PAGE)	0.0			$0	
TOTAL SALARIES AND WAGES (A+B)				$113,859	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$35,638	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$149,496	
PROGRAM SUPPORT				$14,950	
TOTAL LABOR, including PROGRAM SUPPORT				$164,446	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.) See Budget Justification					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL — 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$3,000	
incl. visitor program — 2. FOREIGN				$0	
TOTAL TRAVEL				$3,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				$0	
2. TUITION & FEES				$0	
3. TRAINEE TRAVEL				$0	
4. WORKSHOPS AND SUMMER SCHOOL				$0	
TOTAL PARTICIPANTS () TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$450	
3. CONSULTANT SERVICES				$0	
4. SCIENTIFIC COMPUTING SERVICES				$0	
5. SUBCONTRACTS				$0	
6. OTHER Tuition				$0	
TOTAL OTHER DIRECT COSTS				$450	
H. TOTAL DIRECT COSTS (A THROUGH G)				$167,896	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) PS @ 10.0% Labor and Travel @ 52.0%					
TOTAL INDIRECT COSTS All Other @ 9.42%				$87,114	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$255,010	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$255,010	

DOE F 4620.1 (04-93) All Other Editions Are Obsolete	**U.S. Department of Energy** **Budget Page** (See reverse for Instructions)	OMB Control No. 1910-1400 OMB Burden Disclosure Statement on Reverse

ORGANIZATION AD 2013				**Budget Page No:** 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Cho Ng				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. Dr. Cho Ng	3.00			$35,595	
2. Dr. Greg Schussman	1.80			$17,902	
3. Dr. Zenghai Li	3.00			$33,070	
4. Dr. Liling Xiao	3.00			$29,944	
5. 0	0.00			$0	
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.00			$0	
7. (4) TOTAL SENIOR PERSONNEL (1-6)	10.80			$116,511	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. () POST DOCTORAL ASSOCIATES	0.0			$0	
2. () OTHER PROFESSIONAL (Computer Cluster Manager)	0.0			$0	
3. () GRADUATE STUDENTS	0.0			$0	
4. () UNDERGRADUATE STUDENTS	0.0			$0	
5. () SECRETARIAL - CLERICAL	0.0			$0	
6. (1) OTHER	0.0			$0	
7. () OTHERS (LIST INDIVIDUALLY ON OTHER PERSONNEL PAGE)	0.0			$0	
TOTAL SALARIES AND WAGES (A+B)				$116,511	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$36,468	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$152,980	
PROGRAM SUPPORT				$15,298	
TOTAL LABOR, including PROGRAM SUPPORT				$168,278	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.) See Budget Justification					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$3,075	
incl. visitor program 2. FOREIGN				$0	
TOTAL TRAVEL				$3,075	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				$0	
2. TUITION & FEES				$0	
3. TRAINEE TRAVEL				$0	
4. WORKSHOPS AND SUMMER SCHOOL				$0	
TOTAL PARTICIPANTS () TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$461	
3. CONSULTANT SERVICES				$0	
4. SCIENTIFIC COMPUTING SERVICES				$0	
5. SUBCONTRACTS				$0	
6. OTHER Tuition				$0	
TOTAL OTHER DIRECT COSTS				$461	
H. TOTAL DIRECT COSTS (A THROUGH G)				$171,814	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) PS @ 10.0% Labor and Travel @ 52.0%					
TOTAL INDIRECT COSTS All Other @ 9.42%				$89,147	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$260,961	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$260,961	

DOE F 4620.1	**U.S. Department of Energy**	OMB Control No.
(04-93)	**Budget Page**	1910-1400
All Other Editions Are Obsolete	(See reverse for Instructions)	OMB Burden Disclosure Statement on Reverse

ORGANIZATION				**Budget Page No:** 4	
AD 2014					
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Cho Ng				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Dr. Cho Ng	3.00			$36,841	
2. Dr. Greg Schussman	1.80			$18,529	
3. Dr. Zenghai Li	3.00			$34,227	
4. Dr. Liling Xiao	3.00			$30,992	
5. 0	0.00			$0	
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.00			$0	
7. (4) TOTAL SENIOR PERSONNEL (1-6)	10.80			$120,589	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. () POST DOCTORAL ASSOCIATES	0.0			$0	
2. () OTHER PROFESSIONAL (Computer Cluster Manager)	0.0			$0	
3. () GRADUATE STUDENTS	0.0			$0	
4. () UNDERGRADUATE STUDENTS	0.0			$0	
5. () SECRETARIAL - CLERICAL	0.0			$0	
6. (1) OTHER	0.0			$0	
7. () OTHERS (LIST INDIVIDUALLY ON OTHER PERSONNEL PAGE)	0.0			$0	
TOTAL SALARIES AND WAGES (A+B)				$120,589	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$37,744	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$158,334	
PROGRAM SUPPORT				$15,833	
TOTAL LABOR, including PROGRAM SUPPORT				$174,167	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.) See Budget Justification					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$3,152	
incl. visitor program 2. FOREIGN				$0	
TOTAL TRAVEL				$3,152	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				$0	
2. TUITION & FEES				$0	
3. TRAINEE TRAVEL				$0	
4. WORKSHOPS AND SUMMER SCHOOL				$0	
TOTAL PARTICIPANTS () TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$473	
3. CONSULTANT SERVICES				$0	
4. SCIENTIFIC COMPUTING SERVICES				$0	
5. SUBCONTRACTS				$0	
6. OTHER Tuition				$0	
TOTAL OTHER DIRECT COSTS				$473	
H. TOTAL DIRECT COSTS (A THROUGH G)				$177,792	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) PS @ 10.0% Labor and Travel @ 52.0%					
TOTAL INDIRECT COSTS All Other @ 9.42%				$92,250	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$270,042	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$270,042	

Budget Explanation:

The budget period spans three years, 07/01/2012 through 06/30/2015. The budget assumes a 2.33% escalation labor costs from year 1 to year 2 and 3.50% year 2 to 3, and 2.5% per year for non-labor escalation.

A. Senior Personnel:

Principal Investigator

Cho-Kuen Ng, Principal Investigator and staff scientist of SLAC National Accelerator Laboratory, is an expert in accelerator modeling using high performance computing and will dedicate 25% efforts to the project. As the PI, Dr. Ng will ensure that research goals are met in a timely manner, with scientific integrity, and completed within budgeted amounts. The PI will ensure that project activities and expenditures are in compliance with Stanford University and Department of Energy policy. Dr. Ng will oversee this project.

Zenghai Li, staff scientist of SLAC National Accelerator Laboratory, an expert in RF modeling of accelerator structures and will dedicate 25% effort towards this research.

Greg Schussman, research software developer of SLAC National Accelerator Laboratory, an expert in computational science and will dedicate 15% effort towards this research.

Liling Xiao, staff scientist of SLAC National Accelerator Laboratory, an expert in RF modeling of accelerator structures and will dedicate 25% effort towards this research.

B. Other Personnel:

Research Associates: Research Associates are recruited from programs at Stanford University, and other universities nationwide and worldwide. They are hired for their expertise in the field and their potential to contribute to the research projects. In the three year period, there will be one research associate engaged 50%.

C. Fringe Benefits:

Fringe benefit rate used for this proposal are shown below.

Fringe Benefit Rates	FY12
Regular Benefits-eligible Employees	31.3 %
Post-Doctoral Research Affiliates	22.5 %
Contingent Employees	7.9 %
Graduate Assistants	4.7 %

D. Permanent equipment:

Capital equipment is not required for this project

E. Travel:

Travel costs for the PI will be incurred as domestic travel to conferences to disseminate their findings. As the program progresses, there will be more results to present and would like to interact with other experts. The total travel cost is estimated at $3,000 annually with 2 domestic business trips per year.

F. Trainee costs: None

G. Other Direct Costs:

Publication/documentation/Dissemination: The costs for preparing and publishing the results of the work conducted are estimated at $450 per year.

H. Total direct costs: Indirect costs:

Current SLAC indirect rates for activities funded are indicated below:
Labor and travel: 52%
Procurements: 9.42%
Program Support: 10%

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION AD 2012-2015				**Budget Page No:** 1	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Cho Ng				Requested Duration: 36 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Dr. Greg Schussman	3.60			$32,178	
2. Dr. Kihwan Lee	11.88			$97,915	
3. Dr. Lixin GE	11.88			$108,952	
4. 0	0.00			$0	
5. 0	0.00			$0	
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.00			$0	
7. (3) TOTAL SENIOR PERSONNEL (1-6)	27.36			$239,045	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. () POST DOCTORAL ASSOCIATES	0.00			$0	
2. () OTHER PROFESSIONAL (Computer Cluster Manager)	0.00			$0	
3. () GRADUATE STUDENTS	0.00			$0	
4. () UNDERGRADUATE STUDENTS	0.00			$0	
5. () SECRETARIAL - CLERICAL	0.00			$0	
6. (1) OTHER	0.00			$0	
7. () OTHERS (LIST INDIVIDUALLY ON OTHER PERSONNEL PAGE)	0.00			$0	
TOTAL SALARIES AND WAGES (A+B)				$239,045	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$74,821	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$313,866	
PROGRAM SUPPORT				$31,387	
TOTAL LABOR, including PROGRAM SUPPORT				$345,253	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.) See Budget Justification					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL — 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$9,227	
incl. visitor program — 2. FOREIGN				$0	
TOTAL TRAVEL				$9,227	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				$0	
2. TUITION & FEES				$0	
3. TRAINEE TRAVEL				$0	
4. WORKSHOPS AND SUMMER SCHOOL				$0	
TOTAL PARTICIPANTS () TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$0	
3. CONSULTANT SERVICES				$0	
4. SCIENTIFIC COMPUTING SERVICES				$0	
5. SUBCONTRACTS				$0	
6. OTHER Tuition				$0	
TOTAL OTHER DIRECT COSTS				$0	
H. TOTAL DIRECT COSTS (A THROUGH G)				$354,480	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) PS @ 10.0%; Labor and Travel @ 52.0%					
TOTAL INDIRECT COSTS All Other @ 9.42%				$184,329	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$538,809	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$538,809	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION AD 2012				Budget Page No: 2	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Cho Ng				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Dr. Greg Schussman	1.20			$10,439	
2. Dr. Kihwan Lee	3.96			$31,766	
3. Dr. Lixin GE	3.96			$35,346	
4. 0	0.00			$0	
5. 0	0.00			$0	
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.00			$0	
7. (3) TOTAL SENIOR PERSONNEL (1-6)	9.12			$77,551	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. () POST DOCTORAL ASSOCIATES	0.0			$0	
2. () OTHER PROFESSIONAL (Computer Cluster Manager)	0.00			$0	
3. () GRADUATE STUDENTS	0.0			$0	
4. () UNDERGRADUATE STUDENTS	0.0			$0	
5. () SECRETARIAL - CLERICAL	0.0			$0	
6. (1) OTHER	0.0			$0	
7. () OTHERS (LIST INDIVIDUALLY ON OTHER PERSONNEL PAGE)	0.0			$0	
TOTAL SALARIES AND WAGES (A+B)				$77,551	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$24,274	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$101,825	
PROGRAM SUPPORT				$10,182	
TOTAL LABOR, including PROGRAM SUPPORT				$112,007	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.) See Budget Justification					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$3,000	
incl. visitor program 2. FOREIGN				$0	
TOTAL TRAVEL				$3,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				$0	
2. TUITION & FEES				$0	
3. TRAINEE TRAVEL				$0	
4. WORKSHOPS AND SUMMER SCHOOL				$0	
TOTAL PARTICIPANTS () TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$0	
3. CONSULTANT SERVICES				$0	
4. SCIENTIFIC COMPUTING SERVICES				$0	
5. SUBCONTRACTS				$0	
6. OTHER Tuition				$0	
TOTAL OTHER DIRECT COSTS				$0	
H. TOTAL DIRECT COSTS (A THROUGH G)				$115,007	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) PS @ 10.0%; Labor and Travel @ 52.0%					
TOTAL INDIRECT COSTS All Other @ 9.42%				$59,804	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$174,811	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$174,811	

DOE F 4620.1	U.S. Department of Energy	OMB Control No.
(04-93)	**Budget Page**	1910-1400
All Other Editions Are Obsolete	(See reverse for Instructions)	OMB Burden Disclosure Statement on Reverse

ORGANIZATION AD 2013				**Budget Page No:** 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Cho Ng				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Dr. Greg Schussman	1.20			$10,682	
2. Dr. Kihwan Lee	3.96			$32,506	
3. Dr. Lixin GE	3.96			$36,170	
4. 0	0.00			$0	
5. 0	0.00			$0	
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.00			$0	
7. (3) TOTAL SENIOR PERSONNEL (1-6)	9.12			$79,358	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. () POST DOCTORAL ASSOCIATES	0.0			$0	
2. () OTHER PROFESSIONAL (Computer Cluster Manager)	0.0			$0	
3. () GRADUATE STUDENTS	0.0			$0	
4. () UNDERGRADUATE STUDENTS	0.0			$0	
5. () SECRETARIAL - CLERICAL	0.0			$0	
6. (1) OTHER	0.0			$0	
7. () OTHERS (LIST INDIVIDUALLY ON OTHER PERSONNEL PAGE)	0.0			$0	
TOTAL SALARIES AND WAGES (A+B)				$79,358	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$24,839	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$104,197	
PROGRAM SUPPORT				$10,420	
TOTAL LABOR, including PROGRAM SUPPORT				$114,617	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.) See Budget Justification					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$3,075	
incl. visitor program 2. FOREIGN				$0	
TOTAL TRAVEL				$3,075	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				$0	
2. TUITION & FEES				$0	
3. TRAINEE TRAVEL				$0	
4. WORKSHOPS AND SUMMER SCHOOL				$0	
TOTAL PARTICIPANTS () TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$0	
3. CONSULTANT SERVICES				$0	
4. SCIENTIFIC COMPUTING SERVICES				$0	
5. SUBCONTRACTS				$0	
6. OTHER Tuition				$0	
TOTAL OTHER DIRECT COSTS				$0	
H. TOTAL DIRECT COSTS (A THROUGH G)				$117,692	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) PS @ 10.0%					
Labor and Travel @ 52.0%					
TOTAL INDIRECT COSTS All Other @ 9.42%				$61,200	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$178,892	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$178,892	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION AD 2014				**Budget Page No:** 4	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Cho Ng				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Dr. Greg Schussman	1.20			$11,056	
2. Dr. Kihwan Lee	3.96			$33,644	
3. Dr. Lixin GE	3.96			$37,436	
4. 0	0.00			$0	
5. 0	0.00			$0	
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)	0.00			$0	
7. (3) TOTAL SENIOR PERSONNEL (1-6)	9.12			$82,136	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. () POST DOCTORAL ASSOCIATES	0.0			$0	
2. () OTHER PROFESSIONAL (Computer Cluster Manager)	0.0			$0	
3. () GRADUATE STUDENTS	0.0			$0	
4. () UNDERGRADUATE STUDENTS	0.0			$0	
5. () SECRETARIAL - CLERICAL	0.0			$0	
6. (1) OTHER	0.0			$0	
7. () OTHERS (LIST INDIVIDUALLY ON OTHER PERSONNEL PAGE)	0.0			$0	
TOTAL SALARIES AND WAGES (A+B)				$82,136	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$25,708	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$107,844	
PROGRAM SUPPORT				$10,784	
TOTAL LABOR, including PROGRAM SUPPORT				$118,629	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.) See Budget Justification					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$3,152	
incl. visitor program 2. FOREIGN				$0	
TOTAL TRAVEL				$3,152	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				$0	
2. TUITION & FEES				$0	
3. TRAINEE TRAVEL				$0	
4. WORKSHOPS AND SUMMER SCHOOL				$0	
TOTAL PARTICIPANTS () TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$0	
3. CONSULTANT SERVICES				$0	
4. SCIENTIFIC COMPUTING SERVICES				$0	
5. SUBCONTRACTS				$0	
6. OTHER Tuition				$0	
TOTAL OTHER DIRECT COSTS				$0	
H. TOTAL DIRECT COSTS (A THROUGH G)				$121,781	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) PS @ 10.0%					
Labor and Travel @ 52.0%					
TOTAL INDIRECT COSTS All Other @ 9.42%				$63,326	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$185,106	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$185,106	

Budget Explanation:

The budget period spans three years, 07/01/2012 through 06/30/2015. The budget assumes a 2.33% escalation labor costs from year 1 to year 2 and 3.50% year 2 to 3, and 2.5% per year for non-labor escalation.

A. Senior Personnel:

Principal Investigator

Lixin Ge, research software developer of SLAC National Accelerator Laboratory, an expert in computational science and will dedicate 30% effort towards this research.

Kihwan Lee, research software developer of SLAC National Accelerator Laboratory, an expert in computational science and will dedicate 30% effort towards this research.

Greg Schussman, research software developer of SLAC National Accelerator Laboratory, an expert in computational science and will dedicate 10% effort towards this research.

B. Other Personnel:

Research Associates: Research Associates are recruited from programs at Stanford University, and other universities nationwide and worldwide. They are hired for their expertise in the field and their potential to contribute to the research projects. In the three year period, there will be one research associate engaged 50%.

C. Fringe Benefits:

Fringe benefit rate used for this proposal are shown below.

Fringe Benefit Rates	FY12
Regular Benefits-eligible Employees	31.3 %
Post-Doctoral Research Affiliates	22.5 %
Contingent Employees	7.9 %
Graduate Assistants	4.7 %

D. Permanent equipment:

Capital equipment is not required for this project

E. Travel:

Travel costs for the PI will be incurred as domestic travel to conferences to disseminate their findings. As the program progresses, there will be more results to present and would like to interact with other experts. The total travel cost is estimated at $3,000 annually with 2 domestic business trips per year.

F. Trainee costs: None

G. Other Direct Costs:

Publication/documentation/Dissemination: The costs for preparing and publishing the results of the work conducted are estimated at $450 per year.

H. Total direct costs: Indirect costs:

Current SLAC indirect rates for activities funded are indicated below:

Labor and travel: 52%

Procurements: 9.42%

Program Support: 10%

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Tech-X Corporation HEP				**Budget Page No:** 1	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR John R Cary				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applpicant	by DOE
1. John R Cary 5%				13,115.00	
2. David L Bruhwiler 10%				16,296.00	
3. Peter H Stoltz 10%				13,528.00	
4. Estelle Cormier 15%				12,707.00	
5. Kevin Paul 12%				8,472.00	
6. (3) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				42,713.00	
7. (8) TOTAL SENIOR PERSONNEL (1-6)				106,831.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				106,831.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				34,026.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				140,857.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				2,470.00	
2. FOREIGN					
TOTAL TRAVEL				2,470.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				143,327.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Overhead base 140857 = 84866 G&A base 228193 = 31947 FEE base 140857 = 9860					
TOTAL INDIRECT COSTS				126,673.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				270,000.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				270,000.00	0.00

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Tech-X Corporation HEP				**Budget Page No:** 2	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR John R Cary				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. John R Cary 5%				13,377.00	
2. David L Bruhwiler 10%				16,622.00	
3. Peter H Stoltz 10%				13,799.00	
4. Estelle Cormier 15%				12,961.00	
5. Kevin Paul 12%				8,641.00	
6. (3) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				43,568.00	
7. (8) TOTAL SENIOR PERSONNEL (1-6)				108,968.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				108,968.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				34,706.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				143,674.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				2,470.00	
2. FOREIGN					
TOTAL TRAVEL				2,470.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				146,144.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Overhead base 143674 = 86564 G&A base 232707 =32579 FEE base 143674 = 10057					
TOTAL INDIRECT COSTS				129,200.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				275,344.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				275,344.00	0.00

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Tech-X Corporation HEP				**Budget Page No:** 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR John R Cary				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applpicant	by DOE
1. John R Cary 5%				13,778.00	
2. David L Bruhwiler 10%				17,120.00	
3. Peter H Stoltz 10%				14,213.00	
4. Estellle Cormier 15%				13,351.00	
5. Kevin Paul 12%				8,901.00	
6. (3) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				44,875.00	
7. (8) TOTAL SENIOR PERSONNEL (1-6)				112,238.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				112,238.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				35,748.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				147,986.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				2,470.00	
2. FOREIGN					
TOTAL TRAVEL				2,470.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				150,456.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Overhead base 147986 = 89162 G&A base 239619 =33547 FEE base 147986 = 10359					
TOTAL INDIRECT COSTS				133,068.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				283,524.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				283,524.00	0.00

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Tech-X Corporation HEP				Budget Page No: 4	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR John R Cary				Requested Duration: summary-36 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applpicant	by DOE
1. John R Cary				40,270.00	
2. David L Bruhwiler				50,038.00	
3. Peter H Stoltz				41,540.00	
4. Estelle Cormier				39,019.00	
5. Kevin Paul				26,014.00	
6. (3) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				131,156.00	
7. (8) TOTAL SENIOR PERSONNEL (1-6)				328,037.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				328,037.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				104,480.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				432,517.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				7,410.00	
2. FOREIGN					
TOTAL TRAVEL				7,410.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				439,927.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Overhead G&A FEE					
TOTAL INDIRECT COSTS				388,941.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				828,868.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				828,868.00	0.00

"Community Project for Accelerator Science and Simulation"

DOE Funding Opportunity Number: DE-FOA-0000580
Tech-X Corporation – John Cary, Co-PI
Application Due Date: January 9, 2012

The budgeted direct costs for this project are primarily labor. Labor costs are based on significant past experience with research projects and on the nature and scope of the work being proposed for this particular project. Specifically, the budget includes time for the Co-PI, John Cary. Professor and CEO John Cary is an internationally known computational physicist and original architect of the VORPAL computational framework. He has more than 150 refereed journal articles and conference proceedings or presentations. He has significant experience and publication record in software development as well. Dr. Cary brings significant experience in several areas: a) project management, b) parallel computing, c) performance optimization, d) parallel visualization, e) electromagnetic modeling of superconducting rf (SRF) and dielectric structures, f) developing and working with the parallel VORPAL framework, and g) laser-plasma acceleration of electrons.

The other key personnel include David Bruhwiler, Estelle Cormier-Michel, Ben Cowan, Marc Durant, Paul Mullowney, Kevin Paul, Brian Schwartz and Seth Veitzer, all of whom are members of the VORPAL development team.

- Dr. Bruhwiler brings significant experience in developing algorithms within the parallel VORPAL framework and using them for laser-plasma simulations and other applications. He also has experience in beam dynamics with space charge, electrostatic and electromagnetic PIC modeling of beams and structures, parallel computing and project management.
- Dr. Cormier-Michel is an expert VORPAL developer, with an international reputation in laser plasma accelerator modeling. She has also used VisIt for an award winning 3D movie.
- Dr. Cowan brings significant expertise in designing and modeling dielectric laser accelerator structures. He has emerged as a leader in this field, having presented several invited talks on the subject as well as led or co-led two workshop working groups. He also has a great deal of experience using and developing the VORPAL electromagnetic simulation code.
- Mr. Durant is an expert in the development of SciDAC visualization software VisIt and in the use of VisIt for parallel 3D visualization of large data sets. He is also the lead developer of the VisIt-based graphical user interface for VORPAL, known as VorpalComposer.
- Dr. Mullowney is an expert in code development for GPU and other manycore architectures. He has implemented thread-safe charge and current deposition for PIC on the NVIDIA Fermi card, with significant speedup. He's also used VORPAL for many beam-related problems.
- Dr. Paul is an expert in beam dynamics for muon cooling channels and the modeling of inverse cyclotrons for the capture, cooling and reacceleration of high-emittance muon beams. He has also used VORPAL for parallel laser-plasma simulations.
- Dr. Schwartz has extensive experience with design and characterization of wavelength-scale optical materials and devices. He has developed algorithms for the design of optical metamaterials and has used simulations to find performance-optimized designs of image sensors with wavelength scale features.

- Dr. Veitzer brings significant experience in developing and using VORPAL, including extensive work on modeling rf diagnostics for measuring electron cloud effects. He has strong ties to researchers fielding electron cloud diagnostics at FNAL, LBNL and Cornell, which will be useful for coordination with ongoing rf electron cloud experiments.

We include annual three-day visits for three people to Fermilab, for project-wide collaboration. We will also collaborate on a weekly basis via the WebEx online service, which is covered by Tech-X overhead funds. The detailed budget is included within the required application forms.

Tech-X Corp. overhead rates are competitive with rates at other comparable small businesses. To ensure that all federal accounting procedures are followed, Tech-X has in its Controller's office individuals with extensive knowledge of federal requirements. Also, Tech-X contracts with an independent Certified Public Accountant who specializes in accounting services for small businesses with federal contracts. Tech-X was initially audited in 1999 by the Defense Contract Audit Agency (DCAA), which formally approved the Tech-X overhead rate structure and accounting practices. The most recent annual DCAA review and approval of Tech-X overhead rates occurred in December 2010, and the accounting system was most recently approved by DCAA in September, 2007.

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Tech-X Corporation ASCR				Budget Page No: 1	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR John R Cary				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applpicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. John R Cary 5%				13,115.00	
2. David L Bruhwiler 10%				16,296.00	
3. Estelle Cormier 12.5%				10,488.00	
4. Marc Durant 10.5%				8,947.00	
5. Paul J Mullowney 9.5%				8,500.00	
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (5) TOTAL SENIOR PERSONNEL (1-6)				57,346.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				57,346.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				18,265.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				75,611.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				1,383.00	
2. FOREIGN					
TOTAL TRAVEL				1,383.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				76,994.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Overhead base 75611 = 45556 G&A base 122550 = 17157 FEE base 45556 = 5293					
TOTAL INDIRECT COSTS				68,006.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				145,000.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				145,000.00	0.00

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Tech-X Corporation ASCR				**Budget Page No:** 2	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR John R Cary				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applpicant	by DOE
1. John R Cary 5%				13,380.00	
2. David L Bruhwiler 10%				16,621.00	
3. Estelle Cormier 12.5%				10,698.00	
4. Marc Durant 10.5%				9,126.00	
5. Paul J Mullowney 9.5%				8,670.00	
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (5) TOTAL SENIOR PERSONNEL (1-6)				58,495.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				58,495.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				18,630.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				77,125.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				1,469.00	
2. FOREIGN					
TOTAL TRAVEL				1,469.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				78,594.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Overhead base 77125 = 46467 G&A base 125059 = 17508 FEE base 77125 = 5399					
TOTAL INDIRECT COSTS				69,374.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				147,968.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				147,968.00	0.00

DOE F 4620.1

(04-93)

All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Tech-X Corporation ASCR				Budget Page No: 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR John R Cary				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applpicant	by DOE
1. John R Cary 5%				13,778.00	
2. David L Bruhwiler 10%				17,120.00	
3. Estelle Cormier 12.5%				11,020.00	
4. Marc Durant 10.5%				9,399.00	
5. Paul J Mullowney 9.5%				8,930.00	
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (5) TOTAL SENIOR PERSONNEL (1-6)				60,247.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				60,247.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				19,189.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				79,436.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				1,469.00	
2. FOREIGN					
TOTAL TRAVEL				1,469.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				80,905.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Overhead base 79436 = 47861 G&A base 128767 = 18027 FEE base 79436 = 5561					
TOTAL INDIRECT COSTS				71,449.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				152,354.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				152,354.00	0.00

DOE F 4620.1 (04-93) All Other Editions Are Obsolete	**U.S. Department of Energy** **Budget Page** (See reverse for Instructions)	OMB Control No. 1910-1400 OMB Burden Disclosure Statement on Reverse

ORGANIZATION Tech-X Corporation ASCR				**Budget Page No:**	4
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR John R Cary				Requested Duration:	summary-36 (Months)
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. John R Cary				40,273.00	
2. David L Bruhwiler				50,037.00	
3. Estelle Cormier				32,206.00	
4. Marc Durant				27,472.00	
5. Paul J Mullowney				26,100.00	
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (5) TOTAL SENIOR PERSONNEL (1-6)				176,088.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				176,088.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				56,084.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				232,172.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				4,321.00	
2. FOREIGN					
TOTAL TRAVEL				4,321.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				0.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				236,493.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Overhead G&A FEE					
TOTAL INDIRECT COSTS				208,829.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				445,322.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				445,322.00	0.00

"Community Project for Accelerator Science and Simulation"

DOE Funding Opportunity Number: DE-FOA-0000580
Tech-X Corporation – John Cary, Co-PI
Application Due Date: January 9, 2012

The budgeted direct costs for this project are primarily labor. Labor costs are based on significant past experience with research projects and on the nature and scope of the work being proposed for this particular project. Specifically, the budget includes time for the Co-PI, John Cary. Professor and CEO John Cary is an internationally known computational physicist and original architect of the VORPAL computational framework. He has more than 150 refereed journal articles and conference proceedings or presentations. He has significant experience and publication record in software development as well. Dr. Cary brings significant experience in several areas: a) project management, b) parallel computing, c) performance optimization, d) parallel visualization, e) electromagnetic modeling of superconducting rf (SRF) and dielectric structures, f) developing and working with the parallel VORPAL framework, and g) laser-plasma acceleration of electrons.

The other key personnel include David Bruhwiler, Estelle Cormier-Michel, Ben Cowan, Marc Durant, Paul Mullowney, Kevin Paul, Brian Schwartz and Seth Veitzer, all of whom are members of the VORPAL development team.

- Dr. Bruhwiler brings significant experience in developing algorithms within the parallel VORPAL framework and using them for laser-plasma simulations and other applications. He also has experience in beam dynamics with space charge, electrostatic and electromagnetic PIC modeling of beams and structures, parallel computing and project management.
- Dr. Cormier-Michel is an expert VORPAL developer, with an international reputation in laser plasma accelerator modeling. She has also used VisIt for an award winning 3D movie.
- Dr. Cowan brings significant expertise in designing and modeling dielectric laser accelerator structures. He has emerged as a leader in this field, having presented several invited talks on the subject as well as led or co-led two workshop working groups. He also has a great deal of experience using and developing the VORPAL electromagnetic simulation code.
- Mr. Durant is an expert in the development of SciDAC visualization software VisIt and in the use of VisIt for parallel 3D visualization of large data sets. He is also the lead developer of the VisIt-based graphical user interface for VORPAL, known as VorpalComposer.
- Dr. Mullowney is an expert in code development for GPU and other manycore architectures. He has implemented thread-safe charge and current deposition for PIC on the NVIDIA Fermi card, with significant speedup. He's also used VORPAL for many beam-related problems.
- Dr. Paul is an expert in beam dynamics for muon cooling channels and the modeling of inverse cyclotrons for the capture, cooling and reacceleration of high-emittance muon beams. He has also used VORPAL for parallel laser-plasma simulations.
- Dr. Schwartz has extensive experience with design and characterization of wavelength-scale optical materials and devices. He has developed algorithms for the design of optical metamaterials and has used simulations to find performance-optimized designs of image sensors with wavelength scale features.

- Dr. Veitzer brings significant experience in developing and using VORPAL, including extensive work on modeling rf diagnostics for measuring electron cloud effects. He has strong ties to researchers fielding electron cloud diagnostics at FNAL, LBNL and Cornell, which will be useful for coordination with ongoing rf electron cloud experiments.

We include annual three-day visits for three people to Fermilab, for project-wide collaboration. We will also collaborate on a weekly basis via the WebEx online service, which is covered by Tech-X overhead funds. The detailed budget is included within the required application forms.

Tech-X Corp. overhead rates are competitive with rates at other comparable small businesses. To ensure that all federal accounting procedures are followed, Tech-X has in its Controller's office individuals with extensive knowledge of federal requirements. Also, Tech-X contracts with an independent Certified Public Accountant who specializes in accounting services for small businesses with federal contracts. Tech-X was initially audited in 1999 by the Defense Contract Audit Agency (DCAA), which formally approved the Tech-X overhead rate structure and accounting practices. The most recent annual DCAA review and approval of Tech-X overhead rates occurred in December 2010, and the accounting system was most recently approved by DCAA in September, 2007.

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure Statement on Reverse

ORGANIZATION Regents of University of California				Budget Page No: 1	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Warren Mori				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. Mori, Warren					
2. Tsung, Frank	6.00			$41,400	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)	6.00			$41,400	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	12.00			$60,000	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$101,400	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$32,139	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$133,539	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$6,000	
2. FOREIGN				$3,000	
TOTAL TRAVEL				$9,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$1,817	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$1,000	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER- Telephone Infrastructure Fee				$748	
TOTAL OTHER DIRECT COSTS				$3,565	
H. TOTAL DIRECT COSTS (A THROUGH G)				$146,104	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Modified Total Direct Cost @ 26%. Base: $146,104					
TOTAL INDIRECT COSTS				$78,896	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$225,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$225,000	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Regents of University of California				**Budget Page No:** 2	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Warren Mori				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Mori, Warren					
2. Tsung, Frank	6.00			$42,228	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)	6.00			$42,228	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	12.00			$61,200	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$103,428	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$34,850	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$138,278	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$5,500	
2. FOREIGN				$2,500	
TOTAL TRAVEL				$8,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$1,000	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$1,000	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER- Telephone Infrastructure Fee				$748	
TOTAL OTHER DIRECT COSTS				$2,748	
H. TOTAL DIRECT COSTS (A THROUGH G)				$149,026	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Modified Total Direct Cost @ 26%. Base: $149,026					
TOTAL INDIRECT COSTS				$80,474	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$229,500	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$229,500	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Regents of University of California	**Budget Page No:** 3
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Warren Mori	Requested Duration: 12 (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Mori, Warren					
2. Tsung, Frank	6.00			$43,495	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)	6.00			$43,495	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	12.00			$63,036	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$106,531	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$38,026	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$144,557	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$5,000	
2. FOREIGN				$2,000	
TOTAL TRAVEL				$7,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$692	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$500	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER- Telephone Infrastructure Fee				$748	
TOTAL OTHER DIRECT COSTS				$1,940	
H. TOTAL DIRECT COSTS (A THROUGH G)				$153,497	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Modified Total Direct Cost @ 26%. Base: $153,497					
TOTAL INDIRECT COSTS				$82,888	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$236,385	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$236,385	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Regents of University of California				**Budget Page No:** 4	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Warren Mori				Requested Duration: 36 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Mori, Warren					
2. Tsung, Frank	18.00			$127,123	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)	18.00			$127,123	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	36.00			$184,236	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$311,359	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$105,015	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$416,374	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL — 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$16,500	
2. FOREIGN				$7,500	
TOTAL TRAVEL				$24,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$3,509	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$2,500	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER- Telephone Infrastructure Fee				$2,244	
TOTAL OTHER DIRECT COSTS				$8,253	
H. TOTAL DIRECT COSTS (A THROUGH G)				$448,627	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Modified Total Direct Cost @ 26%. Base: $448,627					
TOTAL INDIRECT COSTS				$242,258	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$690,885	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$690,885	

BUDGET JUSTIFICATION
UCLA

SALARIES AND BENEFITS

Funds are requested to support Co-PI Dr. Frank Tsung at 50% time for 12 months per year. Dr. Tsung is a research physicist. Funds will also support one Post doc at 100% time for 12 months per year. Salary costs include 2% cost of living and proposed merit increases for Year 2 and 3% cost of living for Year 3. The total in salaries for the three years is $311,359.

The benefit rate for Dr. Tsung is 38.5% and 27% for the Post doc. Benefit rate include a 2% increase each year.

SUPPLIES AND EXPENSES

Project related printing charges (including printer hardware), project supplies, tools and hardware incurred during year 1 estimated to be $1,817, $1000 for year 2 and $692 for year 3.

OTHER MISCELENEOUS EXPENSES

Publication cost is based on previous experience. We expect to publish two papers each year. The expected cost is $1,000 for year 1, $1,000 for year 2 and $500 for year 3.

The Technology Infrastructure Fee (TIF) is a consistently-applied direct charge that is assessed to each and every campus activity unit, regardless of funding source, including units identified as individual grant and contract awards. The TIF pays for campus communication services on the basis of a monthly accounting of actual usage data. These costs are charged as direct costs and are not recovered as indirect costs. The TIF charge is based on a full time employee (FTE) and is calculated at $41.58 per FTE per month. The cost is $2,244 for all three years.

TRAVEL

Funds are requested for domestic and foreign travel to participate in conferences and all hands project meetings to present our findings.

Domestic travel funds are requested to participate in two (2) 5 days domestic conferences and one (1) all hands project meeting each year for all 3 years. The cost per trip is $2000 including $600 for Airfare, Lodging & Meals at $140/day, Registration at $400 and Transportation at $300.

Foreign travel funds are requested to participate in one (1) 5 days international conference each year for all 3 years. The cost per trip is $3000 including $1200 for Airfare, Lodging & Meals at $180/day, Registration at $400 and Transportation at $500.

The total domestic and foreign travel cost for all three years is $24,000.

INDIRECT COST

Indirect costs have been applied to all direct costs except graduate student fee remissions, fabrication of specific experimental systems. Information on the UCLA – Federal Government Agreement can be found at website http://www.research.ucla.edu/ocga/sr2/idcinfo.htm. The current F&A Rate Agreement is dated April 27, 2011, and was negotiated with the Department of Health and Human Services (HHS) [Wallace Chan: 415-437-7820]. The cognizant Federal Audit Agency is HHS Office of Inspector General, Region IX, Office of Audit Services, 50 United Nations Plaza, San Francisco, CA 94102 [Lori Ahlstrand: 415-437-8360]. The on-campus Research rate currently in effect is 54%.

The total indirect cost is $242,258 for all three years for a total budget of $690,885.

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Regents of University of California				**Budget Page No:** 1	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Warren Mori				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Mori, Warren					
2. Decyk, Viktor	3.00			$39,150	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)	3.00			$39,150	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	6.00			$27,000	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$66,150	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$19,818	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$85,968	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$5,000	
2. FOREIGN					
TOTAL TRAVEL				$5,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$1,814	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$1,000	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER- Telephone Infrastructure Fee				$374	
TOTAL OTHER DIRECT COSTS				$3,188	
H. TOTAL DIRECT COSTS (A THROUGH G)				$94,156	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Modified Total Direct Cost @ 26%. Base: $94,156					
TOTAL INDIRECT COSTS				$50,844	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$145,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$145,000	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION Regents of University of California				Budget Page No: 2	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Warren Mori				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Mori, Warren					
2. Decyk, Viktor	3.00			$39,933	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)	3.00			$39,933	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	6.00			$27,540	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$67,473	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$21,564	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$89,037	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$4,500	
2. FOREIGN					
TOTAL TRAVEL				$4,500	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$1,128	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$1,000	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER- Telephone Infrastructure Fee				$374	
TOTAL OTHER DIRECT COSTS				$2,502	
H. TOTAL DIRECT COSTS (A THROUGH G)				$96,039	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Modified Total Direct Cost @ 26%. Base: $96,039					
TOTAL INDIRECT COSTS				$51,861	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$147,900	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$147,900	

DOE F 4620.1 (04-93) *All Other Editions Are Obsolete*	**U.S. Department of Energy** **Budget Page** (See reverse for Instructions)	OMB Control No. 1910-1400 OMB Burden Disclosure Statement on Reverse

ORGANIZATION Regents of University of California				Budget Page No: 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Warren Mori				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Mori, Warren					
2. Decyk, Viktor	3.00			$41,131	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)	3.00			$41,131	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	6.00			$28,366	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$69,497	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$23,600	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$93,097	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$4,000	
2. FOREIGN					
TOTAL TRAVEL				$4,000	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$649	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$800	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER- Telephone Infrastructure Fee				$374	
TOTAL OTHER DIRECT COSTS				$1,823	
H. TOTAL DIRECT COSTS (A THROUGH G)				$98,920	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Modified Total Direct Cost @ 26%. Base: $98,920					
TOTAL INDIRECT COSTS				$53,417	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$152,337	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$152,337	

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION: Regents of University of California

Budget Page No: 4

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR: Warren Mori

Requested Duration: 36 (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Mori, Warren					
2. Decyk, Viktor	9.00			$120,214	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)	9.00			$120,214	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (1) POST DOCTORAL ASSOCIATES	18.00			$82,906	
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$203,120	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$64,982	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$268,102	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$13,500	
2. FOREIGN					
TOTAL TRAVEL				$13,500	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST					
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$3,591	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$2,800	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER- Telephone Infrastructure Fee				$1,122	
TOTAL OTHER DIRECT COSTS				$7,513	
H. TOTAL DIRECT COSTS (A THROUGH G)				$289,115	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) Modified Total Direct Cost @ 26%. Base: $289,115					
TOTAL INDIRECT COSTS				$156,122	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$445,237	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				$445,237	

BUDGET JUSTIFICATION

SALARIES AND BENEFITS

Funds are requested to support Co-PI Dr. Viktor Decyk at 25% time for 12 months per year. Dr. Decyk is a research physicist. Funds will also support one Post doc at 50% time for 12 months per year. Salary costs include 2% cost of living and proposed merit increases for Year 2 and 3% cost of living for Year 3. The total in salaries for the three years is $203,120.

The benefit rate for Dr. Decyk is 32% and 27% for the Post doc. Benefit rate are increased by 2% each year.

SUPPLIES AND EXPENSES

Project related printing charges (including printer hardware), project supplies, tools and hardware incurred during year 1 estimated to be $1,814, $1,128 for year 2 and $649 for year 3.

OTHER MISCELENEOUS EXPENSES

Publication cost is based on previous experience. We expect to publish two papers each year. The expected cost is $1,000 for year 1, $1,000 for year 2 and $800 for year 3.

The Technology Infrastructure Fee (TIF) is a consistently-applied direct charge that is assessed to each and every campus activity unit, regardless of funding source, including units identified as individual grant and contract awards. The TIF pays for campus communication services on the basis of a monthly accounting of actual usage data. These costs are charged as direct costs and are not recovered as indirect costs. The TIF charge is based on a full time employee (FTE) and is calculated at $41.58 per FTE per month. The cost is $1,122 for all three years.

TRAVEL

Funds are requested for domestic travel to participate in conference meetings and present our findings.

Domestic travel funds are requested to participate in two (2) 5 days domestic conference each year. The cost per trip is $2500 including $700 for Airfare, Lodging & Meals at $150/day, Registration at $500 and Transportation at $550.

The total **domestic** travel cost for all three years is $13,500.

INDIRECT COST

Indirect costs have been applied to all direct costs except graduate student fee remissions, fabrication of specific experimental systems. Information on the UCLA – Federal Government Agreement can be found at website http://www.research.ucla.edu/ocga/sr2/idcinfo.htm. The current F&A Rate Agreement is dated April 27, 2011, and was negotiated with the Department of Health and Human Services (HHS) [Wallace Chan: 415-437-7820]. The cognizant Federal Audit Agency is HHS Office of Inspector General, Region IX, Office of Audit Services, 50 United Nations Plaza, San Francisco, CA 94102 [Lori Ahlstrand: 415-437-8360]. The on-campus Research rate currently in effect is 54%.

The total indirect cost is $156,122 for all three years for a total budget of $445,237.

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy
Budget Page
Community Project for Accelerator Science and Simulation

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION The University of Texas at Austin				Budget Page No: 1	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Ernesto Esteves Prudencio				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applpicant	by DOE
1. PI	2.50			21,658.00	
2. Postdoctoral Fellow	6.25			29,688.00	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)				51,346.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				51,346.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				12,837.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				64,183.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				11,000.00	
2. FOREIGN					
TOTAL TRAVEL				11,000.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				2,500.00	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				2,500.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				77,683.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 54% of TDC					
TOTAL INDIRECT COSTS				41,949.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				119,632.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				119,632.00	0.00

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

Community Project for Accelerator Science and Simulation

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION The University of Texas at Austin				**Budget Page No:** 2	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Ernesto Esteves Prudencio				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applpicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. PI	**2.50**			22,091.00	
2. Postdoctoral Fellow	**6.25**			30,282.00	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)				52,373.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				52,373.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				13,094.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				65,467.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				11,000.00	
2. FOREIGN					
TOTAL TRAVEL				11,000.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				1,500.00	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				1,500.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				77,967.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 54% of TDC					
TOTAL INDIRECT COSTS				42,102.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				120,069.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				120,069.00	0.00

DOE F 4620.1

(04-93)

All Other Editions Are Obsolete

U.S. Department of Energy

Budget Page

Community Project for Accelerator Science and Simulation

OMB Control No.

1910-1400

OMB Burden Disclosure

Statement on Reverse

ORGANIZATION The University of Texas at Austin

Budget Page No: 3

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Ernesto Esteves Prudencio

Requested Duration: 12 (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applpicant	Funds Granted by DOE
1. PI	**2.50**			22,754.00	
2. Postdoctoral Fellow	**6.25**			31,190.00	
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (2) TOTAL SENIOR PERSONNEL (1-6)				53,944.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				53,944.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**13,487.00**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				**67,431.00**	**0.00**
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				11,000.00	
2. FOREIGN					
TOTAL TRAVEL				11,000.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				1,500.00	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER					
TOTAL OTHER DIRECT COSTS				1,500.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				79,931.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 54% of TDC					
TOTAL INDIRECT COSTS				43,163.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				123,094.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				123,094.00	0.00

DOE F 4620.1
(04-93)
All Other Editions Are Obsolete

U.S. Department of Energy

Cumulative Budget Page

Community Project for Accelerator Science and Simulation

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION The University of Texas at Austin				**Budget Page No:** 4		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Ernesto Esteves Prudencio				Requested Duration: 36 (Months)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted	
	CAL	ACAD	SUMR	by Applpicant	by DOE	
1. PI	**7.50**			66,503.00		
2. Postdoctoral Fellow	**18.75**			91,160.00		
3.						
4.						
5.						
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)						
7. (2) TOTAL SENIOR PERSONNEL (1-6)				**157,663.00**	0.00	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. ( ) POST DOCTORAL ASSOCIATES						
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)						
3. ( ) GRADUATE STUDENTS						
4. ( ) UNDERGRADUATE STUDENTS						
5. ( ) SECRETARIAL - CLERICAL						
6. ( ) OTHER						
TOTAL SALARIES AND WAGES (A+B)				157,663.00	0.00	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**39,418.00**		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				**197,081.00**	**0.00**	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				33,000.00		
2. FOREIGN						
TOTAL TRAVEL				33,000.00	0.00	
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00	
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES				**5,500.00**		
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES						
5. SUBCONTRACTS						
6. OTHER						
TOTAL OTHER DIRECT COSTS				5,500.00	0.00	
H. TOTAL DIRECT COSTS (A THROUGH G)				235,581.00	0.00	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 54% of TDC						
TOTAL INDIRECT COSTS				127,214.00		
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				362,795.00	0.00	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
L. TOTAL COST OF PROJECT (J+K)				362,795.00	**0.00**	

UT Austin Budget Justification (Version December 13, 2011)

Project Title: Community Project for Accelerator Science and Simulation

DOE/Office of Science Program Offices:
Office of High Energy Physics (HEP)
Office of Advanced Scientific Computing Research (ASCR)

Funding Opportunity Number: DE-FOA-0000580

The budget breakdown for the UT Austin portion of this three-year research project follows.

Salaries:
We are requesting 2.5 calendar months of support per year for Dr. Ernesto Esteves Prudencio, the PI (base annual salary of $103,950), and 6.25 months of support per year for a postdoctoral fellow (base annual salary of $57,000.00). We are requesting 2% salary increase for Year 2 and 3% salary increase for year 3. Salaries are based on current salary figures.

Fringe benefits:
Budgeted at 25% for all personnel. Grants and Contracts awards are responsible for the actual fringe benefits incurred by each employee. Fringe benefits costs have been calculated based on historical data. Actual costs for fringe benefits are charged (billed) to the sponsored project at the time the cost is incurred, based on salary, selected benefits package and other variables applicable to the individual employee.

Travel:
We are requesting $6,000 per year for four trips of UT Austin researchers to other institutions also participating in the research project, as well as to annual project meetings, each trip having a duration of three to four days. The meeting budget will cover air ticket, parking, hotel, taxi, rental car, and per diem. We are also requesting $5,000 per year for two trips of UT Austin researchers to conferences in USA, each trip having a duration of five days in the conference city. The conference budget will cover registration fee, air ticket, parking, hotel, taxi, rental car, and per diem.

Materials and Supplies:
We are requesting $2,000 in the first year for a notebook for the post-doc; $500 per year for years 1 and 2, for books. We are also requesting $1,000.00 per year, for years 2 and 3, for journal submissions of research results produced by this project. All materials and supplies will be allocable and needed for this project only. We will have free-of-charge accounts on UT Austin and National Laboratories' supercomputers.

Indirect Costs:
Based on 54% of eligible direct costs per current UT Austin indirect cost policy.

Contents

Community Project for Accelerator Science and Simulation

Lead Institution: Fermi National Accelerator Laboratory
Principal Investigator: Panagiotis Spentzouris
M.S. 203, P.O. Box 500, Batavia, IL 60510
phone: (630) 840-4342; email: spentz@fnal.gov

Co-PIs: J. Cary (TechX), W. Mori (UCLA), C. Ng (SLAC), E. Ng (LBNL), B. Norris (ANL), E. Prudencio (UT Austin)

Senior Researchers: J. Amundson (FNAL), D. Bruhwiler (TechX), P. Colella (LBNL), V. Decyk (UCLA), C. Geddes (LBNL), X.S. Li (LBNL), T. Munson (ANL), J. Qiang (LBNL), E. Stern (FNAL), F. Tsung (UCLA), J-L. Vay (LBNL), S. Wild (ANL), C. Yang (LBNL)

Project Summary

Particle accelerators are critical to scientific discovery both nationally and worldwide. The development and optimization of accelerators are essential for advancing our understanding of the fundamental properties of matter, energy, space and time. In the past ten years, the SciDAC program has produced accelerator modeling tools using high-performance computing (HPC), and these have been employed to tackle some of the most difficult accelerator science problems. These codes obtain good scalability and parallel performance efficiency to several tens of thousands of processors.

In the next decade, the high-energy physics (HEP) community will explore the intensity frontier of particle physics by designing high intensity proton sources for neutrino physics and rare process searches, as well as high intensity muon sources for neutrino physics. It will also be exploring the energy frontier of particle physics by operating the Large Hadron Collider, developing novel concepts and technologies necessary for the design of the next lepton collider, and undertaking R&D for new acceleration technologies.

The proposed project will develop the HPC tools and applications necessary to design Project X, the proposed proton driver at Fermilab, the next lepton collider, with either electron or muon beams, and with either conventional or advanced (plasma, dielectric structure) acceleration technology, and perform R&D at FACET and BELLA. It will build on the successful HPC accelerator modeling tools developed under SciDAC1 and SciDAC2 and augment and evolve them so they can drive and support the accelerator science required for the above applications.

1 HPC Modeling Advances Accelerator Science

The U.S. Department of Energy (DOE)'s Office of High Energy Physics (HEP) promotes a broad, long-term particle physics program by supporting current operations and experiments and research as well as development for future facilities and experiments at three interrelated frontiers of particle physics [1].

- The Energy Frontier directly explores the fundamental constituents and architecture of the universe.
- The Intensity Frontier offers a second, unique investigation of fundamental interactions, accessed via a combination of intense particle beams and highly sensitive detectors,
- The Cosmic Frontier reveals the nature of dark matter and dark energy by using particles from space to explore new phenomena.

These scientific frontiers form an interlocking framework that addresses fundamental questions about the laws of nature and the cosmos. The development and deployment of high-performance-computing (HPC) modeling capabilities is essential to meeting these grand scientific HEP challenges because it enables and catalyzes advancement in accelerator science.

Particle accelerators are critical to scientific discovery in the United States DOE program and indeed the world. Of the 28 facilities listed in the DOE report "Facilities for the Future of Science: A Twenty-Year Outlook", 14 involve accelerators [2]. The development and optimization of accelerators are essential for advancing our understanding of the fundamental properties of matter, energy, space, and time, directly in two out of the three frontiers supported by the HEP program and indirectly in the third (the Cosmic Frontier, where scientific advances depend critically on auxiliary measurements performed using accelerators). Modeling of accelerator components and simulation of beam dynamics are necessary for understanding and optimizing the performance of existing accelerators, for optimizing the design and cost effectiveness of future accelerators, and for discovering and developing new acceleration techniques and technologies.

1.1 Science Challenges and Research Needs

In the next decade, the HEP community will explore the intensity frontier by designing high intensity proton sources for neutrino physics and rare process searches, such as the Project X accelerator at Fermilab, and designing high intensity muon sources for neutrino factories. It will also be exploring the energy frontier by operating the Large Hadron Collider (LHC), developing novel concepts and technologies necessary for the design of the next lepton collider, and, through operating facilities such as BELLA and FACET, undertake R&D for new acceleration technologies.

To enable the realization of the above efforts, we need to support a world-class research and development program to develop new accelerator technologies and scientific approaches, such as

- superconducting technology and accelerator structure design
- accelerator techniques and beam dynamic concepts to control beam losses in high intensity proton sources
- high-gradient normal conducting rf technology
- advanced materials capable of revolutionary increases in breakdown voltages
- muon-based accelerator components and muon cooling concepts
- ultra-high gradient laser wakefield and plasma wakefield accelerator structures.

1.2 Identification

The design, cost optimization, and successful operation of modern accelerators, such as those described above, require the optimization of many parameters, and the understanding and control of many physics processes. This can only be accomplished by employing high fidelity computational accelerator models that efficiently utilize high-performance-computing (HPC) resources. A representation of current HPC accelerator modeling capabilities can be obtained by reviewing the capabilities developed under the Scientific Discovery through Advanced Computing (SciDAC) Accelerator Science and Technology (AST) project (under SciDAC1), and those currently being developed and deployed by the Community Petascale Project for Accelerator Science and Simulation (ComPASS) project (under SciDAC2). The ComPASS codes obtain good scalability and parallel efficiency on thousands to hundreds of thousands of processors and are routinely used to perform single-physics, single-scale simulations on a few thousand processors.

Figure 1: Plasma-based accelerator publications utilizing ComPASS tools.

1.3 Past Accomplishments

In the past nine years, funded by the SciDAC program, the AST project, and its successor, ComPASS [3], have developed a powerful suite of HPC simulation tools which have enabled large scale multi-scale, multi-physics simulations of the most challenging accelerator science projects. The ComPASS collaboration (`https://compass.fnal.gov`) has deployed an HPC accelerator modeling environment for realistic, inclusive simulation of beam dynamics effects (single and multi-particle dynamics, realistic geometry and parameters), and a prototyping environment for realistic simulation of all relevant accelerator component effects (thermal, mechanical, and electromagnetic properties with accurate geometry description). During this nine year period, HPC tools have been applied to major HEP accelerator facilities and future accelerator projects including the Tevatron, PEP-II, LHC, Next Linear Collider (NLC), International Linear Collider (ILC), Project X, and plasma-based acceleration experiments. In the latter case they played a key role in understanding the physics of doubling the energy of a 42 GeV beam at the Stanford Linear Accelerator Center and of low-energy-spread beam production in laser wakefield accelerators. In addition, ComPASS applications have enabled advances in many DOE accelerator facilities and projects outside HEP, such as the Relativistic Heavy Ion Collider (RHIC), the Spallation Neutron Source (SNS), the Linac Coherent Light Source (LCLS), and designs for an electron ion collider.

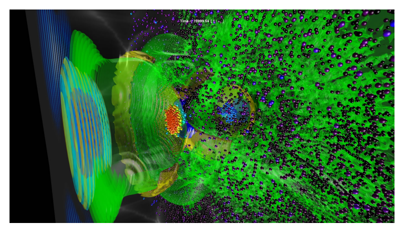

Figure 2: OSIRIS simulation showing the laser pulse (blue and red) driving a plasma wave (red, yellow, and blue), and a subset of the particles, colored by their energy, revealing particle accumulation at the back of the bucket.

There are many success stories of applications utilizing the SciDAC-developed tools that demonstrate the impact of large scale simulations in accelerator science [4]. Here we discuss only a few representative examples, to demonstrate the impact of our codes and applications in different accelerator science domains. Simulations performed with the Synergia framework were used to study emittance growth and beam halo generation in the Fermilab Booster. The model enabled the first-ever simulation of linac microbunch capture, debunching, and acceleration, including beam position feedback, three-dimensional space-charge [157], and multi-bunch impedance effects [145]. These simulations provided guidance to machine operators to reduce losses and maximize intensity and to commission the Booster collimators, which were essential to the success of the neutrino program during the Tevatron Run II. Another example of an application that helped maximize the reach of US HEP experiments is the study of beam-beam and impedance effects at the FNAL Tevatron performed with the BeamBeam3D code. These simulations provided guidance for finding the optimal Tevatron chromaticity setting and helped to increase Tevatron luminosity and minimize losses [150]. Advanced accelerator R&D is another high-impact area for large-scale simulation applications leading to scientific discovery. The accomplishments of the HPC plasma and laser wakefield simulation efforts have led to many publications, including results highlighted in journals such as Science, Nature, and Physical Review Letters, see [8] and Fig. 1. Applications of the OSIRIS, QuickPIC, VORPAL and Warp codes successfully modeled the major U.S. plasma-based accelerator experiments at SLAC and LBNL, and developed key physics understanding of plasma wakefield acceleration (PWFA) and laser wakefield acceleration (LWFA) in the nonlinear blowout regime(see Fig. 2). In some cases, the simulations predicted important effects in plasma acceleration, helping guide the design of the experiments. (for example, the LWFA LOASIS experiment, see Fig. 3) We also applied the ComPASS codes to the design of next-generation lepton collider concepts. Omega3P was used for an end-to-end simulation of the ILC cryomodule consisting of 8 connected superconducting (SRF) cavities. The first-ever calculations of higher-order-modes (HOM) were carried out and provided direct comparison with data measured at the FLASH facility at DESY. The results indicated a strong coupling for beam dynamics in the horizontal and vertical directions. Detailed analysis also showed that the damping factors of HOMs varied among the cavities in the cryomodule due to cavity imperfections [9]. Using measured cavity parameters as inputs, the deformed cavity shape was recovered by solving the inverse problem through an optimization method. The same method was later used to identify the cause of beam breakup in the CEBAF 12-GeV upgrade prototype cryomodule [10, 11]. This is just one example of the applicability of our simulation tools across DOE accelerator facilities, exemplifying HEP stewardship in accelerator science.

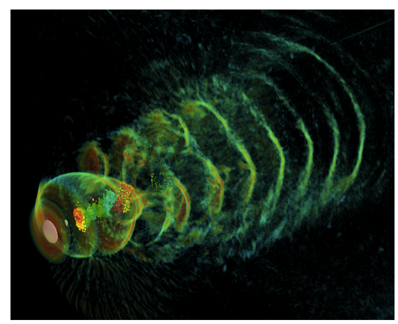

Figure 3: VORPAL simulation showing density wake from a laser pulse in a hydrogen plasma, overlaid with high-energy particles, colored by their momentum.

1.4 Budget and Project Deliverables Overview

The total budget of our proposed work is $2.565M for HEP accelerator science deliverables and the necessary ASCR support for applied mathematics, computer science and uncertainty quantification (UQ). Our proposal involves seven institutions: four national labs, two universities, and one private research company, thus also contributing to the education of new computational scientists and technology transfer. It achieves synergism through strong connections to other projects (see section 5) and efficiency through integration of the different scientific areas required for the success of our program. Our applications cover both HEP frontiers directly related to accelerator science, the energy (section 2) and the intensity (section 3) frontiers, with math, computer science and UQ activities (section 4) that span all applications. We propose $680K for energy frontier applications, aiming to support and drive the research for new technologies (plasma, dielectric, high-gradient rf), $615k for intensity frontier applications (Project X, FNAL proton source, and Project X to muon collider interface, an application that will impact both frontiers), and $1270K for math, computer science and UQ activities that are aimed to algorithmic and infrastructure development that impacts various application areas (Particle-In-Cell, Linear Algebra, performance, and data and visualization). The detailed budgets for these activities are shown in the institutional budget pages and the corresponding statements of work in Appendix B.

2 Energy Frontier

A primary driver for developing new accelerator technology is colliding fundamental particles at the energy frontier. Such accelerators are some of the most expensive machines and tools for scientific discovery in existence. These tools are not only expensive, but they are complex and large. For example, the LHC is close to 30 kilometers in circumference and cost over 10 billion dollars to build. Designing and developing a new accelerator or upgrading an existing one is not only time consuming but is also expensive. It is becoming more evident that the next accelerator at the energy frontier will rely on a new accelerator technology that provides significantly higher gradients and/or a new paradigm such as colliding muons. Because such machines are so complex and expensive to build, computer simulations will undoubtedly play a significant role in discovering a new technology, in studying parameters not yet accessible in a laboratory, and in reducing the time and cost it takes from the conceptual design of an accelerator to operation.

Presently, there are three new technologies and/or paradigms being considered for a new accelerator at the energy frontier. These are plasma based acceleration, dielectric loaded structures, and a muon collider. ComPASS codes and ComPASS researchers have been at the forefront of this research. In this section the status of each is described as well as exciting areas for proposed work.

2.1 Plasma-based acceleration

A leading concept for reducing the size and cost of lepton accelerators at the energy frontier is plasma-based acceleration, [12], [13], [14] where particle space charge forces or radiation pressure from an intense laser pulse drives a plasma wake. The phase velocity of the wake equals the velocity of the driver, which is close to the speed of light, c. Electrons or positrons can be trapped and accelerated with electric field gradients exceeding 50 GeV/m, roughly 1000 times greater than conventional RF accelerator technology. This is called laser wakefield acceleration (LWFA)[12] or more recently laser-plasma acceleration (LPA) for laser-driven accelerators, and plasma wakefield acceleration (PWFA) [13] for the beam-driven case.

Plasma-based acceleration is a rapidly advancing field. For example, PWFA experiments have shown that 50 GeV/m wakefields can be excited over meter-scale pump depletion distances [15]. LPA experiments have produced GeV electron beams in cm-scale distances with good properties [16]. Computer simulations using ComPASS codes supported these experimental successes. These simulations have in some cases modeled the experimental parameters one-to-one in three dimensions and they have also been used to test new ideas, to help design the recently funded FACET and BELLA facilities, and to examine collider concepts based on staging plasma wakefield sections.

The ComPASS codes OSIRIS, VORPAL, QuickPIC and Warp contain all of the current state-of-the-art techniques and algorithms for modeling plasma-based acceleration including the best reduced models. The codes continue to improve in the areas of numerical algorithms, single core performance and parallelization efficiency. New algorithms and ideas developed by the ComPASS team are speeding up simulations further, including the use and further development of reduced models. Much of this work was done under the SciDAC program including the current ComPASS project. New computing hardware (and software developed specifically for that hardware), together with improved algorithms and workflows, could lead to simulations being used for real-time steering of experiments. They could also be used with parallel global optimization algorithms to find optimal laser and particle beam profiles, or to virtually integrate plasma stages with other components in a complex accelerator. The ComPASS codes are very complex and varied. They have also been benchmarked against each other in some test cases.

The ComPASS codes used for plasma-based acceleration scale very well on leadership class facilities. For example, OSIRIS was chosen by the DOE Office of Advanced Scientific Computing Research to be featured in their software effectiveness program. As part of this program, OSIRIS was shown to scale well to the full Jaguar machine (220,000 cores) for strong scaling studies using both test and physics problems. It demonstrated high parallel scalability as well as single core efficiency (through the use of the SSE vector units). For example, on a 3D problem with excellent load balance it achieved .736 PFlops (30% of peak speed). Load imbalance was found to the largest roadblock to strong scaling when modeling LWFA.

To accurately simulate plasma wakefield excitation, one needs to model how a short and intense driver evolves over "large" distances, how the wake is excited and how it evolves, and how the properties of the witness beams evolve as they are trapped and accelerated. In many cases, the excitation of the wake is nonlinear so a particle or kinetic description is needed. The leading kinetic description is the particle-in-cell (PIC) method [17]. In some cases fluid models for the plasma response are useful. There is now a well established hierarchy of methods for modeling plasma based acceleration (many developed within SciDAC). The most "complete" method is the fully explicit, full Maxwell solver, fully relativistic, PIC method. In this method, a large number of charged macro-particles are followed self-consistently with their own electromagnetic fields. Interpolations are performed between the Lagrangian particles positions and momenta and the fields gridded quantities. The ComPASS codes vary in their implementation for parallelization, single core optimization, current deposition, field interpolation, high-order particle shapes, boundary conditions, initialization techniques, and diagnostics.

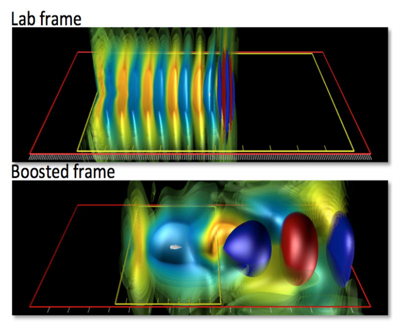

Figure 4: Warp scaled LWFA simulations in the lab (top) and boosted (bottom) frames: laser pulse in blue/red; plasma wakefield in pale blue/yellow.

A method was recently proposed to speed up full PIC simulations by performing the calculation in a Lorentz boosted frame [18], taking advantage of the properties of space/time contraction and dilation of special relativity to render space and time scales (that are separated by orders of magnitude in the laboratory frame) commensurate in a Lorentz boosted frame, resulting in far fewer computer operations (see Fig. 4). The ability to use the technique has been implemented into several ComPASS codes and was used to study stages where the laser is deeply depleted in the weakly nonlinear regime up to 1 TeV [19] and to study the nonlinear bubble regime up to 50 GeV [20]. In the ponderomotive guiding center (PGC) approximation [21], [22], the laser pulse is separated into a central frequency and an "envelope", which is a complex number describing the pulse shape and length. Only the evolution of the envelope is calculated. When advancing the particles, one uses a ponderomotive (i.e. light pressure) force from the laser pulse (permitting larger cells and time steps), together with the self-consistent wakefields. One cannot resolve the wide broadening of the laser spectrum in a strongly depleted laser pulse, but recent progress has lead to some improvements [23]. The quasi-static approximation [21], [24] allows even larger time steps by treating the laser or particle beam driver as static over a single transit time of the surrounding plasma. One calculates the wake for a given driver shape, then uses the potentials and fields of the wake to advance the laser pulse or particle beam forward with very large time steps. For a laser driver this builds on the PGC method. Theoretically this is the fastest method. It is used extensively to model PWFA. More work on the envelope solver will be need to achieve the theoretical speedups for LWFA. However, this technique does not model self-injection. This technique has been used to study how LWFA scales to 100 GeV energies[25], [26] and 25 - 1 TeV PWFA stages [15], [27], [28]. These reduced models have relative advantages and disadvantages depending on the choice of parameters. Uncertainty quantification (see below) will be used to better quantify the merits of various numerical and reduced model choices.

We next describe specific areas of emphasis for LWFA and PWFA.

Laser driven plasma wakefield acceleration

The goal is to design laser plasma accelerator stages in both nonlinear, weakly nonlinear, and quasi-linear regimes with an emphasis to support the BELLA project at LBNL and experiments at other facilities such as LLNL. Common issues include electron beam injection, stable laser propagation over many Rayleigh lengths, dephasing, efficient laser-plasma coupling, efficient beam loading, and staging. Another goal is to extrapolate the simulations to parameter regimes that are currently inaccessible to experiments.

The goal of the BELLA project is to demonstrate efficient acceleration of an electron beam to 10 GeV in a meter-long plasma in the quasi-linear regime. The ultimate goal is to string many of these stages together to produce a TeV beam. By using a similar approach for positron beam, it is projected to build a collider entirely based on laser plasma accelerators. Some of the side challenges to this project are to inject a high quality beam in the first stage of the plasma accelerator and provide coupling between stages which is short enough to keep the collider small and hence relatively inexpensive. Other experiments such as those done in a collaboration between UCLA and LLNL [29] are aimed more at studying LWFA in a nonlinear regime for accelerating electrons including the possibility of self-guiding.

Modeling LWFA requires understanding how the laser couples to the plasma, how a witness beam is accelerated with high efficiency while maintaining beam quality, and how to inject electrons into a wakefield structure. Different injector ideas are currently pursued both theoretically and experimentally and need to be optimized through simulations. Current methods being explored include injection from tailored plasma density, injection through colliding laser pulses and injection via ionization of high Z gases. Exploration of these different methods with simulations will determine which beam properties we can obtain and how sensitive the method is to variations in the system.

Simulations will be performed in order to optimize efficiency in BELLA stages. The goal is to accelerate over pump depletion distances and to optimize the amount of charge accelerated, energy gain and minimize the emittance of the beam. This will include exploring the effects of longitudinal tailoring of the plasma profile and tailoring of the laser pulse shape by using higher order Gaussian modes. Simulations will also be performed to model the joint UCLA/LLNL experiments (and other 100+ TW facilities) in which the goal is to generate mono-energetic electrons at 1-2 GeV energies using self-guiding.

In addition, simulations will be performed using parameters that are currently not accessible. This will include studying staging, the optimum particle beam shape, laser pulse shape, and axial plasma profile to optimize the overall efficiency and beam quality. One also needs high fidelity codes that can be used to develop beam loading scenarios in which 100 pC to 1 nC of electrons and positrons are accelerated over meter or longer distances while maintaining excellent beam quality. In addition, when modeling TeV energies radiation damping will need to be included for some beam loading scenarios. There is much overlap between LWFA and PWFA in the need and code requirements for developing beam loading scenarios. In order to study staging we will need to allow output from ComPASS plasma-based accelerator codes and beam dynamics codes to be used as input to each other.

Beam driven wakefield acceleration

The goal is to study and design plasma wakefield stages driven by electron, positron, and proton beams. For example, there is a PWFA Linear Collider (PWFA-LC) [30] design that uses a conventional 25 GeV electron drive beam accelerator, to produce trains of drive bunches distributed in counter-propagating directions to >20 PWFA cells for both the electron and the positron arms of the collider to reach energy of >500 GeV for each beam. Each cell provides 25 GeV of energy to the main beam in about a meter of plasma. The layout and parameters were chosen to optimize PWFA performance while also providing feasible parameters at the interaction point and a practical design for the main beam injector and the drive beam acceleration and distribution system. The wakes are to be excited in a nonlinear or weakly nonlinear blow-out regime where if the plasma ions remain stationary a uniform ion column results which provides a linear focusing force and a radially independent focusing force for both the driving and accelerated electron beams. There is a small region in a weakly nonlinear wake that can both focus and accelerate positrons.

The work on PWFA driven by electron beams will be closely coupled to experiments at FACET. One of the highest priorities at FACET is to carry out a two bunch experiment in which a drive beam creates a wakefield and a trailing bunch has its energy doubled while maintaining its energy spread and emittance. The ComPASS codes will be also be used to study beam loading scenarios for PWFA-LC parameters for early and late stages in the 20 stage train. This will include researching optimal current profiles for both the drive and trailing beam and enhancing codes to handle very narrow trailing bunches to study beam loading scenarios.

In addition, there has been recent interest in using proton beams (anti-proton beams would be better but it would be difficult to provide such beams at the rep rate needed for a collider) [31] . Current proton beams have energies near 7 TeV and have total beam energy near 100 kJ. If such a bunch could be compressed to efficiently make a wakefield then a trailing electron bunch with more than a nC of charge could be accelerated in a single stage to nearly 1 TeV before dephasing occurs. Currently, no compressed bunches exist so experiments are being considered to study how a long proton bunch self-modulates as it propagates in a tenuous plasma. The physics behind how nonlinear wakefields that are produced by a proton (or a positron) bunch is not the same as for an electron bunch [32] because in one case the plasma electrons are blown out and in the other they are pulled in. ComPASS codes can be used to study how long proton bunches self-modulate (in space and in energy) and how externally injected electrons are accelerated to design near term experiments and to study how compressed bunches (which will not be available in the near term) drive wakes and accelerate trailing bunches. This area is ripe for scientific discovery. In addition, to design experiments one will need to couple the output of a beam dynamics code into a plasma code and to output the beam after it propagates through the plasma back into a beam dynamics code.

Goals for the next three years

To meet the goals described above, will require developing highly optimized quasi-static and full PIC codes that scale to 100,000+ cores and utilize dynamic load balancing. It requires algorithms that can handle cell sizes that are smaller in the transverse direction and can include radiation reaction. These types of simulations also require Maxwell solvers that minimize numerical dispersion and accurately model the betatron motion of accelerated electrons. Boosted frame and reduced model simulations will support parameter scans. Further development for using the boosted frame technique for handling self-injection and nonlinear regimes will be needed. Reduced models require accurate and improved envelope solvers for the laser. Quasi-static codes offer dramatic speed ups for both PWFA and LWFA modeling, but to reach their full potential they will require improvements and further optimization of the predictor corrector loop, and for LWFA modeling improvements in the envelope solver including pipelining of the laser solver.

We will also need to develop PIC algorithms that run on many-core and SIMD accelerators such as GPUs. In the foreseeable future, new computing platforms are likely to consist of a heterogeneous hierarchy of powerful shared memory multicore nodes, with some element of SIMD (vector) processors as part of their design, coupled together with traditional message passing networks. To prevent memory starvation, they will likely have lightweight threads which can hide memory latency. To meet this challenge for PIC codes, new data structures and algorithms will be required. New kernels have already been implemented for key elements of the PIC algorithm [33], [34]. For example, kernels for 2D electrostatic and electromagnetic codes have been tested on a NVIDIA Tesla C2050 and obtained complete loop timings of 1.5 ns/particle/step and 2.5 ns/particle/step respectively. Depending on the hardware these represent speed ups of 28-80. While current GPUs appear to offer the greatest acceleration, one should expect that not only will they evolve significantly but future many-core platforms will also evolve rapidly. As a result algorithms will need to be retuned regularly and should be parameterized as much as possible. In addition, load balancing can be a large problem when simulating nonlinear wakefields. In these wakefields the plasma electrons are blown out and then coalesce at the rear of the bubble. This region have a volume that is only a few cells cubed, leading to load imbalances of 10 or more when 50,000 cores are used (for typical problems). We will improve our codes to scale to large core counts by addressing this issue.

The deliverables for this activity are discussed below. Note that the priorities and activities may change depending on progress and needs.

Year 1. Use suite of ComPASS codes to design and model LWFA experiments at BELLA & LOASIS, UCLA LWFA experiments, PWFA experiments at FACET and possible proton PWFA experiments at FNAL. Explore how codes scale to 100,000+ cores. Explore load balancing strategies across codes. Explore optimization strategies for single node performance. Further investigate the capability of boosted frame for self-injection in plasma gradients and uniform plasmas.

Year 2. Use suite of ComPASS codes to design and model LWFA experiments at BELLA & LOASIS, UCLA LWFA experiments, PWFA experiments at FACET and possible proton PWFA experiments at FNAL. Study injection strategies. Model parameters of envisaged stages of PWFA and LWFA linear collider designs. Integrate beam dynamics and plasma code capability. Investigate and enhance envelope models across codes. Develop hybrid OpenMP/MPI strategies to ensure parallel scalability to 100,000+ cores on physics simulation including load balancing strategies across codes. Add new data structures where needed to run on many-core hardware. Explore the use of mesh refinement where needed. Optimize quasi-static algorithm.

Year 3. Continue to use the suite of ComPASS codes to design and model LWFA experiments at BELLA & LOASIS, UCLA LWFA experiments, and PWFA experiments at FACET. Continue to model parameters of envisaged stages of PWFA and LWFA linear collider designs and model multiple stages. Optimize injection strategies. Experiment with and optimize load balancing strategies. Develop strategies for using codes to design optimized laser and particle beam profiles. Finish development of new envelope solvers. Pipeline the laser solver for quasi-static codes. Merge new algorithms and libraries from PIC applied math efforts into appropriate codes. Further explore mesh refinement.

2.2 Dielectric laser acceleration

A High-Energy Physics research effort is underway to develop particle accelerators based on laser-driven dielectric structures. Dielectric laser acceleration (DLA) structures have the potential of achieving $\sim$ GeV/m accelerating gradients because of the high breakdown threshold of dielectric materials at optical frequencies. Further, DLA structures can be powered with efficient, commercially-developed fiber lasers and can be manufactured at low cost, for instance with lithographic or fiber-drawing techniques. Several DLA topologies are under investigation including a 3D silicon woodpile photonic crystal waveguide and a 2D glass photonic bandgap (PBG) hollow-core optical fiber [35].

The modeling effort will touch on several critical aspects of DLAs. One is the design of efficient power couplers to transport energy from a conventional optical fiber into a complex accelerator structure, without interrupting the particle beam. Another is the understanding and mitigation of wakefield effects and the associated beam break-up concerns. Third, the material nonlinearities have an effect on the accelerator system and must be understood. Finally, achieving the beam quality needed for a collider requires optical injection, so low-beta structures that can accelerate to relativistic energies over many wavelengths must be designed.

Modeling dielectric structures is inherently complex. While the dimensions of a conventional conducting cavity are on the order of a wavelength in each direction, photonic crystal cavities must surround the defect by many lattice periods in each direction to be effective. Hence, the simulation domain for DLA structures is orders of magnitude larger than those required for conventional structures. Even for pure electromagnetic simulations, for instance coupler design, high-performance simulations are necessary. For understanding beam loading, and especially wakefields and beam breakup, a code that incorporates particles is required as well. In addition, parameter scans and optimization will be needed to achieve a design. The ComPASS project contains complementary codes for modeling this problem. The VORPAL computational framework primarily employs the FDTD method with embedded boundaries separating the vacuum and dielectric regions and uses stable, cell-averaging methods [36]. Frequencies are currently obtained using the filter diagonalization method [37]. The ACE3P computational application uses a finite-element approach, with elements aligned to the dielectric-vacuum interfaces. ACE3P uses an eigensolver for mode computations and a time domain solver for wakefield computations.

The ComPASS team has extensive experience in DLA modeling. The band gaps for commercial optical fibers have been computed and compared with beam test experiments [38]. The accelerating and radiated modes in the impedance spectrum have been computed. Appropriate directing of laser power from free space has demonstrated a first viable mechanism of coupling power into the optical fiber that can be achieved readily in an experimental setup [39]. Previous work [40] has shown how hybrid dielectric cavities can be optimized to minimize wakefields and radiative loss of the desired mode. Coupling optimizations have previously been done in Ref. [41]. Another approach is to determine the coupling efficiency using methods analogous to those used to match couplers in conventional microwave accelerators [42, 43], combined with previously developed shape optimization techniques [11].

The work plan and deliverables to meet these challenges is detailed below. General themes include extending the calculations for a structure length on the order of 100 accelerating mode wavelengths. This will allow accurate wakefield computations when some unwanted modes are attenuated due to their high radiation loss from the outer surface of the PBG fiber. Themes also include implementation of better computational algorithms suited to dielectric accelerators.

Year 1. Develop coupling mechanisms for efficient power transmission from laser to photonic structures (fiber and woodpile structure). Implement multi-mode waveguide boundary condition for inhomogeneous medium in ACE3P frequency domain solver. Implementing in VORPAL the complex-envelope FDTD algorithm for the narrow-band field excitations in the DLA structure. Conduct short-range wakefield simulations in both the woodpile and fiber DLA structures to assess the effects of wakefields on beam quality.

Year 2. Optimize coupling mechanisms for efficient power transmission from laser to photonic structures (fiber and woodpile structure). Determine wakefield and radiation in PBG fiber and woodpile structures and compare with measurements. Implement realistic dispersive and nonlinear material properties. Develop transfer map from self-consistent wakefield simulations.

Year 3. Optimize coupler designs for PBG and woodpile structures. Determine wakefield and radiation in woodpile structure and compare with measurements. Optimize the parallel performance of the complex-envelope FDTD algorithm and add GPU capability. Improve the performance of the algorithms for dispersive and nonlinear material response. Implement the model for beam propagation with wakefields in a tracking code to evaluate the effects of beam-breakup instability over a km-scale collider length.

2.3 High Gradient

In order to achieve high-gradient acceleration at room temperature towards a multi-TeV e+e- linear collider, a worldwide collaboration has been established for high-gradient R&D involving the development of new acceleration concepts and the design of various types of accelerator structures. A continuous 5-year plan for the high-gradient collaboration is being planned to further address the important issues crucial to the development of high-gradient accelerator structures [44]. The basic accelerator physics research includes the understanding of the gradient limit for structure operation without rf breakdown, and the suppression of wakefields through appropriate damping mechanisms to maintain beam quality in a linear collider.

The proposed Compact Linear Collider (CLIC) is based on a novel two-beam concept including a drive beam providing the acceleration power and a main beam to be accelerated [45]. A significant challenge facing the proposed two-beam accelerator is the issue of wakefields excited by the transit of an electron or positron bunch in the Power Extraction & Transfer Structure (PETS) of the drive beam linac and in the accelerator structures (AS) of the main beam linac. One overriding concern is the long-range wakefields that can result in cross coupling between the PETS and the accelerator structure and to quantify this effect is critical to the success of the two-beam accelerator scheme. ACE3P has been used for the first-ever simulation (see Fig. 5) of a CLIC coupled structure (1 PETS and 2 AS) and the results show stronger than expected dipole wakefield coupling [46]. Based on these findings, we propose to extend the simulation to numerically quantify this cross coupling accurately in the realistic 3D geometry of the entire system of the two-beam module (4 PETS and 8 AS) to understand the intricate phenomenon of wakefield coupling and to devise measures to mitigate the effect. Any possible trapped modes that can affect the beam quality will be identified in both the drive beam and main beam structures. Due to the tight tolerances required in the machine design, simulation will also help understand the effects of structure misalignments on the wakefields in the coupled structure.

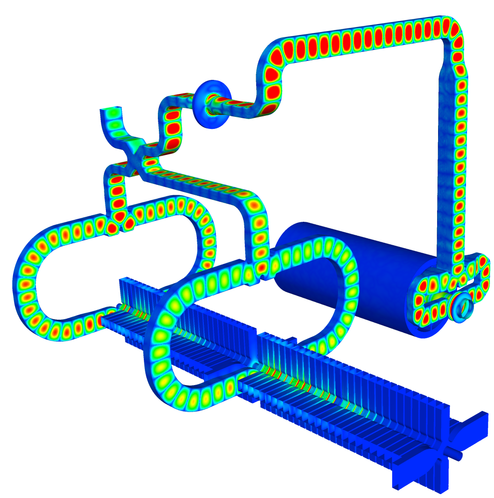

Figure 5: Snapshot of wakefield excited by a drive beam in a coupled structure consisting of a PETS and 2 accelerating structures connected by power coupling waveguides. Note that the two-beam rf module is 4 times the size of this coupled structure.

Another concern with the high gradient accelerator is the generation of dark current, which arises from field emissions of electrons from the surface of an accelerating structure and their subsequent movements whose trajectories are determined by the accelerating rf field. Dark current may lead to beam loading of the accelerator structure and, if captured, may also produce undesirable backgrounds downstream to the detector at the interaction point. Ongoing high-gradient structure tests have been carried out at KEK, CERN and SLAC [47], providing a useful and valuable validation of simulation results [48]. In particular, the field enhancement factor for field emission can be quantified by comparison with the measured energy spectrum of the dark current. Then the simulation effort will be extended to study the effects of dark current in the main beam section of the two-beam module. The capture of dark current downstream may take a long distance that can involve multiple modules, and therefore large-scale simulation is essential to providing insights for the design of the machine. The deliverables are

Year 1 Evaluate beam energy spread and beam loading compensation in a coupled system consisting of a PETS and an AS. Model wakefields in a coupled two-beam system (1 PETS, 2 AS).

Year 2 Evaluate trapped modes in drive beam section and in main beam section of a two-beam module. Simulate wakefield effects in one half of a two-beam module (2 PETS, 4 AS).

Year 3 Model wakefield effects in an entire two-beam module. Simulate dark current effects in main beam section of a two-beam module.

3 Intensity Frontier

The Intensity Frontier (IF) addresses central questions in particle physics that are not directly accessible with current or planned accelerators at the Energy Frontier. Experiments at the IF study rare processes that indirectly probe higher mass scales and exotic physics using intense beams of particles such as neutrinos, muons, kaons and nuclei, providing powerful probes of new phenomena. In the US, the key to long-term leadership at the IF is Project X, a multi-megawatt proton accelerator, that will produce intense beams of neutrinos, muon, and kaons, as well as heavy nuclei. Project X can be coupled to a muon storage ring leading to a neutrino factory, and, ultimately, could be used as the driver for a muon collider, thus extending its importance to the Energy Frontier. ComPASS codes and researchers have been involved in the accelerator science activities necessary to enable the IF program in both the near future (evolving the existing FNAL accelerator complex) and the long-term future (with Project X). In this section we describe our proposed work in this exciting area of accelerator science.

3.1 Fermilab Proton Improvement Plan

Every proton for the domestic United States high energy physics experimental program will be accelerated by the existing, now 40-year-old, Fermilab Linac and Booster until new machines become operational to replace them. The leading replacement candidate, the proposed Fermilab Project X accelerator, is anticipated for completion no sooner than 2020, to serve demands for beams at 3 GeV and lower energy, and no sooner than well into the next decade to serve demand for beams at higher energy. The domestic high energy physics program for the next 15 years is dependent on the viability and vitality of the Fermilab Linac and Booster. Fermilab has established a charge for developing a plan to assure this viability and vitality. Specifically, the charge calls for "delivering 1.8×10^{17} protons/hour (cycling the machine at 12 Hz) by May 1, 2013" and "delivering 2.25×10^{17} protons/hour (at 15 Hz) by January 1, 2016" (more than 2 times the beam rate in current operations) while "ensuring a useful operating life of the proton source through 2025" [49, 50].

Booster intensities and repetition rate are currently limited by radiation due to uncontrolled losses. These losses are a problem both because of prompt radiation levels and equipment activation. To reach the above goals, an improved collimation system must be implemented to limit losses to acceptable levels. We will provide simulations in support of this effort.

Two intensity-dependent effects are important in the Fermilab Booster: space charge and wake fields in the laminated quadrupole magnets. During SciDAC2, we developed a detailed model of wake fields in laminated structures in Synergia and validated it with experimental results (Fig. 6 and Reference [145]). The wake field and space charge calculations are inherently coupled through

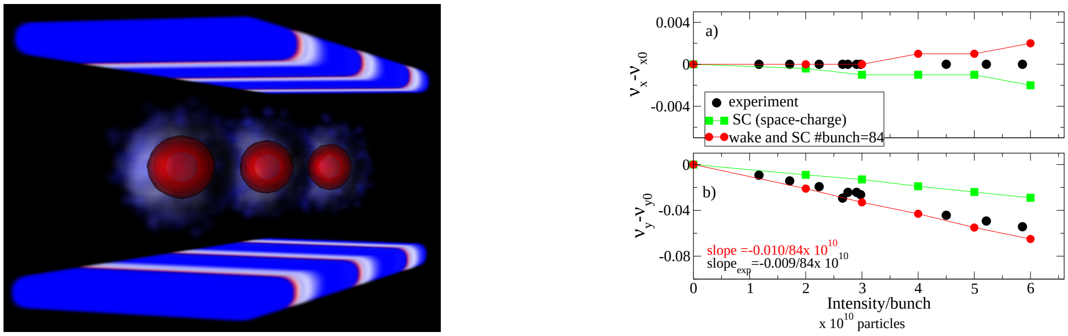

Figure 6: *Left*: Wakefields induced in parallel planes by multiple beam bunches. *Right*: Coherent horizontal (a) and vertical (b) tune shift versus beam intensity. The vertical tune is decreased while the horizontal tune changes very little. The calculation are in good agreement with the experiment, the deviation being within $3\sigma_{meas}$.

the boundary conditions in the space charge field, so our model has to include space charge with compatible boundary conditions. Wake fields link motions of particles within a bunch as well as coupling bunch to bunch motion. We will study both effects. Since collective effects are most important at the lower injection energy, all of our initial simulations will take place at the injection energy. Our later simulations will expand to consider higher energies in the Booster cycle. Our work plan is summarized below.

Year 1. Detailed booster model including space charge, single-bunch wakefields and detailed optics derived from studies, including apertures. Compare simulations to data from beam studies, validate/improve model.

Year 2. Simulations expanded to include multi-bunch effects. Perform simultaneous simulations of all 84 booster bunches. Compare simulations to data from beam studies, validate/improve model. Develop model of collimators and integrate into simulation.

Year 3. Complete simulations with collimators and 84 bunches. Include accelerating phase of booster cycle. Perform simulations at higher energies, especially in the vicinity of transition.

3.2 Fermilab Main Injector at 2MW

In the Project X era the Fermilab Main Injector (MI) will be the driver for the higher-energy portion of the physics program at the intensity frontier. In the near term, this includes the production of intense neutrino and antineutrino beams for the detailed study of oscillation parameters. Longer time-scale plans envision production of muon beams for a neutrino factory and a muon collider. Space-charge and electron cloud effects are expected to play a significant role in limiting the performance of the machine. It is essential to understand these effects in order to minimize losses and maximize the effectiveness of the mitigation systems. With this activity we will provide the necessary guidance for designing such systems, especially the collimator and rf systems.

Electron Cloud

Electron clouds can be formed in particle accelerators under conditions where there is a source to seed the cloud formation and a mechanism to amplify the production of electrons [51]. Seeding can happen through the particle beam's ionization of the residual gas present under imperfect vacuum conditions. Amplification can happen when electrons with energies above a few hundred eV hit the beam chamber walls and produce more electrons than were originally present. Acceleration of these electrons occurs when they are trapped and then released in the potential created by the proton bunches. Formation of electron clouds can cause degradation of vacuum, produce emittance growth and, in the worst cases, cause beam instabilities.

The Project X leadership has requested a simulation effort aimed at reproducing and interpreting the set of electron cloud experiments conducted in the MI, including direct Retarded Field Analyzer (RFA) measurements, and non-destructive traveling wave and pseudo-resonant cavity rf experiments to derive cloud densities. In addition, electron-cloud-induced beam instabilities need to be simulated so that related beam losses can be estimated for a given set of hypotheses.

Previous simulation results have shown that the most critical parameter in this process is the secondary emission yield (SEY) of the beam pipe. The hardware necessary for an in-situ measurement of this SEY in a field free region are planned to be made available for FY13. Note that simulations also very clearly show that the electron fluence at the beam pipe walls depends on the magnetic field configuration. Since it is widely understood that SEY depends on the history of exposure to incident electrons, a result of our previous simulation efforts is a strong endorsement for measuring the SEY in a dipole after the typical "scrubbing" that takes place during normal operation. Once these factors are known, the electric fields produced by the electron cloud can and will be computed in Warp-POSINST and VORPAL. Good agreement between these two codes has been recently obtained.

During past simulations of electron cloud buildup, and especially for Fermilab's MI, an unphysical runaway of electrons accumulation has been observed near boundaries [52]. The origin of the unphysical instability is well understood and is linked to spatial and temporal inaccuracies in the integration of field and particle motion near conductors. Adaptive mesh refinement will be applied on a combination of block Cartesian and conformal patches (that follow the contours of conductors) and specialized particle pushing toward the mitigation of the numerical instability. These techniques are already existent within Warp [53] and will be generalized for the Warp-POSINST package. The package will then be used for buildup and fully self-consistent modeling of the electron cloud effects in Fermilab's MI.

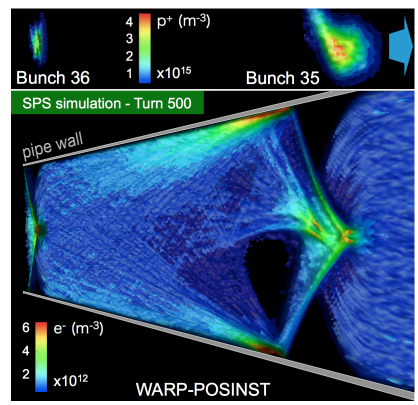

Figure 7: Warp-POSINST simulation of two consecutive bunches (top) interacting with an electron cloud (bottom).

VORPAL simulations of the MI have modeled the formation of electron clouds given a fixed beam. Part of our efforts will include incorporating the electron cloud fields in Synergia's beam dynamics calculations. The Synergia-VORPAL and Warp-POSINST calculations will be complementary. Synergia and VORPAL focus on detailed calculations of individual beam dynamics (including long-term tracking) and electromagnetic field solutions, while Warp-POSINST focuses on a self-consistent approach to the beam-cloud system. Through collaboration of these two approaches, we will be able to investigate the importance of self-consistency and the effects of long-term tracking. In addition, QuickPIC, which is primarily used for plasma-based acceleration modeling (see section 2), will be used for long-term tracking and validation of the other approaches, when applicable. QuickPIC will be extended or coupled to Synergia, to enable more accurate modeling of the machine dynamics. Predictive simulations may ultimately necessitate following hundreds of bunches at very high resolution and statistics, and runs for tens of thousand of turns, which calls for very large-scale simulations using hundred of thousands of CPUs.

VORPAL simulations of traveling wave and pseudo-resonant cavity rf diagnostics of electron clouds relevant to experiments in the MI will be developed utilizing a plasma dielectric numerical model. This model has a number of advantages over PIC models with respect to these experiments because one must have very high temporal and spatial resolution over large distances (tens of meters) and long times (beam revolution scales). We will develop and perform detailed plasma dielectric models of rf diagnostic experiments in the MI that will include CAD-based models of beam pipe geometry so that the effects of reflections and attenuation of rf on diagnostic signals can be computed. In addition, we will integrate PIC simulations of cloud buildup with long-time-scale plasma dielectric simulations to capture the effects of non-uniform cloud densities on rf diagnostic experimental results. Deliverables and milestones for this activity are discussed below.

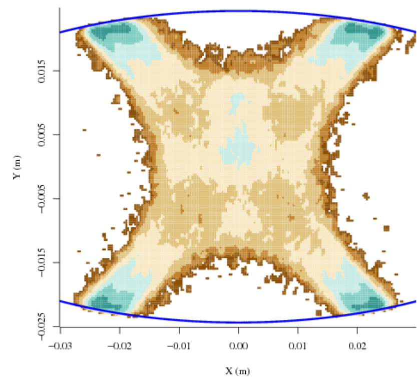

Figure 8: VORPAL simulation of electron cloud formation in a MI quad during the pinch phase.

Year 1 Support of the analysis of the electron cloud experiments in the MI, including the simulation of the electron fluence at the RFA for current operational conditions, and simulations of table top experiments to measure reflections and attenuation of rf in the presence of dielectrics. Application of adaptive mesh refinement and specialized particle pushing to mitigation of numerical instability near conductors. Enhance QuickPIC lattice modeling capabilities.

Year 2 Support for experiment and simulation of electron-cloud-induced beam instabilities, via an interface between VORPAL and/or POSINST electron cloud field maps and Synergia. Enhancement of adaptive macro-particle management (reduction and coalescence of macro-particles). Establish validation procedure and cases, validate implementation with QuickPIC comparisons. Support MI pseudo-resonant cavity rf experiments to predict cloud densities by developing detailed simulations using VORPAL.

Year 3 Complete the Synergia electron cloud module. Identifying losses in Synergia simulations combining space charge and electron cloud effects (see below). Fully self-consistent modeling of electron cloud buildup and its effect on bunch trains in MI using quasi-static or/and Lorentz boosted frame mode. Integrated PIC and plasma dielectric modeling of traveling wave rf diagnostics of electron clouds using realistic beam pipe geometries and variable magnetic field configurations, over tens of meters of pipe.

Space Charge

In the Project X era, the MI will be required to run with a total beam power of 2.1 MW, which is about seven times larger than the beam power produced during current operations. The power increase is achieved by increasing the number of bunches in the machine by $\sim 12\%$, reducing the cycle time from 2.2 s to 1.4 s, and increasing the individual bunch intensity from 0.9×10^{11} to 3.1×10^{11} protons. All this has to occur while keeping beam losses below 1 kW.

Space-charge effects from the increased bunch intensity will change the tune of bunch particles. This, along with magnet imperfections and impedance effects will almost certainly increase losses due to particles moving into resonantly unstable phase space regions, where their amplitude will grow sufficiently that they will be lost at an aperture restriction. Understanding these effects requires a high performance computing environment running a multi-physics simulation that includes particle tracking with magnetic field errors, realistic models of machine apertures, space charge, and impedance. In order for a computer simulation of a particle accelerator to model meaningful particle losses, the simulation has to run long enough to correspond to a macroscopically significant time scale. The MI beam circulates approximately 90,000 times/second. It will be a goal to simulate several seconds of MI real time running with multiple beam and machine configurations. In addition, the MI beamline is not uniform, but contains sections with different transverse shapes. The space charge calculation is the most computationally expensive part of the simulation. Deliverables and milestones for this activity are discussed below:

Year 1 Perform space charge simulations of the MI and determine the space charge solver that gives the best performance given the trade-offs between computational speed and correctness given the boundary conditions.

Year 2 Continue running our simulation adding detailed machine aperture to the machine mode and determine the effects of these apertures in generating localized machine losses. Consider additional effects such as magnet ramping for acceleration, machine impedance and multiple bunches.

Year 3 Integrate space charge simulations with electron cloud simulations described above. Run simulations of the MI that synthesize the effects of space charge, electron cloud, and apertures to determine a detailed map of location and magnitude of particle losses in the accelerator.

3.3 Project X linacs design

In the Reference Design of Project X, the linear accelerator consists of two main parts which are the continuous wave (CW) linac and the pulsed linac [54]. The CW linac accelerating anti-protons (H^-) to 3 GeV spans the first portion of the linear accelerator providing beams for rare process programs, and the pulsed linac accelerates relativistic H^- from 3 to 8 GeV before they are injected into the main injector for the neutrino program. The schematic of the 3 GeV CW linac and the pulsed linac is shown in Fig. 9. The CW linac adopts superconducting RF (SRF) technology for the accelerating cavities operating at different frequencies (162.5 MHz, 325 MHz and 650 MHz) to increase the beam energy using a total of more than 200 cavities and 30 cryomodules. The pulsed linac operating at 1.3 GHz is based on the ILC SRF technology with about 250 cavities in 28 cryomodules. One main goal of the Project X R&D is to mitigate risks associated with possible technical, cost and schedule uncertainties. Extensive simulation of the SRF cavities in the CW and pulsed linacs will help identify potential problems of the cavity designs before they are fabricated for production, which can significantly reduce the risks involved in the R&D.

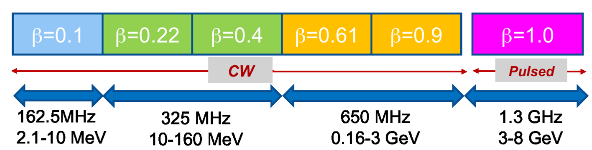

Figure 9: Schematic of Project X 3 GeV CW linac and 8 GeV pulsed linac.

The design of the SRF cavities needs to take into account beam-excited wakefields and higher-order-modes (HOMs) so that their effects on the beam quality as well as on cryogenic power losses are properly controlled. In order to maintain the HOM effects below certain thresholds, normally an SRF cavity is equipped with HOM dampers to extract the beam-excited power from the cavity. As proposed for the ILC linac, the ILC 9-cell SRF cavity was designed with HOM couplers located at both ends of the cavity to damp the first several dipole bands; it was shown experimentally that the HOM couplers can effectively lower the damping factors of the dipole modes. However, the HOM damper is a vulnerable, expensive, and complicated component requiring additional hardware such as cables, feedthroughs, connectors, loads, etc. The experience at SNS has shown that HOM dampers may limit the cavity performance and reduce operation reliability because of problems arising from multipacting and the damage of feedthroughs [55]. Indeed, SNS linac does not show the necessity of the HOM couplers at current operation parameters. Thus we propose to evaluate the HOM wakefields of the Project X SRF cavities and cryomodules to determine if HOM dampers are needed for the machine operation.

Previous studies showed that the properties of HOMs of SRF cavities are affected by fabrication errors and the tuning of the accelerator mode which leads to cavity imperfection deviating from the ideal cavity design, resulting in dipole mode frequency shift and scatter in damping factor

(Q_{ext}) among the cavities. This phenomenon was observed in the ILC TTF modules and ACE3P simulation results corroborated well with the measurements (see Fig. 10) [9]. Cavity imperfection also contributed to the beam breakup (BBU) at currents well below the designed threshold observed in the prototype cryomodule of the CEBAF 12-GeV Upgrade [10, 11]. Furthermore, cavity imperfection in random azimuthal orientation will change the dipole mode polarizations resulting in x-y coupling of the HOMs [56]. The detailed analysis of the excitation of HOMs, both monopole and dipole, in the Project X linac SRF cavities will be performed in the presence of cavity cell imperfections and misalignments and statistical variations to assess the BBU condition.

The analysis of HOM and wakefield effects for the Project X SRF cavities is similar to that carried out for the ILC using ACE3P. During SciDAC2, ACE3P's frequency-domain eigensolver Omega3P was used to perform the first-ever calculations of the HOMs in the ILC TTF cryomodule (Fig. 11). Simulation results qualitatively agreed with measurements at DESY (except for cavity imperfection) [57]. ACE3P's time-domain module T3P was used to carry out the first-ever simulation of a beam transit through the entire ILC TTF cryomodule by which one can determine possible trapped modes between cavities and estimate the power coupling out from the HOM couplers. Both approaches will be employed for the studies of HOM effects for the Project X SRF cavities. While the treatment of non-relativistic beam ($\beta < 1$) in the CW linac can be extended straightforwardly for Omega3P calculations in the frequency domain, new boundary conditions will be developed in T3P to handle $\beta < 1$ beam excitation.

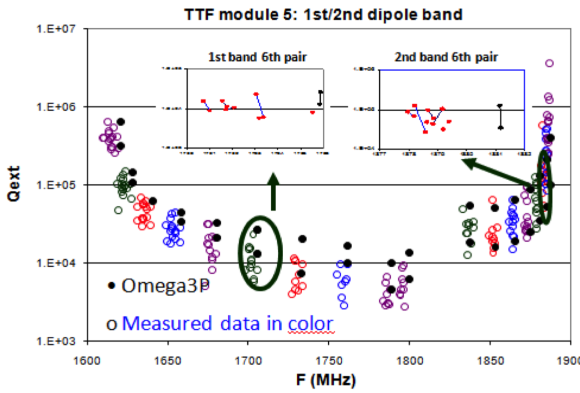

Figure 10: Comparison between ideal cavity results from Omega3P (black dots) and measurements from 8 cavities in TTF Module 5 (in color).

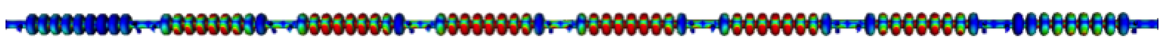

Figure 11: Trapped mode Omega3P calculation in the 3^{rd} dipole band of the ILC TTF cryomodule

In this proposal, we will focus most of our simulation work in the CW linac. The 1.3 GHz SRF cavity design has been studied extensively both experimentally and computationally, and therefore there is a good understanding of the performance of this cavity. In contrast, the low β cavities at 650 MHz are novel 5-cell designs with an elliptical equator and their reliability can be assessed through simulation. It is essential to calculate the HOM wakefields in the presence of cavity imperfections and misalignments, and to determine in the worst scenario if HOM dampers are required to satisfy the BBU threshold and to limit the cryogenic losses. The simulation procedure will be applied in a similar manner to the 1.3 GHz 9-cell SRF cavity and the 325 MHz spoke SRF cavities. The deliverables are

Year 1. Calculate monopole and dipole HOM spectra in 650 MHz cryomodules. Develop wakefield computational technique in ACE3P for non-relativistic beam excitation.

Year 2. Simulate 650 MHz cryomodules including cavity imperfection and misalignment to assess BBU condition. Evaluate beam-generated power and its effects on cryogenic losses in 650 MHz cryomodules.

Year 3. Simulate 1.3 GHz cryomodule including cavity imperfection and misalignment to assess BBU condition. Calculate monopole and dipole HOM spectra in 325 MHz cryomodules.

3.4 Project X to Muon Collider

A future muon collider (MC) or a neutrino factory (NF) requires a primary beam of short intense bunches of ∼10 GeV protons at frequencies between 15 Hz and 60 Hz and power of ∼4 MW. With the baseline proton energy set at 8 GeV, this requires $\sim 2 \times 10^{14}$ protons at 15 Hz or $\sim 5 \times 10^{13}$ at 60 Hz. At extraction onto a target to produce a high-intensity muon pulse, these protons would need to be compressed to ∼1 m long bunches. The most likely proton driver for such an accelerator complex would be an upgrade to the planned Project X facility. On the other hand, the proton bunch parameters and timing of the bunch train of Project X will be inappropriate for the pion target/source of the MC or NF. In its current incarnation, the Fermilab Project X linac would produce 3 GeV CW proton beam at 1 mA, with varying bunch structures [58]. To extend this to a MC or NF source beam, one might begin by adding a linac extension to 8 GeV; a pulsed 3-8 GeV linac is considered as a Project X component to provide beam at ∼250 kW for the Fermilab Main Injector program. To obtain 4 MW at 8 GeV both the CW linac and the pulsed linac must be upgraded to support acceleration of 5 mA H- beam at a ∼10% duty cycle. This would provide 4 MW but not the desired time structure. Formation of short intense bunches requires accumulation of beam from the linac in a storage ring and compression of that beam to short bunches. This storage ring will have to tolerate energy spread and space charge forces far in excess of what has been addressed in previous rings. The changing longitudinal structure (probably two orders of magnitude in bunch length) on relatively short time scales (tens of μs) are challenges that no accelerator design code has yet had to address. The necessary peak proton current is $\sim 10^{14}$ protons in ∼1 ns, RMS.

There are many conceptual ideas on how to design this interface and the Muon Acceleration Program (MAP) collaboration is expected to select a few for study during their Winter 2012 meeting. All of these designs appear to be inherently nonlinear, so standard computational tools will not be adequate for their simulation and optimization. The Synergia framework is well suited for this work, especially because losses from beam halo are a significant concern and, hence, very large numbers of macroparticles will be required. Because the design effort is in the early stages of development, this activity will require close collaboration with experts from both the Project X team and members of MAP. This will be the first major ComPASS involvement with MAP research. We hope to establish a successful collaboration which could lead to more involvement in the future. The deliverables for this activity are discussed below.

Year 1. Work with MAP researchers to incorporate different design ideas in Synergia and perform initial simulations to evaluate them. Begin building detailed model and optimization infrastructure.

Year 2. Extend Synergia capabilities to handle the challenging beam characteristics (rapidly changing spatial scales). Synergia is already capable of handling bunch merging.

Year 3. Optimize selected designs using project developed tools and evaluate their performance.

4 Applied Math, Computer Science, Uncertainty Quantification

4.1 Visualization and data interoperability

Visualization and data analysis have been critical to scientific discovery in accelerator physics. They generally allow one to study field and particle interactions in complex geometries, to understand the critical physics during particle acceleration, and to identify potential problems during the design process. In particular, visualization and data analysis have helped find surface magnetic hot-spots or regions of multipactoring in conventional accelerator cavities, aided in determining which particles are trapped and accelerated in self-injection in laser-plasma acceleration, and allowed observation of the generation of halo particles in beam dynamics. The ComPASS team plans to continue visualization and data analysis work through unification and advancing techniques and tools, at the same time advancing data description to improve interoperability among ComPASS computational applications.

This team has significant experience in visualization using existing tools. Award winning visualizations span the entire period of the SciDAC effort. Fig. 12 shows field-cavity interactions due to a short particle bunch; it led to an OASCAR award in the 2010 SciDAC Conference [59]. Fig. 13 is one image from a cavity visualization movie that won an OASCR visualization award in 2008. Fig. 14 is an image from a laser-plasma acceleration movie that not only received an OASCR visualization award in 2011, but was also picked up in the popular press. The ComPASS team also has a history of interacting with the data and visualization efforts supported by OASCR. For example, Marc Durant of Tech-X is a co-author on the latest VisIt publication [60]. VORPAL I/O patterns were used [61] as a benchmark for improving HDF5 performance.

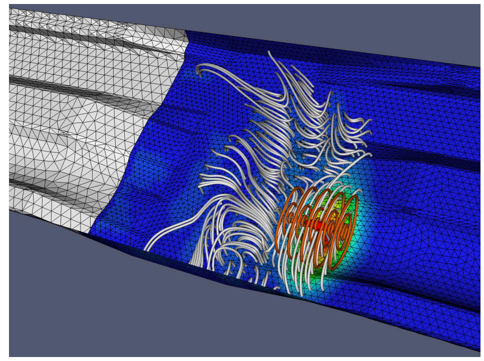

Figure 12: Snapshot of wakefield due to a beam transit in a Cornell ERL vacuum chamber, generated by ParaView from ACE3P simulation. The electric and magnetic fields are represented by white and red lines, respectively. The refined mesh region of the moving window is shown in blue.

There now exist powerful tools, such as VisIt [60] and ParaView [62], for visualization of the large datasets generated from high-performance computations through use of parallel visualization backends. However, use of these tools is hampered in the accelerator community through the complexities involved in importing the data into tools such as VisIt and creating the desired visualizations using these powerful tools. This has been ameliorated by the development of *VizSchema* [63], a generic schema for data description for the purposes of visualization, but at this point there is a need to ensure that all ComPASS codes can either write or have their data files modified to be VizSchema compliant so that VisIt visualization is available throughout the project, and there is a need to facilitate standard visualizations.

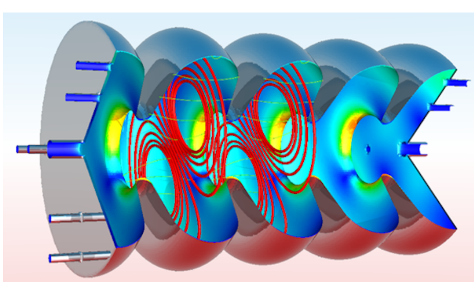

Figure 13: Visual inspection of a VORPAL modeled crab cavity from Ref. [64]. This image is from a movie that won a 2008 OASCR visualization award.

A second thrust will be to improve the interoperability of ComPASS codes through data exchange via files. This would facilitate, e.g., the particles output from a detailed laser-plasma simulation to be used as input to a tracking code, whether for optics or through materials. Alternatively, one could take the fields from an EM cavity simulation, create the resulting map, and use that in a tracking code [65]. There is also the task of inter-code comparison, i.e. benchmarking/verification exercises. For these tasks to be routine, there needs to be developed a general semantic schema for describing accelerator data, as is common in other fields. For example, neutron science has the NEXUS format [66], and the climate and forecast communities share the NetCDF Climate and Forecast (CF) Metadata Conventions [67]. Developing a semantic schema for accelerators would have consequences beyond the accelerator community, as such a schema would be valuable to many other fields, e.g., fusion, where there is the use of particles, in particular electrons, and various ionized species.

The basic idea is to use a self-describing file format, which has the capability to name a dataset within the file and include metadata within the file that defines the physical meaning of that dataset. A consumer of that dataset can then examine the file and determine through the metadata whether the particular physical data it needs is present, what form it is in, and how to extract it. Examples of consumers include other simulation codes and visualization and analysis tools.

Foundational work for developing a semantic data schema is the visualization data schema, VizSchema [63]. This schema lays out how one can mark up a dataset for the purposes of visualization. For such purposes, one needs to know the mesh that the data lives on and then the type of mesh, how it is defined, and so forth. One also needs to know whether the data represents a collection of scalar fields or a vector field. VizSchema was designed to be able to provide all of this information. Moreover, VizSchema was designed to be minimally prescriptive. By that it is meant that the code developer has wide latitude in how data is written out; the markups then permit the data to be interpreted. VizSchema has been highly successful and widely used.

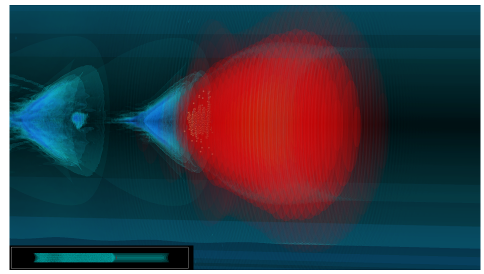

Figure 14: Visualization of the laser-plasma acceleration calculation of Ref. [68]. This image was from a movie that won a 2011 OASCR visualization award and was cited by Wired magazine [69].

The VizSchema approach reduces code maintenance. Historically, the VisIt team and others have been producing data readers on nearly a one-per-code basis, with the result that there are now 116 data readers to be maintained. In contrast, VizSchema is/can be used by a number of codes (VORPAL, FACETS, NIMROD, Synergia) in the computational accelerator community and beyond, such that for this large set of codes there is only one data reader.

The next stage is to develop a semantic metadata schema that describes the physical meanings of the datasets within a file. Such metaschema would be able to indicate that a particular dataset represents, say electrons, by particle (or fluids), with the particles laid out in a certain order, and the particle data having the meaning of, say, positions, velocities, and weights. Or the electrons might be represented by a fluid or by continuum kinetics (Vlasov). In any of these cases, the semantic metadata would define how the data is to be interpreted, with sufficient specificity that someone knowledgeable about that representation would be able to translate it into another one.

The ComPASS project will also be addressing challenges in visualization and analysis of larger systems, whether conventional, e.g., the Project X cryomodule (see section 3.3), staged, plasma-based accelerators, or complex dielectric-based accelerators. Moving in this direction will increase the size of datasets and the geometric complexity, in come cases involving orders of magnitude difference in scales, with the different directions not aligned with Cartesian axes. Thus visualization tools will need a means of moving along the curved design orbit of accelerators.

Year 1. Develop semantic metadata schema for self-describing data files. Test (and generalize as needed) visualization metadata schema (VizSchema) to allow VisIt to import files from currently non-compliant accelerator codes. Develop a ParaView plugin which takes an extracted set of segments from a well-formed path, computes their connectivity and orders them for generating plots of variables vs. path length.

Year 2. Generalize converters/modifiers to be able to add visualization metadata as needed to the output of all ComPASS computational applications. Modify computational applications as needed to directly provide marked up data. Extend the ParaView plugin to accept an arbitrary number of paths, with user options to stack multiple variables vs. path length series in the same plot.

Year 3. Generalize converters/modifiers to be able to add semantic metadata as needed to the output of all ComPASS computational applications, thus easing data exchange between ComPASS applications. Develop a ParaView interactor to improve user navigation of extremely long or geometrically complex large scale accelerator datasets.

4.2 Nonlinear parameter optimization

In accelerator design and operation, one aims to find the machine parameters that produce the best beam quality and/or minimize particle losses. These optimal parameters can significantly reduce accelerator construction and operational costs and provide the best performance for user experiments.

4.2.1 Local optimization of expensive problems

Accelerator design optimization problems typically depend on the output of a computationally expensive simulation (e.g., a VORPAL run) for which derivatives of the output with respect to the design variables are noisy and often unavailable. Through systematic parameterization of surfaces and other dimension reductions, typical problems depend on up to tens of parameters and must be solved with so-called derivative-free optimization methods [70].

The primary consideration for these problems is that the expense of evaluating the objective or constraints allows for relatively few sequential evaluations. Consequently we will explore model-based methods (such as NEWUOA [71], BOBYQA [72], ORBIT [73, 74]), which have been shown to be effective at reducing objectives in as few evaluations as possible [75]. In addition to parallelization strategies, we will explore exploiting additional structure in the problem, such as RMS objectives based on sums of squared residuals depending on simulation outputs. When such structure is present, algorithms such as Argonne's POUNDerS (Practical Optimization Using No Derivatives for Squares) have been shown to require many fewer simulation evaluations than blackbox alternatives [76, 77]. POUNDerS is available in TAO, the Toolkit for Advanced Optimization [78].

In cases where multiple simultaneous objectives are present (e.g., in laser plasma modeling, minimizing both the energy spread and RMS particle-based quantities), we will leverage the research in the SciDAC3 Institute for Sustained Performance, Energy, and Resilience (SUPER) [79] and explore multi-objective optimization [80, 81, 82, 83].

4.2.2 Global optimization

The purpose of global optimization in nonlinear accelerator beam dynamics optimization is to find the set of parameters resulting in the best performance of the accelerator (defined by the merit function) within all the potential feasible solutions. As mentioned above, the objective function for large scale beam dynamics simulation is computationally expensive (i.e., time consuming), even on next generation high-performance supercomputers. In this study for global optimization, we will develop a multi-start cluster algorithm with the above local model based optimization algorithm and the expected improvement [84] to balance the exploitation and the global exploration. Even though the multi-start algorithm is an incomplete heuristic global optimization method, it provides a great opportunity for multi-level parallelization and significantly extends the scalability of the current accelerator application code to a level beyond a hundred thousand processors.

4.3 Performance Analysis and Optimization

To ensure performance portability and code maintainability on existing and future HPC platforms, we will employ the performance and reliability methodology and tools developed in the SUPER Institute or available through platform vendors and the larger performance community to the set of accelerator codes involved in this project. Our goals are to ensure both performance portability and resilience of new parallel algorithms developed as part of this project, as well as to improve the performance of existing implementations that are leveraged through the use of numerical libraries. A key component of our approach is the integration of advanced performance analysis capabilities and autotuning into the development of new algorithms and the improvement of existing implementations. To be truly effective, the performance evaluation and key optimizations must be automated, so that performance testing and improvement can become an integral component of the accelerator software development process. Ultimately performance testing and certain types of tuning will be integrated into regression and unit testing frameworks for accelerator codes, starting with VORPAL in year 1, followed by QuickPIC in year 2, and finally Synergia in year 3. We will develop common methods for performance regression testing, so that other existing and new codes can incorporate these capabilities in their development.

For the measurement and analysis capabilities, we will rely on the approaches and software being developed in SUPER, while simultaneously ensuring that specific accelerator software needs are considered through the involvement of PI Norris, who is also the Argonne SUPER PI.

Beyond performance characterization, partly or fully automating the generation of highly optimized versions of key kernels will improve both application performance and the developers' productivity. Several components are required to provide these code generation capabilities: (i) a mechanism for defining the computation at a sufficiently high level, (ii) application-specific library optimizations, and (iii) automatic tuning of generated kernels and (re)integration into larger code bases. Next we discuss our proposed approach to providing each of these components.

High-level computation specifications. Existing implementations of key kernels, e.g., matrix-vector products, can be generated from higher-level (e.g., Matlab-like) representations. Previous work in generating optimized code for composed linear algebra operations [85] demonstrates that the generated code performance can greatly exceed that of collections of calls to prebuilt libraries. The key challenges are to associate different underlying matrix and vector representations with the high-level kernel specification. Another challenge is code generation for distributed memory architectures, including hybrid CPU/GPU systems. Part of our research will be to identify key kernels and devise a high-level representation that can be associated with different (manually specified) data structures. Another issue is seamlessly integrating the tuned versions into the rest of the code base, which is typically implemented in Fortran, C, or C++. In previous work we have shown that high- level computation specifications can be embedded in existing C or Fortran codes by expressing them through annotations specified as structured comments [86]. Because of better utilization of spatial and temporal locality in the presence of fusible matrix and vector operations, the performance of code generated from such high-level specifications is almost always significantly better than that of compiled C or Fortran code and for composed operations, it far exceeds that of multiple calls to optimized numerical libraries. We will implement new code generation capabilities targeting emerging many-core and hybrid multicore/accelerator architectures.

Application-specific library optimizations. Given a high-level computation representation and a detailed architectural description (e.g., obtained through microbenchmarks), we will generate multiple kernels by using different performance-improving transformations. Ideally this will be done in a specific application context, e.g., using a representative sample of input sizes and values.

Integration with autotuning capabilities. The generated tuned code versions would be evaluated by using an empirical autotuning approach. Empirical autotuning presents a challenging optimization problem – the search space is extremely large and thus cannot be explored exhaustively. We will employ the derivative-free global optimization techniques being developed as part of the DOE Math/CS CACHE Institute [87] and the multiobjective optimization approaches in the SciDAC SUPER Institute [79] to produce better (closer to optimal) results while exploring just a tiny fraction of the parameter space. By producing customized builds of key subsets of numerical algorithms (e.g., linear algebra kernels) that reflect actual application inputs, we will be able to exploit multicore and hybrid resources more effectively. We will generalize this idea to more types of operations and enable kernel specialization (e.g., based on problem size) during autotuning.

4.4 Particle-In-Cell Methods

Particle-in-cell (PIC) methods [88] are ubiquitous in accelerator modeling. The basic approach taken in PIC methods was extended to the distributed-memory multiprocessors that appeared in the late 1980's by using MPI and domain-decomposition methods [89] (e.g. slicing the domain into 1D, 2D, or 3D domains) that took advantage of the structure of the problems arising in beam dynamics. Recent developments in computer architectures involving deep memory hierarchies and greater memory latency and limited bandwidth compared to floating point throughput have forced a reconsideration of the data structures and the pure-MPI approach. Under SciDAC2, we investigated CUDA-based GPU and hybrid OpenMP-MPI updates to the architecture of UPIC and Synergia as a step toward PIC implementations optimized for new computing architectures.

Another recent development is that of new algorithmic ideas for PIC methods, such as adaptive mesh refinement [53, 90]; potential-theoretic based methods for solving Poisson's equation on structured grids [91]; and methods for reducing self-forces and unphysical noise, and increasing the accuracy of calculations with large dynamic ranges [92, 93]. These methods have been viewed as less competitive, due to the higher program complexity and floating-point counts, relative to traditional uniform-grid PIC.

These two developments motivate the development of a new generation of computational libraries and frameworks for PIC methods. These will be leveraged by the cross-cutting support of PIC by the FASTMath SciDAC Institute and support of PIC on many-core architectures by the UCLA Institute for Digital Research and Education (IDRE). The results of these efforts will be integrated by Fermilab into the Synergia framework, allowing the comparison and/or combination of the results in a production beam dynamics framework. This effort will emphasize the support of electrostatic PIC which is used throughout the project, but will also include developing skeleton codes and experimentation of strategies for electromagnetic PIC.

The proposed work is driven by aforementioned memory/FLOP characteristics of recent and future computing hardware which make it desirable to reconsider some of the basic data structures and mathematical approaches to the field solutions for PIC methods. Memory on GPUs, for example, has more than an order of magnitude greater bandwidth than on the CPU, but the floating point throughput is even higher. Memory is improving, just not as fast as FLOPS. In this computing environment, the traditional data structures used in PIC codes may no longer be effective. The low computational intensity [94], defined as the number of flops per main memory access, of both the particle operations and the field solves used in current PIC codes could lead to performance that will be best measured by what fraction of peak memory bandwidth and not FLOPS that can be achieved. Processor heterogeneity, due either to the presence of multiple types of processors on a node, or run-time variation of the clock time to manage thermal loads, makes the locally-static bulk-synchronous load balancing used by most high-end codes infeasible.

We will explore data structures and parallelization strategies for PIC on hybrid architectures, using the UCLA UPIC Framework [33, 34, 95] as an experimental platform. The UPIC Framework is highly optimized; key pieces already run well on GPUs. We will explore a nested architecture intended to support domain decompositions for PIC codes on emerging high performance computing architectures. There will be one library for the outermost domain, which will use MPI. The innermost domain might have multiple versions, possibly using multiple languages, but it might turn out that many-core and GPUs could be programmed in the same language (*e.g.*, OpenACC). The goal is to have the libraries for the innermost domain be interchangeable as much as possible, so that the same code base could be used on different architectures. The many-core and GPU implementations will produce the same results, but not in the same way. It is possible for multiple libraries to eventually merge, as software matures. Skeleton (compact) applications will be developed to test the libraries and illustrate their use by others. The libraries will be included in the Synergia framework as a real-world application.

We will also provide enhancement of the Chombo framework [96], which is supported as part of the FASTMath Institute, with beam dynamics codes as the target application. The best ideas that result from the research and exploration using UPIC as new analytical approaches in [94] will be used. One key priority for Chombo will be the development of high-order structured-grid adaptive Poisson solvers based on the AMR MLC solver described in [91]. This approach has a computational intensity that is an order of magnitude or more greater than traditional global FFT or multigrid methods. Furthermore, they extend to structured adaptive mesh refinement (AMR) meshes in a way that naturally eliminates the spurious self–force problems associated with more conventional AMR discretizations. We will also develop a particle framework that will provide support for more flexible domain decomposition and on-the-fly load balancing. This will require the use of lightweight performance measurement tools similar to those that already exist in Chombo to measure performance at runtime. We will also consider methods (including those developed in skeleton codes) to improve the data locality of particle operations. These will include new algorithms that improve the accuracy (and increase the computational intensity) of particle operations, as well as exploring the possibilities afforded by the potential-theoretic field solvers for hiding the cost of particle data movement by more tightly integrating the particle operations with the field solver. Such methods would be much more complicated to implement than the traditional PIC methods, and therefore would need to be designed carefully to provide the flexibility to support the range of requirements in the accelerator community, while hiding the complex programming details from the applications user. At the low levels, we will use a variety of implementation techniques. The roofline model in [94] provides guidelines for what techniques can be used effectively on a given processor architecture, based on the computational intensity of the operation. We will also develop appropriate metrics for performance between the approaches developed within UPIC and Chombo which will vary depending on the application code. The best will be incorporated in the libraries.

In Year 1, we will develop many-core and GPU modules for nested decompositions for 2D skeleton code developed at UCLA and evaluate feasibility of three-level decompositions with MPI/many-core/GPUs within UPIC. We will also implement and evaluate dynamic load balancing with fine partitions which can be needed in beam dynamics codes. In the FASTMath component of the project, we will release versions of the AMR MLC solver that support the usage patterns for structured-grid Vlasov-Poisson as it appears in accelerator modeling. This implementation will take advantage of the higher computational intensity of the MLC algorithm to maximize data locality, minimize global communications, and hide communications at all levels. We will also make an initial design of a programming interface for PIC methods that is portable, broadly capable of expressing PIC algorithms as they arise in accelerator modeling, and maximizes data locality while minimizing the extent to which the applications developer must provide platform-specific code. The Fermilab Synergia team will act as a testbed for the FASTMath programming interface and evaluate performance. In Year 2, the UCLA component of the project will extend nested domain decompositions to 3D skeleton code and add dynamic load balancing to nested decompositions for the 2D skeleton code. In FASTMath, we will implement a particle library to the specification developed in Year 1, and test its performance for use cases arising in accelerator modeling on a variety of platforms. We will also begin to extend the AMR MLC algorithms developed in Year 1 to support complex boundary geometries, using variations on the ideas in [90, 97]. The Fermilab team will continue to work with the FASTMath interfaces as well as interfacing to the 3D portion of the UCLA library. In Year 3, both components of the PIC effort will release their particle libraries, and bring them to production status in Synergia, as well as assist in incorporating into other accelerator modeling production codes such as QuickPIC. We will also make changes to both the AMR MLC solvers and the particle libraries in response to further requirements identified by the accelerator modeling community.

4.5 Linear Algebra

In the simulation of large accelerator systems such as the Project Xcryomodule and the entire CLIC accelerator module using the finite-element electromagnetic suite ACE3P, consisting of different modules in frequency and time domains, there are two classes of numerical linear algebra problems. The first is consisted of eigenvalue problems, which come from discretizing Maxwell's equations in the frequency domain. Depending on the accelerator cavity to be studied or designed, the eigenvalue problems can be linear or nonlinear (in the eigenvalue). The second consists of large sparse systems of linear equations. Because of the need to perform high-fidelity modeling and simulation, the matrix sizes can be very large. For example, calculating the eigenmodes for the ILC cryomodule required a finite-element mesh of 3 million finite elements, corresponding to 20 million degrees of freedom and 1 billion non-zeros in the matrices. Over the last decade, collaboration between computational scientists at SLAC and applied mathematicians in the TOPS project ("Towards Optimal PDE Solvers" in SciDAC1 and "Towards Optimal Petascale Simulations" in SciDAC2) have resulted in the development and integration of several state-of-the-art numerical linear algebra algorithms and software packages into the accelerator modeling suite ACE3P.

For linear eigenproblems, which arise in computing the eigenmodes of a closed accelerator cavity (without external damping), work under the SciDAC2 ComPASS contributed an exact shift-invert Lanczos (ESIL) algorithm (see, e.g., [98]) into ACE3P's frequency-domain eigensolver Omega3P for computing some of the extreme eigenvalues. The ESIL algorithm requires the solution of sparse linear systems. This has led to further optimization of SuperLU_DIST [99], which is an efficient parallel sparse linear solver for distributed-memory machines based on direct methods. Other sparse direct solvers, such as WSMP [100] and MUMPS [101], have also been investigated. We have also developed an algebraic sub-structuring method for solving sparse eigenproblems [102].

When an accelerating cavity is coupled to an external system through a waveguide, an appropriate boundary condition must be imposed at the truncated waveguide port to properly terminate the propagation of electromagnetic power at the boundary. The propagation characteristics depend on the frequency (eigenvalue) of the cavity mode adding a nonlinear term to the eigenproblem representing a closed cavity without any external coupling. We have incorporated several algorithms into Omega3P for tackling such problems. These have included the second-order Arnoldi reduction for quadratic eigenproblems, as well as the self-consistent iterations and the nonlinear Arnoldi method for more general nonlinear eigenproblems.

Despite the successes of collaboration between SLAC and TOPS, accelerator physicists and computational mathematicians are facing new challenges because of the increasing use of multi-/many-cores in the current and the next generation of parallel computer architectures, as well as the relatively decreasing memory footprint. The consequence of the architectural evolution is that millions of cores may have to be employed in order to accommodate the increasing problem size. The current eigensolvers in ACE3P will therefore face performance and scalability issues. Improvements in performance and scalability on such architectures will require changing the data structures, redesigning, and rewriting the eigensolvers. This work will be carried out in collaboration with the FASTMath SciDAC Institute.

Solution of large sparse systems of linear equations is another bottleneck we have to overcome. Sparse linear systems arise in several ways. They are at the heart of ESIL for solving linear eigenproblems. They also come up in solving the Maxwell's equations in the time domain.

When the linear systems are ill-conditioned, such as those arising in ESIL, we use direct methods, which are based on Gaussian elimination. Previous work has included the incorporation of SuperLU_DIST and other sparse direct solvers in ACE3P. There are two challenges. First, applying Gaussian elimination to a sparse matrix generates fill (which are zero elements in the original matrix that become nonzero). Thus, the amount of memory required can be much more than what is required for storing the original matrix. Second, SuperLU_DIST is designed to handle nonsymmetric matrices storing both the upper and lower triangular factors, but our matrices are symmetric (and some of them can be complex).

To tackle the first challenge, we developed and implemented under SciDAC2 a hybrid solver PDSLin, based on domain decomposition. In terms of accelerator cavity modeling, domain decomposition essentially partitions a finite element mesh into independent subdomains separated by *interfaces*. Existing hybrid solvers differ in the way they treat subdomains and their interfaces. In PDSLin, each subdomain is independently processed using SuperLU_DIST to enhance scalability. The Schur complement, which represents the interface after the subdomains have been processed, can be solved using a number of methods. However, the Schur complement tends to be dense, so applying sparse direct methods may not be efficient and scalable. In almost all hybrid solvers, it is handled using a preconditioned iterative method. There are several ways to construct the preconditioner. For example, one can apply incomplete factorization to the Schur complement and use the resulting incomplete factors as preconditioners. Alternatively, one can form an inexact Schur complement, e.g., by discarding some of the non-zeros, and then compute an exact factorization of the inexact (sparse) Schur complement. Both approaches have been implemented in PDSLin.

The preliminary implementation of our hybrid algorithm has been integrated into Omega3P at SLAC and has produced promising results. For a highly-indefinite symmetric linear system with about 18 millions of unknowns from Omega3P, our hybrid solver can scale beyond 4,000 processors, solving the system in 1 minute, a significant improvement over existing state-of-the-art solvers. The performance of PDSLin depends on how the Schur complement is treated, as demonstrated by examples for which the preconditioners we have constructed are not good enough.

We propose to continue our work on PDSLin in two directions: we will (i) investigate better ways to construct preconditioners for the Schur complement, and (ii) develop a version of PDSLin that can take advantage of multicore architectures. Since PDSLin is using SuperLU_DIST for factoring the subdomains, and multicore capabilities will be developed by the FASTMath SciDAC Institute for SuperLU_DIST and various Krylov solvers, our work will focus on adding shared memory parallelism in computing the Schur complement (or its approximations) and the preconditioner.

As already mentioned, SuperLU_DIST (and hence PDSLin) is designed for sparse nonsymmetric matrices and hence does not exploit symmetry (in terms of storage) when applied to symmetric matrices. To tackle the second challenge, we will investigate better sparse direct solvers that will exploit symmetry explicitly in order to reduce the storage requirement substantially. There are plans in the FASTMath SciDAC Institute to develop to a new parallel sparse symmetric linear solver. We expect to work with the FASTMath team to tailor the symmetric solver for accelerator cavity modeling.

Our collaborative work with FASTMath on symmetric linear solvers will benefit another important area of the modeling effort: the determination and optimization of the cavity shape. We are using a PDE-constrained optimization approach, in which the so-called Karush-Kuhn-Tucker (KKT) linear systems must be solved. The KKT linear systems are symmetric and indefinite but have special structures. Hence, we will also work with the FASTMath team to produce symmetric linear solvers that take advantage of the special structures.

Finally, instead of solving Maxwell's equations in the frequency domain, we solve them in the time domain. While the frequency domain approach allows the solution of discrete eigenmodes in an accelerator cavity, in the time domain one can obtain the continuous spectrum of broadband excitation due to the transient form of the transit of a charged particle bunch. The resulting sparse linear systems are solved using iterative methods, whose accuracy and performance depends on the choice of preconditioners. The accelerator physicists will work with the applied mathematicians to construct physics-based preconditioners [103], such as approximating an operator using a lower-order one and implementing workload balancing for domain decomposition on multicore architectures.

Tasks. Year 1: Develop and evaluate linear solvers, including preconditioning techniques, for hybrid architectures. Year 2: Develop eigensolvers for hybrid architectures and develop symmetric linear solvers. Year 3: Performance and scalability studies of linear and eigensolvers.

4.6 Fluid Dynamics

A central design issue for laser-wakefield accelerators is the formation of the density, temperature and species profiles in the initial capillary discharge. These properties are critical to guiding the laser pulse and control of the electron beam phase in the wake. The mathematical representation of this process consists of the time-dependent equations of gas dynamics with complex constitutive behavior: ionization physics, including multiple fluid components; diffusive transport; separate electron and ion temperatures; and coupling to magnetic fields. Furthermore, critical design parameters are associated with three-dimensional effects in complex geometries, such as the placement of fill tubes.

We propose to develop a three-dimensional simulation capability to provide a high-resolution representation of these processes, including appropriate models for all of the relevant physical processes. This work will be based on the embedded-boundary method for simulating partial differential equations in complex geometries [97, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113]. In this approach, an irregular boundary is represented on a rectangular grid by intersecting each rectangular cell with the boundary. This leads to a natural finite-volume discretization of the solution to the PDE in the irregular domain(s) defined by the boundary. Typically, this approach is combined with block-structured adaptive mesh refinement (AMR), in which the grid resolution is locally adjusted as a function of space and time to maintain a uniform level of accuracy [114, 115]. The refined regions are are organized into rectangular patches of several hundred to several thousand grid cells per patch. Thus, one can use discretizations appropriate for rectangular grids and the overhead in managing the small amount of irregular data is amortized over relatively large amounts of floating point work on regular arrays. Further efficiency gains can be realized for time-dependent problems by refining in time as well as in space. All of these capabilities are fully parallelizable, and scale to 1000's of processors using a flat MPI model. We will leverage the embedded-boundary AMR tools developed under the SciDAC program, and supported as cross-cutting technologies as part of the FASTMath Institute. In addition, under SciDAC2, we developed prototype 1D simulation capabilities in collaboration with the BELLA team, producing the basic design for the extension of the high-order Godunov methods that are the basis of our gas dynamics solvers to the case of multicomponent ionized fluids with diffusive transport and wall heat transport coupling. We will extend these core capabilities to provide a fully three-dimensional high-temperature gas dynamics codes for simulating the capillary discharges required by the BELLA experiment and other projects. In Year 1, we will complete the implementation of physics models in 1D and use these to benchmark existing codes, then develop the initial implementation of the full-physics, 3D code. In Year 2, we will validate the code and participate in its application to design problems for BELLA. This will likely involve significant changes in the code, both in response to the need for changes in the model suggested by the validation process, and to improve parallel scaling of this complex multiphysics code. In Year 3, we will continue to support the use of the code by the LWFA community, and address scaling issues on multicore and heterogeneous systems.

4.7 Uncertainty Quantification (UQ)

Uncertainty is pervasive in the assessment of nature. As computational power increases and becomes available, modelers should incorporate uncertainty in the models they construct for the analysis of *realistic* phenomena. Uncertainty can result from incomplete information about phenomena and their environment (e.g. initial and boundary conditions), or from variability in measured data. Probability logic [116, 117] together with Bayesian model updating [118, 119, 120] provides a framework for dealing with uncertainties. Let D be some reference data available for analyzing a phenomenon, with the objective of, e.g., performing predictions afterwards. When scientists lack complete understanding of a phenomenon, they tend to propose different combinations of physical principles, equations, parameterizations, and conditions, for modeling D. Any one proposed combination of assumptions can be seen as a hypothesis (an educated guess), which usually involves a vector $\boldsymbol{\theta}$ of parameters whose values are not known a priori. Any deterministic sample $\boldsymbol{\theta}$ corresponds to a unique model (deterministic or stochastic), while a hypothesis corresponds to a family of (infinitely many) models. Given D and candidate hypotheses competing for consistency with it, Bayesian analysis allows one to statistically calibrate the hypotheses, *quantitatively* rank them, obtain an information theoretical interpretation [121] (which data set is more informative, which hypothesis "learns" more), and average post-calibration predictions of quantities of interest (QoIs, usually scalars). At its core, it is based on the Bayes' formula $\pi_{\text{post}}(\boldsymbol{\theta}|D) = \pi_{\text{like}}(D|\boldsymbol{\theta}) \cdot \pi_{\text{prior}}(\boldsymbol{\theta})/\pi(D)$, where $\pi_{\text{prior}}(\boldsymbol{\theta})$ is the *prior* probability density function (pdf) characterizing uncertainties in $\boldsymbol{\theta}$, $\pi_{\text{like}}(D|\boldsymbol{\theta})$ is the *likelihood* pdf describing how likely D is according to model $\boldsymbol{\theta}$, $\pi(D)$ is the *model evidence* indicating how likely D is according to the hypothesis, and $\pi_{\text{post}}(\boldsymbol{\theta}|D)$ is the *posterior* pdf of uncertainties. Bayesian analysis *quantitatively* reveals, *under uncertainty*, which hypotheses are more consistent with D, deserving further thinking. However, it usually requires the calculation of high dimensional integrals of pdfs involving complex models and multiple modes. One way to tackle these difficulties is to combine state-of-the-art parallel sampling algorithms with HPC [122, 123, 124, 125].

Since UQ is a new activity in the ComPASS project, is laborious (not "off-the-shelf"), and will involve cross-teaching between UQ specialists and physicists, we will confine our UQ efforts to laser-plasma acceleration (LPA), with a hierarchy of relatively fast simulation tools and models. Due to lack of complete understanding of LPA experimental states, physicists use best guesses and a limited parameterization of initial, boundary, laser and plasma conditions, for modeling available D. Due to computational constraints, they might also employ reduced models or do simulations in Lorentz boosted frames. LPA can thus clearly benefit from the *quantitative analysis of models under uncertainty* outlined above. All UQ activities will be carried in interaction with the QUEST SciDAC Institute, under the lead of QUEST Co-PI Prudencio, whose research, with collaborators, focuses on statistically robust, scalable, load-balanced and fault-tolerant parallel stochastic algorithms for the Bayesian assessment of mathematical models of complex engineering and natural systems. Such research is applied through the QUESO MPI/C++ *research library* [126] from UT Austin, being developed under the lead of Prudencio. QUESO can *handle simultaneous Markov chains or Monte Carlo sequences, each of them eventually requiring parallelism for model evaluations at any given parameter vector sample.* QUESO only requires the number of random parameters and QoIs to fit in the memory of any computing node, thus allowing the analysis of thousands of parameters and QoIs, enough even for state-of-the-art UQ algorithms.

Regarding deliverables, UQ will involve the understanding of all assumptions and the selection of uncertainties to be explored, calibration data and likelihood structure to be used, and QoIs to be predicted after calibration. It will also require a C++ application to "control" both codes (QUESO and model code), code linking, sanity checks, long runs, analysis, and looping for improving overall conclusions. The running and analysis of LPA codes are also laborious. We will begin with "simple" calibrations and acquire experience. "Fast" models are those that run under 30 seconds at any given parameter vector sample with a fixed number of processors per sample, e.g. 64. We will manufacture data with OSIRIS, VORPAL, and Warp 3D simulations with high-resolution, high-order particle shapes, and limited number of particles-per-cell. We will then rank reduced models, which could include a) 2D and 3D boosted-frame time-explicit PIC; b) 2D lab-frame time-explicit PIC; c) 2D and 3D laser envelope ponderomotive guiding center (PGC) PIC; d) 3D quasistatic with PGC with the QuickPIC code. QoI options are beam energy, energy spread, and transverse emittance. Y2 and Y3 plans are tentative, and might be tuned as our research progresses.

Y1 deliverables: data manufacturing with 3D complex simulations; selection of fast models, few random parameters per model, and likelihood structure; QUESO under modifications to incorporate statistically more robust algorithms. Milestone: calibration and ranking of fast models.

Y2 deliverables: advance the analysis of Y1, e.g. manufacture more data or expand the number of random parameters; QUESO under modifications to use fault-tolerant versions of MPI (for small MTBFs, key for 10^5 core concurrency). Milestone: calibration, ranking and QoI predictions.

Y3 deliverables: selection of reference data for the emulation of complex models; QUESO under modifications to incorporate Gaussian process emulation of complex models. Milestone: Gaussian process emulation of complex models, as well as QoI predictions.

5 Management Plan

The success of the SciDAC3 ComPASS program will require the coordination between the research team, the SciDAC3 Institutes, the accelerator science community, and DOE sponsors. Our organizational structure emphasizes this coordination and provides strong management focus on, and accountability for, the execution of our plans (Fig. 15). The management plan of the project incorporates the necessary elements to enable, support, and manage these interactions.

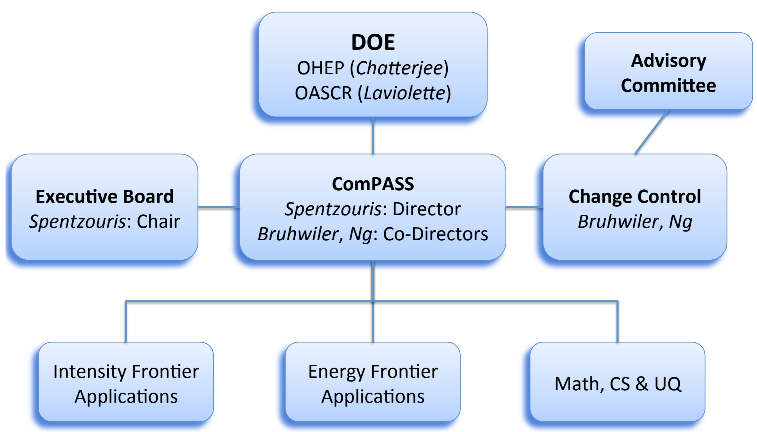

Figure 15: ComPASS management structure.

5.1 Roles and responsibilities

The Project Director (PD) The Principal Investigator (PI) of ComPASS (Spentzouris) serves as the PD, who is responsible for executing the project plan, directing and overseeing the project, and ensuring that deliverables and functionality are achieved as defined in the ComPASS proposal, the funding documentation, and subsequent plans. The PD is also responsible for the management of all project assigned resources, serves as the primary liaison between the project's Executive Board and DOE, and escalates decisions and issues as needed.

The Executive Board (EB) Overall responsibility for devising the ComPASS strategic plan and ensuring good communication within the ComPASS project, the partners of the project, and the DOE sponsors is vested to the ComPASS EB, whose members are the co-PIs of the collaborating institutions as listed in the proposal, and is chaired by the PD. The board assists the PD in executing the strategic plan of the project. The EB sets the project's strategies, goals and milestones in coordination with our DOE sponsors (the HEP and ASCR program managers), and develops the tactical plans for meeting them. It sets priorities, decides on fund allocation, and ensures that work is completed on schedule. At the end of each project year, the EB develops a rolling two-year roadmap for both modeling capabilities development and applications.

The co-Director for Science (DS) The DS acts as the primary liaison with the accelerator science stakeholders (accelerator projects, experiments, and the community at large), monitors status of scientific activities, and chairs the scientific Advisory Committee when it meets on scientific priorities. The DS also participates in the Change Control process and advises the PD and EB on changes in scientific deliverables. This is a rotating position with a one-year term. David Bruhwiler will serve as the first DS of ComPASS.

The co-Director for Computation (DC) The DC is the primary liaison with the SciDAC institutes and centers, monitors status of math and computer science (CS) activities within the project, and chairs the Advisory Committee when it meets on such activities. The DS also participates in the Change Control process, and advises the PD and EB on changes in math and CS deliverables. This is a rotating position (one year term). Esmond Ng will serve as the first DC of ComPASS.

The Scientific Advisory Committee (SAC) The SAC monitors the scientific progress of the project and provides leadership in setting directions and priorities. The Committee participates in project meetings with users and stakeholders and project reviews. The SAC consists of representatives of our stakeholders in the accelerator science community and experts in applied mathematics, computer science and uncertainty quantification. The names of the committee members are listed in Appendix A. The SAC organizes an annual meeting, possibly inviting other experts as needed to review progress and obtain input on future directions. The SAC also provides recommendations to the EB to ensure that project resources are allocated to best serve the needs of the HEP program. The objective of this process is to achieve the greatest scientific benefit from the project's resources through broad input from the community. In addition to the annual meeting, the PD can call for additional SAC meetings if additional input is needed.

Change Control Process Any project participant or other concerned party (stakeholder, collaborator) may raise Change Requests. The Project Director and co-Directors will ensure they are captured and proactively manage them to conclusion. An initial review will be made to examine the need for the change, how it could be achieved and what the consequences would be. Based on those conclusions, the recommended action would be proposed. Minor changes within scope can be approved by the Project Director. Also, any change affecting deliverables and project priorities will be reviewed in consultation with the Advisory Committee and the relevant stakeholders. Finally, changes of scope will require the approval of the EB, then communicated for approval to our DOE sponsors (OASCR and OHEP managers).

5.2 Project outreach, monitoring, and reporting

The Project will maintain a unified web presence including project web pages, a document repository, and a code meta-repository. The project web pages will be an expanded version of the current ComPASS website (`https://compass.fnal.gov`) using a new content management system (CMS). The project CMS will be a portal for the accelerator physics community, including an overview of the ComPASS project, news items and meeting information. The document repository will contain results and progress of our research, including technical documents and reports. The code meta-repository is a new feature, whose goal is to enhance the visibility and availability of our codes to the community. Each code in the project will be described, including a general overview as well as capabilities and requirements. For each entry there will be information on availability, which could range from links to source and/or binary downloads, information on installed versions for supercomputer installations, and contact information for requests, as appropriate. Where applicable, links to documentation, bug databases, mailing lists, and code repositories will be given.

The Program Director (PD) serves as the principal contact with the DOE. Each institution receiving funds under this grant has a co-PI. The co-PIs assume responsibility for the work carried out at their institutions and submit quarterly reports to the PD. The EB holds regular (bi-weekly) meetings, chaired by the PD to discuss, monitor, and coordinate project activities. The PD will submit progress reports to DOE semi-annually and is responsible for tracking the overall grant budget. The EB will organize full collaboration meetings prior to the submission of project reports.

5.3 Coordination with the NP Accelerator Modeling SciDAC Team

We will coordinate with the accelerator modeling SciDAC project, "Advanced Simulations for Present and Future Nuclear Science Accelerator Facilities," with lead PI Yuhong Zhang of Jefferson Lab, which is supporting the DOE Office of Nuclear Physics (NP). In particular, we will ensure that the two efforts are not in any way overlapping, and we will work to maximize mutual benefit to R&D programs of HEP, NP and ASCR.

Both projects include co-Directors of Science and of Computation. For the NP project, these are David Bruhwiler (Tech-X) and Xiaoye Li (LBL), respectively. By mutual agreement, the DS and DC for the two projects will form a Liaison Committee (LC). The LC will communicate regularly via email and telecon and will meet formally after each annual project-wide meeting.

This approach proved successful during the proposal writing stage. For example, two accelerator physics topics that are common to both proposals include SRF cavity modeling and particle tracking with space charge. In both cases, the NP and HEP proposals are directing resources to completely different accelerator facilities, and algorithmically the efforts are completely distinct. However, efforts to achieve higher concurrency with SciDAC codes are synergistic and promise mutual benefit to the programs of both DOE offices.

5.4 Links to SciDAC Institutes

The SciDAC3 ComPASS program will have very strong links to the SciDAC3 Applied Math, Computer Science and Uncertainty Quantification (UQ) Institutes. This is evident from the fact that several participants in this proposal are also members of the SciDAC3 Institutes. Phil Colella, Daniel Graves, Xiaoye Li, Todd Munson, Esmond Ng, Brian Van Straalen, and Chao Yang are members of FASTMath. Moreover, Colella and Ng are members of the FASTMath Executive Committee (Colella is not supported by this proposal, but he will be working closely with Graves, Schwartz, and Van Straalen). Boyana Norris and Stefan Wild are members of SUPER. Ernesto Prudencio is a Co-PI of QUEST. As a result of these links, the applied math, computer science and UQ requirements in ComPASS will be communicated to the SciDAC3 Institutes effectively. Similarly, relevant tools developed by the Institutes will be made available to the ComPASS team promptly. However, it should be noted that the work described in section 4 is tailored specifically for the accelerator physics codes.

References

[1] Particle Physics Project Prioritization Panel, US particle physics: Scientific opportunities, a strategic plan for the next ten years, text available at `http://science.energy.gov/~/media/hep/pdf/files/pdfs/p5_report_06022008.pdf`, 2008.

[2] S. Abraham, Spencer Abraham announces department of energy 20-year science facility plan, text available at `http://www.er.doe.gov/Sub/Newsroom/News_Releases/DOE-SC/2003/Energy%2020-Year%20Science20Facility%20Plan.htm`, 2003.

[3] P. Spentzouris et al., J. Phys. Conf. Ser. **125**, 012005 (2008).

[4] ComPASS Collaboration, Community petascale project for accelerator science and simulation, `http://compass.fnal.gov/scidac-breakthroughs`, `http://compass.fnal.gov/talks-and-publications`, 2008.

[157] J. Amundson, W. Pellico, P. Spentzouris, T. Sullivan, and L. Spentzouris, Nucl. Instrum. Meth. **A570**, 1 (2007).

[145] A. Macridin, P. Spentzouris, J. Amundson, L. Spentzouris, and D. McCarron, Phys.Rev.ST Accel.Beams **14**, 061003 (2011).

[150] E. G. Stern, J. F. Amundson, P. G. Spentzouris, and A. A. Valishev, Phys. Rev. ST Accel. Beams **13**, 024401 (2010).

[8] Many, Nucl. Instrum. Meth. **A570**, 1 (2007).

[9] C. Ng et al., State of the art in em field computation, in *Proceedings of EPAC 2006*, 2006.

[10] Z. Li et al., Analysis of the cause of high external q modes in the jlab high gradient prototype cryomodule renascence, Technical Memorandum SLAC-PUB-13266, SLAC National Accelerator Laboratory, Batavia, Illinois, 2008.

[11] V. Akcelik et al., J. Comput. Phys. **227**, 1722 (2008).

[12] T. Tajima and J. Dawson, Physical Review Letters **43**, 267 (1979).

[13] P. Chen, J. M. Dawson, R. W. Huff, and T. Katsouleas, Phys. Rev. Lett. **54**, 693 (1985).

[14] E. Esarey, P. Sprangle, J. Krall, and A. Ting, Plasma Science, IEEE Transactions on **24**, 252 (1996).

[15] I. Blumenfeld et al., Nature **445**, 741 (2007).

[16] W. Leemans et al., Nature Physics **2**, 696 (2006).

[17] C. Birdsall and A. Langdon, *Plasma physics via computer simulation*, Adam-Hilger, 1991.

[18] J.-L. Vay, Physical Review Letters **98**, 130405/1 (2007).

[19] J.-L. Vay, C. G. R. Geddes, E. Cormier-Michel, and D. P. Grote, Physics of Plasmas **18**, 123103 (2011).

[20] S. F. Martins, R. A. Fonseca, W. Lu, W. B. Mori, and L. O. Silva, Nature Physics **6**, 311 (2010).

[21] P. Mora and T. M. Antonsen, Jr., Phys. Plasmas **4**, 217 (1997).

[22] D. Gordon, W. Mori, and T. M. Antonsen, Jr., IEEE Trans. Plasma Sci. **28**, 1135 (2000).

[23] B. M. Cowan et al., Journal of Computational Physics **230**, 61 (2011).

[24] C. Huang et al., J. Comput. Phys. **217**, 658 (2006).

[25] C. G. R. Geddes et al., J. Phys. Conf. Ser. **125**, 012002 (2008).

[26] M. Tzoufras et al., J. Plasma Phys., submitted (2012).

[27] C. Huang et al., Contributed to Particle Accelerator Conference (PAC 05), Knoxville, Tennessee, 16-20 May 2005.

[28] C.-K. Huang and W. Tsung, F.and Mori, IEEE TRANSACTIONS ON PLASMA SCIENCE **36** (2008).

[29] B. Pollock et al., Physical Review Letters **107**, 45001 (2011).

[30] A. Seryi et al., Contributed to Particle Accelerator Conference (PAC 09), Vancouver, BC, Canada, 4-8 May 2009.

[31] A. Caldwell, K. Lotov, A. Pukhov, and F. Simon, (2008).

[32] S. Lee, T. C. Katsouleas, R. G. Hemker, E. S. Dodd, and W. B. Mori, Phys. Rev. **E64**, 045501 (2001).

[33] V. K. Decyk and T. V. Singh, Comp. Phys. Comm. **182**, 641 (2011).

[34] X. Kong, M. C. Huang, C. Rena, and V. K. Decyk, Comp. Phys. Comm. **230**, 1676 (2011).

[35] X. Lin, Phys. Rev. ST Accel. Beams **4**, 051301 (2001).

[36] G. Werner and J. Cary, Journal of Computational Physics **226**, 1085 (2007).

[37] G. Werner and J. Cary, Journal of Computational Physics **227**, 5200 (2008).

[38] R. England et al., Experiment to demonstrate dcceleration in optical photonic bandgap structures, in *Proc. Particle Accelerator Conference*, 2011.

[39] C.-K. Ng et al., Phys. Rev. ST Accel. Beams **13**, 121301 (2010).

[40] C. Bauer, G. Werner, and J. Cary, Journal of Applied Physics **104**, 053107 (2008).

[41] B. Cowan et al., Compact couplers for photonic crystal laser-driven accelerator structures, in *Proceedings of the First International Particle Accelerator Conference, Kyoto, Japan*, 2011.

[42] J. England et al., Coupler studies for pbg fiber accelerators, in *Proc. Particle Accelerator Conference*, 2011.

[43] Z. Wu, C. Ng, C. McGuinness, and E. Colby, Design of on-chip power transport and coupling components for a silicon woodpile accelerator, in *Proc. Particle Accelerator Conference*, 2011.

[44] Joint MAP & High Gradient RF Collaboration Workshop, 2011, see `https://sites.google.com/a/lbl.gov/rf-workshop/home/`.

[45] S. van der Meer, CLIC-NOTE-68.

[46] A. Candel et al., Numerical verification of the power transfer and wakefield coupling in the clic two-beam accelerator, in *Proc. Particle Accelerator Conference*, 2011.

[47] S. Matsumoto et al., 100 mw x-band test facility in kek, in *Proceedings of EPAC 2008*, 2008.

[48] Z. Li et al., Dark current simulation for the clic t18 high gradient structure, in *Proc. Particle Accelerator Conference*, 2011.

[49] Fermilab Proton Improvement Plan, see `http://www-ad.fnal.gov/proton/PIP/PIP_index.html`.

[50] V. Lebedev, D. McGinnis, W. Pellico, and B. Webber, Proton source improvement plan, Technical Memorandum FNAL/Beams-Doc 3781, Fermi National Accelerator Laboratory, Batavia, Illinois, 2011.

[51] F. Zimmermann, Phys. Rev. ST Accel. Beams **7** (2004).

[52] M. A. Furman, 2010, LBNL Center for Beam Physics Technical Notes 364, 367 & 392.

[53] J.-L. Vay et al., Physics of Plasmas **11**, 2928 (2004).

[54] S. Nagaitsev, Project x reference design and r&d plan, in *Talk at 2011 Fall Project X Collaboration Meeting*, 2011.

[55] S.-H. Kim, Sns superconducting linac operational experience and upgrade path, in *Proc. Particle Accelerator Conference*, 2007.

[56] L. Xiao et al., Effects of elliptically deformed cell shape in the cornell erl cavity, in *Proc. 15th Int. Conf. on RF Superconductivity*, 2011.

[57] R. Lee et al., Multi-cavity trapped mode simulation, in *Talk at Wake Fest 07 - ILC Wakefield Workshop*, 2007.

[58] The Project-X Collaboration, Project x-reference design report v1.0, text available at `http://ProjectX-docdb.fnal.gov/cgi-bin/RetrieveFile?docid=776;filename=RDR-v0.9.pdf;version=1`, 2010.

[59] `http://computing.ornl.gov/workshops/scidac2010/viz_night_winners.pdf`.

[60] H. Childs et al., Visit: An end-user tool for visualizing and analyzing very large data, text available at `http://www.mcs.anl.gov/uploads/cels/papers/scidac11/final/childs_hank.pdf`, 2011.

[61] M. Howison, Q. Koziol, D. Knaak, J. Mainzer, and J. Shalf, Tuning hdf5 for lustre file systems, in *Proceedings of Workshop on Interfaces and Abstractions for Scientific Data Storage*, 2010.

[62] ParaView, see `http://www.paraview.org/`.

[63] S. Shasharina et al., Vizschema–visualization interface for scientific data, in *IADIS International Conference, Computer Graphics, Visualization, Computer Vision and Image Processing*, page 49, 2009.

[64] T. Austin, J. Cary, G. Werner, and L. Bellantoni, Validation of broadly filtered diagonalization method for extracting frequencies and modes from high-performance computations, in *Journal of Physics: Conference Series*, volume 180, page 012003, IOP Publishing, 2009.

[65] D. Abell, PRSTAB **9**, 052001 (2006).

[66] R. Osborne, M. Koennecke, and et al, Nexus user manual, text available at `http://download.nexusformat.org/doc/html/UserManual.html`, 2011.

[67] B. Eaton, J. Gregory, B. Drach, K. T. S. Hankin, and et al, Netcdf climate and forecast (cf) metadata conventions, text available at `http://cf-pcmdi.llnl.gov/documents/cf-conventions/1.6/cf-conventions.html`, 2011.

[68] E. Cormier-Michel et al., Simulation **1**, 1 (2010).

[69] E. Cormier, J. R. Cary, D. L. Bruhwiler, and D. Kindig, Colliding laser pulses launch an electron beam into a plasma accelerator, text available at `http://www.wired.com/wiredscience/2011/08/science-simulation-videos/?pid=1743`, 2011.

[70] A. R. Conn, K. Scheinberg, and L. N. Vicente, *Introduction to Derivative-Free Optimization*, MPS/SIAM Series on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2009.

[71] M. J. Powell, The NEWUOA software for unconstrained optimization without derivatives, in *Large-Scale Nonlinear Optimization*, edited by G. D. Pillo and M. Roma, pages 255–297, Springer, 2006.

[72] M. J. Powell, The bobyqa algorithm for bound constrained optimization without derivatives, Technical Report DAMTP 2009/NA06, University of Cambridge, 2009.

[73] S. M. Wild, R. G. Regis, and C. A. Shoemaker, SIAM J. Sci. Comput. **30**, 3197 (2008).

[74] S. M. Wild and C. A. Shoemaker, SIAM J. Optimization **21**, 761 (2011).

[75] J. J. Moré and S. M. Wild, SIAM Journal on Optimization **20**, 172 (2009).

[76] M. Kortelainen et al., Physical Review C **82**, 024313 (2010).

[77] M. Kortelainen et al., Nuclear energy density optimization: Large deformations, Preprint ANL/MCS-P1977-1111, Mathematics and Computer Science Division, 2011.

[78] S. Benson, L. McInnes, J. Moré, T. Munson, and J. Sarich, TAO users manual (Revision 1.10.1), Technical Memorandum ANL/MCS-TM-242, Argonne National Laboratory, Argonne, Illinois, 2010.

[79] Scidac-3 institute for sustained performance, energy, and resilience (super), `http://super-scidac.org`, 2011.

[80] C. Audet, G. Savard, and W. Zghal, SIAM Journal on Optimization **19**, 188 (2008).

[81] A. L. Custódio, J. F. A. Madeira, A. I. F. Vaz, and L. N. Vicente, SIAM Journal on Optimization **21**, 1109 (2011).

[82] I. Das and J. E. D. Jr., Structural Optimization **14**, 63 (1997).

[83] R. Steuer, *Multiple Criteria Optimization: Theory, Computation and Application*, John Wiley & Sons, New York, 1986.

[84] D. R. Jones, M. Schonlau, and W. J. Welch, Journal of Global Optimization **13**, 455 (1998).

[85] B. Norris, A. Hartono, E. Jessup, and J. Siek, Generating empirically optimized composed matrix kernels from MATLAB prototypes, in *Proceedings of the International Conference on Computational Science 2009*, 2009, Also available as Preprint ANL/MCS-P1581-0209.

[86] A. Hartono, B. Norris, and P. Sadayappan, Annotation-based empirical performance tuning using Orio, in *Proceedings of the 23rd IEEE International Parallel & Distributed Processing Symposium*, Rome, Italy, 2009, Also available as Preprint ANL/MCS-P1556-1008.

[87] Optimization algorithms and software for communication avoidance and communication hiding at the extreme scale (CACHE Institute), `https://ftg.lbl.gov/projects/cache`, 2011.

[88] R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles*, McGraw-Hill, 1981.

[89] P. C. Liewer and V. K. Decyk, J. Computational Phys. **85**, 302 (1989).

[90] P. McCorquodale, P. Colella, D. P. Grote, and J.-L. Vay, J. Comput. Phys. **201**, 34 (2004).

[91] P. McCorquodale, P. Colella, G. Balls, and S. Baden, Communications in Applied Mathematics and Computational Science **2**, 57 (2007).

[92] G.-H. Cottet and P. D. Koumoutsakos, *Vortex methods: theory and practice*, Cambridge University Press, 2000.

[93] B. Wang, G. H. Miller, and P. Colella, SIAM J. for Sci. Computing (2011), to appear.

[94] S. W. Williams, The roofline model, in *Performance Tuning of Scientific Applications*, edited by D. H. Bailey, R. F. Lucas, and S. W. Williams, CRC Press, 2010.

[95] V. K. Decyk, Comp. Phys. Comm. **177**, 95 (2007).

[96] P. Colella et al., Chombo Software Package for AMR Applications - Design Document, unpublished, 2000.

[97] P. Schwartz, M. Barad, P. Colella, and T. Ligocki, Journal of Computational Physics **211**, 531 (2006).

[98] Y. Saad, *Numerical Methods for Large Eigenvlaue Problems*, SIAM, 2nd edition, 2011.

[99] X. S. Li and J. W. Demmel, ACM Trans. on Mathematical Software **29**, 110 (2003).

[100] A. Gupta and M. Joshi, Wsmp: A high-performance shared- and distributed-memory parallel sparse linear equations solver, 2001, IBM Research Report.

[101] P. Amestoy, I. Duff, and J.-Y. L'Excellent, Comput. Methods in Appl. Mech. Eng. **184**, 501 (2000).

[102] C. Yang et al., SIAM J. Sci. Comput. **27**, 873 (2005).

[103] L. Lee et al., J. Phys.: Conf. Ser. **125**, 012077 (2008).

[104] W. F. Noh, CEL: A time-dependent, two-space-dimensional, coupled Eulerian - Lagrangian code, in *Fundamental Methods in Hydrodynamics*, edited by B. Alder, S. Fernbach, and M. Rotenberg, volume 3 of *Methods in Computational Physics*, pages 117–180, Academic Press, 1964.

[105] I. L. Chern and P. Colella, A conservative front-tracking method for hyperbolic conservation laws, Technical Report UCRL-97200, Lawrence Livermore National Laboratory, 1987.

[106] J. Bell, P. Colella, and M. Welcome, Conservative front-tracking for inviscid compressible flow, in *AIAA 10th Computational Fluid Dynamics Conference. Honolulu*, pages 814–822, 1991.

[107] M. J. Berger and R. J. Leveque, Stable boundary conditions for cartesian grid calculations, Technical Report 90-37, ICASE, 1990.

[108] R. B. Pember, J. B. Bell, P. Colella, and W. Y. Crutchfield, Journal of Computational Physics **120**, 278 (1995).

[109] A. S. Almgren, J. B. Bell, P. Colella, and T. Marthaler, A cell-centered cartesian grid projection method for the incompressible Euler equations in complex geometries, in *Proceedings of the AIAA 12th Computational Fluid Dynamics Conference,*, San Diego, California, 1995.

[110] H. Johansen and P. Colella, J. Comput. Phys. (1998).

[111] P. Colella, Volume–of–fluid methods for partial differential equations, in *Godunov Methods: Theory and Applications*, pages 161–177, Kluwer, 2001.

[112] P. McCorquodale, P. Colella, and H. Johansen, J. Comput. Phys. **173**, 620 (2001).

[113] P. Colella, D. T. Graves, B. Keen, and D. Modiano, J. Comput. Phys. **211**, 347 (2006).

[114] M. Berger and J. Oliger, J. Comput. Phys. **53**, 484 (1984).

[115] M. J. Berger and P. Colella, J. Comput. Phys. **82**, 64 (1989).

[116] R. T. Cox, *The Algebra of Probable Inference*, Johns Hopkins Univ. Press, Baltimore, MD, 1961.

[117] E. T. Jaynes, *Probability Theory: The Logic of Science*, Cambridge University Press, 2003.

[118] J. L. Beck and L. S. Katafygiotis, ASCE Journal of Engineering Mechanics **124**, 455 (1998).

[119] J. A. Hoeting, D. Madigan, A. E. Raftery, and C. T. Volinsky, Statistical Science **14**, 382 (1999).

[120] C. P. Robert, *The Bayesian Choice: From Decision-Theoretic Foundations to Computational Implementation*, Springer Science+Business Media, LLC, 2007.

[121] M. Muto and J. L. Beck, J. Vib. and Cont. **14**, 7 (2008).

[122] S. H. Cheung and J. L. Beck, Computer Methods in Applied Mechanics and Engineering (2011), Accepted for publication.

[123] S. H. Cheung, T. A. Oliver, E. E. Prudencio, S. Prudhomme, and R. D. Moser, Reliab. Eng. Syst. Saf. **96**, 1137 (2011).

[124] E. E. Prudencio and S. H. Cheung, International Journal for Uncertainty Quantification (2011, to appear).

[125] S. H. Cheung and E. E. Prudencio, (2011, submitted).

[126] E. E. Prudencio and K. W. Schulz, The parallel C++ statistical library QUESO: Quantification of uncertainty for estimation, simulation and optimization, in *Proceedings of the Workshops of the Euro-Par 2011 Conference*, edited by P. D'Ambra *et al.*, Lecture Notes in Computer Science, Springer, 2011, to appear.

[154] J. Amundson et al., J.Phys.Conf.Ser. **125**, 012001 (2008).

[153] D. Dechow, P. Stoltz, J. Amundson, P. Spentzouris, and B. Norris, Conf.Proc. **C0806233**, TUPP088 (2008).

[129] L. Curfman McInnes et al., Conf.Proc. **C070625**, 3552 (2007).

[130] M. A. Furman, 1998, LBNL-41482/LHC-PR-180.

[131] M. A. Furman and M. T. V. Pivi, Phys. Rev. ST-AB **5**, 124404 (2003).

[132] D. Grote, A. Friedman, J.-L. Vay, and I. Haber, The warp code: modeling high intensity ion beams, in *AIP Conference Proceedings*, number 749, pages 55–8, 2005.

[133] J.-L. Vay, M. A. Furman, and M. Venturini, Direct numerical modeling of e-cloud driven instability of a bunch train in the cern sps, in *Proc. Particle Accelerator Conference*, New York, NY, 2011, WEP154.

[134] J.-L. Vay, Physics of Plasmas **15**, 056701 (2008).

[135] C. G. R. Geddes et al., Nature **431**, 538 (2004).

[8] C. G. R. Geddes et al., Physical Review Letters **100** (2008).

[137] C. G. R. Geddes et al., Laser plasma particle accelerators: Large fields for smaller facility sources, in *SciDAC Review 13*, page 13, 2009.

[138] E. Cormier-Michel et al., Physical Review E **78** (2008).

[139] J.-L. Vay, C. G. R. Geddes, E. Cormier-Michel, and D. P. Grote, Physics of Plasmas (Letter) **18**, 030701 (2011).

[140] R. Storn and K. Price, Journal of Global Optimization **11**, 341 (1997).

[141] C. Nieter and J. R. Cary, J. Comput. Phys. **196**, 538 (2004).

[142] A. Taflove and S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method*, Artech House, Boston, third edition, 2005.

[143] K. S. Yee, IEEE Trans. Antennas Propag. **14**, 302 (1966).

[144] K. Amyx et al., Gpu-accelerated 3d electromagnetic particle-in-cell implementations in vorpal, 2012.

A Scientific Advisory Committee

Ilan Ben-Zvi	BNL
Eric Colby	SLAC
Lori Diachin	LLNL
Omar Ghattas	UTA
Chan Joshi	UCLA
Wim Leemans	LBNL
Bob Lucas	USC
Sergei Nagaitsev	FNAL
Vladimir Shiltsev	FNAL

B Statements of Work

Description of statements of work follow in alphabetical order.

Argonne National Laboratory – Statement of Work

POC: Boyana Norris

ANL is requesting funds to support work in computer science, with a focus on performance analysis and tuning, and numerical approaches to parameter optimization (to be funded by ASCR).

Performance Analysis and Optimization

To ensure performance portability and code maintainability on existing and future HPC platforms, we will employ the performance and reliability methodology and tools developed in the SciDAC-3 Institute for Sustained Performance, Energy, and Resilience (SUPER) [79] or available through platform vendors and the larger performance community to the set of accelerator codes involved in this project. Our goals are to ensure both performance portability and resilience of new parallel algorithms developed as part of this project, as well as to improve the performance of existing implementations that are leveraged through the use of numerical libraries. A key component of our approach is the integration of advanced performance analysis capabilities and autotuning into the development of new algorithms and the improvement of existing implementations. To be truly effective, the performance evaluation and key optimizations must be automated, so that performance testing and improvement can become an integral component of the accelerator software development process. Ultimately performance testing and certain types of tuning will be integrated into regression and unit testing frameworks for accelerator codes, starting with VORPAL in year 1, followed by QuickPIC in year 2, and finally Synergia in year 3. We must develop common methods for performance regression testing, so that other existing and new accelerator codes can incorporate these capabilities in their development.

For the measurement and analysis capabilities, we will rely on the approaches and software being developed in SUPER, while simultaneously ensuring that specific accelerator software needs are considered through the involvement of PI Norris who is the Argonne SUPER PI.

Beyond performance characterization, automating the generation of highly optimized versions of key kernels will improve both application performance and the developers' productivity. Furthermore, this approach enables the "customization" of general-purpose numerical libraries for specific applications by generating versions that are optimized for specific input and use characteristics. Several components are required to provide these code generation capabilities.

- A mechanism for defining the computation at a sufficiently high level.
- Application-specific library optimizations.
- Automatic tuning of generated kernels and (re)integration into larger code bases.

Next we discuss our proposed approach to providing each of these components.

High-level computation specifications. Existing implementations of key kernels, e.g., matrix-vector products, can be generated from higher-level (e.g., Matlab-like) representations. Previous work in generating optimized code for composed linear algebra operations [85] demonstrates that the generated code performance can greatly exceed that of collections of calls to prebuilt libraries. The key challenges are to associate different underlying matrix and vector representations with the high-level kernel specification. Another challenge is code generation for distributed memory architectures, including hybrid CPU/GPU systems. Part of our research will be to identify key kernels and devise a high-level representation that can be associated with different (manually specified) data structures. Another issue is seamlessly integrating the tuned versions into the rest of the code base, which is typically implemented in Fortran, C, or C++. In previous work we have shown that high- level computation specifications can be embedded in existing C or Fortran codes by expressing them through annotations specified as structured comments [86]. Because of better utilization of spatial and temporal locality in the presence of fusable matrix and vector operations, the performance of code generated from such high-level specifications is almost always significantly better than that of compiled C or Fortran code and for composed operations, it far exceeds that of multiple calls to optimized numerical libraries. We will implement new code generation capabilities targeting emerging manycore and hybrid multicore/accelerator architectures.

Application-specific library optimizations. Given a high-level computation representation and a detailed architectural description (e.g., obtained through microbenchmarks), we will generate multiple kernels by using different performance-improving transformations. Ideally this will be done in a specific application context, e.g., using a representative sample of input sizes and values.

Integration with autotuning capabilities. The generated tuned code versions would be evaluated by using an empirical autotuning approach. Empirical autotuning presents a challenging optimization problem – the search space is extremely large and thus cannot be explored exhaustively. We will employ the derivative-free global optimization techniques being developed as part of the DOE Math/CS CACHE Institute [87] and the multiobjective optimization approaches in the SciDAC SUPER Institute [79] to produce better (closer to optimal) results while exploring just a tiny fraction of the parameter space. By producing customized builds of key subsets of numerical algorithms (e.g., linear algebra kernels) that reflect actual application inputs, we will be able to exploit multicore and hybrid resources more effectively. We will generalize this idea to more types of operations and enable kernel specialization (e.g., based on problem size) during autotuning. The resilience toolset being developed in SUPER builds on the autotuning ideas to provide mechanisms for detecting and responding to soft errors. We will integrate resilience approaches into the development of new algorithms to improve resilience along with performance on leadership architectures.

Local Optimization of Expensive Problems

Accelerator design optimization problems typically depend on the output of a computationally expensive simulation (e.g., a VORPAL run) for which derivatives of the output with respect to the design variables are noisy and often unavailable. Through systematic parameterization of surfaces and other dimension reductions, typical problems depend on up to tens of parameters and must be solved with so-called derivative-free optimization methods [70].

We will consider several types of optimization problems. In laser plasma modeling, first we wish to simultaneously optimize energy spread, RMS quantities, and particle distribution (which requires expensive simulations). A second type of optimization problem involves changing the accelerator cavity shape to minimize the maximum surface temperature. To support future accelerator design, nonlinear beam dynamics-based optimization can be used to determine the best accelerator machine parameters.

The primary consideration for these problems is that the expense of evaluating the objective or constraints allows for relatively few sequential evaluations. Consequently we will explore model-based methods (such as NEWUOA [71], BOBYQA [72], ORBIT [73, 74]), which have been shown to be effective at reducing objectives in as few evaluations as possible [75]. In addition to parallelization strategies, we will explore exploiting additional structure in the problem, such as RMS objectives based on sums of squared residuals depending on simulation outputs. When such structure is present, algorithms such as Argonne's POUNDerS (Practical Optimization Using No Derivatives for Squares) have been shown to require many fewer simulation evaluations than blackbox alternatives [76, 77]. POUNDerS is available in TAO, the Toolkit for Advanced Optimization [78].

In cases where multiple simultaneous objectives are should be pursued (e.g., in laser plasma modeling minimizing both the energy spread and RMS particle-based quantities), we will leverage the research in the SUPER SciDAC Institute and explore multi-objective optimization [80, 81, 82, 83]. In ComPASS, the Argonne optimization work will focus on providing an interface and solver software for the local solution of the hybrid multistart approach that will be developed jointly with LBNL.

<u>Tasks</u>:

- YEAR 1:
  - Identify performance test cased for VORPAL and QuickPIC. These will include test problems with excellent load balance as well as typical physics runs.
  - Identify performance bottlenecks in VORPAL (both parallel and single-node) and produce a report.
  - Begin development of common methods and software for performance regression testing of all codes.
  - Investigate effectiveness of local optimization methods for laser plasma modeling.
- YEAR 2:
  - Identify performance bottlenecks in QuickPIC using test problem(s) defined in Year 1.
  - Implement manual and automated transformations in VORPAL based on the findings in Year 1.
  - Continue development of common methods and software for performance regression testing of all codes.
  - Investigate the use of POUNDerS as the local optimization approach in a hybrid method for global optimization of nonlinear beam dynamics.
- YEAR 3:
  - Analyze Synergia performance, including its use of external libraries such as PETSc.
  - Develop performance optimization strategies for Synergia, interacting with PETSc and other underlying numerical software teams as necessary.
  - Complete development of common methods and software for performance regression testing of all codes.
  - Complete integration of local methods into hybrid multistart global optimization method (with LBNL).

Fermi National Accelerator Laboratory – Statement of Work

POC: Panagiotis Spentzouris

Fermilab is requesting funds to support work in accelerator physics, particle-in-cell library development, and to provide domain expertise in data and visualization and parameter optimization capability development. Fermilab is also requesting funds for project management and coordination.

Fermilab will participate in accelerator physics applications for Intensity Frontier (Fermilab Proton Improvement Plan, Project X) and Energy Frontier (beam-driven plasma acceleration), working in close collaboration with personnel from LBNL, Tech-X and UCLA. Under the SciDAC program, Fermilab has developed state-of-the-art beam dynamics capabilities in Synergia. Synergia is a multi-language, extensible, parallel PIC framework which allows state-of-the-art optimized numerical libraries, solvers, and physics models to be employed to simulate complex simulation scenarios. We have established close collaboration with accelerator designers and machine physicists, that ensure that the Synergia will meet the needs of the above projects.

Software development at Fermilab will focus on new techniques and technologies for scalable solvers and Particle In Cell (PIC) algorithms and providing domain expertise to the development of data, visualization and parameter optimization capabilities. Under SciDAC2, Fermilab has acquired significant expertise in PIC and solver development, including hybrid and GPU environments. We will work in close collaboration with personnel from ANL, LBNL, Tech-X, and UCLA to extend and improve these capabilities. In addition to contributing to the development of general-purpose libraries developed by the collaboration, we will extend the Synergia framework with new capabilities to support accelerator physics applications described above.

Accelerator Physics (to be funded by HEP)

Proton Improvement Plan Fermilab Booster intensities and repetition rate are currently limited by radiation due to uncontrolled losses. These losses are a problem both because of prompt radiation levels and equipment activation. An improved collimation system must be implemented to limit losses to acceptable levels while increasing beam intensities and repetition rates to increase the protons per hour by a factor of 2.3, as called for by the Fermilab Proton Improvement Plan [49, 50]. In order to design the collimation system, the source and cause of losses during the machine cycle must be identified. We will develop the necessary Synergia applications and provide the simulations necessary to support this effort.

Two intensity-dependent effects are important in the Fermilab Booster: space charge and wake fields in the laminated quadrupole magnets. During SciDAC2, we developed a detailed model of wake fields in laminated structures in Synergia and validated it with experimental results [145]. This is the first time that a comprehensive model of impedance and space-charge for all 84 bunches was utilized in Fermilab Booster simulations. The wake field and space charge calculations are inherently coupled through the boundary conditions of the space charge field, so our model must include space charge with compatible boundary conditions. Wake fields give rise to interactions between particles within a bunch as well as from bunch to bunch. We will model and study both effects. Since collective effects are most important at the lower injection energy, all of our initial simulations will take place at the injection energy. Our later simulations will expand to consider higher energies in the Booster cycle, to provide information of the loss pattern during the complete cycle.

Tasks:

- YEAR 1:
  - Detailed booster model including space charge, single-bunch wakefields and beam optics including apertures derived from studies. Compare simulations to data from beam

studies, validate/improve model.

- YEAR 2:
  - Simulations expanded to include multi-bunch effects. Perform simultaneous simulations of all 84 booster bunches. Compare simulations to data from beam studies, validate/improve model. Develop model of collimators and integrate into simulation.
- YEAR 3:
  - Complete simulations with collimators and 84 bunches. Include accelerating phase of booster cycle into simulations. Perform simulations at higher energies, especially in the vicinity of transition.

Project X Main-Injector In the Project X era the Fermilab Main Injector (MI) will be the driver for the higher-energy portion of the physics program at the intensity frontier. In the near term, this program includes the production of intense neutrino and antineutrino beams for the detailed study of oscillation parameters. Longer time-scale plans envision production of muon beams for a neutrino factory and a muon collider. Space-charge and electron cloud effects are expected to play a significant role in limiting the performance of the machine. It is essential to understand these effects in order to minimize losses and maximize the effectiveness of the mitigation systems. With this activity we will provide the necessary guidance for designing such systems, especially the collimator and rf systems.

Fermilab, in collaboration with Tech-X, has developed detailed models of electron cloud generation experiments at the MI using the VORPAL framework and has applied these models to study and analyze experimental results. In addition, we are in the process of developing a detailed model of the MI, including measured fringe-fields and apertures, in order to study space-charge and electron cloud-induced instabilities and losses. We will extend these capabilities, incorporating results from electron cloud experiments to improve the model, and incorporate new libraries to improve the numerical performance. We will also incorporate electron cloud effects in Synergia, benchmark with WARP and QuickPIC, and ultimately deploy these capabilities to study losses and design mitigation systems for the MI.

Tasks:

- YEAR 1:
  - Support for the analysis of electron cloud experiments in the MI, including the simulation of the electron fluence at the RFA for current operating conditions, and simulations of table top experiments to measure reflections and attenuation of rf in the presence of dielectrics.
  - Perform space charge simulations of the MI and determine the space charge solver that gives the best performance given the trade-offs between computational speed and correctness given the boundary conditions and other factors.
- YEAR 2:
  - Support for experiments and simulation of electron-cloud-induced beam instabilities, via an interface between VORPAL and/or POSINST electron cloud field maps and Synergia. Establish validation procedure and cases, validate implementation with QuickPIC comparisons.
  - Continue our program of space charge simulations, adding detailed aperture specifications to the machine mode and determine the effects of their contribution to generating localized machine losses. Consider additional effects such as magnet ramping for acceleration, machine impedance and multiple bunches.
- YEAR 3:
  - Enhance adaptive macro-particle management (*i.e.,* reduction and coalescence of macro-

particles) for VORPAL electron cloud simulations.
  - Integrate space charge simulations with electron cloud simulations described above. Perform simulations of the MI incorporating the effects of space charge, electron cloud, fringe fields, and apertures to determine a detailed map of location and magnitude of particle losses in the accelerator.

Beam-Plasma Accelerators There has been recent interest in using proton beams [31]. Current proton beams have energies near 7 TeV and have total beam energy near 100 kJ. If such a bunch could be compressed to efficiently make a wakefield, a trailing electron bunch with more than a nC of charge could be accelerated in a single stage to nearly 1 TeV before dephasing occurs. Currently, no such compressed bunches exist, so experiments are being considered to study how a long proton bunch self-modulates as it propagates in a tenuous plasma. Fermilab, in collaboration with UCLA, has been studying the possibility of performing such experiments at Fermilab using either MI or Booster proton beams. In order to design, explore and optimize parameters for such experiments, it is imperative that we develop integrated modeling capabilities that combine plasma modeling with conventional beam dynamics codes. Such capabilities will be also useful for studying operating conditions in other beam-driven experiments such as those performed in the FACET facility. The Synergia framework incorporates all the necessary beam dynamics capabilities and it is easily extendable. We will take advantage of these features of Synergia to interface it with the UCLA codes OSIRIS and QuickPIC, to develop the necessary capabilities and deploy them for the design of proton-driven plasma experiments at Fermilab.
Tasks:
- YEAR 1:
  - Develop Synergia interface to OSIRIS.
  - Develop Synergia interface to QuickPIC.
- YEAR 2:
  - Develop a model for self-modulating proton-driven plasma experiment for MI beam parameters using a section of the FNAL Tevatron lattice.
- YEAR 3:
  - Optimize self-modulation experiment.
  - Develop compressed proton beam experiment concepts for beam from the FNAL Booster, for a proof-of-principle experiment design.

Project X to Muon Collider There are many conceptual ideas on how to design this interface, and the Muon Acceleration Program (MAP) collaboration is expected to select a few for study during their Winter 2012 meeting. All of these designs appear to be inherently nonlinear, so standard computational tools will not be adequate for their simulation and optimization. The Synergia framework is well suited for this work, and the TAU library for parallel nonlinear optimization will be used with Synergia to enable systematic design and optimization. We will perform this work in collaboration with Tech-X. Since the design effort is in the early stages of development, this activity will require close collaboration with experts from the Project X team, members of MAP, and ComPASS team members at Fermilab.
Tasks:
- YEAR 1:
  - Work with MAP researchers to identify promising ring design ideas.
  - Use Synergia to simulate one or more ring designs.
  - Identify Synergia development needs.
- YEAR 2:
  - Implement new capabilities in Synergia, based on Year 1 results.

  - Develop improved merit functions for nonlinear optimization.
- YEAR 3:
  - Implement new capabilities in Synergia, based on Year 2 results.
  - Work with Project X and MAP researchers to refine design concepts.
  - Optimize selected designs using project developed tools, evaluate their performance.

Particle-in-Cell and Infrastructure (to be funded by ASCR)

Particle in Cell Development Recent (and anticipated future) developments in computing hardware have created new challenges for the efficient use of the particle-in-cell methods that are ubiquitous in accelerator simulation. The existence of multiple hierarchies of access to memory has made simple extrapolations of existing single-level, purely MPI-based parallelism less efficient than they were are the previous generation of leadership-class computing hardware. The change in the memory access to FLOP ratios are even forcing us to reevaluate some of the underlying numerical algorithms in our PIC implementations. During SciDAC2, we have performed initial investigations in adapting Synergia for GPUs (in collaboration with UCLA) and many-core processors (in collaboration with LBNL.) We will continue and expand these collaborations to participate in the development of general purpose libraries for PIC methods in accelerator physics adapted to the new era of computing hardware. Fermilab will participate in interface development and full integration with a full beam-dynamics package, Synergia. We will also perform real-world profiling and optimization and compare and combine the approaches developed by computational scientists at Fermilab and UCLA and applied mathematicians at LBNL.
Tasks:
- YEAR 1:
  - Work in collaboration with UCLA to develop many-core and GPU optimization for Synergia.
  - Work with LBNL to act as a testbed for the FASTMath PIC library programming interface and evaluate performance.
- YEAR 2:
  - Interface Synergia to the 3D portion of the PIC library developed by UCLA and compare results with native optimizations. Provide feedback for PIC library design.
  - Interface Synergia to FASTMath PIC library. Profile real-world performance and collaborate with FASTMath on optimizations.
- YEAR 3:
  - Work on UCLA and FASTMath library interfaces in Synergia to bring them to end-user, production use.
  - Profile real-world performance of both libraries and work on possible combinations of functionality.
  - Contribute to releases of libraries.

Infrastructure Many high performance computing topics fall at the intersection of computer science, applied math and the application domain. Topics such as these require expertise from all three domains to be combined in order to create working application domain solutions at the leading edge of computer science and applied math research. The Fermilab group has developed a track record of working with computer science and applied math groups from ANL, Tech-X, and LBNL under previous SciDAC grants[129, 153, 154]. During SciDAC3, we will work with computer scientists at Tech-X on requirements for and optimization of visualization metadata. We will also work with computer scientists and applied mathematicians at ANL on global parameter optimization.
Tasks:

- YEAR 1:
  - Provide requirements for semantic metadata schema for self-describing data files in collaboration with Tech-X. Implement schema in Synergia.
  - Interface Synergia to initial global optimization libraries in collaboration with ANL.
- YEAR 2:
  - Provide requirements for semantic metadata schema for self-describing data files in collaboration with Tech-X. Implement schema in Synergia.
  - Compare other project-developed optimization approaches in Synergia, using basic interface developed in Year 1.
- YEAR 3:
  - Provide requirements for semantic metadata schema for self-describing data files in collaboration with Tech-X. Implement schema in Synergia.
  - Perform production global optimization in Synergia simulations of Fermilab Main Injector and Booster.

Project management, support and outreach (to be funded by HEP)

The Fermilab PI, Panagiotis Spentzouris, serves as the Program Director (PD) of the project and serves as the principal contact with the DOE. The PD will submit progress reports to DOE semi-annually and is responsible for tracking the overall grant budget and project issues and progress. He will chair bi-weekly meetings of the Executive Board (EB), whose members are the co-PIs of the collaborating institutions.

Fermilab will be responsible for supporting and coordinating the project infrastructure and outreach. The project will maintain a unified web presence including project web pages, a document repository, and a code meta-repository. The project web pages will be an expanded version of the current ComPASS website (`https://compass.fnal.gov`) using a new content management system (CMS). The expanded pages and their content will be designed and maintained by a Fermilab outreach specialist, from the Outreach Office of the Fermilab Computing Division. The project CMS will be a portal for the accelerator physics community, including an overview of the ComPASS project, news items and meeting information. The document repository will contain results and progress of our research, including technical documents and reports.

The code meta-repository is a new feature, whose goal is to enhance the visibility and availability of our codes to the community. Each code in the project will be described, including a general overview as well as capabilities and requirements. For each entry there will be information on availability, which could range from links to source and/or binary downloads, information on installed versions for supercomputer installations, and contact information for requests, as appropriate.
Tasks:

- YEAR 1:
  - PD maintains and tracks Project WBS, coordinates project activities, chairs bi-weekly EB meetings,compiles and submits reports to DOE and coordinates with DOE offices.
  - Select CMS, design and implement Project web pages and code meta-repository.
- YEAR 2:
  - PD maintains and tracks Project WBS, coordinates project activities, chairs bi-weekly EB meetings,compiles and submits reports to DOE and coordinates with DOE offices.
  - Maintain and update web pages and code meta-repository.
- YEAR 3:
  - PD maintains and tracks Project WBS, coordinates project activities, chairs bi-weekly EB meetings,compiles and submits reports to DOE and coordinates with DOE offices.
  - Maintain and update web pages and code meta-repository.

Lawrence Berkeley National Laboratory – Statement of Work

POC: Esmond G. Ng

LBNL is requesting funds to support work in accelerator physics and applied mathematics.

Accelerator Physics (to be funded by HEP)

Electron Clouds LBNL has developed state-of-the-art simulation tools for the computer modeling of the buildup of electron clouds and their interaction with positively charged beams. The buildup code POSINST [130, 131] and the Particle-In-Cell accelerator code Warp [132] have been integrated into one common framework, allowing for three-dimensional fully self-consistent simulations of the electron cloud buildup and its effect on the beam dynamics simultaneously, therefore including the memory of electron clouds between bunches, hence multi-bunch effects. Such simulations have been performed for 1000 turns of up to three trains of 72 bunches each circling in the CERN SPS ring [133]. For moderately high resolution and statistics, 8 CPUs were used per RF bucket, for a total of 5-10 hours runs using 11,520 CPUs on Franklin at NERSC.

During past simulations of electron cloud buildup, and especially for Fermilab's Main Injector, an unphysical runaway of electrons accumulation has been observed near boundaries [52]. The origin of the unphysical instability is well understood and is linked to spatial and temporal inaccuracies in the integration of field and particle motion near conductors. The LBNL team proposes to apply adaptive mesh refinement on a combination of block Cartesian and conformal patches (that follow the contours of conductors) and specialized particle pushing toward the mitigation of the numerical instability. These techniques are already existent within Warp [53] and will be generalized for the Warp-POSINST package. The package will then be used for buildup and fully self-consistent modeling of the electron cloud effects in Fermilab's main injector. The large number of macroelectrons that are produced during the buildup process sometimes necessitate active particle management via culling (available in Posinst) or coalescence. Different algorithms will be experimented and compared against each other, and the best will be implemented for production in Warp-POSINST.

The new tools will be applied to the fully self-consistent modeling of electron cloud buildup and its effect on bunch trains in the Main Injector. Predictive simulations may ultimately necessitate following hundreds of bunches at very high resolution and statistics for tens of thousand of turns, which calls for very large-scale simulations using hundred of thousands of CPUs. These simulations will be performed in either the quasistatic or the Lorentz boosted frame mode [134], and in both modes for comparison if time permits. Computing capabilities that exist or are being developed in the SciDAC3 institutions (e.g. Poisson solver with adaptive mesh refinement), when confirmed to offer better performance and/or usability than the equivalent capabilities in Warp-POSINST, will be adopted and used in place of the latter.

Tasks:

- YEAR 1:
  - apply and evaluate adaptive mesh refinement and specialized particle pushing to mitigation of numerical instability near conductors
- YEAR 2:
  - enhancement of adaptive macro-particle management (splitting and culling/coalescence of macro-particles)
- YEAR 3:

- fully self-consistent modeling of electron cloud buildup and its effect on bunch trains in Main Injector using quasistatic or/and Lorentz boosted frame mode

Laser-Plasma Accelerators The LBNL simulation effort in laser-plasma acceleration (LPA) will continue to develop state of the art simulation tools and use these to explore forefront physics. Recent highlights include the physics of high quality electron bunches [135], controlled injection and detailed benchmarking with experiments [8, 137], reduction of unphysical kinetic effects in PIC [138]. The simulations require the highest performance computing (often 100's of thousands of hours and >10k processors) due to the separation of scales between the micron laser period and meter scale accelerator length. Full scale 10 GeV stage designs relevant to the BELLA PW laser have been enabled by Lorentz boost technique and its application [18, 139], and by collaboration on Envelope reduced models [23]. This includes work with the VORPAL and Warp codes as well as algorithm development and physics models used to improve the codes.

LBNL will model and design laser plasma accelerator (LPA) stages to produce high quality 10 GeV beams in meter-scale plasmas, techniques to improve electron beam quality, and staging of multiple LPAs while maintaining beam quality and geometric gradient. This supports HEP investment in the BELLA project and related LOASIS experiments at LBNL, as well as future collider concepts and stewardship of accelerator technology for light sources. Uncertainty quantification will be conducted to better understand model and input uncertainties. Code development focuses on improvements to VORPAL in collaboration with Tech-X and to Warp. Reduced models will be developed for faster compute time and greater accuracy, such as envelope models which better tolerate laser depletion. The boosted frame method will be further developed, benchmarked, and used for production simulations. Methods for more accurately modeling phase space will be explored, including mesh refinement [53], which are important to modeling high brightness beams over long propagation distances for colliders. Validation against experiments will be conducted, facilitated by close interaction with the LOASIS laser facility of LBNL, including experiments by SciDAC investigators and other group members. Several smaller codes are also used for algorithm and model development.

Tasks:

- YEAR 1:
  - model 10 GeV stages for BELLA, start injection work
  - begin uncertainty quantification on 100 MeV, externally injected LPAs
- YEAR 2:
  - use simulations to evaluate options for controlled injection, continue 10 GeV simulations
  - pursue uncertainty quantification on 100 MeV, externally injected LPAs
- YEAR 3:
  - simulate staging of multiple LPAs
  - development of envelope models for deep depletion
  - complete uncertainty quantification on 100 MeV, externally injected LPAs

Nonlinear Parameter Optimization Parallel nonlinear beam dynamics optimization plays an important role in designing next generation accelerators. It provides the means to identify the best accelerator machine parameters that results in the best performance of the accelerator. This can not only lower the technical risk in the construction of new accelerator but also reduce the potential cost of the accelerator. In our previous study at LBNL, we have explored two optimization methods, one is an evolutionary based method; i.e., differential evolution method [140], the other is the trust region based method [72].

The differential evolution method is a relative simple but powerful stochastic optimization method. It will find the optimal Pareto front in a single simulation. The trust region algorithm developed recently by Powell is a deterministic method that provides an effective way to handle expensive black-box objective function. In our case, the objective function is from the parallel beam dynamics simulation results. In this proposal, we will first parallelize the trust region bease algorithm for a single objective function optimization. Next, we will implement a multi-start cluster algorithm with above local model based optimization algorithm and the expected improvement [84] to balance the exploitation and the global exploration. Then we will implement a parallel multiple objective optimization using the differention evolution method or the hybrid method.

Tasks:

- YEAR 1:
  - parallelize a trust region based optimization algorithm and integrate with beam dynamics optimization
- YEAR 2:
  - implement a parallel incomplete global optimization package
- YEAR 3:
  - implement a parallel multi-objective optimization package

Applied Mathematics (to be funded by ASCR)

Numerical Linear Algebra Collaboration between applied mathematicians at LBNL and computational scientists at SLAC over the last decade has resulted in the development and integration of state-of-the-art numerical linear algebra algorithms and software packages into the accelerator modeling suite ACE3P for the simulation of electromagnetics systems. Our work has focused on eigenvalue calculations and the solution of large sparse linear systems.

- Incorporation of an exact shift-invert Lanczos algorithm into ACE3P's frequency-domain eigensolver Omega3P for computing some of the extreme eigenvalues.
- Further optimization of SuperLU_DIST, which was subsequently incorporated into the exact shift-invert Lanczos code.
- Development of an algebraic sub-structuring method for solving sparse eigenvalue problems.
- Incorporation of the second-order Arnoldi reduction into ACE3P for solving quadratic eigenvalue problems, which arise in the modeling of an accelerating cavity when it is coupled to an external system through a waveguide.
- Inclusion of the self-consistent iterations and the nonlinear Arnoldi method for general nonlinear eigenvalue problems
- Development of a hybrid linear solver, PDSLin, which is based on domain decomposition techniques: the problem is subdivided into subdomains, with an interface connecting the subdomains, and a sparse direct method is applied to the subdomains and a preconditioned iterative method is applied to the Schur complement; the preconditioner can be an approximation of the Schur complement.

We will build on the successes and continue our collaboration with SLAC. Our proposed work will focus on improving the performance and scalability of eigensolvers and linear solvers on the current and the next generations of parallel computer architectures that use multi-/many-cores. In particular, there is a need to balance the workload and reduce the amount of communication. The work will require changing the data structure, redesigning, and rewriting the eigensolvers and linear solvers. We will also investigate improving the reliability and numerical quality of our solvers, particularly PDSLin in the context of solving large sparse linear systems arising from the simulation of electromagnetics systems. This work will be carried out in close collaboration with the FASTMath SciDAC Institute, including the incorporation of a new parallel sparse symmetric solver to be developed by FASTMath to reduce the memory requirement in solving large sparse linear systems arising in simulation of electromagnetics systems.

Tasks:
- YEAR 1:
  - development of linear solvers for multi-/many-core architectures
  - investigation of the reliability of linear solvers (PDSLin, in particular)
- YEAR 2:
  - development of eigenvalue solvers for multi-/many-core architectures
  - development of sparse symmetric linear solvers for accelerating cavity modeling
- YEAR 3:
  - continued development of sparse symmetric linear solvers
  - hardening of linear and eigenvalue solvers in ACE3P

High-Speed Gas Dynamics for Laser-Wakefield Accelerators A central design issue for laser-wakefield accelerators is the formation of the density, temperature and species profiles in the initial capillary discharge. These properties are critical to guiding the laser pulse and control of the electron beam phase in the wake. The mathematical representation of this process are the time-dependent equations of gas dynamics with complex constitutive behavior: ionization physics, including multiple fluid components; diffusive transport; separate electron and ion temperatures; and coupling to magnetic fields. Furthermore, critical design parameters are associated with three-dimensional effects in complex geometries, such as the placement of fill tubes. In this work, we propose developing a three-dimensional simulation capability to provide a high-resolution representation of these processes, including appropriate models for all of the relevant physical processes. This work will be based on the embedded-boundary method for simulating partial differential equations in complex geometries. In this approach, an irregular boundary is represented on a rectangular grid by intersecting each rectangular cell with the boundary. This leads to a natural finite-volume discretization of the solution to the PDE in the irregular domain(s) defined by the boundary. Typically, this approach is combined with block-structured adaptive mesh refinement (AMR), in which the grid resolution is locally adjusted as a function of space and time to maintain a uniform level of accuracy. Our implementation will be based on the core embedded-boundary AMR tools that are part of the Chombo framework and supported as cross-cutting technologies as part of the FASTMath Institute. We will extend these core capabilities to provide a fully three-dimensional high-temperature gas dynamics code to simulate capillary discharges required by the BELLA experiment and other such projects.

Tasks:
- YEAR 1:
  - Completion of the 1D full-physics capability begun under SciDAC2 to benchmark the basic discretization methodology against other existing 1D codes with the same physics models.
  - Develop the initial implementation of the full-physics, 3D code.
- YEAR 2:
  - validate the code and participate in its application to design problems for BELLA. This will likely involve significant changes in the code in response to the need for changes in the model suggested by the validation process.
  - Address parallel scaling issues arising from the complex multiphysics character of the code.

- YEAR 3:
  - Continue to support the use of the code by the LWFA community.
  - Address scaling issues on multicore and heterogeneous systems.

Particle-In-Cell Methods We will enhance the Chombo framework which is supported as part of the FASTMath Institute to support beam dynamics codes. One key priority will be the development of high-order structured-grid adaptive Poisson solvers based on the AMR method of local corrections (MLC) solver. This approach has a computational intensity that is an order of magnitude or more greater than traditional global FFT or multigrid methods. Furthermore, they extend to structured adaptive mesh refinement (AMR) meshes in a way that naturally eliminates the spurious self–force problems associated with more conventional AMR discretizations. We will also develop a particle framework that will provide support for more flexible domain decomposition and on-the-fly load balancing. This will require the use of lightweight performance measurement tools similar to those that already exist in Chombo to measure performance at runtime. We will also develop methods to improve the data locality of particle operations. These will include new algorithms that improve the accuracy (and increase the computational intensity) of particle operations, as well as exploring the possibilities afforded by the potential-theoretic field solvers for hiding the cost of particle data movement by more tightly integrating the particle operations with the field solver. Such methods would be much more complicated to implement than the traditional PIC methods, and therefore would need to be designed carefully to provide the flexibility to support the range of requirements in the accelerator community, while hiding the complex programming details from the applications user. At the low levels, we will use a variety of implementation techniques. The roofline model in [94] provides guidelines for what techniques can be used effectively on a given processor architecture, based on the computational intensity of the operation. We will also develop appropriate metrics for performance between the approaches developed here and those developed as part ofthe UCLA UPIC library, with the best approaches will be incorporated in both libraries.
Tasks:

- YEAR 1:
  - Release versions of the AMR MLC solver that support the usage patterns for structured-grid Vlasov-Poisson as it appears in accelerator modeling.
  - Develop the initial design of a programming interface for PIC methods that is portable, broadly capable of expressing PIC algorithms as they arise in accelerator modeling, and maximizes data locality while minimizing the extent to which the applications developer must provide platform-specific code.
- YEAR 2:
  - implement a particle library to the specification developed in Year 1, and test its performance for use cases arising in accelerator modeling on a variety of platforms.
  - Begin to extend the AMR MLC algorithms developed in year 1 to support complex boundary geometries.
- YEAR 3:
  - Release the particle libraries, and bring them to production status in Synergia, as well as assist in incorporating into other accelerator modeling production codes such as Quick-PIC.
  - Complete the extensions of AMR MLC solver to support complex boundary geometries.
  - Make changes to both the AMR MLC solvers and the particle libraries in response to further requirements identified by the accelerator modeling community.

SLAC National Accelerator Laboratory – Statement of Work

POC: Cho Ng

SLAC is requesting funds to support work in accelerator physics and applied mathematics & computer science.

Accelerator Physics (to be funded by HEP)

Project X Linacs Design The design of the Project X SRF cavities needs to take into account of beam-excited wakefields and higher-order-modes (HOMs) so that their effects on the beam quality as well as on cryogenic power losses are properly controlled. In order to maintain the HOM effects below certain thresholds, normally an SRF cavity is equipped with HOM dampers to extract the beam-excited power from the cavity. However, the HOM damper is a vulnerable, expensive and complicated component requiring additional hardware such as cables, feedthroughs, connectors, loads, etc. The experience at SNS has shown that HOM dampers may limit the cavity performance and reduce operation reliability because of problems arising from multipacting and the damage of feedthroughs [55]. Indeed, SNS linac does not show the necessity of the HOM couplers at current operation parameters. Thus we propose to evaluate the HOM wakefields in the Project X SRF cavities and cryomodules to determine if HOM dampers are needed for the machine operation.

We will focus most of our simulation work of the Project X CW linac. The 1.3 GHz SRF cavity design in the pulsed linac has been studied extensively both experimentally and computationally, and therefore there is a good understanding of its performance. In contrast, the low β cavities at 650 MHz are novel 5-cell designs with an elliptical equator and their reliabilities can be assessed through simulation. It is essential to calculate the HOM wakefields in the presence of cavity imperfections and misalignments, and to determine in the worst scenario if HOM dampers are required to satisfy the BBU threshold and to limit the cryogenic losses. The simulation procedure will be applied in a similar manner to the 1.3 GHz 9-cell cavity and the 325 MHz spoke cavities. While the treatment of non-relativistic beam ($\beta < 1$) in the CW linac can be extended straight-forwardly for Omega3P calculations in the frequency domain, new boundary conditions will be developed in the time domain code T3P to handle $\beta < 1$ beam excitation.

Tasks:

- YEAR 1:
  - Calculate monopole and dipole HOM spectra in 650 MHz cryomodules.
  - Develop wakefield computational technique in ACE3P for non-relativistic beam excitation.
- YEAR 2:
  - Simulate 650 MHz cryomodules including cavity imperfection and misalignment to assess BBU condition.
  - Evaluate beam-generated power and its effects on cryogenic losses in 650 MHz cryomodules.
- YEAR 3:
  - Simulate 1.3 GHz cryomodule including cavity imperfection and misalignment to assess BBU condition.
  - Calculate monopole and dipole HOM spectra in 325 MHz cryomodules.

High Gradient A significant challenge facing the CLIC two-beam accelerator is the issue of wakefields excited by the transit of an electron or positron bunch in the Power Extraction &

Transfer Structure (PETS) in the drive linac and the accelerator structures in the main linac (AS). One overriding concern is the long-range wakefields that can result in cross coupling between the PETS and the accelerator structure. ACE3P has been used for the first-ever simulation (see Fig. 5) of a CLIC coupled structure (1 PETS and 2 AS) and the results show stronger than expected dipole wakedfield coupling [46]. Based on these findings, we propose to extend the simulation to numerically quantify this cross coupling accurately in the realistic 3D geometry of the entire two-beam module (4 PETS and 8 AS) to understand the intricate phenomenon of wakefield coupling and to devise measures to mitigate the effect. Any possible trapped modes that can affect the beam quality will be identified in both the drive beam and main beam structures. Due to the tight tolerances required in the machine design, simulation will also help understand the effects of structure misalignements on the wakefields.

Another concern with the high gradient accelerator is the generation of dark current, which arises from field emissions of electrons from the surface of an accelerating structure and their subsequent movements whose trajectories are determined by the accelerating rf field. Dark current may lead to beam loading of the accelerator structure and, if captured, may also produce undesirable backgrounds downstream to the detector at the interaction point. Then the simulation effort will be focused on studing the effects of dark current in the main beam section of the two-beam module. The capture of dark current downstream may take a long distance that can involve multiple modules, and therefore large-scale simulation is essential to providing insights for the design of the machine.

Tasks:

- YEAR 1:
  - Evaluate beam energy spread and beam loading compensation in a coupled system consisting of a PETS and an AS.
  - Model wakefields effects in a coupled two-beam system (1 PETS, 2 AS).
- YEAR 2:
  - Evaluate trapped modes in drive beam section and in main beam section of a two-beam module.
  - Simulate wakefield effects in one half of a two-beam module (2 PE TS, 4 AS).
- YEAR 3:
  - Model wakefield effects in an entire two-beam module.
  - Simulate dark current effects in main beam section of a two-beam module.

Dielectric Laser Acceleration The first experimental effort will be focused on the beam excitation in dielectric laser acceleration (DLA) structures. The band gaps calculated using ACE3P corroborated well with commercial optical fibers measured during beam tests at SLAC [38]. We propose to extend the calculations to a structure length at the order of 100's of wavelengths of the accelerating mode in order to obtain a correct account of the wakefield when the unwanted modes are attenuated due to their high radiation loss from the outer surface of the PBG fiber.

The efficient coupling of laser power into a DLA structure is a challenging problem, conceptually and computationally. It has been demonstrated for the 2D PBG waveguide structure uniform in the longitudinal direction that one can determine power coupling from free space by studying the radiation from the propagation of the accelerating mode in the PBG [39]. For the 3D woodpile structure where the geometry is periodic in the longitudinal direction, one needs to determine the coupling efficiency form the coupling waveguide using methods analogous to those used to match couplers in conventional microwave accelerators [42, 43]. The frequency domain solver in ACE3P will be used to carry out large-scale high precision calculations for these coupler designs.

Several code development efforts in ACE3P are needed to handle port mode excitation in inhomogeneous medium and to terminate wave propagation in free space. The absorbing boundary condition at the inhomogeneous waveguide port requires the implementation of multi-mode propagation in inhomogeneous medium. The scattering matrix formulation in ACE3P frequency domain solver needs to be modified to accommodate the unbounded elbeit weak radiated nature of the accelerating mode from the DLA structure. Shape optimization techniques [11] already existing in ACE3P will be improved for automatic and efficient to obtain the coupler dimensions for its optimal matching.

Tasks:

- YEAR 1:
  - Develop coupling mechanism for optimal power transmission from laser to PBG fiber.
  - Implement multi-mode waveguide boundary condition for inhomogeneous medium in ACE3P frequency domain solver.
- YEAR 2:
  - Develop efficient power coupling mechanism in woodpile structure.
  - Determine wakefield and radiation in PBG fiber and compare with measurements.
- YEAR 3:
  - Optimize coupler designs for PBG and woodpile structures.
  - Determine wakefield and radiation in woodpile structure and compare with measurements.

Applied Mathematics & Computer Science (to be funded by ASCR)

Numerical Linear Algebra Collaboration between computational scientists at SLAC and applied mathematicians at LBNL over the last decade has resulted in the development and integration of state-of-the-art numerical linear algebra algorithms and software packages into the accelerator modeling suite ACE3P for the simulation of electromagnetics systems. Our work has focused on eigenvalue calculations and the solution of large sparse linear systems.

- Incorporation of an exact shift-invert Lanczos algorithm into ACE3P's frequency-domain eigensolver Omega3P for computing some of the extreme eigenvalues.
- Development of an algebraic sub-structuring method for solving sparse eigenvalue problems.
- Incorporation of the second-order Arnoldi reduction into ACE3P for solving quadratic eigenvalue problems, which arise in the modeling of an accelerating cavity when it is coupled to an external system through a waveguide.
- Included the self-consistent iterations and the nonlinear Arnoldi method for general nonlinear eigenvalue problems
- Development of preconditioning techniques for solving sparse linear in ACE3P's time-domain solver.

We will build on the successes and continue our close collaboration with LBNL. Our proposed work will focus on improving the performance and scalability of eigensolvers and linear solvers on the current and the next generations of parallel computer architectures that use multi-/many-cores. In particular, there is a need to balance the workload and reduce the amount of communication. The work will require changing the data structure, redesigning, and rewriting the eigensolvers and linear solvers. We will improve the physics-based preconditioners used in the finite-element method used for electromagnetic simulation, such as approximating an operator using a lower-order one based on the finite-element basis functions, and developing accurate work-load balancing for graph-based mesh partitioners [103] and hybridization approaches to reduce memory footprint and improve scalability with OpenMP/MPI in multi-core architectures. This work will be carried out in close collaboration with the FASTMath SciDAC Institute, particularly those members at LBNL.

Tasks:

- YEAR 1:
  - Evaluate and test linear solvers for multi-/many-core architectures.
  - Develop physics-based preconditioning techniques for linear systems in ACE3P's time-domain module.
- YEAR 2:
  - Evaluate and test eigenvalue solvers for multi-/many-core architectures.
  - Continue development of physics-based preconditioning techniques for linear systems to improve work-load balance in ACE3P's time-domain module.
- YEAR 3:
  - Incorporate FASTMath's sparse symmetric linear solvers into ACE3P's frequency-domain module.
  - Study performance and scalability of linear and eigenvalue solvers in ACE3P.

Visualization and Data Interoperability In the simulation of the entire CLIC two-beam module and the Project X cryomodule, there are a couple of challenges in analyzing the results. First, the size of the datasets will increase by almost of an order of magnitude to hundreds of TBytes. Second, the complex geometry involved in the simulation makes it difficult to extract the relevant information from the results. For example, it is required to devise effective techniques in order to visualize the fields of HOMs in the Project X cryomodules whose geometries are of high aspect ratio. In order to speed up the analysis of mode structure along the cryomodule, a new capability of assembling different curved segments will be incorporated in ParaView [62] to show scalar variables such as field distributions along the integrated path.

Tasks:

- YEAR 1:
  - Develop a ParaView plugin which takes an extracted set of segments from a well-formed path, computes their connectivity and orders them for generating plots of variables vs. path length.
- YEAR 2:
  - Extend the ParaView plugin to accept an arbitrary number of paths, with user options to stack multiple variables vs. path length series in the same plot.
- YEAR 3:
  - Develop a ParaView interactor to improve user navigation of extremely long or geometrically complex large-scale accelerator datasets.

Tech-X Corporation – Statement of Work

POC: John R. Cary

Tech-X is requesting funds to support work in accelerator physics and applied mathematics.

A significant fraction of the Tech-X effort involves use and further development of VORPAL, which is a parallel framework for modeling time-domain particle and field dynamics, with many boundary conditions and algorithms. Electromagnetic simulations in VORPAL use the finite-difference time-domain (FDTD) method, discretizing the fields on a uniform, orthogonal Yee mesh and explicitly evolving them in time [141, 142, 143], using the local nature of the FDTD update to scale efficiently in parallel. Frequencies are currently obtained using the filter diagonalization method [37]. On the Franklin supercomputer at NERSC, VORPAL shows close to linear scaling out to 16,384 processors. Also, VORPAL supports electromagnetic simulations with metallic boundaries on graphics processing units, and implementation of dielectric and particle features is underway [144]. VORPAL is used for several types of physical problems, including: a) laser-plasma accelerators, b) dielectric laser-driven structures, c) rf cavities, including high-order modes, multipactor and thermal effects, d) electron cloud physics, and many others.

Accelerator Physics (to be funded by HEP)

Laser-Plasma Acceleration Tech-X will work in collaboration with LBNL to model and design laser plasma accelerator (LPA) stages for high-quality electron and positron bunches with 10 GeV scale energy gain in meter-scale plasmas. The work will emphasize resonant injection of high-quality electron bunches via two and three pulse colliding pulse (CPI) and field-induced tunneling ionization of high-Z ions. ASCR developed tools for parallel nonlinear optimization (DAKOTA or TAU) will be used with VORPAL to enable systematic design and optimization. In addition to supporting the BELLA project and related LOASIS experiments at LBNL, the work is directly relevant to future lepton collider concepts and to HEP stewardship of accelerator technology. Software development will focus on improvements to VORPAL speed and scaling, including algorithmic improvements, numerical techniques and porting to next-generation supercomputers.

Tasks:

- YEAR 1:
  - Start 2D and 3D simulations of controlled injection for ∼10 GeV stages
  - Demonstrate improved strong scaling of 3D PIC in VORPAL on 100,000 cores
- YEAR 2:
  - Continue 2D and 3D simulations of controlled injection for ∼10 GeV stages
  - Implement workflow for use of VORPAL with parallel optimization library (DAKOTA or TAO)
- YEAR 3:
  - Use parallel nonlinear optimization to systematically improve beam properties
  - ASCR tools (DAKOTA or TAO) enable concurrent use of 1 million cores with high efficiency

Dielectric Laser Acceleration Tech-X will work on the design and modeling of dielectric laser-driven accelerator (DLA) structures, in collaboration with the DLA group at SLAC. The work will focus on extending computational capabilities from modeling single structures to modeling collider-scale acceleration lengths. To this end, we will improve algorithms for power coupler design, essential to staging individual segments. We will also implement realistic dielectric models to capture material effects that may accumulate over significant propagation lengths. In addition, we will use the particle capability of VORPAL to self-consistently assess the effects of short range wakefields.

Tasks:

- YEAR 1:
  - Prototype improved algorithms for accelerating waveguide and power coupler design, including the complex-envelope FDTD algorithm.
  - Conduct short-range beam-driven wakefield simulations for the photonic crystal fiber and woodpile structures, using the fully self-consistent PIC capabilities of VORPAL.
- YEAR 2:
  - Implement realistic dispersive and nonlinear material properties in VORPAL.
  - Develop analytic approximations for the integrated wakefield effect on a particle bunch over an accelerator segment.
- YEAR 3:
  - Optimize the parallel performance and add GPU capability for the complex-envelope FDTD algorithm dispersive and nonlinear material updates.
  - Incorporate the model for beam propagation with wakefields into a tracking code so that we can evaluate the effects of beam-breakup instability over a km-scale collider length, consisting of many thousands of accelerator segments.

Electron Cloud Modeling The primary thrust of this work is to support rf diagnostics of electron clouds in the Main Injector. In order to provide detailed models for these experiments, we will develop new, more accurate numerical models of electron clouds and perform large simulations requiring LCF resources with accurate models of beam pipe geometries to better interpret rf experimental data.

Tasks:

- YEAR 1:
  - Verify plasma dielectric model with spatially and temporally changing magnetic field configurations in VORPAL through quantified comparisons with equivalent PIC models with particles and embedded boundaries.
  - Complete detailed simulations of lossy cavities with dielectrics in support of tabletop experiments at FNAL, by predicting rf characteristics due to reflections and losses in travelling wave and resonant cavity tabletop beam pipe experiments underway at FermiLab.
- YEAR 2:
  - Develop and perform detailed simulations of resonant cavity rf experiments in the Main Injector using modulated plasma dielectric models of electron clouds using VORPAL. Simulation predictions of frequency shifts and side band measurements will be compared with experimental data to derive experimental electron cloud densities.
- YEAR 3:
  - Develop and perform simulations of travelling wave rf diagnostics on meter spatial scales, but with detailed representations of beam pipe geometries and spatially variable magnetic fields. Modulated plasma dielectric models will be used to generate synthetic spectra to derive electron cloud densities in experimental data.
  - Develop and perform simulations of travelling wave rf diagnostics over tens of meters of

realistic Main Injector beam pipe including the effects of rf reflections and attenuation, spatially variable magentic field configurations, temporal and spatial evolution of cloud densities, and plasma modulation at beam revolution frequencies.

Project X to Muon Collider There are many conceptual ideas on how to design this interface, and the Muon Acceleration Program (MAP) collaboration is expected to select a few for study during their Winter 2012 meeting. All of these designs appear to be inherently nonlinear, so standard computational tools will not be adequate for their simulation and optimization. The Synergia framework is well suited for this work, and the TAU library for parallel nonlinear optimization will be used with Synergia to enable systematic design and optimization. Because the design effort is in the early stages of development, this activity will require close collaboration with experts from the Project X team, members of MAP, and ComPASS team members at Fermilab. Tech-X has a successful history of collaborating with Fermilab on the use of Synergia, including the generation and use of 3D nonlinear cavity mappings.

Tasks:

- YEAR 1:
  - Work with MAP researchers to define a range of proton beam requirements
  - Implement use of Synergia with parallel nonlinear optimization library TAO
- YEAR 2:
  - Use Synergia to simulate one or more ring designs
  - Use parallel optimization with Synergia to begin improving designs
- YEAR 3:
  - Generate 3D nonlinear rf cavity maps and use them in Synergia
  - Optimize selected designs using project developed tools, evaluate their performance

Applied Mathematics (to be funded by ASCR)

Visualization and Data Analysis Tech-X will lead the effort to allow universal visualization of accelerator data with the VisIt visualization application and to develop semantic metadata to simplify the interchange of data among accelerator applications. The first task area will consist of ensuring that the VizSchema metadata is applicable and can be post-facto applied to the HDF5 data produced by the ComPASS accelerator physics computational applications. Utilities for doing so will be developed. The second is to mark up data with sufficient information such that exchange between accelerator codes is possible, then to implement the markups and test the data exchange.

Tasks:

- YEAR 1:
  - Visualization metadata schema (VizSchema) tested and generalized as needed to allow VisIt to import files from currently non-compliant accelerator codes.
  - Semantic metadata schema for self-describing data files developed.
- YEAR 2:
  - Converters/modifiers to be able to add visualization metatdata as needed to the output of all ComPASS computational applications developed.
  - VORPAL modified as needed to directly provide marked up data.
- YEAR 3:

  - Converters/modifiers generalized to be able to add semantic metadata as needed to the output of all ComPASS computational applications, thus easing data exchange between ComPASS applications. Test exchange of data between codes.

Performance Tech-X will work with Argonne to identify performance bottlenecks in VORPAL and to share the knowledge gained with the rest of the ComPASS team. The specific areas of interest are in electromagnetics (EM) and EM particle-in-cell methods. The goal is to identify the optimal data structures and/or methods for autotuning to find the best data structures.

Tasks:

- YEAR 1:
  - Major performance bottlenecks identified for VORPAL for explicit EM updates and EM-PIC.
- YEAR 2:
  - VORPAL modified as needed to use performance enhancing data structures and/or algorithms for explicit electromagnetics.
  - Design for incorporating autotuning completed.
- YEAR 3:
  - VORPAL modified as needed to use performance enhancing data structures and/or algorithms for particle in cell.
  - Autotuning incorporation completed.

Uncertainty Quantification The UQ effort is directed towards laser-plasma accelerator modeling with externally injected electron beams and no dark current (i.e. no self-injection of electrons from the plasma). This limits the laser intensity to order unity (normalized), which means a density channel will be required to guide the pulse. To make the simulations as fast as possible, we will consider 100 MeV scale parameters, which implies mm scale plasma interaction lengths. The "reference code" at Tech-X will be 3D lab-frame, time-explicit PIC simulations using VORPAL. Comparison with the reference code results from UCLA and LBNL (i.e. 3D lab-frame OSIRIS and WARP simulations) will provide estimates of uncertainty in the resulting "manufactured data". The ComPASS team has many "hypothesis" codes, including use of the boosted-frame, a variety of reduced models, as described in the proposal text, and also approximations such as using only two spatial dimensions. The hypothesis codes will be run via the QUESO library from UT Austin, and must be run many thousands of times; hence, it is essential to make the problem run time as small as possible. By the end of the third year, the team will have developed Gaussian process emulation techniques that will enable the future treatment of larger-scale problems, including UQ of simulation results in comparison with experimental data.

Tasks:

- YEAR 1:
  - Generate manufactured data with reference code (3D lab-frame VORPAL simulations) of 100 MeV-scale LPA with externally injected bunches; compare with results from other RCs
  - Use QUESO with one hypothesis code for calibration against manufactured data
- YEAR 2:
  - Generate additional manufactured data with reference code for the same physical problem; compare with results from other RCs for refined uncertainty estimates
  - Use QUESO with the same (or perhaps another) hypothesis code for calibration against manufactured data

- YEAR 3:
  - Generate additional manufactured data with reference code for the same physical problem
  - Develop Gaussian process emulation techniques for this problem domain

The University of Texas at Austin – Statement of Work

COMMUNITY PROJECT FOR ACCELERATOR SCIENCE AND SIMULATION

POC: Ernesto Esteves Prudencio

UT Austin will collaborate on activities related to quantification of uncertainties present in laser plasma acceleration (LPA), with the final goal of helping the LPA team to systematically characterize and propagate uncertainties in models for laser-plasma phenomena. More specifically, UT Austin will, in collaboration with LPA physicists, (i) understand uncertainties present in reference data or in laser-plasma model parameters, (ii) understand/propose possible candidate competing laser-plasma models, as well as quantities of interest (QoIs) to be predicted with calibrated models, (iii) properly represent the uncertainties and the competing models for the application of Bayesian analysis, (iv) research statistically robust, scalable, load balanced, and fault tolerant parallel stochastic algorithms, (v) code them in the Quantification of Uncertainty for Estimation, Simulation and Optimization (QUESO) MPI/C++ research library from UT Austin, (vi) help to link QUESO with model codes, (vii) help to run the resulting executables on parallel HPC platforms for either calibration or prediction exercises, (viii) help to analyze the results, and (ix) understand/propose actions, e.g. which models to continue to work with, which data sets to improve, which uncertainties to reduce.

We propose the following participants from UT Austin:

- Ernesto Esteves Prudencio (21% = 2.5 months/year), who is a Co-PI in the QUEST SciDAC Institute, to lead UT Austin on its UQ efforts (parallel stochastic algorithms research, software design and software development) and on its interactions with LPA members of the research project; and
- one post-doc (52% = 6.25 months/year), to contribute on all these UT Austin activities as well.

Specific tasks and milestones are as follows, per year (to be funded by ASCR):

- YEAR 1:
  - Help performing Bayesian analysis of simple laser-plasma models and evaluate the results.
  - Research ways to improve the statistical robustness of model evidence calculations.
  - Begin improving QUESO towards using fault-tolerant versions of MPI.
- YEAR 2:
  - Help improving the Bayesian analysis of simple laser-plasma models, including prediction of QoIs, and evaluate the results.
  - Continue researching statistically robust model evidence calculations.
  - Continue improving QUESO towards using fault-tolerant versions of MPI.
- YEAR 3:
  - Improve QUESO towards having capabilities for constructing Gaussian process emulators of complex models.
  - Help develop emulators of complex laser-plasma models.
  - Continue improving QUESO towards having fault-tolerant stochastic algorithms.

University of California at Los Angeles – Statement of Work

POC: Warren B. Mori

The University of California at Los Angeles (UCLA) is requesting funds from HEP to support work in accelerator physics research and from ASCR to support work in particle-in-cell skeleton code and library development, in code performance optimization, and in uncertainty quantification.

UCLA will participate in Energy Frontier (plasma based acceleration) and in Intensity Frontier (e-cloud modeling capability for Fermilab Proton Improvement Plan, Project X) activities working in close collaboration with personnel from FNAL, LBNL, and Tech-X. It will enhance and use its state-of-the-art collection of particle-in-cell codes, including participating in applied math and computer science activities that propose to develop new data structures and parallelization strategies for many core architectures, to optimize the quasi-static method, and to explore the use of uncertainty quantification for laser wakefield acceleration. This work will done in collaboration with personnel from FNAL, LBNL, Tech-X, ANL, and UT Austin.

The UCLA codes and capabilities of relevance to ComPASS are: OSIRIS, QuickPIC, and UPIC. Using previous SciDAC awards as a key source of funding these codes have been used to make Scientific Discovery that has led to publications in over 35 Physical Review Letters, in 3 Nature articles, and in 2 Nature Physics articles. The UCLA codes are highly optimized and scale very well on both strong and weak scaling studies. For example, OSIRIS was chosen by the DOE Office of Advanced Scientific Computing Research to be featured in their software effectiveness program. As part of this program, on a strong scaling study OSIRIS was shown to scale effectively to the full Jaguar machine (220,000 cores) on both test and physics problems. It also demonstrated high single core efficiency (through the use of the SSE vector units). For example, a 3D problem with excellent load balance and with 1.86×10^{12} particles, .517 PFlops (25% of peak speed and 150 ns/particle/step) and .736 PFlops (30% of peak speed and 280ns/particle/step) were achieved on Jaguar cores for linear and quadratic particle shapes respectively.

Codes and data analysis

We next briefly describe the UCLA codes and capabilities of relevance to ComPASS that will be used and enhanced as part of this project.

OSIRIS:

OSIRIS is a state-of-the-art, fully explicit, multi-dimensional, fully parallelized, fully relativistic, PIC code which also includes a set of sophisticated diagnostic and visualization packages. . OSIRIS is now an extremely mature code that has been run on well over 100 Million core hours. It is highly optimized on a single core and it scales extremely well to over 300,000 cores. It has options for several FDTD field solvers, for field interpolation, and for current smoothing and compensation. It can run using a moving window to efficiently model short pulses and it has Perfecly Matched Layers for absorbing EM waves at the boundaries. It can launch lasers from a moving antenna for use in boosted frame simulations. The parallelization is done either using domain decomposition with MPI across all cores or by using a hybrid approach where MPI is used across nodes and OpenMP on a node. It also has the infrastructure in place for dynamic load balancing using the MPI decomposition. It has field ionization based on the ADK and above threshold models, it has radiation reaction forces if needed, and it has a relativistic two body Coulomb collision model.

QuickPIC:

QuickPIC is a highly efficient, fully parallelized, fully relativistic, three-dimensional particle-in-cell code for simulating particle or laser beam driven wakefield acceleration . The algorithm is based on the quasi-static approximation which effectively allows one to use larger time steps to advance the beam or laser driver. This algorithm has been shown to provide excellent agreement with full PIC codes such as OSIRIS when used appropriately. For the laser driver, the ponderomotive guiding center approximation is used. QuickPIC is built upon the UPIC Framework. Dynamic load balancing with 1D domain decomposition is available. A field ionization module based on the ADK model is implemented. With a novel pipelining algorithm , QuickPIC achieves good strong scaling to 10,000 cores on platforms at NERSC and at ORNL. A basic version of QuickPIC is appropriate for e-cloud modeling.

UPIC:

The UCLA Parallel PIC Framework (UPIC) is a unified environment for the rapid construction of new parallel PIC codes . UPIC contains support for electrostatic, Darwin, and fully electromagnetic field solvers, as well as relativistic particles. The field solvers are spectral (FFT) based. It supports several boundary conditions including conducting and open (Vacuum) boundary conditions for the electrostatic solver (using HockneyÕs scheme). Dynamic load balancing for both particles and fields have been implemented. UPIC supports both distributed memory parallelism using MPI and shared memory parallelism using pthreads, or both. We have also begun development of UPIC for the next generation of hardware expected to be used in future exascale computers, e.g., GPU clusters We have built compact applications and modular libraries with hierarchical domain decompositions using mixed shared and distributed memory programming models. These kernels have achieved speeds of 1.5ns/particle/step and 2.5 ns/particle/step for 2D electrostatic and electromagnetic loops respectively which are within factors of 2 of the asymptotic limits of no particle movement. So far, these have been implemented in OpenMP, OpenCL, CUDA, and MPI. The lessons learned and some kernels will directly impact the development for QuickPIC and OSIRIS to run on a cluster of GPUs.

Visualization and Data Analyis (visXD):

UCLA and its collaborators have developed our own sophisticated set of data analysis and visualization routines that can be used on QuickPIC and OSIRIS output. We have added full particle tracking and data analysis capability for our massively parallel codes, which allows one to follow individual orbits across processor boundaries, and keeps detailed time history of all relevant quantities, e.g, position, momentum and energy, and fields on the particle. Interesting particles can be tagged at any point in a run . An identical run can be restarted and then run to completion to get the tracks. The particle tracks can also be used to generate the synchrotron radiation spectra. We use parallel HDF5 so that our data can also be analyzed by tools being developed across ComPASS.

Accelerator Physics (to be funded by HEP)

<u>**Plasma based acceleration**</u> With the construction of FACET and BELLA, with the existence of numerous 100 + TW laser facilities, with new theoretical developments, with new plasma based accelerator concepts such as proton driven PFWA, and with the code infrastructure developed under SciDAC 1 and 2, the future is ripe for scientific discovery. Just as in the past, ComPASS codes (the complete hierarchy) will be essential for making the anticipated advances and discovery. The hierarchy of codes will have to be further developed to take advantage of current and next generation leadership class computing facilities. UCLA will use its codes to model LWFA experiments (at

UCLA, and other facilities in which UCLA is a collaborator such as at LLNL, and even BELLA). It will facilitate the study key physics in nonlinear and weakly nonlinear LFWA regimes with an emphasis in developing self-injection schemes and beam loading scenarios for both e- and e+. It will use its codes to model PWFA experiments at FACET as well as study key physics for linear collider parameters including staging. In collaboration with FNAL (see FNAL work statement) it will also use its codes to model possible self modulated proton driven PWFA experiments using either the MI or Booster proton beams and of proton driven PFWA experiments using a compressed beam. This work will include coupling UCLA plasma codes to the FNAL Synergia code. It will also work to improve the algorithms in its codes so they model the necessary problems and they can run effectively (and optimally) on 100,000+ cores on physics problems and this will require addressing dynamic load balancing issues and on next generation many core platforms.

Tasks:

- YEAR 1:
  - Use OSIRIS and QuickPIC to design and interpret 1-10 GeV LWFA experiments.
  - Use UCLA codes to design and interpret PWFA and related experiments at FACET, and possible proton driven PFWA experiments at FNAL.
  - Experiment with load balancing strategies for OSIRIS. Improve performance of predictor corrector loop of QuickPIC. Test variety of numerical options for boosted frame simulations with an emphasis towards self-injection studies.
  - Work with FNAL to develop Synergia interfaces to OSIRIS and QuickPIC. Improve the beam initialization packages in OSIRIS.
- YEAR 2:
  - Continue to support the designing and interpretation LWFA and PWFA experiments.
  - Model parameters for LWFA and/or PWFA linear collider parameters including beam loading.
  - Scale QuickPIC to 100,000+ cores. Improve laser solver in QuickPIC.
  - Develop a model for self-modulating proton-driven plasma experiment for MI beam parameters using a section of the FNAL Tevatron lattice.
- YEAR 3:
  - Continue to support designing and interpreting LWFA and PWFA experiments.
  - Incorporate new PIC data structure and load balancing strategies into OSIRIS and QuickPIC. Scale OSIRIS 500,000+ cores. Continue to improve envelope solver for QuickPIC. Improve boosted frame capabilities where needed.
  - Model possible self-modulation proton PFWA experimental parameters. Model compressed proton PFWA parameters.

Project X Main-Injector In the Project X era the Fermilab Main Injector (MI) will be the driver for the higher-energy portion of the physics program at the intensity frontier. Space-charge and electron cloud effects are expected to play a significant role in limiting the performance of the machine. It is essential to understand these effects in order to minimize losses and maximize the effectiveness of the mitigation systems. Particle-in-cell codes which are also used for plasma based acceleration are also very useful for modeling electron cloud effects.

UCLA will improve and optimize a basic version of QuickPIC that has been used in the past for studying e-cloud effects. We will work with FNAL to include accurate particle advances for the beam particles using the machine lattice, will help FNAL personnel run the code to run benchmarks against WARP for selected problems, and we will add options to QuickPIC for non rectangular pipes if needed.

Tasks:

- YEAR 1:
  - Incorporate necessary beam advance algorithms (for general lattices) into basic QuickPIC.
- YEAR 2:
  - Use QuickPIC in the e-cloud modeling validation pr ocess.
- YEAR 3:
  - Incorporate general pipe geometries into QuickPIC.

Particle-in-Cell and Infrastructure (to be funded by ASCR)

Particle in Cell Development We propose to continue to explore data structures and parallelization strategies for PIC on hybrid architectures, using the UCLA UPIC Framework as an experimental platform. The UPIC Framework is highly optimized; key pieces that already run well on GPUs. We will work to improve these skeleton codes and incorporate these strategies into Synergia and QuickPIC. We also propose to develop modular libraries for managing nested domain decompositions for PIC codes on emerging high performance computing architectures. There will be one library for the outermost domain, which will use MPI. The innermost domain will have multiple versions, for example, a CUDA version for GPUs or an OpenMP version for Intel Multi-Core processors. The OpenMP and CUDA implementations will produce the same results, but not in the same way. These implementations will be written so they are as interchangeable as possible, and so they can be merged if a more general programming model such as OpenCL or OpenACC becomes easier to use.

Another important issue to explore is dynamic load balancing. We already have dynamic load balancing in the UPIC Framework. The scheme there uses domains which are based on grid points. Extending the domains to include fractional grid points allows for finer load balancing at the expense of using additional guard cells. Using domains which are fractions of a cell is similar to domain cloning where adjacent nodes have duplicate fields but not duplicate particles, however, it has precise control over and minimizes the duplication. For partitions which are rapidly evolving, the success depends on how rapidly new domain boundaries can be determined. The UPIC Framework already contains a function to calculate new partitions that works reasonably well. We will experiment with extending this to include fractional grids.

The 2D case will be used for experimentation. Once a solid architecture is in place for the 2D case, we will implement the winning design in a 3D code. This may uncover new problems that also need to be addressed. We will then incorporate this approach into our production codes, such as QuickPIC and help others in incorporating it into other codes.

Tasks:

- YEAR 1:
  - Work in collaboration with FNAL to develop many-core and GPU optimization for Synergia.
  - Develop OpenMP, CUDA modules for nested decompositions for 2D Skeleton code.
  - Evaluate feasibility of 3 level decompositions with MPI/OpenMP/CUDA.
  - Implement and evaluate dynamic load balancing with fine partitions.
  - Extend parallel repartitioning algorithm to include fine partitions.
- YEAR 2:
  - Extend nested domain decompositions to 3D Skeleton code.
  - Add dynamic load balancing to nested decompositions for 2D Skeleton code.

- YEAR 3:
  - Incorporate modular MPI/OpenMP/CUDA libraries into production codes such as QuickPIC.
  - Extend dynamic load balancing to 3D Skeleton code.
  - Contribute to releases of libraries.

Performance optimization (to be funded by ASCR) QuickPIC is a very sophisticated code includes 2D and 3D field solves and different partitions for plasma and beam particles and requires a predictor and corrector loop. Unlike a standard PIC code the field solver is not negligible compared to particle advance. The fields can be solved using several gauges. It also uses a novel pipelining algorithm for improved parallel scalability. We believe there is room to optimize the code. We propose to use SUPER performance evaluation tools to identify performance bottlenecks and then to address them.

Tasks:

- YEAR 1:
  - Identify performance test problems for QuickPIC.
- YEAR 2:
  - Use the SUPER performance evaluation tools to identify performance bottlenecks.
- YEAR 3:
  - Work to address performance bottlenecks for QuickPIC.

Uncertainty Quantification (to be funded by ASCR) The UQ effort is directed towards laser wakefield accelerator modeling with externally injected electron beams and no dark current (see UT Austin and Tech-X work statements). We will consider 100 MeV scale parameters for a proof of concept exercise. The work will include generating and comparing reference "data" by running OSIRIS, VORPAL, and WARP in 3D in the lab-frame, time-explicit mode. Full PIC codes in the boosted frame mode and reduced models (The hypothesis codes) will be run via the QUESO library from UT Austin. UCLA will assist in generating reference data and providing hypothesis codes.

Tasks:

- YEAR 1:
  - Use OSIRIS to generate manufactured data.
  - Use QUESO with 2D OSIRIS (or boosted frame) for calibration against manufactured data.
- YEAR 2:
  - Generate additional manufactured data with OSIRIS.
  - Use QUESO with QuickPIC (or OSIRIS boosted frame).
- YEAR 3:
  - Generate additional manufactured data with OSIRIS.
  - Use QUESO with OSIRIS in boosted frame (or QuickPIC)
  - Help to summarize results.

C Biographical Sketches

Biographical sketches of the senior personnel follow in alphabetical order.

James F. Amundson

Computing Division	Phone: (630) 840-2430
Fermi National Accelerator Laboratory	Fax: (630) 840-2783
P.O. Box 500	E-mail: `amundson@fnal.gov`
Batavia, IL 60510	`http://home.fnal.gov/~amundson`

Education

Ph.D. in Physics, University of Chicago, 1993
B.S., *Summa cum Laude*, in Physics, University of Minnesota 1989

Positions

Computational Physics Developer, Fermi National Accelerator Laboratory,
January 2002 – present
Computer Professional, Fermi National Accelerator Laboratory,
September 1998 – January 2002
Postdoctoral Research Associate, Michigan State University,
September 1996 – August 1998
Visiting Assistant Professor of Physics, University of Wisconsin, Madison,
January 1994 – August 1996
Postdoctoral Research Associate, University of Wisconsin, Madison,
September 1993 – December 1993

Teaching Experience

US Particle Accelerator School, "Modern Computational Accelerator Physics," 2007 and 2011
University of Wisconsin, Madison, "Introductory Physics for Engineers" (three courses), 1994-1996

Professional Activities

Project Leader, Maxima Project (`http://maxima.sf.net`), 2000 - 2005.

Selected Recent Publications and Presentations

[145] A. Macridin, P. Spentzouris, J. Amundson, L. Spentzouris and D. McCarron, "Coupling impedance and wake functions for laminated structures with an application to the Fermilab Booster," Phys. Rev. ST Accel. Beams **14**, 061003 (2011).

[146] C. S. Park, J. Amundson, J. Johnstone, L. Michelotti, V. Nagaslaev and S. Werkema, "Space charge effect of the high intensity proton beam during the resonance extraction for the Mu2e experiment at Fermilab," FERMILAB-CONF-11-102-CD.

[147] E. Stern, J. Amundson, P. Spentzouris, J. Qiang and R. Ryne, "Simulations of space charge in the Fermilab Main Injector," FERMILAB-CONF-11-087-CD.

[151] J. F. Amundson, A. Macridin, P. Spentzouris and E. G. Stern, "Advanced computations of multi-physics, multi-scale effects in beam dynamics," J. Phys. Conf. Ser. **180**, 012002 (2009).

[149] S. A. Veitzer *et al.* [SciDAC-COMPASS Collaboration], "Computation of electron cloud diagnostics and mitigation in the main injector," J. Phys. Conf. Ser. **180**, 012007 (2009).

[150] E. G. Stern, J. F. Amundson, P. G. Spentzouris and A. A. Valishev, "Fully 3D Multiple Beam Dynamics Processes Simulation for the Tevatron," Phys. Rev. ST Accel. Beams **13**, 024401 (2010) [arXiv:0906.0513 [physics.acc-ph]].

[151] J. F. Amundson, A. Macridin, P. Spentzouris and E. G. Stern, "Recent Advances in the Synergia Accelerator Simulation Framework," FERMILAB-CONF-09-180-APC-CD, May 2009. *Presented at Particle Accelerator Conference (PAC 09), Vancouver, BC, Canada, 4-8 May 2009.*

[152] J.F Amundson, P. Spentzouris and E.G. Stern, "Simulation Studies of the Interplay Between Space-Charge and Impedance Effects of the Fermilab Main Injector," *Invited Talk Presented at 42nd ICFA Advanced Beam Dynamics Workshop on High-Intensity, High-Brightness Hadron Beams, Nashville, TN, August 2008.*

[153] D. R. Dechow, P. Stoltz, J. F. Amundson, P. Spentzouris and B. Norris, "Software Components for Electron Cloud Simulation," *In the Proceedings of 11th European Particle Accelerator Conference (EPAC 08), Magazzini del Cotone, Genoa, Italy, 23-27 Jun 2008, pp TUPP088.*

[154] J. F. Amundson, D. Dechow, L. McInnes, B. Norris, P. Spentzouris and P. Stoltz, "Multiscale, multiphysics beam dynamics framework design and applications," J. Phys. Conf. Ser. **125**, 012001 (2008).

[155] J. F. Amundson, P. Spentzouris, J. Qiang, R. D. Ryne and D. R. Dechow, "SciDAC Frameworks And Solvers For Multi-Physics Beam Dynamics Simulations," *In the Proceedings of Particle Accelerator Conference (PAC 07), Albuquerque, New Mexico, 25-29 Jun 2007, pp 894.*

[156] D. McCarron, J. F. Amundson, W. Pellico, P. Spentzouris, R. E. Tomlin and L. K. Spentzouris, "Measurement And Simulation Of Space-Charge Dependent Tune Separation In Fnal Booster," *In the Proceedings of Particle Accelerator Conference (PAC 07), Albuquerque, New Mexico, 25-29 Jun 2007, pp 772.*

[157] J. Amundson, W. Pellico, P. Spentzouris, T. Sullivan and L. Spentzouris, "An experimentally robust technique for halo measurement," Nucl. Instrum. Meth. A **570**, 1 (2007).

[158] I. Hofmann *et al.*, "Benchmarking of simulation codes based on the Montague resonance in the CERN proton synchrotron," *In the Proceedings of Particle Accelerator Conference (PAC 05), Knoxville, Tennessee, 16-20 May 2005, pp 330.*

[159] J. F. Amundson, P. Spentzouris, J. Qiang and R. Ryne, "Synergia: An accelerator modeling tool with 3-D space charge," J. Comput. Phys. **211**, 229 (2006).

Collaborators for the past four years

Ji Qiang and Robert Ryne, LBNL; John Cary, Seth Veitzer, Peter Stoltz, Doug Dechow, Tech-X; Lois Curfman McInnes and Boyana Norris, ANL; Roman Samulyak, BNL, Alex Valishev, Fermilab; Juan Gonzalez, Accelogic LLC.

David L. Bruhwiler
Tech-X Corporation, Boulder, CO
bruhwiletxcorp.com – 303-448-0732

Education and Training

- University of Colorado (Boulder, CO)
  Ph.D. Astrophysical, Planetary and Atmospheric Sciences, 1990.
- Carleton College (Northfield, MN)
  B.A. Physics and Astronomy, magna cum laude, 1986.

Research and Professional Experience

2001–present	Vice President of Accelerator Technology, Tech-X Corp.
1997–2001	Research Scientist, Tech-X Corporation
1995–1997	Engineering Specialist, Northrop Grumman Corp.
1992–1995	Research Scientist, Grumman Aerospace Corp.
1990–1991	Research Associate, University of Colorado, Boulder
1986–1990	Research Assistant, University of Colorado, Boulder

Related and Recent Publications

- G I Bell, D L Bruhwiler, I Pogorelov et al., *Vlasov and PIC Simulations of a Modulator Section for Coherent Electron Cooling*, Proc. Particle Accel. Conf., MOP067 (2011).
- B M Cowan, D L Bruhwiler, E Cormier-Michel, E Esarey, C G R Geddes, P Messmer and K Paul *Characteristics of an envelope model for laser-plasma accelerator simulation*, J. Comput. Phys. **230**, 61 (2011).
- W P Leemans, E Esarey, C G R Geddes, Cs Toth, C B Schroeder, K Nakamura, A J Gonsalves, D Panasenko, E Cormier-Michel, G R Plateau, C Lin, D L Bruhwiler and J R Cary *Progress on laser plasma accelerator development using transversely and longitudinally shaped plasmas*, Comptes Rendus Physique **10**, 130 (2010).
- C G R Geddes et al., *Laser Plasma Particle Accelerators: Large Fields for Smaller Facility Sources*, SciDAC Review **13**, 13 (2009).
- D L Bruhwiler, J R Cary, B Cowan, K Paul, C G R Geddes, P J Mullowney, P Messmer, E Esarey, E Cormier-Michel, W P Leemans and J-L Vay *New Developments in the Simulation of Advanced Accelerator Concepts*, Proc. Adv. Accel. Concepts Workshop, Eds. C B Schroeder, W P Leemans and E Esarey, 29 (AIP, 2009).
- K Paul, D L Bruhwiler, B Cowan, J R Cary, C Huang, F S Tsung, W B Mori, E Cormier-Michel, C G R Geddes, E Esarey, S Martins, R A Fonseca and L O Silva *Benchmarking the codes VORPAL, OSIRIS and QuickPIC with Laser Wakefield Acceleration Simulations*, Proc. Adv. Accel. Concepts Workshop, Eds. C B Schroeder, W P Leemans and E Esarey, 315 (AIP, 2009).
- C G R Geddes, D L Bruhwiler, J R Cary et al. *Laser wakefield simulations towards development of compact particle accelerators*, J. Physics: Conf. Series **78**, 012021 (2007).
- D L Bruhwiler, T Antonsen, J R Cary et al. *Towards the petascale in electromagnetic modeling of plasma-based accelerators for high-energy physics*, J. Physics: Conf. Series **46**, 215 (2006).
- C G R Geddes, Cs Toth, J van Tilborg, E Esarey, C B Schroeder, D L Bruhwiler, C Nieter, J R Cary and W P Leemans *High-quality electron beams from a laser wakefield accelerator using plasma-channel guiding*, Nature **431**, 538 (2004).

- D L Bruhwiler D A Dimitrov, J R Cary et al. *Particle-in-cell simulations of tunneling ionization effects in plasma-based accelerators*, Phys. Plasmas **10**, 2022 (AIP, 2003).

Synergistic Activities

- 2003, 2007, 2011; Program Committee, Particle Accelerator Conf.
- 2009–present; Program Committee, Adv. Accel. Concepts Workshop
- 2006, 2012; Working Group Leader for Computational Phys., AAC Workshop
- 2008–2010; Executive Committee, NERSC Users Group
- 1986–present; American Physical Society; Beams, Plasma and Comp. Physics Div.'s
- Proposal Referee; Department of Energy, for Offices of HEP and BES
- Journal Referee; Phys. Rev., Phys. Plasmas, J. Comp. Phys., IEEE Trans. Plasma Sci.

Collaborators

D.T. Abell, G.I. Bell, I. Ben-Zvi, J.R. Cary, E. Cormier-Michel, D. Dimitrov, E. Esarey, A.V. Fedotov, C.G.R. Geddes, B. Hidding, W.P. Leemans, V.N. Litvinenko, P. Messmer, P.J. Mullowney, S. Nagaitsev, C. Nieter, K. Paul, C.B. Schroeder, S. Shasharina, D.N. Smithe, P. Spentzouris, P.H. Stoltz, A. Valishev, S.A. Veitzer, G.R. Werner

Thesis advisors: J.R. Cary

Advisees: None

John R. Cary
Tech-X Corporation, Boulder, CO
carytxcorp.com – 303-448-7727

Education and Training

- University of California (Berkeley, CA)
  Ph.D. Physics, 1979.
  M.A. Physics, June 1975.

- University of California (Irvine, CA)
  B.A. Physics cum laude, June 1973
  B.A. Mathematics, March 1973

Research and Professional Experience

1994–present	CEO and co-founder, Tech-X Corporation
1984–present	Associate Professor, Professor, Department Chair, Director, University of Colorado, Boulder
1980–1984	Institute for Fusion Studies, University of Texas, Austin
1978–1980	Member of the Technical Staff, Los Alamos National Lab
Additional Affiliations:	
2011–present	Associate Editor, Reviews of Modern Physics
2010–present	Member, Executive Committee, Division of Plasma Physics, American Physical Society
various times	Associate Editor for Physical Review E and Physical Review Letters; Chair of Publications Committee, Public Information Committee, Nominations Committee. for the Division of Plasma Physics of the American Physical Society

Related and Recent Publications

- T M Austin, J R Cary, S Ovtchinnikov, G R Werner, and L Bellantoni, *Validation of frequency extraction calculations from time-domain simulations of accelerator cavities*, Comput. Sci. Disc. **4** 015004 (2011).
- E Cormier-Michel, E Esarey, C G R Geddes, C B Schroeder, K Paul, P J Mullowney, J R Cary, and W P Leemans, *Control of focusing fields in laser-plasma accelerators using higher-order modes*, Phys. Rev. ST Accel. Beams **14**, 031303 (2011).
- C A Bauer, G R Werner, and J R Cary, *A second-order 3D electromagnetics algorithm for curved interfaces between anisotropic dielectrics on a Yee mesh*, J. Comput. Phys. 230, 2060-2075 (2011).
- T.M Austin, J.R Cary, D.N Smithe, C Nieter, *Alternating Direction Implicit Methods for FDTD Using the Dey-Mittra Embedded Boundary Method*, The Open Plasma Physics Journal, **3**, pp. 29-35, 2010

Synergistic Activities

- Lead PI, SciDAC project, FACETS (Framework Application for Core-Edge Transport Simulations)
- Institutional PI, SciDAC project, CommPASS (Community of Petascale Simulation Software)

Collaborators

T.M. Austin, G. Bateman, C.A. Bauer, L. Bellantoni, J.A. Carlsson, I.W. Choi, E. Cormier-Michel, E. Esarey, C.G.R. Geddes, S.J. Hahn, A. Hakim, A. J. Brizard, A.H. Kritz, S.E. Kruger, P.L.G. Lebrun, J. Lee, W.P. Leemans, M. Miah, P.J. Mullowney, C. Nieter, S. Ovtchinnikov, K.H. Pae, A.Y. Pankin, K. Paul, A. Pletzer, T. Rafiq, T.D. Rognlien, C.B. Schroeder, S. Shasharina, D.N. Smithe, K.G. Sonnad, P.H. Stoltz, S. Vadlamani, S.A. Veitzer, G.R. Werner

Thesis advisors: A.N. Kaufman (UC-B)

Advisees: B. Goode, J. Lee, K. Sonnad, S.E. Hendrickson, P.H. Stoltz, W.E. Gabella, D.L. Bruhwiler, P.H. Rusu

Phillip Colella

Mail Stop 50A-1148 Lawrence Berkeley National Laboratory Berkeley, CA 94720
PColella@lbl.gov

Colella has developed high-resolution and adaptive numerical algorithms for partial differential equations and numerical simulation capabilities for a variety of applications in science and engineering. He has also participated in the design of high-performance software infrastructure for scientific computing, including software libraries, frameworks, and programming languages. Over the last 20 years, he has led a number of multi-disciplinary and / or multi-institutional algorithm and software development projects in high-performance computing and has participated in strategic planning / policy activities on computational science for DOE and the National Academies. Honors and awards include the IEEE Sidney Fernbach Award for high-performance computing in 1998, the SIAM/ACM prize (with John Bell) for computational science and engineering in 2003, election to the US National Academy of Sciences in 2004, and election to the inaugural class of SIAM Fellows in 2009.

Education and Training

University of California, Berkeley, A.B. in Applied Mathematics, 1974.
University of California, Berkeley, M.A. in Applied Mathematics, 1976.
University of California, Berkeley, Ph.D. in Applied Mathematics, 1979.

Research and Professional Experience

Senior Scientist; Group Leader, Applied Numerical Algorithms Group, Lawrence Berkeley National Laboratory, 1996-present.
Professor in Residence, Electrical Engineering and Computer Science Department, University of California, Berkeley, 2010-present.
Senior Mathematician, Lawrence Livermore National Laboratory, 1995-1996.
Faculty member, Mechanical Engineering Department, University of California, Berkeley: Associate Professor 1989-1992; Professor 1992-1995; Professor in Residence 1995-1998.
Mathematician; Group Leader, Applied Mathematics Group, Lawrence Livermore National Laboratory, 1986-1988.
Mathematician, Lawrence Berkeley National Laboratory, 1978-1986.

Research Interests

Discretization methods for partial differential equations (PDE): finite volume methods and adaptive mesh refinement on structured grids, particle methods, volume-of-fluid methods for complex geometries and moving fronts, analysis-based fast solvers for potential theory. Analysis-based splittings of stiff PDE; software frameworks and programming environments for high-performance computing; applications to scientific and engineering problems represented using PDE.

Selected Relevent Publications

1. B. Wang, G. Miller, and P. Colella, "A particle-in-cell method with adaptive phase-space remapping for kinetic plasmas", to appear in SIAM J. on Sci. Comput., (2011).
2. P. Colella, M.R. Dorr, J.A.F. Hittinger, and D.F. Martin "High-Order Finite-Volume Methods in Mapped Coordinates", Journal of Computational Physics 230, p. 2952-2976 (2011).
3. P. McCorquodale and P. Colella, "A high-order finite-volume method for conservation laws on locally refined grids", Communications in Applied Mathematics and Computational Science 6, No. 1, 1-25 (2011).

4. F. Miniati and P. Colella, "Block-structured adaptive mesh and time refinement for hybrid, hyperbolic + N-body systems", J. Comput. Phys 227, p. 400-430 (2007).
5. P. McCorquodale, P. Colella, G. Balls, and S. B. Baden , "A Local Corrections Algorithm for Solving Poisson's Equation in Three Dimensions". Communications in Applied Mathematics and Computational Science 2, p. 57-81 (2007).
6. P. Schwartz, M. Barad, P. Colella, and T. J. Ligocki, "A Cartesian grid embedded boundary method for the heat equation and Poisson's equation in three dimensions", J. Comput. Phys. 211, p. 531-550 (2006).
7. P. Colella, D. T. Graves, B. Keen, and D. Modiano, "A Cartesian grid embedded boundary method for hyperbolic conservation laws", J. Comput. Phys. 211, p. 347-366 (2006).
8. M. Barad and P. Colella, "A fourth-order accurate adaptive mesh refinement method for Poisson's equation", J. Comput. Phys. 209, p. 1-18 (2005).
9. P. McCorquodale, P. Colella, D. P. Grote and J.-L. Vay, "A node-centered local refinement algorithm for Poisson's equation in complex geometries", J. Comput. Phys. 201, p. 34-60 (2004).
10. J.-L. Vay, P. Colella, J. W. Kwan, P. McCorquodale, D. Serafini, A. Friedman, D. P. Grote., G. Westenskow, J.-C. Adam, A. Héron, and I. Haber. "Application of adaptive mesh refinement to particle-in-cell simulations of plasmas and beams", Physics of Plasmas 11, p 2928-2934 (2004)

Synergistic Activities

Panel member, National Academies study on the Science Justification for High End Computing, 2006-2008.

Panel member, DOE Joint ASCAC / BERAC Panel on Climate Modeling, 2007.

Member, DOE OFES Fusion Simulation Project Planning committee, 2008-2009.

Lead PI, SciDAC Applied Partial Differential Equations Center, 2001-2011.

Lead PI, DOE HPCCP Computational Fluid Dynamics and Combustion Dynamics Project (1992-1997)

Collaborators (non-LBNL)

M. Adams (Columbia), B. Alder (LLNL), D. Arnett (Univ. of Ariz.), E. Ateljevich (CA Dept. of Water Resources), S. Baden (UC San Diego), D. Bader (ORNL), G. Balls (UC San Diego), E. Bierly (AGU), A. Bourlioux (Univ. Montreal), D. Calhoun (CEA-Saclay), A. Choudhary (Northwestern), R. Cohen (LLNL), J. Cracraft (AMNH), J. Compton (LLNL), J. Demmel (UC Berkeley), M. Dorr (LLNL), J. Drake (ORNL), J. Dutton (PSU), S. Edwards (Harvard), D. Erickson (ORNL), I. Foster (ANL), B Gross (GFDL), S. Guzik (LLNL), J. Hack (ORNL), L. Hernquist (Harvard), J. Hittinger (LLNL), L. Howell (LLNL), C. Jablonowski (U. Mich.), P. Jones (LANL), G. Keller (MATRIC), J. Lyons (NDU), G. Miller (UC Davis), F. Miniati (ETHZ), W. Nevins (LLNL), P. Norgaard (Princeton), P. Papadopoulos (UC Berkeley), N. Patel (UC Berkeley), J. Percelay (UC Berkeley), M. Rezac (KSU), T. Rognlien (LLNL), R. Samtaney (KAUST), E. Sarachik (U. Washington), M. Sekora (Princeton), P. Sharma (UC Berkeley), Q. Shu (CA Dept. of Water Resources), R. Smith (Yale), J. Stone (Princeton), W. Tang (PPPL), S. Weidman (NRC), T. Weisgraber (LLNL), D. Williams (LLNL), J. Wooley (UC San Diego), S. Woosley (UC Santa Cruz) Z. Xu (LLNL). **Students and Postdocs:** Robert Crockett (Tech-X Corporation), Bei Wang (Princeton Univ.)

Estelle Cormier-Michel
Tech-X Corporation, Boulder, CO
ecormiertxcorp.com – 303-996-7524

Education and Training

University of Strasbourg, France	Physics	Master degree, 2000
University of Paris Sud, Orsay, France	Astro-particle physics	Ph.D., 2003

Research and Professional Experience

- *2010–present: Research Scientist, Tech-X Corporation.* Since joining Tech-X, Dr. Cormier-Michel has been involved in simulations of colliding-pulse injection for laser plasma accelerators (LPA), and simulations of future LPA experiments with reduced models recently developed in the VORPAL framework. She has also been involved in the development of a new montecarlo simulation package for application to muon cooling in an inverse cyclotron.

- *2004–2010: Postdoctoral fellow, Nevada Terawatt Facility, University of Nevada Reno and Lawrence Berkeley National Laboratory.* During her postdoctoral work Dr. Cormier-Michel studied LPA both theoretically and numerically with particle-in-cell (PIC) codes. In particular, she modified and used the PIC code PSC to study the effect of numerical noise in LPA simulations. Her work also included simulation and design of current and future experiments of the LOASIS program at LBNL with the VORPAL framework.

Selected publications

[1] E. Cormier-Michel et al., "Control of focusing fields in laser-plasma accelerators using higher-order modes," PRST-AB **14**, 031303 (2011).

[2] E. Cormier-Michel et al., "Unphysical kinetic effects in particle-in-cell modeling of laser wakefield accelerators," Phys. Rev. E **78**, 016404 (2008).

[3] E. Cormier-Michel et al., "Predictive design and interpretation of colliding pulse injected laser wakefield experiments," in *Proceedings of PAC '11* (2011).

[4] E. Cormier-Michel et al., "Scaled simulations of a 10 GeV laser wakefield accelerator," in *Advanced Accelerator Concepts*, edited by C. B. Schroeder, W. P. Leemans, and E. Esarey (AIP, New York, 2009), vol. 1086, p. 297.

[5] J.-L. Vay et al., "Effects of hyperbolic rotation in Minkowski space on the modeling of plasma accelerators in a Lorentz boosted frame," Phys. Plasmas **18**, 030701 (2011).

[6] B. M. Cowan et al., "Characteristics of an envelope model for laser-plasma accelerator simulation," J. Comput. Phys. **230**, 61 (2011).

[7] C. G. R. Geddes, "Laser-plasma particle accelerators: Large fields for smaller facilities," SciDAC review **13**, 13 (2009).

[8] C. G. R. Geddes et al., "Plasma-density-gradient injection of low absolute-momentum-spread electron bunches," Phys. Rev. Let. **100**, 215004 (2008).

[9] K. T. Phuoc et al., "Betatron radiation from density tailored plasmas," Physics of Plasmas **15**, 063102 (2008).

[10] E. Esarey et al., "Thermal effects in plasma-based accelerators," Phys. Plasmas **14**, 056708 (2007).

Collaborators and co-editors

Eric Esarey (LBNL), Cameron Geddes (LBNL), Serguei Kalmykov (U. Nebraska), Wim Leemans (LBNL), O. Rubel (LBNL), Carl Schroeder (LBNL), Bradley Shadwick (U. Nebraska), Donald Umstadter (U. Nebraska), Jean-Luc Vay (LBNL)

Graduate and postdoctoral advisors and advisees

Graduate Advisor: Alain Cordier, University of Paris XI at Orsay, France
Postdoctoral Advisors: Thomas Cowan, Institute of Radiation Physics at Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany. Wim Leemans and Cameron Geddes at Lawrence Berkeley National Laboratory, Berkeley, CA
Post-graduate Advisees: none

Benjamin M. Cowan
Tech-X Corporation, Boulder, CO
benctxcorp.com – 303-996-7521

Education and Training

University of Chicago	Physics	B.A., 1999
Stanford University	Accelerator and optical physics	Ph.D., 2007

Research and Professional Experience

- *2007–present: Research Scientist, Tech-X Corporation.* Since joining Tech-X, Benjamin Cowan has been involved in a number of accelerator design and simulation projects. These have included development of coupling structures and analysis of fabrication error for three-dimensional photonic crystal accelerator structures. He has also developed a reduced model for laser wakefield acceleration as part of the VORPAL PIC code and performed simulations in a Lorentz boosted frame, and developed algorithms for computing short-range wakefields in RF cavities.

  Dr. Cowan has emerged as a leader in the field of dielectric laser acceleration. He presented invited talks on photonic crystal-based accelerators at the 2008 Advanced Accelerator Concepts Workshop and the 2009 workshop on the Physics and Applications of High Brightness Electron Beams. He also served as co-leader of the high gradient and laser structure-based acceleration working group at the 2010 Advanced Accelerator Concepts Workshop, and the leader of the Accelerator Applications working group at the 2011 Dielectric Laser Accelerator Workshop.
- *2000–2007: Research Assistant, Advanced Accelerator Research Department, SLAC National Accelerator Laboratory.* For his doctoral work at SLAC, Dr. Cowan developed simulations of two- and three-dimensional photonic bandgap optical accelerator structures, including mode properties and beam dynamics. He also developed microfabrication techniques for optical accelerator structures, performed experiments on ultrafast optical breakdown in silicon, and assisted with the Laser Electron Acceleration Program experiments.

Selected publications

[1] B. M. Cowan, "Three-dimensional dielectric photonic crystal structures for laser-driven acceleration," Phys. Rev. ST Accel. Beams **11**, 011301 (2008).

[2] B. M. Cowan, "Two-dimensional photonic crystal accelerator structures," Phys. Rev. ST Accel. Beams **6**, 101301 (2003).

[3] B. M. Cowan et al., "Characteristics of an envelope model for laser-plasma accelerator simulation," J. Comput. Phys. **230**, 61 (2011).

[4] B. M. Cowan et al., "Optical accelerator structures," in *Thirteenth Advanced Accelerator Concepts, Santa Cruz, CA, 2008*, edited by C. B. Schroeder, W. P. Leemans, and E. Esarey (American Institute of Physics, Melville, NY, 2009), pp. 56–64.

[5] B. M. Cowan et al., "Compact couplers for photonic crystal laser-driven accelerator structures," in *Proceedings of the First International Particle Accelerator Conference, Kyoto, Japan, 2010* (JACoW, 2010), p. 4077.

[6] B. Cowan, "Three-dimensional photonic crystal laser-driven accelerator structures," in *Twelfth Advanced Accelerator Concepts, Lake Geneva, WI, 2006*, edited by M. Conde and C. Eyberger (American Institute of Physics, Melville, NY, 2006), pp. 844–850.

[7] B. Cowan, "Microfabrication of laser-driven accelerator structures," in *Advanced Accelerator Concepts: Tenth Workshop, Mandalay Beach, CA, 2002*, edited by C. E. Clayton and P. Muggli (American Institute of Physics, Melville, NY, 2002), pp. 324–330.

[8] B. M. Cowan, "Optical damage threshold of silicon for ultrafast infrared pulses," in *Laser-Induced Damage in Optical Materials, Boulder, CO, 2007*, edited by G. J. Exarhos et al. (SPIE, Bellingham, WA, 2007), vol. 6720 of *Proceedings of SPIE*, pp. 67201M–1.

[9] B. Cowan, "Optical damage threshold of silicon for ultrafast infrared pulses," in *Twelfth Advanced Accelerator Concepts, Lake Geneva, WI, 2006*, edited by M. Conde and C. Eyberger (American Institute of Physics, Melville, NY, 2006), pp. 837–843.

[10] T. Plettner et al., "Visible-laser acceleration of relativistic electrons in a semi-infinite vacuum," Phys. Rev. Lett. **95**, 134801 (2005).

Collaborators and co-editors

Kyle Bunkers (U. Nebraska), Robert Byer (Stanford), Eric Colby (SLAC), R. Joel England (SLAC), Eric Esarey (LBNL), Cameron Geddes (LBNL), Serguei Kalmykov (U. Nebraska), Wim Leemans (LBNL), Chris McGuinness (Stanford), Robert Noble (SLAC), Tomas Plettner (KLA-Tencor), Carl Schroeder (LBNL), Christopher Sears (KLA-Tencor), Bradley Shadwick (U. Nebraska), James Spencer (SLAC), Donald Umstadter (U. Nebraska), Jean-Luc Vay (LBNL), Dieter Walz (SLAC), Rodney Yoder (Manhattanville College)

Graduate and postdoctoral advisors and advisees

Graduate advisor: Robert H. Siemann (deceased); no postdoctoral advisor; no advisees

Marc Durant

Software Developer II, Tech-X Corporation

Relevant Experience

Marc Durant's background is in artificial intelligence, application development, and human perception and cognition. Before joining Tech-X he worked at the NSA on a distributed model checking tool designed to automate and streamline code reviews of Java source code. He has experience with application development in multiple languages on Mac, Linux, and Windows. Mr. Durant is currently a Software Developer II at Tech-X.

Mr. Durant is one of the primary developers of the Composer Toolkit project, which is a C++ framework specifically targeted at developing user interfaces for simulation codes. The Composer Toolkit provides input file editing, run management, and embedded visualization of data using VisIt. Mr. Durant is also a primary developer of Vorpal Composer, a user interface for Vorpal that uses the Composer Toolkit.

Mr. Durant has worked extensively with the VisIt software and with the VisIt development team. He maintains the VizSchema database reader plugin for VisIt that reads HDF5 data files with standardized metadata markup.

Education and Training

- Cornell University, School of Engineering. B.S. in Computer Science, May 2000

Research and Professional Experience

- Software Developer II, Tech-X Corp. Since October 2008
- Software Developer, User Interfaces. Sona Mobile, Boulder. October 2007-August 2008
- Independent Contractor, Durant Logic Research. Contracted to National Security Agency. June 2004-December 2006
- Cryptographic Analyst / Software Developer, National Security Agency. June 2001-April 2004

Publications

1. Hank Childs, et. al. (Marc Durant contributing). VisIt: An End-User Tool For Visualizing and Analyzing Very Large Data. *Proceedings SciDAC 2011*, Denver, CO July 10-14, 2011.
2. Svetlana Shasharina, John R. Cary, Marc Durant, Scott Kruger, Seth Andrew Veitzer. VizSchema - a standard approach for visualization of computational accelerator physics data. *Proceedings of the 10th International Computational Accelerator Physics Conference (ICAP)*, San Francisco, USA, 2009.
3. Cameron G. R. Geddes, et. al. (Marc Durant contributing). Large Fields for Smaller Facility Sources. *SciDAC review*, Issue 13, Summer 2009.
4. Svetlana Shasharina, John R. Cary, Seth Veitzer, Paul Hamill, Scott Kruger, Marc Durant, and David A. Alexander. VizSchema ■ Visualization Interface for Scientific Data. *IADIS International Conference, Computer Graphics, Visualization, Computer Vision and Image Processing*, 2009, page 49.

Miguel A. Furman
Senior Scientist, Lawrence Berkeley National Laboratory
Accelerator and Fusion Research Division
mafurman@lbl.gov
http://mafurman.lbl.gov

Research Interests

Fast and accurate integration techniques to solve multiparticle Newton-Maxwell equations. Electron-cloud effect for intense beams in storage rings; beam-beam effects in high energy physics colliders.

Education and Training

- University of California, Santa Cruz, Ph.D. in Physics, 1977.
- Post-doc, Lawrence Berkeley Lab. Physics Division Theoretical Physics Group, 1977-79.
- Post-doc, Columbia University Physics Dept., 1979-83.

Research and Professional Experience

- Visiting Assistant Professor, Physics Dept., University of California, Santa Cruz, 1983-84.
- Consultant, Fairchild Advanced Research Division, Palo Alto, California (VLSI Tools and Architectures), 1983-84.
- Staff Scientist/Physicist, Lawrence Berkeley National Laboratory, Accelerator and Fusion Research Division, 1984 – 2007.
- Senior Scientist/Physicist, Lawrence Berkeley National Laboratory, Accelerator and Fusion Research Division, 2007 – present.
- Group Leader, LBNL Center for Beam Physics Theory Group, 1998 – 2009.

Honors and Awards

- Member, International Committee on Future Accelerators (ICFA) Beam Dynamics Panel, 2004-11
- Fellow of the American Physical Society, Nov. 2007
- American Physical Society Outstanding Referee, Feb. 2008.

Selected Publications

1. M. A. Furman and W. C. Turner, "Beam-Beam Simulation for Separated Beams in the LHC," Proc. EPAC00 (Vienna, 26-30 June 2000), p. 1196.
2. M. A. Furman, "The electron-cloud effect in the arcs of the LHC," LBNL-41482/CBP Note 247/LHC Project Report 180, May 20, 1998.
3. M. A. Furman and M. T. F. Pivi, "Probabilistic Model for the Simulation of Secondary Electron Emission," PRST-AB **5**, 124404 (2002).

4. R. Cimino, I. R. Collins, M. A. Furman, M. Pivi, F. Ruggiero, G. Rumolo, and F. Zimmermann, "Can Low Energy Electrons Affect High Energy Physics Accelerators?," Phys. Rev. Lett. **93**, 014801 (2004).

5. M. A. Furman, I. Kourbanis and R. M. Zwaska, "Status of Electron-Cloud Build-Up Simulations for the Main Injector," Proc. PAC09 (Vancouver, BC, 4-8 May 2009), paper TH5PFP032.

Selected Synergistic Activities
Initiator and co-developer of the electron-cloud buildup code POSINST.

Collaborators within the Past 48 Months
C. Celata, G. Penn, J.-L. Vay, M. Venturini, J. Qiang, R. Ryne (Lawrence Berkeley National Laboratory); J. Fox, M. Pivi (SLAC); R. De Maria, Y. Papaphilippou and G. Rumolo,W. Höfle, F. Zimmermann (CERN); P. Stoltz, S. Veitzer, J. Cary (Tech-X); R. Zwaska, I. Kourbanis (FNAL); M. Palmer, G. Dugan, J. Crittenden, M. Billing, K. Sonnad and many others (Cornell Univ.); K. Harkay (ANL); R. H. Cohen, A. Friedman and D. P. Grote (LLNL); K. Ohmi (KEK).

Lixin Ge
SLAC National Accelerator Laboratory
Advanced Computations Department
2575 Sand Hill Road
Menlo Park, CA 94025
email: lge@slac.stanford.edu

Education and Training

Ph.D., Computational Aerodynamics,	Beijing University of Aeronautics and Astronautics, China, 1997
M.Sc., Applied Mathematics,	Jilin University, China, 1993
B.Sc., Applied Mathematics,	Jilin University, China, 1990

Research and Professional Experience

2002 -	Computational Scientist, SLAC National Accelerator Laboratory
2001 - 2002	Research Assistant, Stanford University
1999 - 2000	Postdoctoral Fellow, Department of Computer Science, University of Kentucky, Lexington
1997 - 1999	Computational Scientist, Institute of Applied Physics and Computational Mathematics, China
1993 - 1997	Research Assistant, Beijing University of Aeronautics and Astronautics, China
1990 - 1993	Research Assistant, Jilin University, Changchun, China

Dr. Lixin Ge obtained her Ph. D. in Computational Aerodynamics from Beijing University of Aeronautics and Astronautics, China in 1997. Her Ph.D. thesis is developing a 3D Navier-Stokes equations solver which includes mesh generation, high order finite difference algorithms, large linear solvers and visualization for results analysis. She parallelized this serial 3D Navier-Stokes solver while working at the Institute of Applied Physics and Computational Mathematics in China. She developed a family of high order difference schemes and studied different solvers to solve large-scale matrices when she was a postdoctoral fellow in the University of Kentucky. She has been with the SLAC National Accelerator Laboratory since 2002. Dr. Lixin Ge's main research interests in SLAC are high performance electromagnetic code development, adaptive mesh refinement, and modeling of RF accelerator structures. She has been involved in the parallel finite element advanced simulation code suit ACE3P's development, especially Track3P, a 3D parallel multipacting and dark current simulation code, which has been successfully benchmarked with experiments and used to predict multipacting activities in many accelerator projects, such as ICHIRO cavity, TTFIII couplers in the International Linear Colldider (ILC), FRIB Half Wave Resonator and Quarter Wave Resonator. By collaborating with RPI, she successfully applied adaptive mesh refinement on several cavity simulations, substantially improving simulation performance. She is currently involved in the parallel adaptive h-p refinement code design and development without file transfer among different software packages, load balancing and error estimators based on hierarchical finite element basis functions, and mesh correction tools for curved surface. She is also involved in the RF design of the muon cooling cavity, and the design and optimization of the compact crab cavity for the LHC upgrade.

Selected Publications

1. Lixin Ge and Zenghai Li, "ultipacting analysis for the half-spoke resonator crab cavity for LHC", Proceedings of 2011 Particle Accelerator Conference, New York, NY, USA.

2. X.-J. Luo, M. S. Shephard, L.-Q. Lee, L. Ge and C. Ng, "Moving Curved Mesh Adaptation for Higher Order Finite Element Simulations", J. of Engineering with Computers 27, 41 (2011).
3. Lixin Ge, Zenghai Li, Kwok Ko, John Popielarski, Walter Hartung, Jeremiah Holzbauer, "Multipacting Simulation amd analysis for the FRIB Superconducting Resonators Using Track3P", 25th International Linear Accelerator Conference (LINAC10), Tsukuba, Japan, 12-17 Sep 2010.
4. Lixin Ge, Zenghai Li, Cho-Kuen Ng, Kwok Ko, Robert B. Palmer, D. Li, "Multipacting simulation for muon collider cavity", PAC09-WE5PFP020, May 2009.
5. Lixin Ge, C. Adolphaen, K. Ko, L.-Q. Lee, Z. Li, C. Ng, G. Schussman, F. Wang, B. Rusnak, "Multipacting simulations of TTF-III power coupler components", Particle Accelerator Conference, 2007. PAC. IEEE, 25-29 June 2007, Albuquerque, NM.
6. Lixin Ge, Liequan Lee, Zenghai Li, Cho Ng and Kwok Ko, "Adaptive mesh refinement for high accuracy wall loss determination in accelerating cavity design", SLAC-PUB-10496.
7. Z. Li, N. Folwell, L. Ge, A. Guetz, V. Ivanov, M. Kowalski, L.-Q. Lee, C.-K. Ng, G. Schussman, R. Uplenchwar, M. Wolf, L. Xiao and K. Ko, "High Performance Computing in Accelerator Design and Analysis", Nucl. Instru. Meth. A558, 168 (2006).
8. Lixin Ge and Jun Zhang, "Symbolic computation of high order compact difference schemes for three dimensional linear elliptic partial differential equations with variable coefficients", Journal of Computational and Applied Mathematics, Vol. 143, No. 1, pp. 9-27 (2002).
9. Lixin Ge and Jun Zhang, "High accuracy iterative solution of convection diffusion equation with boundary layers on nonuniform grids", Journal of Computational Physics, Vol. 171, No. 2, pp. 560-578 (2001).
10. Lixin Ge and Jun Zhang, "Accuracy, robustness, and efficiency comparison in iterative computation of convection diffusion equation with boundary layers"„ Numerical Methods for Partial Differential Equations, Vol. 16 (4), 379-394 (2000).

Collaborators (last 48 months) and Co-Editors (last 24 months)

Mark Shephard, RPI,
Bob Rimmer, Thomas Jefferson National Lab,
Haipeng Wang, Thomas Jefferson National Lab,
Geoff Waldschmidt, Argonne National Laboratory,
John Popielarski, Michigen State University,
Derun Li, Lawrence Berkeley National Laboratory,
Daniel L. Bowring, Lawrence Berkeley National Laboratory

Graduate and Postdoctoral Advisors and Advisees:

Chunxuan Lee, Computational Aerodynamics, Beijing University of Aeronautics and Astronautics, Beijing, China, thesis advisor,
Jun Zhang, Computer Science, University of Kentucky, Lexington, KY

Cameron G.R. Geddes
Staff Physicist, Lawrence Berkeley National Laboratory
cgrgeddes@lbl.gov

Research Interests

Intense laser matter interaction applied to laser driven particle acceleration, high energy particle colliders, and radiation sources. Advanced numerical methods, and use of high performance computing to understand and design experiments.

Education and Training

- Swarthmore College & Physics, B.A. in Physics 1997
- University of California Berkeley, M.A. in Physics, 2003
- University of California Berkeley, Ph.D. in Physics, 2005

Research and Professional Experience

- Staff Physicist, Lawrence Berkeley National Laboratory, Accelerator and Fusion Research Division, 2008 – present
- Research Scientist, Lawrence Berkeley National Laboratory, Accelerator and Fusion Research Division, 2006 – 2008
- Term Scientist, Lawrence Berkeley National Laboratory, Accelerator and Fusion Research Division, 2005
- Physicist contractor, Polymath Research 1999-2000
- Term Scientist, Lawrence Livermore Nat'l Lab Plasma group, 1997 – 1999

Honors and Awards

- Am. Phys. Soc. John Dawson Award for Excellence in Plasma Physics Research, 2010.
- Outstanding Performance Awards, LBNL, 2005 and 2007.
- Am. Phys. Soc. Rosenbluth award for outstanding doctoral dissertation, 2006.
- Hertz Thesis prize for outstanding doctoral dissertation, 2005.
- Am. Phys. Soc. Apker award for best undergraduate thesis in physics, 1997.

Selected Publications

1. J.-L. Vay, C. G. R. Geddes, E. Cormier-Michel, and D. P. Grote. Effects of hyperbolic rotation in Minkowski space on the modeling of plasma accelerators in a Lorentz boosted frame. *Physics of Plasmas* 18, 030701 (2011) (press releases at LBNL, NERSC, DOE)

2. J.-L. Vay, C. G. R. Geddes, E. Esarey, C. B. Schroeder, W. P. Leemans, E. Cormier-Michel, and D. P. Grote. Modeling of 10 GeV-1 Tev laser-plasma accelerators using Lorentz boosted simulations. *Physics of Plasmas* 18, 123103 (2011)

3. A. J. Gonsalves, K. Nakamura, C. Lin, D. Panasenko, S. Shiraishi, T. Sokollik, C. Benedetti, C. B. Schroeder, C. G. R. Geddes, J. van Tilborg, J. Osterhoff, E. Esarey, C. Toth , W. P. Leemans, *Tunable laser plasma accelerator based on longitudinal density tailoring,* Nature Physics (2011).

4. C. B. Schroeder, E. Esarey, C. Geddes, C. Benedetti, and W. P. Leemans, *Physics considerations for laser-plasma linear colliders,* PRSTAB 13, 1010301 (2010)

5. C.G.R. Geddes, E. Cormier-Michel, E.H. Esarey, C.B. Schroeder, J-L. Vay, W.P. Leemans, and the LOASIS team, LBNL; D.L. Bruhwiler, J.R. Cary, B. Cowan, M. Durant, P. Hamill, P. Messmer, P. Mullowney, C. Nieter, K. Paul, S. Shasharina, S. Veitzer, and the VORPAL development team, Tech-X; G. Weber, O. Rubel, D. Ushizima, Prabhat, and E.W. Bethel, VACET; and J. Wu, SciDAC Scientific Data Management Center, *Laser Plasma Particle Accelerators: Large Fields for Smaller Facility Sources*, SciDAC Review 13, pp. 13 (2009).

6. C.G.R. Geddes, D.L. Bruhwiler, J.R. Cary, W.B. Mori, J-L. Vay, S.F. Martins, T. Katsouleas, E. Cormier-Michel, W.M. Fawley, C. Huang, X. Wang, B. Cowan, V.K. Decyk, E. Esarey, R.A. Fonseca, W. Lu, P. Messmer, P. Mullowney, K. Nakamura, K. Paul, G.R. Plateau, C.B. Schroeder, L.O. Silva, Cs. Toth, F.S. Tsung, M. Tzoufras, T. Antonsen, J. Vieira and W.P. Leemans, *Computational studies and optimization of wakefield accelerators,* J. Phys. Conf. Series V 125 pp. 12002/1-11 (2008).

7. C.G.R. Geddes, K. Nakamura, G.R. Plateau, Cs. Toth, E. Cormier-Michel, E. Esarey, C.B. Schroeder, J.R. Cary, and W.P. Leemans, *Stable low momentum spread electron bunches from plasma density gradient injection,* PRL V 100, 215004 (2008).

8. E. Cormier-Michel, B.A. Shadwick, C.G.R. Geddes, E. Esarey, C.B. Schroeder, and W.P. Leemans , *Unphysical kinetic effects in laser wakefield accelerators modeled with particle-in-cell codes,* Phys. Rev. E. V 78, 016404 (2008).

9. W. P. Leemans, B. Nagler, A. J. Gonsalves, Cs. Toth, K. Nakamura,3, C. G. R. Geddes, E. Esarey, C. B. Schroeder, S. M. Hooker, *GeV electron beams froma centimetre-scale accelerator/* Nature Physics, V 2, pp. 696.

10. C. G. R. Geddes, Cs. Toth, J. van Tilborg, E. Esarey, C. B. Schroeder, D. Bruhwiler, C. Nieter, J. Cary, W. P. Leemans, *High-quality electron beams from a laser wakefield accelerator using plasma-channel guiding,* Nature, Sept 30 2004, pp 538-41.

Selected Synergistic Activities

- Experimentalist on controlled injection and laser guiding experiments at the LOASIS facility of LBNL. SciDAC codes used to predict and interpret experiments.
- Collaborator on development and use of VORPAL and WARP codes, and related algorithms.

Collaborators within the Past 48 Months
A. J. Gonsalves, K. Nakamura, C. Lin, S. Shiraishi, T. Sokollik, C. Benedetti, J. van Tilborg, J. Osterhoff, E. Esarey, W. Fawley, W. Leemans,C. Schroeder, C. Toth, J.-L. Vay (Lawrence Berkeley National Laboratory, AFRD); G. Weber, O. Rubel, D. Ushizima, Prabhat, and E.W. Bethel (Lawrence Berkeley National Laboratory, CRD); J. Barnard,M. Marinak (Lawrence Livermore National Laboratory); D. Bruhwiler, J. Cary, E. Cormier-Michel, B. Cowan, M. Durant, P. Messmer, P. Mullowney, C. Nieter, K. Paul, S. Shasharina, P. Stoltz, S. Veitzer (Tech-X) (NERSC) M. Krishnan (Alameda Applied Sciences)
Doctoral Advisor: Dr. Wim Leemans, Lawrence Berkeley National Lab, USA. Prof. Jonathan Wurtele, University of California, Berkeley, USA.

Daniel T. Graves
Applied Numerical Algorithms Group
Lawrence Berkeley National Laboratory
1 Cyclotron Road, M/S 50A-1148
Berkeley, CA 94720
`https://commons.lbl.gov/display/ dtgraves@lbl.gov/Dan+Graves` ; `dtgraves@lbl.gov`

Education and Training

Ph.D. in Mechanical Engineering, December 1996
University of California, Berkeley
Dissertation: "A Second Order Projection Method for Rapidly Rotating Flows"
Chair: Prof. Phillip Colella.

B.S. in Mechanical Engineering, June 1989
University of New Hampshire

Research and Professional Experience

Research Scientist 1998 - present
Applied Numerical Algorithms Group, Lawrence Berkeley National Laboratory

Postdoc 1997 - 1998
Center for Computational Sciences and Engineering, Lawrence Berkeley National Laboratory

Publications

1. R.K. Crockett, P. Colella, and D.T. Graves. *A Cartesian grid embedded boundary method for solving the Poisson and heat equations with discontinuous coefficients in three dimensions.* Journal of Computational Physics Vol 230 pp. 2451-1469, 2011.
2. A. Nonaka, D. Trebotich, G. H. Miller, D. T. Graves, and P. Colella *A Higher-Order Upwind Method for Viscoelastic Flow* Comm. App. Math. and Comp. Sci., 4(1):57-83 (2009)
3. Martin, D.F., Colella, P., and Graves, D.T. *A Cell-Centered Adaptive Projection Method for the Incompressible Navier-Stokes Equations in Three Dimensions*, Journal of Computational Physics Vol 227 (2008) pp. 1863-1886.
4. D. T. Graves, D Trebotich, G. H. Miller, P. Colella, *An efficient solver for the equations of resistive MHD with spatially-varying resistivity*, Journal of Computational Physics Vol 227 (2008) pp.4797-4804.
5. P. Colella, D. T. Graves, B. Keen, D. Modiano. *A Cartesian Grid Embedded Boundary Method for Hyperbolic Conservation Laws*, Journal of Compuational Physics, Vol. 211, Issue 1, Jan. 2006, pp. 347-366.

Collaborators (48 months) and Co-Editors (24 months)

M. Adams (Columbia University), E. Ateljevich (Cal. Dept. of Water Resources), M. Barad (NASA), R. Crockett (Tech X), G. Miller (University of California, Davis), R. Samtaney (KAUST University)

Ki Hwan Lee
SLAC National Accelerator Laboratory
Advanced Computations Department
2575 Sand Hill Road
Menlo Park, CA 94025
email: kilee@slac.stanford.edu

Education and Training

Ph.D.,	Aeronautics/Astronautics, Stanford University, 2010
M.S.,	Physics, Aeronautics/Astronautics, Stanford University, 2001
B.S.,	Physics, University of California, Los Angeles, 1999

Research and Professional Experience

2010 - present	Computational Scientist, SLAC National Accelerator Laboratory
2008 - 2010	Engineering Analyst, Engineering Analysis Inc.
2007 - 2008	Aerospace Engineer, NASA Ames
2002 - 2007	Research Assistant, Stanford

Dr. Ki H. Lee has been working in the SLAC Advanced Computations Department (ACD) since 2010. His main research interests are computational sciences, multiphysics simulations, and optimization. His main contribution includes multiphysics simulations of highly nonlinear superconducting and normal conducting cavities for the integrated effect of electromagnetic, thermal and structural loads; imperfection studies of ERL cavity using adjoint-based optimization methodology. He is involved in the development of the parallel finite element advanced simulation tools at ACD/SLAC for multiphysics simulations and optimization where his main focus is on the development and application of these tools to accelerator modeling.

Selected Publications

1. Liling Xiao, Kwok Ko, Ki Hwan Lee, Cho-Kuen Ng, Matthias Liepe, Nicholas Ruben Alexander Vallesm, "Effects of Elliptically Deformed Cell Shape in the Cornell ERL Cavity", 15th International Conference on RF Superconductivity, Chicago in IL, July 25 29, 2011.
2. Ki Hwan Lee, "Design Optimization of Periodic Flows using a Time-Spectral Discrete Adjoint Method", Ph.D. Thesis, June. 2010, Stanford University, CA, USA.
3. Seongim Choi, Mark Potsdam, Ki Hwan Lee, Gianlucca Iaccarino, Juan Alonso, "Helicopter Rotor Design Using a Time-Spectral and Adjoint-Based Method", 12th AIAA/ISSMO Multidisciplinary and Optimization Conference Sep. 10-12, 2008, British Columbia, Canada.
4. Seongim Choi, Ki Hwan Lee, Juan Alonso, "Preliminary Study on Time-Spectral and Adjoint-Based Design Optimization of Helicopter Rotors", Specialist Conference on Aeromechanics, San Francisco, CA, January 23 25, 2008.
5. Ki Hwan Lee, Juan Alonso, Edwin Van der Weide, "Mesh Adaptation Criteria for Unsteady Periodic Flow using a Discrete Adjoint Time-Spectral Formulation", 44th AIAA Aerospace Sciences Meeting and Exhibit, AIAA, Reno, NV, January 2006.

Collaborators (last 48 months) and Co-Editors (last 24 months)

Matthias Liepe, Cornell University,
Nicholas Ruben Alexander Valles, CLASSE,
Gary Chen, Thomas Jefferson National Lab,
Haipeng Wang, Thomas Jefferson National Lab,

Seongim Choi, KAIST, Korea,
Mark Potsdam, US Army Research,
Gianluca Iaccarino, Stanford University

Graduate and Postdoctoral Advisors and Advisees:

Juan Alonso, Stanford University, thesis advisor

Xiaoye Sherry Li

Lawrence Berkeley National Laboratory, 1 Cyclotron Rd, Mail Stop 50F1650, Berkeley, CA 94720-8139
http://crd.lbl.gov/~xiaoye ; xsli@lbl.gov

Education and Training

Tsinghua University, China, B.S. (Highest Honors), Computer Science, 1986.
Penn State University, M.S. Computer Science and M.A. Mathematics, 1990.
University of California, Berkeley, Ph.D. Computer Science, 1996

Research and Professional Experience

Staff Computer Scientist, Lawrence Berkeley National Laboratory, 2001 – present
Computer Systems Engineer, Lawrence Berkeley National Laboratory, 1996 – 2001
Visiting Associate Researcher, University of California, Berkeley, 1998 – 2005
Consultant, Xerox Palo Alto Research Center, 1994 – 1996

Publications

1. J. W. Demmel, S. C. Eisenstat, J. R. Gilbert, X. S. Li and J. W. H. Liu, *A Supernodal Approach to Sparse Partial Pivoting*, SIAM J. Matrix Anal. Appls., vol. 20 (3), 720-755, 1999.
2. J. W. Demmel, J. R. Gilbert and X. S. Li, *An Asynchronous Parallel Supernodal Algorithm for Sparse Gaussian Elimination*, SIAM J. Matrix Anal. Appls., vol. 20 (4), 915-952, 1999.
3. M. Baertschy and X. S. Li, *Solution of a Three-Body Problem in Quantum Mechanics Using Sparse Linear Algebra on Parallel Computers*, Proceedings of SC2001, November 10–16, 2001, Denver, Colorado.
4. X. S. Li and James W. Demmel, *SuperLU_DIST – A Scalable Distributed-Memory Sparse Direct Solver for Unsymmetric Linear Systems*, ACM Trans. Math. Software, Vol. 29, No. 2, pp. 110-140, June 2003.
5. X. S. Li, *An Overview of SuperLU: Algorithms, Implementation, and User Interface*, ACM Trans. Math. Software, Vol. 31, No. 3, September 2005, pp. 302-325,
6. X. S. Li, *Evaluation of sparse factorization and triangular solution on multicore architectures*, Proceedings in VECPAR08 8th International Meeting High Performance Computing for Computational Science, June 24-27, 2008, Toulouse, France.
7. I. Yamazaki and X.S. Li, *On techniques to improve robustness and scalability of the Schur complement method*, Proc. of VECPAR 2010, 9th International Meeting High Performance Computing for Computational Science, June 22-25, 2010, Berkeley, California.
8. J. Qiang and X. Li, *Particle-Field Decomposition and Domain Decomposition in Parallel Particle-In-Cell Beam Dynamic Simulations*, Computer Physics Communications, 181, 2024-2034, 2010.
9. Xiaoye S. Li and Meiyue Shao, ”A Supernodal Approach to Incomplete LU Factorization with Partial Pivoting”, ACM Trans. Mathematical Software, Vol. 37, No. 4, Article 43, 2011.
10. Shen Wang, Xiaoye Li, Jianlin Xia, Yingchong Situ, and Maarten V. de Hoop, *Efficient parallel algorithms for Hierarchically SemiSeparable matrices*, SIAM J. Scientific Computing, submitted, 2011.

Honors

Invited Topical Lecture, “Factorization-based sparse solvers and preconditioners”, SIAM Annual Meeting, 2010.
Associate Editor, ACM Transaction on Mathematical Software (2006-present)
Associate Editor, SIAM Journal on Scientific Computing (2006-2010)

Synergistic Activities

Organizer, Fifth Bay Area Scientific Computing Day, March 13, 2004.
Program Committee Member, SC01, SC04, SC08, SC10, HiPC 2003/2007, IPDPS 2004, IASTED PDCN 2004-2006, VECPAR'08, VECPAR'10, CSC'09.
ACM Senior Member, SIAM Member.

Collaborators (48 months) and Co-Editors (24 months)

Patrick Amestoy (ENSEEIHT-IRIT), Zhaojun Bai (UC Davis), David Bailey (LBNL), Elaine Chan (LBNL), Maarten de Hoop (Purdue Univ.) James Demmel (UC Berkeley), Iain Duff (RAL and CERFACS), Weiguo Gao (Fudan Univ.) Ming Gu (UC Berkeley), Alex Hexemer (LBNL), David Keyes (Columbia Univ./KAUST), Li-Quan Lee (SLAC), Jean-Yves L'Excellent (ENS, Lyon) Osni Marques (LBNL), Esmond Ng (LBNL), Ji Qiang (LBNL), Robert Ryne (LBNL), Panayot Vassilevski (LLNL), Jianlin Xia (Purdue Univ.), Ichitaro Yamazaki (LBNL), Chao Yang (LBNL).

Graduate Students and Postdoctoral Associates (5 years)

Emmanuel Agullo (gs, INRIA), Pietro Cicotti (gs, UC San Diego), Slim Chourou (postdoc, LBNL), Artem Napov (postdoc, LBNL), Abhinav Sarje (postdoc, LBNL), Meiyue Shao (gs, Univ. of Umea), Shen Wang (gs, Purdue Univ.) Jianlin Xia (gs, Purdue Univ.), Ichitaro Yamazaki (postdoc, LBNL), Eric Zhang (UC Berkeley), Yeliang Zhang (gs, Google).

Zenghai Li
SLAC National Accelerator Laboratory
Advanced Computations Department
2575 Sand Hill Road
Menlo Park, CA 94025
email: lizh@slac.stanford.edu

Education and Training

Ph.D.,	Accelerator Physics, the College of William and Mary, 1995.
M.S.,	Accelerator Physics, China Institute of Atomic Energy, 1985.
B.S.,	Physics, Hebei University, China, 1982.

Research and Professional Experience

1997 - present	Staff Physicist, SLAC National Accelerator Laboratory
1995 - 1997	Research Associate, Stanford Linear Accelerator Center
1991 - 1995	Graduate Research Assistant, Thomas Jefferson National Accelerator Facility
1989 - 1991	Visiting Scientist, LAMPF, Los Alamos National Laboratory
1985 - 1989	Research Engineer, China Institute of Atomic Energy

Dr. Zenghai Li has been working in the SLAC Advanced Computations Department (ACD) since May 1995. His main research interests are accelerator physics, RF accelerator structures, and computational electromagnetics. He has been involved in the R&D of many accelerator projects, especially the Next Linear Accelerator (NLC), the International Linear Collider (ILC), the SLAC Linac Coherent Light Source (LCLS), and the Large Hadron Collider (LHC) projects. His main contributions to these projects include the RF design of the X-band Damped Detuned Structures (DDS) for the NLC; the optimization of the HOM damping for the Low Loss 9-cell superconducting cavity for the ILC; the design and optimization of the Low Surface Field superconducting cavity shape for the ILC; the RF design of the S-band RF gun and the injector S-Band accelerator structures for the LCLS; and using the advanced shape determination tools to determine the cause of the high Q modes in one of the CEBAF upgrade prototype SRF cavities. He is currently involved in the X-Band RF gun and structure design for an X-Band test accelerator at SLAC, the RF design of the muon cooling cavity for the Muon Collider project, the design and optimization of the compact Crab Cavity for the LHC upgrade, and the RF optimization of the SRF deflecting cavity cryomodule for the APS upgrade (SPX). He is involved in the development of the parallel finite element advanced simulation tools at ACD/SLAC for electromagnetic simulations where his main focus is on applying these tools to accelerator modeling. He was the co-instructor for the "Computational accelerator physics" class for the US Particle Accelerator School in 1999, 2000, 2002 and 2005.

Selected Publications

1. Zenghai Li et al., "On the Importance of Symmetrizing RF Coupler Fields for Low Emittance Beams", proceedings of PAC2011, New York, 2011.
2. Lixin Ge and Zenghai Li, "Multipacting Analysis for the Half-Wave Spoke Resonator Crab cavity for LHC", proceedings of PAC2011, New York, 2011.
3. Zenghai Li et al., "Compact 400-MHz Half-wave Spoke Resonator Crab Cavity for the LHC Upgrade", proceedings of IPAC2010, Kyoto, Japan, 2010.
4. Lixin Ge, Zenghai Li, Kwok Ko, John Popielarski, Walter Hartung, and Jeremiah Holzbauer, "Multipacting Simulation and Analysis for the FRIB Superconducting Resonators Using

Track3P", proceedings of LINAC2010, Tsukuba, Japan, 2010.

5. Z. Li and C. Adolphsen, "A New SRF Cavity Shape with Minimized Surface Electric and Magnetic Fields for the ILC", proceedings of LINAC08, Victoria, Canada, 2008.
6. Z. Li, V. Akcelik, L. Xiao, L. Lee, C. Ng, and K. Ko, SLAC, H. Wang, F. Marhauser, J. Sekutowicz, C. Reece, and R. Rimmer, TJNAF, "Analysis of the Cause of High External Q Modes in the JLab High Gradient Prototype Cryomodule Renascence", SLAC-PUB-13266, June, 2008.
7. Z. Li et al., "Towards Simulation of Electromagnetics and Beam Physics at the Petascale", invited talk, Proceedings of 2007 Particle Accelerator Conference, Albuquerque, 2007.
8. Z. Li et al., "Optimization of the Low Loss SRF Cavity For the ILC", proceedings of 2007 Particle Accelerator Conference, Albuquerque, 2007.
9. Z. Li et al., "Coupler Design for the LCLS Injector S-Band Structures", Proc. of PAC2005, Knoxville.
10. L. Xiao, R.F. Boyce, D. Dowell, Z. Li, C. Limborg-Deprey, J.F. Schmerge, "Dual Feed RF Gun Design for the LCLS", Proc. of PAC2005, Knoxville.

Synergistic Activities

Teaching, Computational accelerator physics, US Particle Accelerator School
- Vanderbilt University, January, 1999
- SUNY at Stony Brook, June 2000
- Yale University, June 2002
- Cornell University, June 2005

DOE SBIR reviewer
PRSTAB journal reviewer
IEEE Transactions on Nuclear Science journal reviewer

Collaborators (last 48 months) and Co-Editors (last 24 months)

Bob Rimmer (TJNAF), Haipeng Wang (TJNAF), ROngli Geng (TJNAF), Alireza Nassiri (ANL), Genfa Wu (ANL), Geoff Waldschmidt (ANL), Wei Gai (ANL), John Power, (ANL), Jean R. Delayen (ODU), Subashini De Silva (ODU), John Popielarski (MSU), Derun Li (LBNL), Daniel L. Bowring (LBNL), Peter McIntosh (Cockcroft Institute), Graeme Burt (Lancaster University), Erk Jenson (CERN), Walter Wuensch (CERN), Alexej Grudiev (CERN), Rama Calada (CERN), Frank Zimmerman (CERN)

Graduate and Postdoctoral Advisors and Advisees:

Joseph Bisognano, SRC University of Wisconsin - Madison, thesis advisor,
Roger Miller, SLAC National Accelerator Laboratory

Paul Mullowney
Principal Mathematician, Tech-X Corporation
paulm@txcorp.com

Research Interests

Since joining Tech-X corporation in September of 2006, Dr. Mullowney has worked on the plasma simulation code VORPAL as well as various projects in GPU computing. He recently developed scalable, GPU-accelerated finite difference time domain (FDTD) solvers for electromagnetic simulations in the VORPAL framework. These features were released in VORPAL 5.0. He also made recent contributions to the PETSc open source library. Here, he added GPU-accelerated kernels for various preconditioner and sparse matrix vector multiplication algorithms. Lastly, Dr. Mullowney has been a primary developer of the Tech-X GPULib software library. This includes extensive development of GPU kernels for doing direct and iterative solves of linear systems as well as the library interface to MATLAB.

Education and Training

- Boston University, B.A. *cum laude* in Physics and Mathematics, May 1999
- University of Colorado at Boulder, Ph.D. in Applied Mathematics, December 2004
- Postdoctoral Fellow, University of Canterbury, Christchurch, Department of Mathematics and Statistics, June. 2005 – June. 2006

Research and Professional Experience

- Principal Mathematician, Tech-X Corporation, Boulder, CO, since January 2012
- Research Mathematician, Tech-X Corporation, Boulder, CO, 9/2006 – 12/2011

Selected Publications

1. "Computational Models of Germanium Point Contact Detectros", P.J. Mullowney et al, Nuclear Instruments and Methods in Physics Research Section A, 662, 33-44 (2012)
2. "The Effect of Surface Charge on the Performance of a P-type Point Contact HPGe Detector", R.J. Cooper et al, Nuclear Instruments and Methods in Physics Research Section A, 2011, Submitted for publication.
3. "GPU acceleration of out of core solver for electromagnetic scattering simulations", P. Messmer, P.J. Mullowney, M. Koch, Aces Journal, 2010, Accepted for publication.
4. "Chaotic Advection and the Emergence of Tori in the Kuppers-Lortz State," P.J. Mullowney, K.J. Julien, and J.D. Meiss, *Chaos*, 18, 3, 033104 (2008).
5. "GPULib: GPU Computing in High-Level Languages," P. Messmer and P.J. Mullowney and B. Granger, *Computing in Science Engineering*, 10, 5, 70-73 (2008).
6. "Parameter estimation for a leaky integrate-and-fire neuronal model from ISI data," P.J. Mullowney and S. Iyengar, *J. Comp. Neuro.*, **24**, 2, 179-194, (2008).

7. "Parameter Inference in the Ornstein-Uhlenbeck Process." S. Iyengar. and P.J. Mullowney. Revised/Resubmitted in *Annals of Applied Statistics*, (2009).

8. "The role of variance in capped-rate stochastic growth models." P.J. Mullowney and A.F. James. *Journal of Theoretical Biology*, **244**, 2, 228-238 (2007).

9. "Blinking Rolls: Chaotic Advection in a Three-Dimensional Flow with an Invariant." P.J. Mullowney, J.D. Meiss, and K.J. Julien. *SIAM Journal of Applied Dynamical Systems*, **4**, 1, 159-186 (2005)

Selected Synergistic Activities

- PI on GPU PETSc project, for porting PETSc Krylov solves to next-generation heterogeneous architectures.

Collaborators and Co-editors within the Past 48 Months
D. Radford, Oak Ridge National Laboratory (ORNL); R. Cooper, Oak Ridge National Laboratory (ORNL); S. Kizchner, Goddard Space Flight Center (GSFC); B. Smith, Argonne National Laboratory (ANL); B. Joo, Jefferson Laboratory (JLab);
Doctoral Advisor: Keith Julien and James Meiss, University of Colorado at Boulder
Postdoctoral Advisor: Satish Iyengar, University of Canterbury, Christchurch and University of Pittsburgh

Todd S. Munson
Computation Institute
University of Chicago
Chicago, IL 60637
Phone: (630) 252-4279 · Fax: (630) 252-5986
Email: `tmunson@ci.uchicago.edu` · `http://www.mcs.anl.gov/~tmunson`

Professional Preparation

- Argonne National Laboratory, Postdoc, Mathematics and Computer Science Division, 2000 – 2002
- University of Wisconsin at Madison, Ph.D. Computer Science, 2000
- University of Wisconsin at Madison, M.S. Computer Science, 1996
- University of Nebraska at Omaha, B.S. Computer Science (summa cum laude), 1995

Professional Experience

- 2010–present: *Senior Fellow*, Computation Institute, University of Chicago
- 2006–present: *Computational Scientist*, MCS Division, Argonne National Laboratory
- 2004–2010: *Fellow*, Computation Institute, University of Chicago
- 2004–2006: *Assistant Scientist*, MCS Division, Argonne National Laboratory
- 2002–2004: *Enrico Fermi Scholar*, MCS Division, Argonne National Laboratory
- 2000–2002: *Postdoctoral Fellow*, MCS Division, Argonne National Laboratory

Honors and Awards

- Kavli Frontiers Fellow, National Academy of Sciences, 2007
- Presidential Early Career Award for Scientists and Engineers, Executive Office of the President of the United States, 2006
- Early Career Scientist and Engineer Award, United States Department of Energy, 2006
- Beale-Orchard-Hayes Prize, Mathematical Programming Society, 2003
- Enrico Fermi Scholar, Argonne National Laboratory, 2002–2004
- Outstanding Graduate Student Research Award, University of Wisconsin at Madison, 2000
- Distinguished Graduate Fellow in CS, University of Wisconsin at Madison, 1999–2000

Five Relevant Publications

1. M. Ferris and T. Munson, *Semismooth Support Vector Machines*, **Mathematical Programming**, 101 (2004), pp. 185-204.
2. M. Ferris and T. Munson, *Interior Point Methods for Massive Support Vector Machines*, **SIAM Journal on Optimization**, 13 (2003), pp. 783-804.
3. S. Benson, L. C. McInnes, J. Moré, T. Munson, and J. Sarich, *Toolkit for Advanced Optimization (TAO) Users Manual*, Technical Report ANL/MCS-TM-242 - Revision 1.10.1, Argonne National Laboratory, 2011, see `http://www.mcs.anl.gov/tao`.
4. S. Benson and T. Munson, *Flexible Complementarity Solvers for Large-Scale Applications*, **Optimization Methods and Software**, 21 (2006), pp. 155-168.
5. S. Leyffer and T. Munson, *Solving Multi-leader-common-follower Games*, **Optimization Methods and Software**, 25 (2010), pp. 601-623.

Five Other Significant Publications

1. T. Munson, F. Facchinei, M. Ferris, A. Fischer, and C. Kanzow, *The Semismooth Algorithm for Large Scale Complementarity Problems*, **INFORMS Journal on Computing**,

13 (2001), pp. 294-311.

2. M. Ferris and T. Munson, *Complementarity Problems in GAMS and the PATH Solver*, **Journal of Economic Dynamics and Control**, 24 (2000), pp. 165-188.
3. T. Munson, *Mesh Shape-Quality Optimization using the Inverse Mean-Ratio Metric*, **Mathematical Programming**, 110 (2007), pp. 561-590.
4. J. Moré and T. Munson, *Computing Mountain Passes and Transition States*, **Mathematical Programming**, 101 (2004), pp. 151-182.
5. E. Dolan, J. Moré, and T. Munson, *Optimality Measures for Performance Profiles*, **SIAM Journal on Optimization**, 16 (2006), pp. 891-909.

Synergistic Activities

- **Editorial Boards**: Mathematical Programming Computation (technical editor, 2008–present), Mathematical Methods of Operations Research (associate editor, 2008–present)
- **Co-Chair**: Institute for Computational Economics, 2005 – present
- **TAO**: Lead developer of the Toolkit for Advanced Optimization (TAO), designed to solve large-scale optimization problems on high-performance distributed architectures. TAO solvers have been used to solve computational science problems in a wide variety of areas; details can be found in the impact section and `www.mcs.anl.gov/tao`.
- **MINOTAUR**: The Mixed-Integer Nonlinear Optimization Toolkit (MINOTAUR) is a toolkit for solving mixed-integer optimization problems to global optimality that contains many algorithms, underestimation techniques, and relaxation methods.

Collaborators and Co-editors (48 Months)

M. Anitescu (Argonne), J.-Q. Chen (Argonne), J. Elliott (U Chicago), H.-R. Fang (Minnesota), M. Ferris (UW Madison), I. Foster (Argonne), M. Franklin (Argonne), D. Fullerton (U Illinois), Evan Gawlik (Stanford), D. Hanson (Argonne), K. Judd (Hoover Institution), S. Kortum (U Chicago), J. Lee (Argonne), S. Leyffer (Argonne), J. Linderoth (UW Madison), J. Luedtke (UW Madison), L. McInnes (Argonne), A. Miller (U Bordeaux), J. Moré (Argonne), L. Moyer (U Chicago), F. Perez Cervantes (U Chicago), J. Sarich (Argonne), S. Shetty (Tennessee State University), B. Smith (Argonne), L. Wang (Argonne), D. Weisbach (U Chicago).

Advisors: Michael Ferris (thesis advisor), Jorge Moré (postdoc supervisor)

Advisees: Jieqiu Chen (Iowa), Sou-cheng Choi (Stanford), Joshua Elliott (McGill), Haw-ren Fang (Maryland), Ashutosh Mahajan (Lehigh), Zhen Xie (Emory)

Cho-Kuen Ng
SLAC National Accelerator Laboratory
Advanced Computations Department
2575 Sand Hill Road
Menlo Park, CA 94025
email: cho@slac.stanford.edu

Education and Training

Ph.D., Physics,	University of Illinois at Urbana-Champaign, 1986
M.S., Physics,	University of Illinois at Urbana-Champaign, 1982
B.Sc., Physics,	University of Hong Kong, First Class Honors, 1981

Research and Professional Experience

2007 - present	Co-PI of SciDAC ComPASS project
2008 - present	Staff Scientist, SLAC National Accelerator Laboratory
2006 - 2008	Acting Head, Advanced Computations Department, SLAC
2001 - 2006	Deputy Head, Advanced Computations Department, SLAC
1991 - 2001	Physicist, Stanford Linear Accelerator Center
1988 - 1991	Postdoctoral Research Associate, Cornell University
1986 - 1988	Postdoctoral Research Associate, University of Durham, England

Dr. Cho Ng obtained his Ph. D. in High Energy Physics from the University of Illinois at Urbana-Champaign in 1986. After postdoctoral work in particle phenomenology at the University of Durham, England and in computational plasma physics at Cornell University, he has been with the SLAC National Accelerator Laboratory since1991. Dr. Ng's research focuses on electromagnetic simulations of particle acclerators, in particular in the area of wakefield computations of accelerator cavities and beamline components using high performance computing. He has contributed to many accelerator projects including the design and analysis of the PEP-II, NLC, ILC, SPEAR3 and LCLS at SLAC. Currently, Dr. Ng is the institutional PI of the SciDAC ComPASS project and is leading a multi-disciplinary team of physicists and computational scientists in developing parallel finite-element electromagnetic codes for large- scale accelerator applications.

Selected Publications

1. X.-J. Luo, M. S. Shephard, L.-Q. Lee, L. Ge and C. Ng, "Moving Curved Mesh Adaptation for Higher Order Finite Element Simulations", J. of Engineering with Computers 27, 41 (2011).
2. C.-K. Ng, R. J. England, L.-Q. Lee, R. Noble, V. Rawat and J. Spencer, "Transmission and Radiation of an Accelerating Mode in a Photonic Bandgap Fiber", PRSTAB 13, 121301 (2010).
3. L.-Q. Lee, A. Candel, C. Ng and K. Ko, "On Using Moving Windows in Finite Element Time Domain Simulation for Long Accelerator Structures", J. Comput. Phys. 229, 9235 (2010).
4. A. Candel, A. Kabel, L.-Q. Lee, Z. Li, C. Ng, G. Schussman and K. Ko, "State of the Art in Electromagnetic Modeling for the Compact Linear Collider", J. Phys. Conf. Ser. 180, 012004 (2009).
5. A. Akcelik, K. Ko, L.-Q. Lee, Z. li, C.-K. Ng and L. Xiao, "Shape Determination for Deformed Electromagnetic Cavities", J. Comput. Phys. 227, 1722 (2008).
6. C. Ng et al., "Design and Optimization of Large Accelerator Systems through High-Fidelity Electromagnetic Simulations", J. Phys. Conf. Ser. 125, 012003 (2008).

7. C.-K. Ng, V. Akcelik, A. Candel, S. Chen, N. Folwell, L. Ge, A. Guetz, H. Jiang, A. Kabel, L.-Q. Lee, Z. Li, E. Prudencio, G. Schussman, R. Uplenchwar, L. Xiao and K. Ko, "State of the Art in EM Field Computation", invited talk at European Particle Accelerator Conference, Edinburgh, Scotland, June 26-30 2006.
8. C.-K. Ng, N. Folwell, A. Guetz, V. Ivanov, L.-Q. Lee, Z. Li, G. Schussman and K. Ko, "Simulating Dark Current in NLC Structures", Nucl. Instru. Meth. A558, 192 (2006).
9. Z. Li, N. Folwell, L. Ge, A. Guetz, V. Ivanov, M. Kowalski, L.-Q. Lee, C.-K. Ng, G. Schussman, R. Uplenchwar, M. Wolf, L. Xiao and K. Ko, "High Performance Computing in Accelerator Design and Analysis", Nucl. Instru. Meth. A558, 168 (2006).

Synergistic Activities

Member, Organization Committee, International Particle Accelerator Conference, 2009 & 2012
Visiting scientist, Laboratory for High Energy Physics (KEK), Japan, 1995
Consultant, AET Associates, 1993-1997
DOE SBIR reviewer
DOE Early Career Award reviewer

Collaborators (last 48 months) and Co-Editors (last 24 months)

E. Ng (LBNL),
M. Shephard (RPI),
I. Yamazaki (LBNL),
Bob Rimmer (TJNAF),
Haipeng Wang (TJNAF),
Alireza Nassiri (ANL),
Genfa Wu (ANL),
Matthias Liepe (Cornell),
Joseph Dey (FNAL),
Ioanis Kourbanis (FNAL)

Graduate and Postdoctoral Advisors and Advisees:

L.M. Jones (UIUC), thesis advisor, deceased,
A.D Martin (Durham University, England),
R.N. Sudan (Cornell), deceased

Esmond G. Ng
Lawrence Berkeley National Laboratory, Computational Research Division
One Cyclotron Road, Mail Stop 50F1650, Berkeley, CA 94720-8139
EMail: EGNg@lbl.gov

Education and Training

University of Waterloo	Mathematics	BMath	1978
University of Waterloo	Mathematics	MMath	1979
University of Waterloo	Computer Science	PhD	1983

Awards and Patents

- Natural Sciences and Engineering Research Council of Canada, Postgraduate Scholarships (1978-1982).
- United States Patent #5,815,413, "Integrated Method for Chaotic Time Series Analysis" (with Lee M. Hively), issued Sept. 29, 1998.

Research and Professional Experience

Lawrence Berkeley Nat'l Lab	Appl. Math. & Sci. Comput. Dept. Head	Oct 2011 – present
Lawrence Berkeley Nat'l Lab	Senior Scientist	Jan 1999 – present
Lawrence Berkeley Nat'l Lab	Scientific Computing Group Lead	Jan 1999 – present
Oak Ridge Nat'l Lab	Computational Methods Group Lead	Apr 1994 – Jan 1999
Univ. of Tennessee, Knoxville	Adjunct Professor	Jan 1992 – Jan 1999
Oak Ridge Nat'l Lab	Senior Research Staff	Oct 1985 – Jan 1999
Univ. of Waterloo	Research Assistant Professor	Jan 1983 – Sep 1985

Selected Publications

1. Chao Yang, Weiguo Gao, Zhaojun Bai, Xiaoye S. Li, Lie-Quan Lee, Parry Husbands, Esmond Ng. "An Algebraic Sub-structuring Algorithm for Large-scale Eigenvalue Calculation", SIAM J. Sci. Comput. 27, No. 3 (2005), pp. 873-892.
2. Volkan Akcelik, George Biros, Omar Ghattas, David Keyes, Kwok Ko, and Lie-Quan Lee, and Esmond G. Ng. "Adjoint Methods for Electromagnetic Shape Optimization of the Low-Loss Cavity for the International Linear Collider", Proceedings of SciDAC 2005. J. Physics: Conference Series 16 (2005), pp. 435-445, IOP.
3. Ingyu Lee, Padma Raghavan, Esmond G. Ng. "Effective Preconditioning Through Ordering Interleaved With Incomplete Factorization", SIAM J. Matrix Anal. Appls., Vol. 27, No. 4 (2006), pp. 1069-1088.
4. Patrick R. Amestoy, Xiaoye S. Li, and Esmond G. Ng. "Diagonal Markowitz Scheme With Local Symmetrization", SIAM J. Matrix Anal. Appl., Vol. 29, Issue 1 (2006), pp. 228-244.
5. Philip Sternberg, Esmond Ng, Chao Yang, Pieter Maris, James Vary, Masha Sosonkina, and Hung Viet Le. "Accelerating Full Configuration Interaction Calculations for Nuclear Structure", SC '08 Proceedings (2008).
6. Haim Avron, Esmond Ng, and Sivan Toledo. "Using Perturbed QR Factorizations to Solve Linear Least-Squares Problems", SIAM J. Matrix Anal. Appls., Vol. 31 (2009), pp. 674-693.
7. P. Maris, M. Sosonkina, J. Vary, E.G. Ng, and C. Yang. "Scaling of ab-initio nuclear physics calculations on multicore computer architectures", Procedia Computer Science, Vol. 1 (2010), pp. 97-106.
8. J.P. Vary, H. Honkanen, Jun Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de Teramond, P. Sternberg, E.G. Ng, and C. Yang. "Hamiltonian light-front field theory in a basis function approach", Phys. Rev. C, Vol. 81, 035205 (2010). (arXiv:0905.1411v1)

9. I. Yamazaki, X.S. Li, and E.G. Ng. "Preconditioning Schur complement systems of highly-indefinite linear systems for a parallel hybrid solver", Numer. Math. Theor. Meth. Appl., Vol. 3 (2010), pp. 352-366.
10. S.L. Cornford, D.F. Martin, D.T. Graves, D.F. Ranken, A.M. LeBrocq, R.M. Gladstone, A.J. Payne, E.G. Ng, and W.H. Lipscomb, "Adaptive Mesh, finite-volume modeling of marine ice sheets", J. Comput. Phys. (2011). Submitted.

Synergistic Activities

Editorial Boards: SIAM Journal on Matrix Analysis and Applications (1997-2008); SIAM Journal on Scientific Computing (2009-present); IEEE Transaction on Parallel and Distributed Systems (2001-2004); Bulletin of Computational Applied Mathematics (2011-present)

SIAM Committee Work: Vice Chair, SIAM Activity Group on Supercomputing (2006-2008); Member, SIAM Program Committee (2009-present)

Co-chair, International Conferences on Preconditioning Techniques for Large Sparse Matrices for Scientific and Industrial Applications (2001, 2003, 2005, 2007, 2009, 2011)

Recent conference chairs/co-chairs: 2010 DOE Applied Mathematics Program Meeting; 2011 Householder Symposium XVIII; 2011 Euro-Par (High Performance and Scientific Applications Track)

Review Panel - Joint Doctoral Program in Computational Science, San Diego State Univ/Clairmont Graduate Univ (2011)

Collaborators (last 48 months) and Co-Editors (last 24 months)

U Adiga (Okonisys), FJ Asturias (Scripps), H Avron (Tel-Aviv U), Z Bai (UC Davis), SJ Brodsky (SLAC), JR Cary (U Colorado Boulder), DH Chen (Baylor College of Medicine), W Chiu (Baylor College of Medicine), SL Cornford (Bristol), M Cosnard (INRIA), GF de Teramond (U Costa Rica), J Frank (Columbia), RM Glaeser (UC Berkeley), L Grigori (INRIA), M Haranczyk (LBNL), A Harindranath (Saha Inst. of Nuclear Physics), H Honkanen (Iowa State U), W Jiang (Purdue U), K Ko (SLAC), HV Le (Ames Lab), LQ Lee (SLAC), I Lee (Troy U), D Leith (Wadsworth Center), J Li (Iowa State U), XS Li (LBNL), WH Lipscomb, DF Martin (LBNL), P Maris (Iowa State U), LC McInnes (ANL), WB Mori (UCLA), C Ng (SLAC), PA Penczek (U Texas), A Pinar (SNL), T Puzyn (U Gdanski), R Ryne (LBNL), M Sosonkina (Ames Lab), P Spentzouris (FNAL), P Sternberg (ILOG), S Toledo (Tel-Aviv U), JP Vary (Iowa State U), C Yang (LBNL)

Graduate and Postdoctoral Advisors and Advisees:

HM Aktulga (LBNL), C Calderon (Numerica Corp), JA George (U. Waterloo, thesis advisor), P Sternberg (ILOG), I Yamazaki (U. Tennessee)

Boyana Norris
Computer Scientist, Argonne National Laboratory
http://www.mcs.anl.gov/~norris, norris@mcs.anl.gov

Research Interests

High-performance and high-productivity scientific computing, source analysis and transformation systems, domain-specific languages and environments, automatic differentiation, performance analysis and tuning.

Education and Training

- Wake Forest University, B.S. *summa cum laude* in Computer Science, May 1995
- University of Illinois at Urbana-Champaign, Ph.D. in Computer Science, January 2000
- Postdoctoral Fellow, Argonne National Laboratory, Mathematics and Computer Science Division, Nov. 1999 – Sept. 2001

Research and Professional Experience

- Computer Scientist, Argonne National Laboratory, Mathematics and Computer Science Division, since Mar. 2006
- Assistant Computer Scientist, Argonne National Laboratory, Mathematics and Computer Science Division, Oct. 2001 – Mar. 2006
- Senior Fellow, Computation Institute, University of Chicago and Argonne National Laboratory, since Apr. 2004

Selected Publications

1. S. H. K. Narayanan, B. Norris, and P. D. Hovland. Generating performance bounds from source code. *Proceedings of the First International Workshop on Parallel Software Tools and Tool Infrastructures (PSTI 2010)*, 9 2010.
2. B. Norris, A. Hartono, E. Jessup, and J. Siek. Generating empirically optimized composed matrix kernels from Matlab prototypes. *Proceedings of the International Conference on Computational Science 2009*, 2009.
3. A. Hartono, B. Norris, and P. Sadayappan. Annotation-based empirical performance tuning using Orio. *Proceedings of the 23rd IEEE International Parallel & Distributed Processing Symposium*, 2009.
4. K. A. Huck, O. Hernandez, V. Bui, S. Chandrasekaran, B. Chapman, A. D. Malony, L. C. McInnes, and B. Norris. Capturing performance knowledge for automated analysis. *International Conference for High Performance Computing, Networking, Storage and Analysis (SC'08)*, 2008.
5. W. Elwasif, B. Norris, B. Allan, and R. Armstrong. Bocca: A development environment for HPC components. in *Proceedings of HPC-GECO/CompFrame'07, October 21-22, 2007, Montreal, Québec, Canada*. ACM, 2007.

6. D. R. Dechow, B. Norris, and J. Amundson. The Common Component Architecture for particle accelerator simulations. in *Proceedings of HPC-GECO/CompFrame'07, October 21-22, 2007, Montreal, Québec, Canada.* ACM, 2007.

7. E. T. Ong, J. Walter Larson, B. Norris, R. L. Jacob, M. Tobis, and M. Steder. A multilingual programming model for coupled systems. *International Journal for Multiscale Computational Engineering* 6:39–51, 2008.

8. B. Norris, A. Hartono, and W. Gropp. Annotations for Productivity and Performance Portability. in *Petascale computing: Algorithms and applications.* Chapman & Hall / CRC Press, Taylor and Francis Group, Computational Science, 2007.

9. B. Norris. Software architecture issues in scientific component development. *Applied Parallel Computing: 7th International Conference, PARA 2004, Lyngby, Denmark, June 20-23, 2004. Revised Selected Papers*, vol. 3732, pp. 629–636. Springer Berlin / Heidelberg, Lecture Notes in Computer Science, 2006.

Selected Synergistic Activities

- Designer and co-developer of multiple tools for improving application developer productivity (ADIC, Bocca, CCA infrastructure) and for understanding and improving performance of scientific applications (Pbound, PerfExp, Orio).
- SIAM Activity Group on Supercomputing, Secretary (2006–2008), Vice-chair (2010–2012).

Collaborators and Co-editors within the Past 48 Months
B. Allan, Sandia National Laboratories (SNL); R. Armstrong, SNL; J. Amundson, Fermilab; D. Bailey, LBL; D. Bernholdt, Oak Ridge National Laboratory (ORNL); S. Bhowmick, University of Nebraska at Omaha; J. Cary, Tech-X Corp and University of Colorado at Boulder; J. Chame, University of Southern California (USC); B. Chapman, University of Houston; T. Dahlgren, Lawrence Livermore National Laboratory (LLNL); J. Demmel, University of California at Berkeley; J. Dongarra, University of Tennessee; W. Elwasif, Oak Ridge National Laboratory (ORNL); T. Epperly, LLNL; R. Fowler, University of North Carolina (UNC); S. Gray, ANL; W. Gropp, University of Illinois at Urbana-Champaign (UIUC); D. Gunter, LBL; M. Hall, University of Utah; P. Hargrove, LBL; A. Hartono, Intel; J. Hollingsworth, University of Maryland; P. Hovland, ANL; E. Jessup, University of Colorado at Boulder (UCB); J. Larson, ANL; R. Lucas, (USC); A. Malony, University of Oregon; J. Mellor-Crummey, Rice University; P. Messmer, Tech-X Corporation; S. Moore, University of Tennessee; A. Morris, University of Oregon; L. McInnes, ANL; S. Peckham, UCB; A. Pothen, Old Dominion University; D. Quinlan, LLNL; P. Ricker, UIUC; P. Sadayappan, Ohio State University; J. Shalf, LBL; S. Shende, University of Oregon; J. Siek, UCB; J. Shin, HP; B. Smith, ANL; A. Snavely, San Diego Supercomputing Center; E. Strohmaier, LBL; M. M. Strout, Colorado State University; B. de Supinski, LLNL; J. Utke, University of Chicago; B. Van Straalen, LBL; S. Williams, LBL; P. Worley, ORNL; K. Yellick, LBL.
Doctoral Advisor: Michael T. Heath, University of Illinois at Urbana-Champaign (UIUC)
Postdoctoral Advisor: William Gropp, Argonne National Laboratory (currently at UIUC)
Post-graduate Advisees: Li Li (N/A), Sri Hari Krishna Narayanan (ANL), Qian Zhu (ANL)

Kevin Paul
Tech-X Corporation, Boulder, CO
kpaultxcorp.com – 720-974-1854

Education and Training

University of Illinois at Urbana-Champaign	Theoretical High-Energy Particle Physics	Ph.D., 2002
Illinois State University	Physics	B.S., 1996

Research and Professional Experience

- *August 2006–present: Research Scientist, Tech-X Corporation.* Since joining Tech-X, Kevin Paul has been involved in the development of modern beam tracking codes and Tech-X Corporation's electromagnetic PIC code, VORPAL. Most recently, he leads the Tech-X Corporation awarded SBIR Phase II to study inverse cyclotrons for their use in producing intense muon beams with the PIC code VORPAL.

- *August 2004–August 2006: Research Assistant, Muons, Inc., Batavia, IL.* Kevin Paul continued work on muon beam physics and accelerator physics as part of the Neutrino Factory and Muon Collider Collaboration (now, MAP), focusing on RF phase-energy rotation of pion beams and the muon helical cooling channel.

- *August 2002–August 2004: Research Assistant, University of Illinois at Urbana-Champaign, Urbana, IL.* Kevin Paul worked on muon beam physics and accelerator physics as part of the Neutrino Factory and Muon Collider Collaboration, studying pion production and capture.

Selected publications

[1] K. Paul, E. Cormier-Michel, T. L. Hart, and D. J. Summers, "VORPAL Simulations of Muon Cooling with an Inverse Cyclotron," Proceedings for the 2011 International Particle Accelerator Conference (San Sebastian, Spain) (2011).

[2] K. Paul, E. Cormier-Michel, T. Hart, and D. Summers, "Recent Developments in Simulations of an Inverse Cyclotron for Intense Muon Beams," Proceedings for the 2010 Advanced Accelerator Concepts Workshop (Annapolis, MD) (2010).

[3] J. S. Berg et al. (ISS Accelerator Working Group), "Accelerator design concept for future neutrino facilities," JINST **4**, P07001 (2009), `0802.4023`.

[4] K. Paul, C. Huang, D. L. Bruhwiler, W. B. Mori, F. S. Tsung, E. Cormier-Michel, C. G. R. Geddes, B. Cowan, J. R. Cary, E. Esarey, et al., "Benchmarking the codes vorpal, osiris, and quickpic with laser wakefield acceleration simulations," ADVANCED ACCELERATOR CONCEPTS: Proceedings of the Thirteenth Advanced Accelerator Concepts Workshop **1086**, 315 (2009), URL `http://link.aip.org/link/?APC/1086/315/1`.

[5] K. Paul, D. A. Dimitrov, R. Busby, D. L. Bruhwiler, D. Smithe, J. R. Cary, J. Kewisch, D. Kayran, R. Calaga, and I. Ben-Zvi, "Half-cell rf gun simulations with the electromagnetic particle-in-cell code vorpal," ADVANCED ACCELERATOR CONCEPTS: Proceedings of the Thirteenth Advanced Accelerator Concepts Workshop **1086**, 334 (2009), URL `http://link.aip.org/link/?APC/1086/334/1`.

[6] J. R. Cary et al., "COMPASS, the COMmunity Petascale Project for Accelerator Science and Simulation, a broad computational accelerator physics initiative," J. Phys. Conf. Ser. **78**, 012009 (2007).

[7] R. P. Johnson et al., "A six-dimensional muon beam cooling experiment," (2006), prepared for European Particle Accelerator Conference (EPAC 06), Edinburgh, Scotland, 26-30 Jun 2006.

[8] R. P. Johnson, M. Alsharo'a, C. Ankenbrandt, E. Barzi, K. Beard, S. A. Bogacz, Y. Derbenev, L. D. Frate, I. Gonin, P. M. Hanlet, et al., "Recent innovations in muon beam cooling," BEAM COOLING AND RELATED TOPICS: International Workshop on Beam Cooling and Related Topics - COOL05 **821**, 405 (2006), URL `http://link.aip.org/link/?APC/821/405/1`.

[9] K. Paul, R. P. Johnson, T. J. Roberts, D. Neuffer, and Y. Derbenev, "Using high-pressure gas in the front end of a muon source," Nucl. Phys. Proc. Suppl. **155**, 273 (2006).

[10] K. Paul, R. Johnson, and V. Yarba (Neutrino Factory and Muon Collider), "Summary of the low-emittance muon collider workshop (6-10 February 2006)," (2006), presented at Fermilab User's Meeting, Batavia, Illinois, 31 May-1 June 2006.

Collaborators and co-editors

Georg Bollen (MSU/FRIB), Eric Esarey (LBNL), Cameron Geddes (LBNL), Terrence Hart (U. Mississippi), Harold Kirk (BNL), Dave Morrisey (MSU/FRIB), Robert Palmer (BNL), Stefan Schwarz (MSU/FRIB), Donald Summers (U. Mississippi), Jean-Luc Vay (LBNL)

Graduate and postdoctoral advisors and advisees

Graduate Advisor: Scott Willenbrock, University of Illinois at Urbana-Champaign
Postdoctoral Advisor: Deborah Errede, University of Illinois at Urbana-Champaign
Post-graduate Advisees: none

Ernesto Esteves Prudencio
Institute for Computational Engineering and Sciences (ICES)
The University of Texas at Austin
prudenci@ices.utexas.edu

Research Interests

Statistically robust, scalable, load-balanced and fault-tolerant parallel stochastic algorithms for the quantification of uncertainty present in experimental data, in models and in their predictions.

Education and Training

- ITA, Brazil, B.Sc. in Electronics Engineering, December 1990.
- UNICAMP, Brazil, M.Sc. in Applied Mathematics, January 2001.
- CU Boulder, CO, Ph.D. in Computer Science (Numerical Analysis), February 2005.

Research and Professional Experience

- Research Associate, University of Texas at Austin, TX, 2008-present.
- Research Software Developer, Stanford Linear Accelerator Center, CA, 2005-2008.
- Software Engineer, Integris Brazil (Bull Technologies), 1998-1999.
- Solution Architect, Software and Hardware Developer, IBM Brazil, 1990-1998.

Selected Publications

1. K. Miki, S. H. Cheung, E. Prudencio, and P. Varghese, *Bayesian Uncertainty Quantification of Recent Shock Tube Determinations of the Rate Coefficient of Reaction H+O2→OH+O*, 2011, submitted.
2. E. Prudencio and K. Schulz, *The Parallel C++ Statistical Library 'QUESO': Quantification of Uncertainty for Estimation, Simulation and Optimization*, Proceedings of the Workshops of the Euro-Par 2011 Conference, Pasqua D'Ambra *et al.*, eds., Lecture Notes in Computer Science, Springer, 2011, to appear.
3. E. Prudencio and S. H. Cheung, *Parallel Adaptive Multilevel Sampling Algorithms for the Bayesian Analysis of Mathematical Models*, International Journal for Uncertainty Quantification, 2011, to appear.
4. S. H. Cheung, T. A. Oliver, E. Prudencio, S. Prudhomme and R. D. Moser, *Bayesian Uncertainty Analysis with Applications to Turbulence Modeling*, Reliability Engineering and System Safety Journal, 96 (9), pp. 1137–1149, 2011.
5. E. Prudencio, A. Candel, L. Ge, A. Kabel, K. Ko, L. Lee, Z. Li, C. Ng and G. Schussman, *Parallel 3D finite element numerical modeling of DC electron guns*, SLAC-PUB-13097 (2008).
6. E. Prudencio and X.-C. Cai, *Parallel multilevel restricted Schwarz preconditioners with pollution removing for PDE-constrained optimization*, SIAM J. Sci. Comp., 29 (2007), pp. 964–985.

7. E. Prudencio, R. Byrd, and X.-C. Cai, *Parallel full space SQP Lagrange-Newton-Krylov-Schwarz algorithms for PDE-constrained optimization problems*, SIAM J. Sci. Comp., 27 (2006), pp. 1305–1328.

8. K. Ko, N. Folwell, L. Ge, A. Guetz, L. Lee, Z. Li, C. Ng, E. Prudencio, G. Schussman, R. Uplenchwar, and L. Xiao, *Advances in electromagnetic modeling through high performance computing*, Physica C, 441 (2006), pp. 258–262.

9. E. Prudencio and X.-C. Cai, *Robust multilevel restricted Schwarz preconditioners and applications*, in Domain Decomposition Methods in Science and Engineering XVI, O. B. Widlund and D. E. Keyes, eds., vol. 55 of Lecture Notes in Computational Science and Engineering, Springer-Verlag, 2006, pp. 155–162.

10. C. Ng, V. Akcelik, A. Candel, S. Chen, N. Folwell, L. Ge, A. Guetz, H. Jiang, A. Kabel, L. Lee, Z. Li, E. Prudencio, G. Schussman, R. Uplenchwar, L. Xiao and K. Ko, *State of the art in EM field computation*, in Proceedings of EPAC 2006.

Selected Synergistic Activities

- Co-PI at recently granted "Quantification of Uncertainty in Extreme Scale Computations (QUEST)" US DOE SciDAC Institute (SNL Lead), Sep. 2011 - Aug. 2016.
- Co-organizer of seven UQ related mini-symposia: one at the 14th SIAM Conference on Parallel Processing for Scientific Computing in Seattle (February 2010), one at the 6th SIAM Conference on Computational Science and Engineering in Reno (February 2011), one at the 11th US National Congress in Computational Mechanics in Minneapolis (July 2011), two at the 1st SIAM Conference on Uncertainty Quantification in Raleigh (April 2012), and two at the 10th World Congress in Computational Mechanics in Sao Paulo, Brazil (July 2012).
- Main designer and one of the main developers of the research statistical MPI/C++ library QUESO (Quantification of Uncertainty for Estimation, Simulation and Optimization), at the PECOS Center at UT Austin, under the PSAAP Program of US DOE NNSA.
- Presentations at conferences and mini-symposia around the world; review of papers for Journals; member of SIAM, SIAG, IEEE Computer Society, EMI and SSA.

Collaborators and Co-editors within the Past 48 Months

- John Aidun (Sandia NM), Mihai Anitescu (ANL), Ivo Babuska (UT), Xiao Chuan Cai (CU Boulder), Thomas Carraro (Heidelberg U.) Sai Hung Cheung (NTU), Michael Eldred (Sandia NM), David Fuentes (UT/MD Anderson), Omar Ghattas (UT), David Goldstein (UT), Richard Lehouq (Sandia NM), Fabio Nobile (EPFL), Martin Mai (KAUST), Tess Moon (UT), Robert Moser (UT), John Tinsley Oden (UT), Todd Oliver (UT), Michael L. Parks (Sandia NM), Serge Prudhomme (UT), Karl Schulz (UT), James Stewart (Sandia NM), Laura Swiler Painton (Sandia NM), Raul Tempone (KAUST), Phillippe Varghese (UT).
- **Doctoral Advisor (no Postdoctoral Advisor):** Xiao-Chuan Cai, CU Boulder
- **Post-graduate Advisees (partial responsibility):** Sai Hung Cheung (UT), Kenji Miki (UT), Todd Oliver (UT), Gabriel Terejanu (UT)

Ji Qiang
Staff Scientist, Lawrence Berkeley National Laboratory
jqiang@lbl.gov

Research Interests

Large-scale particle simulations, physics of beams, numerical methods, high performance computing for scientific applications.

Education and Training

- University of Electronic Science and Technology (China), B.S., 1991
- University of Illinois at Urbana-Champaign, M.S., 1995
- University of Illinois at Urbana-Champaign, Ph.D., 1997

Research and Professional Experience

- Staff Scientist, Lawrence Berkeley National Laboratory, Accelerator and Fusion Research Division, 2002 – present
- Term staff member, Los Alamos National Laboratory, LANSCE, 2000 – 2002
- Postdoctoral Fellow, Los Alamos National Laboratory, LANSCE, 1998 – 2000

honors and awards

- Outstanding Performance Award, Lawrence Berkeley National Laboratory, University of California, 2003.
- Interdisciplinary fellowship, University of Illinois at Urbana-Champaign, 1995.

Selected Publications

1. J. Qiang, X. Li, Particle-field decomposition and domain decomposition in parallel particle-in-cell beam dynamics simulation, *Computer Physics Communications* 181, 2024 (2010)
2. J. Qiang. Particle-In-Cell/Monte Carlo Simulation of Ion Back Bombardment in a High Average Current RF Photo-Gun, *Nuclear Instruments & Methods in Physics Research A* 614, 1 (2010)
3. J. Qiang, R. D. Ryne, M. Venturini, A. A. Zholents, I. V. Pogorelov, High resolution simulation of beam dynamics in electron linacs for x-ray free electron lasers, *Phys. Rev. ST Accel. Beams* 12, 100702 (2009)
4. J. Qiang, D. Todd, D. Leitner, A 3D model for ion beam formation and transport simulation, *Computer Physics Communications* 175, 416 (2006)
5. J. Qiang, M. Furman, R. Ryne, A Parallel Particle-In-Cell Model for Beam-Beam Interactions in High Energy Ring Colliders, *J. Comp. Phys.* 198, 278 (2004)

Selected Synergistic Activities

- Primary developer of the IMPACT code suite, a parallel particle-in-cell code for simulating high intensity, high brightness beams in linear and circular accelerators.
- Primary developer of the BeamBeam3D code, a parallel paraticle-in-cell code for studying colliding beams in high energy colliders.

Collaborators within the Past 48 Months
Robert Ryne (LBNL), Marco Venturini (LBNL), John Corlett (LBNL), John Byrd (LBNL), Jun Feng (LBNL), Gang Huang (LBNL), Hongzhang Shan (LBNL), Z. Huang (SLAC), T. Ohkawa (J-PARC), Stefan Paret (LBNL), Xiaoye Li (LBNL), Alexander Zholents (ANL), Miguel Furman (LBNL), Juhao Wu (SLAC), Ilya Pogorelov (Tech-X).
Doctoral Advisor: Prof. Clifford Singer, UIUC.
Postdoctoral Advisor: Robert Ryne, Lawrence Berkeley National Laboratory

Greg L. Schussman
SLAC National Accelerator Laboratory
Advanced Computations Department
2575 Sand Hill Road, Mail Stop 33
Menlo Park, CA 94025
email: schussman@slac.stanford.edu

Education and Training

University of California, Davis	Computer Science and Engineering	B.S.	1998
University of California, Davis	Electrical Engineering	B.S.	1998
University of California, Davis	Computer Science	Ph.D.	2003

Research and Professional Experience

SLAC National Accelerator Laboratory	Scientific Visualization R&D	2003 – present
Lawrence Livermore National Laboratory	Scientific Visualization R&D	1996, 1997
University of California, Davis	Computer Graphics Research	1996 – 2003

Dr. Greg Schussman's research interests include scientific visualization, especially of large time varying vector data and of time varying line-based datasets, computer graphics empasizing high quality rendering and GPU computation, computational geometry aimed at computer graphics, and high performance computing. He has expertise in the areas of large scale visualization, stereoscopic animations, line-based rendering techniques, and software development centered around optimization, testing, and algorithm design. He has regularly contributed high resolution and stereo animations of the Advanced Computations Department's results to the SLAC display at the annual Supercomputing conferences. His visualization identified, for the first time, mode rotation in an accelerator cavity. He created a custom wakefield animation shown to U.S. Secretary of Energy, Spencer Abraham during a SLAC visit. Dr. Schussman was awarded the SciDAC OASCR for Outstanding Achievement in Scienti c Visualization at the 2010 SciDAC Conference in Chattanooga, Tennessee.

Selected Publications

1. G.L. Schussman, "Visualizing Electromagnetic Field and Particle Simulations in Accelerators with ParaView", Proceedings of 2009 Ultrascale Visualization Workshop,IEEE Supercomputing, (2009).
2. A.E. Candel, A.C. Kabel, K. Ko, L. Lee, Z. Li, C.-K. Ng, G.L. Schussman, I. Ben-Zvi, J. Kewisch, "Parallel 3D Finite Element Particle-in-Cell Simulations with Pic3P", Particle Accelerator Conference, (2009).
3. K.-L. Ma, G.L. Schussman, B. Wilson, "Visualization for Computational Accelerator Physics", In The Visualization Handbook, (C. Johnson and C. Hansen, eds.), (2005).
4. G. Schussman, K-L. Ma, "Anisotropic Volume Rendering for Extremely Dense, Thin Line Data", Proceedings of IEEE Visualization (2004).
5. N.L. Max, G.L. Schussman, R. Miyazaki, K. Iwasaki, T. Nishita, "Diffusion and Multiple Anisotropic Scattering for Global Illumination in Clouds", Proceedings of WSCG (2004).
6. G.L. Schussman, "Interactive and Perceptually Enhanced Visualization of Large, Complex Line-Based Datasets", Ph.D. thesis, University of California, Davis, (2003).
7. G.L. Schussman, K.-L. Ma, "Scalable Self-Orienting Surfaces: A Compact, Texture-Enhanced Representation for Interactive Visualization of 3D Vector Fields", Proceedings of Pacific Graphics (2002).

8. V. Ivanov, G.L. Schussman, M. Weiner, “Particle Tracking Algorithms for 3D Parallel Codes in Frequency and Time Domains”, Proceedings Applied Computational Electromagnetics (ACES) (2002).
9. K.-L. Ma, G.L. Schussman, B. Wilson, K. Ko, J. Qiang, R.D. Ryne, “Advanced Visualization Technology for Terascale Particle Accelerator Simulations”, Proceedings of Supercomputing (2002).
10. G.L. Schussman, N.L. Max, “Hierarchical Perspective Volume Rendering using Triangle Fans”, Proceedings of the International Workshop on Volume Graphics in Volume Graphics, Springer-Verlag, (2001).

Collaborators (last 48 months)

I. Ben-Zvi (Brookhaven National Laboratory),
J. Kewisch (Brookhaven National Laboratory),
I. Syratchev (CERN)

Graduate and Postdoctoral Advisors and Advisees:

K.-L. Ma (U.C. Davis), thesis advisor,
B. Hammann (U.C. Davis)

Brian T. Schwartz
Research Scientist, Tech-X Corporation
btschwartz@txcorp.com

Research Interests

Computational electromagnetics, photonics, plasma physics, and accelerator physics.

Education and Training

- Swarthmore College, B.A. with Honors in Physics, 1997
- University of Colorado at Boulder, Ph.D. in Electrical & Computer Engineering, 2005

Research and Professional Experience

- Research Scientist, Tech-X Corporation, since Oct. 2009
- Research Associate, University of Colorado at Boulder, 2009
- Senior Optoelectronic Engineer, OmniVision-CDM Optics, 2006 – 2009
- Research Assistant, University of Colorado at Boulder, 1999 – 2005
- Manufacturing Engineer, New Focus, Inc., 1997 – 1999

Selected Publications

1. B.T. Schwartz, D.L. Bruhwiler , V. Litvinenko, *et al.* Simulations of a Single-Pass Through a Coherent Electron Cooler for 40 Gev/n Au^{+79}. *Proceedings of the Particle Accelerator Conference*, 2011.
2. B.T. Schwartz, D.L. Bruhwiler , V. Litvinenko, et al. Massively Parallel Simulation of Anisotropic Debye Shielding in the Modulator of a Coherent Electron Cooling System and subsequent Amplification in a Free Electron Laser. *J. Physics*: Conf. Series, SciDAC 2010.
3. Z. Li, M. Mohammed, X. Chen, E. Dudley, K. Meng, L. Shang, A. Mickelson, R. Joseph, M. Vachharajani, B. Schwartz, and Y. Sun. Reliability Modeling and Management of Nanophotonic On-Chip Networks. *IEEE Transactions on Very Large Scale Integration Systems (TVLSI)*, 99, 1, (2011).
4. E.R. Dowski *et al*, Arrayed Imaging Systems and Associated Methods, World Intellectual Property Organization, Pub. No. WO/2008/020899 (2008).
5. Z. A. Sechrist,, B. T. Schwartz, J. H. Lee, J. A. McCormick, R. Piestun, W. Park, and S. M. George, Modification of Opal Photonic Crystals Using Al_2O_3 Atomic Layer Deposition, *Chemistry of Materials* **18** (15), 3562-3570 (2006).
6. B. T. Schwartz and R. Piestun. Dynamic properties of photonic crystals and their effective refractive index. *J. Opt. Soc. Am.* B **22**, 2018-2026 (2005).

7. B. T. Schwartz and R. Piestun. Waveguiding in air by total external reflection from ultralow index metamaterials. *Appl Phys Lett,* **85**, 1 (2004).

8. B. T. Schwartz and R. Piestun. Total external reflection from metamaterials with ultralow refractive index. *J. Opt. Soc. Am.* B **20**, 2448-2453 (2003).

Selected Synergistic Activities

None

Collaborators and Co-editors within the Past 48 Months

R.L. Byer, Stanford University; X. Chen, University of Colorado at Boulder (CU); E.R. Colby, SLAC; Dudley, E, CU; R.J. England, SLAC; Y. Hao, Brookhaven National Laboratory (BNL); Li, Z, CU; V.N. Litvinenko, BNL; C. McGuinness, Stanford University; Mickelson, A. R., CU; Mohamed, M, CU; R.J. Noble, SLAC; S. Reiche, Paul Scherrer Institut; Shang, L, CU; J.E. Spencer, SLAC; Vachharajani, M., CU; G. Wang, BNL.

Doctoral Advisor: Rafael Piestun, University of Colorado at Boulder

Peter O. Schwartz
Mail Stop 50A-1148 Lawrence Berkeley National Laboratory Berkeley, CA 94720
poschwartz@lbl.gov

As a member of the Chombo development team, Schwartz has developed high-resolution and adaptive numerical algorithms for partial differential equations and numerical simulation capabilities for several applications in science and engineering. In particular, he has developed a simulation tool for reaction-diffusion systems in molecular biology, software infrastructure for computational geometry, and the core hydrodynamic modeling capability in REALM (River,Land, and Estuary Model), the modeling tool of the Delta Modeling Section of the California Department of Water Resources.

Education and Training

University of California, Berkeley, B.S. in Mathematics, 1987.

The Ohio State University, Ph.D. in Mathematics, 1994.

Research and Professional Experience

Research Scientist, Applied Numerical Algorithms Group, Lawrence Berkeley National Laboratory, 2008-present.

Computer Science Engineer, Applied Numerical Algorithms Group, Lawrence Berkeley National Laboratory, 2004-2008.

Post-Doctoral Fellow, Applied Numerical Algorithms Group, Lawrence Berkeley National Laboratory, 2001-2004.

Research Interests

Discretization methods for conservation laws: adaptive mesh refinement on structured grids, volume-of-fluid methods for complex geometries and moving fronts. Analysis-based splittings of stiff PDE, computational geometry, and optimization.

Selected Relevent Publications

- E. Ateljevich, P. Colella, D.T. Graves, T.J. Ligocki, J. Percelay, P.O. Schwartz, Q. Shu "CFD Modeling in the San Francisco Bay and Delta" 2009 Proceedings of the Fourth SIAM Conference on Mathematics for Industry (MI09), pp. 99-107 (2010).
- Schwartz, P., and Colella P., "A Second-Order Accurate Method for Solving the Signed Distance Function Equation", Communications in Applied Mathematics and Computational Science, Vol. 5 (2010), No. 1, 81-97.
- T.J. Ligocki, P.O. Schwartz, J. Percelay, P. Colella, "Embedded boundary grid generation using the divergence theorem, implicit functions, and constructive solid geometry", 2008 J. Phys.: Conf. Ser. 125 012080.
- P.O. Schwartz, M. Barad, P. Colella, T.J. Ligocki,"A Cartesian Grid Embedded Boundary Method for the Heat Equation and Poisson's Equation in Three Dimensions", Journal of Computational Physics, Volume 211, Issue 2, Pages 385-786 (2006)
- Schwartz, P., Adalsteinsson, D., Colella, P., Arkin, A.P., Onsum, M., "Numerical computation of diffusion on a surface", Proc. Nat. Acad. Sci., Vol. 102 (2005), pp. 11151-11156.
- D. Trebotich, G. H. Miller, P. Colella, D. T. Graves, D. F. Martin and P. O. Schwartz, A Tightly Coupled Particle-Fluid Model for DNA-Laden Flows in Complex Microscale Geometries, Computational Fluid and Solid Mechanics 2005, 1018-1022. Also available as Lawrence Livermore National Laboratory technical report UCRL-CONF-208132.
- D. Trebotich, T. Deschamps and P. Schwartz, Air-Flow Simulation in Realistic Models of the Trachea, Technical Proceedings of the 26th Annual International Conference IEEE Engineering in Medicine and Biology Society, pp. 3933-3936, San Francisco, Sept 2004. Also available as Lawrence Livermore National Laboratory technical report UCRL-CONF-208522.
- T. Deschamps, P. Schwartz, D. Trebotich, P. Colella, D. Saloner and R. Malladi, Vessel Segmentation and Blood Flow Simulation Using Level-Sets and Embedded Boundary Methods, Technical Proceedings of the 18th Conference and Exhibition for Computer Assisted Radiology and Surgery, Chicago, June 2004. Also available as Lawrence Livermore National Laboratory technical report UCRL-CONF-208523.
- J. Rosenthal, P. Schwartz, "Gambling systems and multiplication invariant measures" *Advances in Applied Mathematics*, vol. 22, pp.303-311 (1999).
- G.O. Roberts, J. Rosenthal, P. Schwartz, "Convergence Properties of Perturbed Markov Chains, "*Journal of Applied Probability*, vol. 35, pp. 1-11 (1998).
- M. Akcoglu, R. Jones, P. Schwartz, "Variation in Probability, Ergodic Theory, and Analysis,"*Illinois Journal of Mathematics*, vol. 42:1 (1998).
- P. Schwartz, "A Cocycle Theorem with an Application to Rosenthal Sets, "*Proceedings of the American Mathematical Society* vol. 124:12, pp. 3689-3698 (1996).

Collaborators

M. Akcoglu (University of Toronto), E. Ateljevich (CA Dept. of Water Resources), P.Colella (LBL), R. Jones (Depaul University), T.J. Ligocki (LBL), G. Miller (UC Davis), J. Percelay (UC Berkeley),J.,Rosenthal (Unitversity of Toronto),G. Roberts (Oxford),D. Trebotitch (LLNL), Q. Shu (CA Dept. of Water Resources).

Panagiotis Spentzouris

Dr. Panagiotis Spentzouris of the Fermi National Accelerator Laboratory (Fermilab) is the head of the Accelerator and Detector Simulation Department of the laboratory's Computing Division and the lead Principal Investigator of the SciDAC2 Community Project for Accelerator Science and Simulation. After four years at Columbia University, Dr. Spentzouris went to Fermilab, where his main research focus has been computational physics, with emphasis on beam dynamics, and neutrino physics. He is the co-architect of Synergia, a parallel PIC beam dynamics framework which utilizes state-of-the-art numerical libraries, solvers, and physics models. He leads his research team in applying Synergia to many accelerator science problems.

Education

- Ph.D., Physics, Northwestern University, USA, 1994
- Physics Diploma, University of Athens, Greece, 1987

Professional Experience

- 2007 - present Scientist II, Fermi National Accelerator Laboratory
- 2003 - 2007 Scientist, Fermi National Accelerator Laboratory
- 1998 - 2003 Associate Scientist, Fermi National Accelerator Laboratory
- 1997 - 1998 Associate Research Scientist, Columbia University
- 1994 - 1997, Postdoctoral Research Associate, Columbia University

Selected Recent Publications and Presentations

1. A. Macridin, P. Spentzouris, J. Amundson, L. Spentzouris and D. McCarron, "Coupling impedance and wake functions for laminated structures with an application to the Fermilab Booster," Phys. Rev. ST Accel. Beams **14**, 061003 (2011).
2. E. Stern, J. Amundson, P. Spentzouris, J. Qiang and R. Ryne, "Simulations of space charge in the Fermilab Main Injector," FERMILAB-CONF-11-087-CD.
3. E. G. Stern, J. F. Amundson, P. G. Spentzouris and A. A. Valishev, "Fully 3D Multiple Beam Dynamics Processes Simulation for the Tevatron," Phys. Rev. ST Accel. Beams **13**, 024401 (2010)
4. J. F. Amundson, A. Macridin, P. Spentzouris and E. G. Stern, "Advanced computations of multi-physics, multi-scale effects in beam dynamics," J. Phys. Conf. Ser. **180**, 012002 (2009).
5. P. Spentzouris, J. Cary, L. C. McInnes, W. Mori, C. Ng, E. Ng and R. Ryne, "Community petascale project for accelerator science and simulation: Advancing computational science for future accelerators and accelerator technologies," J. Phys. Conf. Ser. **125**, 012005 (2008).
6. J. Amundson, W. Pellico, P. Spentzouris, T. Sullivan, Linda Spentzouris, "An Experimentally Robust Technique For Halo Measurement Using The IPM At The Fermilab Booster," Nucl. Instrum. Meth. **A570**, 1 (2007)
7. P. Spentzouris, "Accelerator modeling under SciDAC: meeting the challenges of next-generation accelerator design, analysis, and optimization", Presented at the 9th International Computational Accelerator Physics Conference, ICAP06.
8. Panagiotis Spentzouris, J. Amundson, "Emittance dilution and halo creation during the first milliseconds after injection at the Fermilab Booster." Prepared for 33rd ICFA Advanced Beam Dynamics Workshop: High Intensity High Brightness Hadron Beams (ICFA HB2004). Published in AIP Conf.Proc.773:127-131,2005
9. James F. Amundson, P. Spentzouris, J. Qiang, R. Ryne, "Synergia: an accelerator modeling tool with 3-D space charge," J. Comput. Phys. **211**, 229 (2006)

10. J. Amundson, J. Lackey, P. Spentzouris, G. Jungman, L. Spentzouris, "Calibration of the FNAL booster ionization profile monitor,"Phys. Rev. ST Accel.Beams **6** 102801 (2003)
11. K. Ko, Robert D. Ryne, P. Spentzouris, "Report of the Snowmass T7 Working Group on high performance computing." Prepared for APS / DPF / DPB Summer Study on the Future of Particle Physics (Snowmass 2001). In the Proceedings of APS / DPF / DPB Summer Study on the Future of Particle Physics (Snowmass 2001), Snowmass, Colorado, 30 Jun - 21 Jul 2001, pp T7001.
12. J. Monroe, P. Spentzouris, V. Balbekov, P. Lebrun, G. Penn, C. Kim, E.S. Kim, D.M. Kaplan, "Design and simulation of muon ionization cooling channels for the Fermilab neutrino factory feasibility study," Phys. Rev. ST Accel.Beams **4** 041301 (2001)

Synergistic Activities

Member, Scientific Program Committee, Advanced Accelerator Concept Workshop 2010
Member, Scientific Program Committee, SciDAC conference, 2008, 2010
Member, Scientific Program Committee, Particle Accelerator Conference 2007, 2009
Member, APS/DPB Nominating Committee, 2008, 2009.

Editorial Services to Scholarly Journals

Referee: Journal of Computational Physics; Physical Review Special Topics

Graduate advisor: Heidi Schellman

Students, postdocs, or collaborators for the past four years

PA = postdoc advisor, C = Collaborator, P = Postdoc (former or present), S = Student (former or present)

J. Conrad, C, MIT; D. Mason, S, Fermilab; L. Emery, C, ANL; D. McCarron, S, IIT; D. McGinnes, C, Fermilab; C. Ng, C, SLAC; M. Goncharov, S, MIT; F. Ostiguy, C, Fermilab; M. Palmer, C, Cornell; C.S. Park, P, Fermilab; B. Pellico, C, Fermilab; R. Ryne, C, LBNL; M. Shaevitz, PA, Columbia University;

Eric G. Stern
Computational Physics Developer, Fermi National Accelerator Laboratory
egstern@fnal.gov

Research Interests

Accelerator modeling with high performance computing, space charge solvers, impedance

Education and Training

- The Johns Hopkins University, B.A. Physics, May 1980
- State University of New York at Stony Brook, M.A. in Experimental High Energy Physics, May 1983
- State University of New York at Stony Brook, Ph.D. in Experimental High Energy Physics, May 1986

Research and Professional Experience

- Computational Physics Developer, Fermi National Accelerator Laboratory, since 2005
- Member of Technical Staff (software engineer), Lucent Technologies, 1998–2002
- Research Scientist, Columbia University Nevis Labs, 1992–1998
- Research Associate, University of Pittsburgh, 1987–1992

Selected Publications and Presentations

1. E. Stern, J. Amundson, P. Spentzouris, A. Valishev, Fully 3D Multiple Beam Dynamics Processes Simulations for the Fermilab Tevatron, presented at SciDAC 2010 Breakthroughs, July 11-15, 2010, Chattanooga, TN.
2. E. Stern, J. Amundson, P. Spentzouris, A. Valishev, Fully 3D Multiple Beam Dynamics Processes Simulations for the Fermilab Tevatron, PRST-AB vol.13, no 2 024401
3. E. Stern, J. Amundson, P. Spentzouris, A. Valishev, Fully 3D Multiple Beam Dynamics Processes Simulation for the Tevatron, invited talk TUPBI01, presented at PAC09 May 4–8, Vancouver, CA.
4. E. Stern, J. Amundson, P. Spentzouris, A. Valishev, J. Qiang, R. Ryne, Development of 3D beam-beam simulation for the Tevatron, contributed talk TUDC02 , PAC07, June 24–29, 2007, Albuquerque, NM.

Collaborators and Co-editors within the Past 48 Months: P. Spentzouris (Fermilab), J.F. Amundson (Fermilab), A.A. Valishev (Fermilab), R.D. Ryne (LBNL), J. Qiang(LBNL), J. Gonzalez (Accelogic LLC)

Doctoral Advisor: Michael D. Marx, State University of New York at Stony Brook (deceased)

Jean-Luc Vay
Staff Physicist, Lawrence Berkeley National Laboratory
jlvay@lbl.gov

Research Interests

Advanced numerical methods, high-performance and high-productivity scientific computing, high energy physics colliders, laser wakefield acceleration, heavy ion inertial fusion.

Education and Training

- University of Poitiers (France), B.S. in Physics, 1991
- University of Paris (France), M.S. in Physics, 1992
- University of Paris (France), Ph.D. in Physics, 1996

Research and Professional Experience

- Staff Physicist, Lawrence Berkeley National Laboratory, Accelerator and Fusion Research Division, 2000 – present
  - Principal Investigator LDRD "Lorentz compaction of scales for ultra-efficient simulation of advanced accelerators (and other systems). ", 2007 – 2010
  - Principal Investigator LDRD "Electron Production and Collective Field Generation in Intense Particle Beams", 2003 – 2006
- Term Scientist, Lawrence Berkeley National Laboratory, Accelerator and Fusion Research Division, 1998 – 2000
- Postdoctoral Fellow, Lawrence Berkeley National Laboratory, Accelerator and Fusion Research Division, 1996 – 1998

Selected Publications

1. J.-L. Vay Noninvariance of space- and time-scale ranges under a Lorentz transformation and the implications for the study of relativistic interactions. *Physical Review Letters* 98, 130405 (2007) (press releases at LBNL, PhysicsFocus)
2. J.-L. Vay, C. G. R. Geddes, E. Cormier-Michel, and D. P. Grote. Effects of hyperbolic rotation in Minkowski space on the modeling of plasma accelerators in a Lorentz boosted frame. *Physics of Plasmas* 18, 030701 (2011) (press releases at LBNL, NERSC, DOE)
3. J.-L. Vay, C. G. R. Geddes, E. Esarey, C. B. Schroeder, W. P. Leemans, E. Cormier-Michel, and D. P. Grote. Modeling of 10 GeV-1 Tev laser-plasma accelerators using Lorentz boosted simulations. *Physics of Plasmas* 18, 123103 (2011)
4. J.-L. Vay, C. G. R. Geddes, E. Cormier-Michel, and D. P. Grote. Numerical methods for instability mitigation in the modeling of laser wakefield accelerators in a Lorentz-boosted frame. *Journal of Computational Physics* 230, 5908-5929 (2011)

5. J.-L. Vay. Simulation of beams or plasmas crossing at relativistic velocity. *Physics of Plasmas* 15, 056701 (2008)

6. J.-L. Vay, M. A. Furman, and M. Venturini, Direct Numerical Modeling of E-Cloud Driven Instability of a Bunch Train in the CERN SPS. *Proceedings of 2011 Particle Accelerator Conference PAC 11*, New York NY (2011)

7. J.-L. Vay, J. M. Byrd, M. A. Furman, R. Secondo, M. Venturini, J. D. Fox, C. H. Rivetta, and W. Hofle. Simulation of E-Cloud Driven Instability and its Attenuation using a Feedback System in the SPS. *Proceedings of 1st International Particle Accelerator Conference*, Kyoto, Japan (2010)

8. J.-L. Vay, M. A. Furman, P. A. Seidl, R. H. Cohen, A. Friedman, D. P. Grote, M. Covo-Kireeff, S. M. Lund, A. W. Molvik, P. H. Stoltz, S. Veitzer, and J. P. Verboncoeur. Self-Consistent Simulations of Heavy-Ion Beams Interacting With Electron-Clouds. *Nuclear Instruments and Methods A* 577, 65–69 (2007)

9. J.-L. Vay, P. Colella, J. W. Kwan, P. McCorquodale, D. Serafini, A. Friedman, D. P. Grote., G. Westenskow, J.-C. Adam, A. Héron, and I. Haber. Application of adaptive mesh refinement to particle-in-cell simulations of plasmas and beams. *Physics of Plasmas* 11, 2928 (2004)

10. J.-L. Vay, J.-C. Adam, A. Héron, and I. Haber. Asymmetric PML for the absorption of waves. Application to mesh refinement in electromagnetic particle-in-cell plasma simulations. *Computer Physics Communications* 164,171 (2004)

Selected Synergistic Activities

- Co-developer of Warp Particle-In-Cell accelerator framework and application to the modeling of heavy ion beam injection, acceleration, transport and neutralization in a plasma for warm dense matter experiments and heavy ion inertial fusion.
- Simulations using the package Warp-POSINST of electron cloud instability and its mitigation using a high bandwidth feedback system.

Collaborators within the Past 48 Months
C. Celata, E. Esarey, W. Faltens, W. Fawley, M. Furman, H. Henestroza, C. Geddes, E. Jung, J. Kwan, E. Lee, W. Leemans, M. Leitner, G. Logan, G. Penn, C. Schroeder, R. Secondo, P. Seidl, M. Venturini, W. Waldron (Lawrence Berkeley National Laboratory); J. Barnard, R. Cohen, A. Friedman, D. Grote, S. Lund, W. Sharp (Lawrence Livermore National Laboratory); R. Davidson, M. Dorf, E. Gilson, I. Kaganovitch (Princeton Plasma Physics Laboratory); W. Hofle, G. Rumolo (CERN); J. Fox, C. Rivetta (SLAC National Accelerator Laboratory); D. Bruhwiler, J. Cary, E. Cormier-Michel, B. Cowan, K. Paul, P. Stoltz, S. Veitzer (Tech-X); B. Godfrey, R. Kishek (U. Maryland)

Doctoral Advisor: Prof. Claude Deutsch, University of Paris-Sud, Orsay, France
Postdoctoral Advisor: Edward Lee, Lawrence Berkeley National Laboratory

Stefan M. Wild

Assistant Computational Mathematician
Mathematics and Computer Science Division
Argonne National Laboratory
Argonne, IL 60439-4844
Phone: 630-252-9948
`http://www.mcs.anl.gov/~wild`

Fellow
Computation Institute
University of Chicago
Chicago, IL 60637
Fax: 630-252-5986
Email: `wild@mcs.anl.gov`

Education and Training

- Argonne National Laboratory: Argonne Director's Postdoctoral Fellow, Sept 2008–Aug 2010
- Cornell University, Operations Research: Ph.D., Jan 2009
- Cornell University, Operations Research: M.S., Jan 2007
- University of Colorado-Boulder, Applied Mathematics: M.S., May 2003
- University of Colorado-Boulder, Applied Mathematics: B.S., May 2002

Research and Professional Experience

- *Assistant Computational Mathematician*, Argonne National Laboratory, Mathematics and Computer Science Division, Sept 2010 – present
- *Fellow*, University of Chicago, Computation Institute, Apr 2010 – present
- *Argonne Scholar*, Argonne National Laboratory, Sept 2008 – Aug 2010
- *Instructor*, University of Colorado-Boulder, Dept. Applied Mathematics, May 2004 – Aug 2004

Honors and Awards

- DOE Computational Science Graduate Fellowship (CSGF), 2005–2008
- Best student paper award, Tenth Copper Mountain Conference on Iterative Methods, 2008
- Outstanding (highest designation), International Mathematical Contest in Modeling (MCM), 2002

Selected Publications Relevant to this Proposal

1. M. Bertolli, T. Papenbrock, and S.M. Wild. Occupation Number-based Energy Functional for Nuclear Masses. Mathematics and Computer Science Division, Preprint ANL/MCS-P1966-1011, (2011).
2. R.B. Gramacy, M.A. Taddy, and S. Wild, Variable Selection and Sensitivity Analysis via Dynamic Trees with an Application to Computer Code Performance Tuning, Mathematics and Computer Science Division, Preprint ANL/MCS-P1961-1011, (2011).
3. J. Moré and S. Wild. Estimating Derivatives of Noisy Simulations. *ACM Transactions on Mathematical Software*, Vol. 38(3), to appear, (2011).
4. S. Wild and C. Shoemaker. Global Convergence of Radial Basis Function Derivative-Free Trust Region Algorithms. *SIAM J. Optimization*, Vol. 21(3), pp. 761–781, (2011).
5. P. Balaprakash, S. Wild, and P. Hovland. Can Search Algorithms Save Large-scale Automatic Performance Tuning? *Proceedings of the International Conference on Computational Science (ICCS 2011), Procedia Computer Science,* 4, 2136–2145, 2011.
6. J. Moré and S. Wild. Estimating Computational Noise. *SIAM J. Scientific Computing*, Vol. 33(3), pp. 1292–1314, (2011).
7. M. Kortelainen, T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. Stoitsov, and S. Wild. Nuclear Energy Density Optimization. *Physical Review C*, Vol. 82, 024313, (2010).
8. J. Moré and S. Wild. Benchmarking Derivative-free Optimization Algorithms. *SIAM J. Optimization*, 20, pp. 172–191, (2009).

9. S Wild. MNH: A Derivative-Free Optimization Algorithm Using Minimal Norm Hessians. *Copper Mountain Conference on Iterative Methods*, April 2008.
10. S. Wild, R. Regis, and C. Shoemaker. ORBIT: Optimization by Radial Basis Function Interpolation in Trust-regions. *SIAM J. Scientific Computing*, Vol. 30(6), pp. 3197–3219, (2008).

Synergistic Activities

- *Contributor:* `TAO` (Toolkit for Advanced Optimization) is designed to solve large-scale optimization problems on high-performance distributed architectures. `TAO` solvers have been used to solve computational science problems in a wide variety of areas; details can be found in the impact section of `www.mcs.anl.gov/tao`.
- *DOE CSGF:* Served on the application review committee, on the alumni committee, as a poster judge, and as a practicum sponsor for the DOE Computational Science Graduate Fellowship.
- *Mentoring:* Supervised and mentored students at Argonne (3 Givens Fellows, 1 Research Aide, 1 Predoc) and Cornell (3 Masters of Engineering candidates).
- *Organizer:* Multiple-part minisymposia at SIAM Conferences Computational Science & Engineering (2011) and Optimization (2011); "Derivative-free and Simulation-based Optimization" cluster co-chair for the 2012 International Symposium on Mathematical Programming.
- *Technical Editor:* Mathematical Programming Computation, 2011–

Collaborators Within The Past 48 Months

- H. Aktulga (Lawrence Berkeley), P. Balaprakash (Argonne), A. Baran (Univ. Tennessee), M. Bertolli (Univ. Tennessee), N. Bliznyuk (Texas A&M), A. Bulgac (Univ. Washington), E. Gawlik (Stanford), R. Gramacy (Univ. Chicago), P. Hovland (Argonne), A. Kannan (Argonne), M. Kortelainen (Oak Ridge), J. Larson (Univ. Colorado), T. Lesinski (Univ. Washington), P. Maris (Iowa State), J. McDonnell (Univ. Tennessee), J. Moré (Argonne), T. Munson (Argonne), H. Nam (Oak Ridge), W. Nazarewicz (Univ. Tennessee/Oak Ridge), E. Ng (Lawrence Berkeley), B. Norris (Argonne), T. Papenbrock (Univ. Tennessee/Oak Ridge), J.C. Pei (Univ. Tennessee/Oak Ridge), P.-G. Reinhard (Univ. Erlangen), J. Sarich (Argonne), N. Schunck (Lawrence Livermore), J. Sheikh (Univ. Tennessee/Oak Ridge), C. Shoemaker (Cornell), A. Staszczak (Univ. Tennessee/Oak Ridge), M. Stoitsov (Univ. Tennessee/Oak Ridge), M. Taddy (Univ. Chicago), I. Thompson (Lawrence Livermore), J.P. Vary (Iowa State), C. Yang (Lawrence Berkeley)

Advisors

- Christine Shoemaker (Cornell, Doctoral)
- Jorge Moré (Argonne, Postdoctoral)

Graduate Students and Postdoctoral Associates

- P. Balaprakash (Argonne), A. Kannan (Argonne), S. Wang (Argonne)

Liling Xiao
SLAC National Accelerator Laboratory
Advanced Computations Department
2575 Sand Hill Road
Menlo Park, CA 94025
email: liling@slac.stanford.edu

Education and Training

Ph.D., Electrical Engineering, Southeast University, Nanjing, China, 1993.
M.E., Electrical Engineering, Southeast University, Nanjing, China, 1990.
B.E., Electrical Engineering, Nanjing Institute of Technology, Nanjing, China, 1987.

Research and Professional Experience

2004 - present	Engineering Physicist, SLAC National Accelerator.
2000 - 2001	Visiting Scientist, Argonne National laboratory.
1993 - 2000	Associate Professor, Tsinghua University, Beijing, China.
1995	Visiting Scholar, High Energy Accelerator Research Organization, Japan.

Dr. Liling Xiao's main research interests are microwave and millimeter wave technologies, RF design and measurement of accelerator structures, and RF modeling and simulation. She has been involved in many accelerator projects, such as the International Linear Collider (ILC), the Linac Coherent Light Source (LCLS) at SLAC, the Large Hadron Collider (LHC), and the Cornell Energy Recovery (ERL) Linac. Her main contributions to these projects include the HOM and LOM coupler optimizations for the ILC crab cavity, the dual-feed RF gun design for LCLS, the 800MHz crab cavity baseline design for the LHC upgrade, and studies of SRF cavity imperfection effects in the ERL linac. Currently, she is working on the 53 MHz and 106 MHz RF cavity design for the Project-X main injector, and the SRF deflecting cavity cryomodule simulations and analysis for the APS upgrade (SPX).

Selected Publications

1. L. Xiao, et al., "Effects of Elliptically Deformed Cell Shape in the Cornell ERL Cavity", Proceeding of SRF11, July 25-29, 2011, Chicago, IL, USA.
2. L. Xiao, et al., "Simulation and Optimization of the Project-X Main Injector Cavity", Proceeding of PAC11, March 28 - April 1, 2011, New York, NY, USA.
3. L. Xiao, "Longitudinal Wakefield Study in SLAC Rotatable Collimator Design for the LHC Phase II Upgrade", Proceeding of IPAC10, May 23-28, 2010, Kyoto, Japan.
4. L. Xiao et al., "800MHz Crab Cavity Conceptual Design for the LHC Upgrade", Proceeding of PAC09, Vancouver, Canada, May 4-8, 2009.
5. L. Xiao et al., "HOM and LOM Coupler Optimizations for the ILC Crab Cavity", SLAC-PUB-12635, 2007, Cockcroft-07-38.
6. L. Xiao et al., "Modeling Imperfection Effects on Dipole Modes in TESLA Cavity", SLAC-PUB-12634, 2007.
7. L. Xiao et al., "Dual Feed RF Gun Design for LCLS", SLAC-PUB-11213, 2005.
8. L. Xiao et al., "Field Analysis of a Dielectric-Loaded Rectangular Waveguide Accelerating Structure", Physics Review E65, 2001.
9. L. Xiao et al., "Measurements of High Order Modes in a 30cm Long X-Band Structure", Nuclear Instruments and Methods in Physics Research A, Vol.463/1-2, 2001.

Collaborators (last 48 months) and Co-Editors (last 24 months)

Ali Nassiri (ANL),
Geoff Waldschmidt (ANL),
Genfa Wu (ANL),
Haipeng Wang (JLAB),
Robert Rimmer (JLAB),
Matthias Liepe (Cornell),
Joseph Dey (FNAL)

Graduate and Postdoctoral Advisors and Advisees:

Wenxun Zhang (Southeast University, China), thesis advisor

Chao Yang

Contact Information:
Lawrence Berkeley National Laboratory
MS-50F
One Cyclotron Road
Berkeley, CA 94720
Phone: (510)486-6424
Fax: (510)486-5812
Email: CYang@lbl.gov

Education:

Ph.D., Rice University, 1998 (Computational Science & Engineering)
M.A., The University of Kansas, 1994 (Mathematics)
B.S., Central Missouri State University, 1992 (Mathematics/Computer Science)

Positions:

Staff Computer Scientist, Lawrence Berkeley National Laboratory (2003-Present);
Senior Scientist, ILOG Inc. (2002-2003);
Computer System Engineer III, Lawrence Berkeley National Laboratory (2000-2002);
Householder Fellow in Scientific Computing, Oak Ridge National Laboratory (1999-2000);
Applications Consultant, NEC Systems Laboratory (1998-1999)

Honors and Awards:

- Householder Fellow, Oak Ridge National Laboratory, 1999.
- Ralph Budd Award for the best engineering thesis, Rice University, 1998.
- Jack C. Pollard Fellowship, Rice University, 1996.

Recent Relevant Publications:

1) H. M. Aktulga, C. Yang, E. Ng, P. Maris and J. P. Vary, *Large-scale Parallel Null Space Calculation for Nuclear Configuration Interaction,* to appear in Proceedings of *High Performance Computational Science Conference* , 2011.

2) H. M. Aktulga, C. Yang, E. Ng, P. Maris and J. P. Vary, *On Reducing I/O Overheads in Large-Scale Invariant Subspace Projections*. To appear in Proceedings of *High Performance Scientific Software (part of Euro-PAR 11*), 2011

3) J. P. Vary, H. Honkane, J. Li, S. J. Brodsky, A. Harindranath, G. F. de Teramond, P. Sternberg, E. G. Ng and C. Yang,*Hamiltonian light-front field theory in a basis function approach, Phys. Rev. C* , vol. 81, no. 3. 2010.

4) P. Maris, M. Sosonkina, J. P. Vary, E. Ng and C. Yang. *Scaling of ab-initio nuclear physics calculations on multicore computer architectures, Procedia Computer Science* , vol 1, no. 1, pp 97-106, 2010.

5) J. P. Vary, P. Maris, E. Ng, C. Yang and M. Sosonkina. *Ab initio nuclear structure -- the large sparse matrix eigenvalue problem,* Journal of Physics: Conference Series, 180:012083, 2009.

Other Significant Publications:

6) C. Yang and J. Meza, *Minimizing the Kohn-Sham Total Energy for Periodic Systems,* to appear in *Linear Algebra and Its Applications* , 2011.

7) P. Sternberg, C. Yang, P. Maris, E. Ng, M. Sosonkina, H. V. Le and J. Vary. *,Accelerating Full Configuration Interaction Calculations for Nuclear Structure*, LBNL Report-591E *, SC'08: Proceedings of the 2008 ACM/IEEE conference on Supercomputing*, pp. 1--12, IEEE Press, 2008.

8) L. Lin, C. Yang, J. Lu, L. Ying and W. E., *A Fast Parallel Algorithm for Selected Inversion of Structured Sparse Matrix with Application to 2D Electronic Structure Calculations* , LBNL-2677E , to appear in *SIAM J. Sci. Comp.* , 2011

9) L. Lin, C. Yang, J. C. Meza, J. Lu, L. Ying and W. E., *SelInv - An Algorithm for Selected Inversion of a Sparse Symmetric Matrix* , LBNL-2746E , *ACM Trans. on Math Software* , vol, 37, no. 4, pages 1 -- 19, 2011.

10) C. Yang , W. Gao and J. Meza. *On the Convergence of the Self-consistent Field Iteration for a Class of Nonlinear Eigenvalue Problems*. LBNL Report 63037 , *SIAM J. Matrix Anal. & Appl*., vol 30, no. 4, pp. 1773--1788, 2009.

Collaborators:

Stefano Marchesini, Filipe Maia, Andre Schirotzek, Esmond Ng, Lin Lin, Carolyn Larabell, Mark LeGros (LBNL), Jianliang Qian, Gang Bao, Di Liu (Michigan State), Weinan E (Princeton), James Vary, Pieter Maris, M. Sosonkina, H. Honkane, J. Li (Iowa State), . J. Brodsky (SLAC),A. Harindranath (Saha Institute of Nuclear Physics, India), G. F. de Teramond (Costa Rica), Juan Meza (UC Merced), J. Lu (Courant), L. Ying (UT-Austin), P. Sternberg (IBM/ILOG)

D Description of Facilities and Resources

Description of facilities and resources follow in alphabetical order.

Argonne National Laboratory

Argonne National Laboratory resources include several major parallel computing systems, visualization systems, advanced display environments, collaborative environments, and high-capacity network links. The Laboratory is connected to the outside world with 10 Gbps links to Internet2 and ESnet (to be upgraded to 100 Gbps in 2011).

The Argonne Leadership Computing Facility (ALCF) has a 557 TF IBM Blue Gene/P system for production scientific and engineering computing and a 13.9 TF Blue Gene/P system for systems software development. The large Blue Gene system is principally available to researchers through the DOE INCITE program, but some time is also set aside for Argonne researchers and their collaborators. In 2012, Argonne will also install Mira, a 10 PF IBM Blue Gene/Q system. This supercomputer will be 20 times faster than the Blue Gene/P, running programs at 10 quadrillion calculations a second. Argonne envisions Mira as a stepping stone to exascale-class computers that will be faster than petascale-class computers by a factor of a thousand.

The ALCF also has a 504-node cloud computing system, Magellan, with a peak performance of 40 TF/s. Each node has two quad-core Nehalem 2.66 GHz CPUs, 24 GB RAM, and 500 GB of disk storage. A 160 TB storage system provides high performance file services. The nodes are interconnected using QDR Infiniband.

The "Fusion" Linux cluster, located in Argonne's Laboratory Computing Resource Center, is available to researchers for development and production computing. Fusion, a 26-teraflop cluster supercomputer, is configured with Intel's powerful Nehalem series processors, and the latest quad-data-rate InfiniBand communications fabric. There are 320 nodes, each with two quad-core processors and 36 GB RAM. A 400 TB storage system provides high performance file services.

The Mathematics and Computer Science Division at Argonne also operates a SiCortex SC5832 system comprising 972 six-core compute nodes with 4 GB of memory, for an aggregate of 5832 cores and nearly 4 TB of memory. The system is connected for I/O via several Myrinet 10G links and has capacity to connect 108 such links. The system is available for researchers for development and scalability testing.

The division also has installed a new NVIDIA Tesla C1060 GPU computer as an exploratory testbed for research and development. Each node is built out using 2 GPUs each, each with 240 computing cores per GPU. GPUs are dedicated graphics rendering devices that are probably best known from their use in games for manipulating and displaying computer graphics. The division also has procured several Sun Niagara systems. The Niagara is a massively multithreaded architecture, each node having dual CPUs, each featuring 8 hardware cores with 8 hardware threads, for a total of 128 hardware threads per node. These systems provide a solid indication what system architectures will look like in the 3-5 year timeframe.

Through the University of Chicago/Argonne Computation Institute, Argonne has access to the TeraGrid's visualization facility. The entire facility is a 13.6 TF grid of distributed clusters using Intel McKinley processors with over 6 TB of memory and greater than 600 TB of disk space. The full machine is distributed among several resource providers connected by a dedicated 40 Gb/s link that acts as the backbone for the machine. The CI component of the machine is focused on visualization support. It consists of 16 dual IA-64 nodes for computation, 96 dual Pentium IV nodes with G Force Ti 4600 graphics accelerators for visualization, and 20 TB of storage.

Argonne has substantial visualization devices as well, each of which can be driven by the TeraGrid visualization cluster or by a number of smaller dedicated clusters. These devices include the ActiveMural, which has 11 million pixels, and the portable MicroMural, which has $\tilde{3}$ million pixels.

Fermilab

Fermilab researchers will use local high-performance computer clusters, and other local computing infrastructure for parallel code development, benchmarking, and software verification. We will perform large-scale testing, performance evaluation, and production runs on supercomputers at the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory under the ComPASS SciDAC allocation. The Fermilab resources available to us include:

- The Fermilab Wilson cluster, which is dedicated to accelerator simulations. It has two sets of nodes: 34 quad-socket, eight-core (32 cores/node, 1088 cores total) AMD Opteron CPU based systems and 20 dual-socket, single-core (2 cores/node, 40 cores total) Intel Xeon CPU based systems. All nodes are connected by high speed (double-data-rate) Infiniband network fabric.

- A GPU-accelerated cluster, which is available for development to the ComPASS team at Fermilab. The cluster contains 172 NVidia M2050 GPUs housed in 76 eight-core Intel-based hosts. The host machines are interconnected with a QDR Infiniband full-bisection-bandwidth fabric.

Lawrence Berkeley National Laboratory

LBNL has access to leading-edge computing platforms and services through NERSC as well as several departmental clusters. A Cray XE6 makes up the heart of NERSC's computational capability. The 153,408-core Cray XE6 contains 6,392 nodes with two 12-core AMD processors per node, interconnected by a high-speed torus network to achieve a peak performance of 1.29 petaflops, making it one of the most powerful supercomputers in the world. Each node has either 32 or 64 gigabytes of memory, and the system has 2 petabytes of disk space. NERSC also operates a 38,128-core Cray XT4 with a peak performance of 356 teraflops, and two IBM iDataplex systems with a total of 7,680 Intel Nehalem processors. These clusters are fully instrumented for detailed measurement of communication and power consumption and can be used for trace capture of full-scale HPC applications. NERSC's research in data-intensive computing is grounded in their operation of a major production facility, the PDSF (Parallel Distributed Systems Facility). For data analysis, NERSC has a Sunfire x4640 server with 48 AMD cores and 512 gigabytes of shared memory. All of these systems are connected to a 450 terabyte global parallel filesystem that interconnects all of NERSC for convenience of users producing and analyzing large data sets. Finally, these systems are connected to a High Performance Storage System (HPSS) for archival storage. NERSC's HPSS system has a current capacity of 2.6 petabytes and the ability to grow to 44 petabytes, making it one of the largest unclassified archival storage systems in the world.

We also have access to a number of architectural testbeds at LBNL.

- The Advanced Technologies Group at NERSC has two BEE-3 FPGA boards, each of which contains four Xilinx 155T FPGAs interconnected by RapidIO links, which can be externally connected to multiple InfiniBand and 10GigE Links. The BEE boards are used for cycle-accurate simulation of gate-level chip designs using the RAMP infrastructure.
- LBNL Computing Sciences operates a small cluster of Convey HC1 systems to perform testing of their novel Gather Scatter memory technology and to act as an alternative FPGA-accelerated architectural simulation platform for RAMP.
- LBNL operates a number of other GPU/accelerator computing testbeds. The Computational Research Division has an NVIDIA 8800GTX cluster with 128 cores, 8 sockets (345 single precision megaflops/GPU). NERSC has a pair of NVIDIA Tesla-based systems (Turing and Tesla) that are available publicly. These systems are comprised of a Sun/AMD host containing 256 gigabytes of DRAM connected to an NVIDIA QuadroPlex 2200 S4. Each S4 Tesla-based GPU accelerator contains 1,024 cores per socket (1 teraflop single precision and 345 gigaflops double precision). In April 2010, NERSC fielded a 48-node Fermi GPU cluster called "Dirac" that consists of QDR InfiniBand-connected Nehalem host-nodes to act as a testbed for GPU computing that are integrated with the Magellan/Carver cluster. The GPU accelerated nodes consist of 44 nodes containing NVIDIA C2050 "Fermi" GPUs, and 8 containing NVIDIA C1040 "Tesla" GPUs. Recently added are 2 multi-GPU nodes: 1 node containing 4 Fermi GPUs, and 1 node containing 4 Tesla GPUs. The system includes a complete set of development tools for hybrid computing, including CUDA, OpenCL, and PGI GPGPU-targeted compilers
- One of the two IBM iDataplex systems at NERSC is managed as a cloud computing testbed, running a variety of cluster and cloud computing software for experimenting with scientific computations on a cloud environment.

Access to the LBNL facilities from anywhere in the U.S. or the world is available through ESnet, which provides multiple 10-gigabit Ethernet bandwidth to NERSC. ESnet also provides major backbone links including peering with domestic and international research and education networks. Over the coming year, the ESnet infrastructure will be upgraded to 100 gigabit Ethernet.

SLAC National Accelerator Laboratory

SLAC scientists will use local workstations, computer clusters, and other computing infrastructures for parallel code development, benchmarking, and software verification. We will perform large-scale testing, performance evaluation, and production runs on Offices of Science's high performance supercomputers at National Energy Research Scientific Computing (NERSC) Center at Lawrence Berkeley National Laboratory.

We have an 8-node Linux cluster mainly used as a testbed for the remote and interactive parallel visualization of electromagnetic fields and particles in complex accelerator cavities. This visualization cluster is configured with dual AMD Opteron 64-bit CPUs and a powerful GeForce 7800 GTX graphics card in each node. The nodes are connected with ultra low-latency high-bandwidth Quadrics network.

Currently SLAC has three computer allocations from NERSC, which are shared among different research institutions. The allocations are

- Advanced Modeling for Particle Accelerators - 2.5 million CPU hours
- Community Petascale Project for Accelerator Science and Simulation - 6 million CPU hours
- Frontiers in Accelerator Design: Advanced Modeling for Next Generation BES Accelerators - 7 million CPU hours

Tech-X Corporation

Tech-X Corporation provides state-of-the-art facilities and equipment needed to successfully complete the proposed project. This includes computing, communications, networking, and security. Tech-X provides support personnel including Information Technology and Networking staff to provide reliable, persistent, and secure communications and computing to the project. The existing facilities and equipment are sufficient for the project.

On-site computing facilities at Tech-X include four high-performance, 64-bit parallel computing clusters, running CentOS and Fedora Core Linux. The primary cluster is a 32-node, 256-core Opteron cluster with Infiniband interconnects, with a 26 TB high-performance Lustre file system.

The remaining three 64-bit clusters range from 32 to 96 cores and are supported by approximately 25 TB parallel file systems. One cluster has several nodes integrated with NVIDIA Tesla GPU computing systems. One cluster is always available for customer/client/collaborator testing and evaluation.

Tech-X utilizes a variety of hardware and operating systems–including virtualization–for servers, individual workstations, and development platforms. Numerous GPU and FPGA configurations are available. This environment permits rapid assignment and configuration of resources to project requirements, and development and testing of cross-platform compatibility. The ratio of computers used for software development and scientific research to researchers is nearly 3:1.

Business class internet service provides access to a company-wide GbE/100 network. Multiple internal wireless networks provide for employees' and clients' secure networking needs. Videoconferencing facilities allow off-site collaborations and application sharing.

Network security is achieved through the use of a combination of firewalls, secure access and authentication protocols, anti-intrusion and monitoring software, and a network topology restricting external services, such as web and secure login, to a select subset of computer systems.

Daily backups of critical systems and data occur both on-site directly to mass storage devices, and to off-site repositories. Computing hardware necessary for reestablishment of critical business functions and recovery of critical resources is in place, including RAID replication of data and UPS.

In addition to extensive computing resources on-site at Tech-X, authorized scientists have access to several high-performance and Leadership Computing Facility (LCF) computers. This includes, among others, access to Hopper and Carver at the National Energy Research Scientific Computing Center (NERSC); and Jaguar at the National Center for Computational Sciences (NCCS). Hopper is a Cray XE6 massively parallel processing system with 6392 nodes and 153K total cores. Jaguar, at the NCCS LCF, is a Cray XT4 and XT5 system, with 31,328 and 224,256 compute cores, respectively. Dirac, at NERSC, is a general purpose GPU testbed consisting of 48 nodes with Tesla and Fermi GPUs.

Founded in 1994, Tech-X currently employs approximately 70 employees. The company specializes in computational science and software engineering in the areas of high performance computing and visualization.

Tech-X Corporation occupies over 14,500 square foot of modern office and computing facilities at its Boulder, Colorado, and Buffalo, New York, sites. In 2010, Tech-X opened UK operations in Daresbury, UK. In addition to the University of Colorado, a major national scientific research university, Boulder is home to several national research laboratories (NIST, NCAR, and NOAA). The New York office is proximate to the University at Buffalo, Center for Computational Research, and the New York State Center for Excellence in Bioinformatics and Life Sciences. The UK site is colocated with Daresbury Science and Innovation Campus, in collaboration with The Cockcroft Institute (the National Centre for Accelerator Science and Technology). These sites foster rich scientific communities supporting research.

Tech-X Corporation facilities meet environmental laws and regulations of federal, State of Colorado and New York, and local governments for, but not limited to, the following groupings: airborne emissions, waterborne effluents, external radiation levels, outdoor noise, solid and bulk waste disposal practices, and handling and storage of toxic and hazardous materials.

The University of Texas at Austin

ICES and the ACES building. The Institute for Computational Engineering and Sciences (ICES) is located in the Applied Computational Engineering and Sciences (ACES) building on The University of Texas at Austin main campus. This facility has offices and work areas equipped with desktop computers, printers and copiers, mini-clusters, computational visualization facilities, and extensive network access for faculty, staff, students, and visitors. A large machine room houses supercomputers, servers, and large-scale storage devices. The building has a 196-seat auditorium with Ethernet ports at each seat. The auditorium also furnishes wireless networking, video conferencing and remote learning capabilities. There are eighteen networked seminar rooms with high-resolution audio visual systems, some with video conferencing and video taping facilities.

Networking infrastructure. The ACES building networks are designed to support both bandwidth-intensive computational research and to accommodate new technology when available. The networks are built around high-performance, multilayer Cisco 6509, 2960 and 4003 network switches, with Lucent Gigaspeed copper Ethernet and Multimode Fiberoptic to each desktop and work area. Wireless networking is available throughout the building and courtyard area.

Workstation Environment. The ICES workstation environment encompasses all offices, cubicles, work areas, and laboratories. Over 300 general-purpose workstations are available, including PCs running Linux and Windows, and Macs. Several color printers and scanners are available. File and email service is provided by a number of Linux servers with over twenty terabytes of disk storage. Other Mac and Linux-based computers function as web servers, LDAP authentication servers, domain name servers, directory servers, application servers, and compute servers.

On-site Linux-Based Clusters. ICES systems and networking team currently supports seven Linux-based Clusters with others in the planning and design stages. The Center for Subsurface Modeling has a 184 core cluster (Bevo2). The Center for Computational Visualization has a 64 core rendering cluster (Prism2). The Center for Computational Materials has a 16-node compute cluster (Deanston). The Center for Computational Molecular Sciences has a 40-node (Muskoka) cluster. The Center for Computational Life Sciences and Biology has two clusters; a 184 core cluster (Junior), and a 512 core cluster (Stampede). The Computational Mechanics Group has a 256 core cluster (Reynolds).

Off-site Supercomputing Facilities. ICES has access to supercomputing facilities via high-speed networking at the Texas Advanced Computing Center (TACC) at the J. J. Pickle Research Center, eight miles north of the main campus. At TACC, the two primary HPC production systems include: the Lonestar cluster with 1,888 Dell M610 PowerEdge blade servers, and peak performance of each 302 Tflop/s; and a Sun Constellation Linux cluster, Ranger, one of the most powerful computers for open academic research in the world. Ranger has 62,976 AMD Opteron processing cores, 123 TB of memory, 1.73 PB of on-line disk storage, and a peak performance of 579 Tflop/s. As part of Lonestar system described above, ICES researchers also have priority access to approximately 18 million CPU hours in a separate queue at TACC. Compute cycles in this queue are managed by the Institute with allocations awarded on a quarterly basis.

The long-term storage solution at TACC is a Sun Microsystems StorageTek Mass Storage Facility, called Ranch. Ranch utilizes Sun's Storage Archive Manager Filesystem for migrating files to/from a tape archival system with a current storage capacity of 10 PB. A single Sun StorageTek SL8500 Automated Tape Library houses all of the offline archival storage. Each SL8500 library contains 10,000 tape slots and 64 tape drive slots. Each tape is capable of holding 1 TB of uncompressed data.

TACC systems also include Corral, deployed in 2009, to support data-centric services. Corral consists of 1.2 PB of online disk and a number of servers providing high-performance storage or all types of digital data. It supports MySQL and Postgres databases, a high-performance parallel file system, web-based access, and other network protocols for storage and retrieval of data to and from sophisticated instruments.

ACES Visualization Laboratory. The ACES Visualization Laboratory provides an end-to-end infrastructure for data-intensive and display-intensive computing and is available to all UTA investigators as well as UT System and Teragrid users. The lab includes a Dell visualization cluster, Stallion, with 24 nodes and a 15×5 307 megapixel tiled display, a Sony 9M pixel flat projection system (Bronco) driven by a high-end Dell workstation, and Mustang a 73-inch Mitsubishi DLP flat-panel TV with active 3D stereo capabilities. These systems provide a unique environment for interactive and immersive visual exploration.

UCLA Campus Research Cyberinfrastructure

IDRE Hoffman2 Shared Research Cluster:

The Shared Hoffman2 Cluster has 64-bit nodes with an Ethernet network and Infiniband interconnect, that includes a scheduler, GCC and the best performing compiler for C, C++, Fortran 77, 90 and 95 on the current Shared Cluster architecture, applications and software libraries that offer languages, compilers and software specific to Chemistry, Chemical Engineering, Engineering, Mathematics, Visualization, Programming and an array of miscellaneous software. Hoffman2 additional resources for researchers include complete system administration for contributed cores, cluster access through a 10Gb network interconnect to the campus backbone, high performance home and scratch storage space, capability to run large parallel jobs that can take advantage of the cluster's InfiniBand interconnect, and web access to the Hoffman2 Cluster through the UCLA Grid Portal, and access to the BlueArc storage system. The Hoffman2 has visualization nodes to allow visualization codes to directly access Hoffman2's storage and compute resources over Infiniband.

Plasma Simulation Group and IDRE GPU Cluster-Dawson2:

UCLA's Dawson2 cluster, comprises 96 HP ProLiant SL390 G7 systems, each having dual socket Intel Xeon X5650 processors, 3 Nvidia M2070 Graphics processors, and 48 GB of main memory giving peak performance of 150 double precision Trillion Floating Point Operations per sec (TFLOPS). On Linpack it achieved 70 TFLOPS making it 148 in the June Top500 list. The cluster uses QDR Infiniband networking and 160 Terabytes of high performance common disk space from Panasas for communication and storage respectively. This cluster is primarily for simulations of high energy density plasma science. It is also available for broader campus efforts in computational science.

The IDRE Data Centers and Facilities:

The Math Sciences Data Center:

The UCLA Math Sciences data center, which is shared with the campus administrative systems unit, houses research computing clusters, including part of the main Hoffman2 shared cluster. The Math Sciences data center also provides backend services to the Visualization Portal and Modeling Lab. Approximately 2,700 square feet of the Math Sciences data center's 5,000 square feet are dedicated to supporting IDRE research computing. The compute resources in this facility and the IDRE data center are networked through 10gigabit Ethernet as well as wide-area Infiniband fabric. The Math Sciences facility is a Tier 3 data center space with greater than 600kW of power with full UPS and motor generator backup and 170 tons of redundant air conditioning capacity. The facility has strong physical security, which includes 24 x 7 staff monitoring and physical presence in the center. In addition to the cluster nodes our central Blue Arc-based storage appliance, currently three-quarters of a petabyte, and online Tivoli tape backup system are housed here.

The IDRE Performance Optimized Data Center (POD):

The Math Sciences Data Center has been extended through the innovative use of the HP Performance Optimized Data Center (POD) making available for researchers an additional 1,535 nodes and 18,000+ cores. The POD is a retrofitted 40' by 8' shipping container that has been extensively modified to support more than 1,500 compute nodes with associated network and interconnect equipment. The POD provides 600KW of power and 170 tons of air conditioning in a highly efficient manner that is roughly 40% better than a conventional data center at a fraction of the cost. The IDRE CNSI Data Center: Located in the California Nanosystems Institute (CNSI) building, the IDRE data center consists of 2,500 square feet of Tier 2 data center space equipped with 200KW of power and 60 tons of air conditioning. The IDRE facility has space for 400 compute nodes. The data center is connected via a redundant, 10Gb fiber connection to the campus backbone through two Cisco 6509 switches in addition to four fiber-linked Infiniband connections to UCLA's Math Sciences data center where there is space for 500 more nodes.

IDRE Visualization Portal:

UCLA's Visualization Portal, used for both instruction and research, has particular foci on scientific visualizations and historical architectural reconstructions. Current Portal research projects span the sciences, arts, humanities, urban planning projects, and medicine. The Institute for Digital Research and Education (IDRE) oversees Portal projects in scientific visualization and computational simulation.

The UCLA GRID:

The Grid is a computing infrastructure that integrates distributed, individually managed computational resources and presents a common user interface to these resources by providing coordinated resource-sharing in a dependable way and according to agreed-upon policies. Because the Grid integrates a large number of resources, an individual researcher can access the best resources available at any particular point in time. The Grid distributes resource-usage for maximum efficiency. The UCLA Grid Portal Software (UGP) and the UCLA Grid Architecture bring computational clusters together into a Grid. The hardware resources that make up the Grid consist entirely of computational clusters, each of which consists of a head node, compute nodes, storage nodes, network resources, software, and data resources. Individual computational clusters can be quite large, containing hundreds of nodes. By incorporating the concepts of pooled resources and Pool Users, the UCLA Grid Portal facilitates sharing resources on a broad level. The UCLA Grid Portal is software that provides a web-based Grid Portal and allows users to interact with distributed computing clusters at the campus or institutional level. A hierarchy of Grids can be created to share even great resources. The University of California has deployed the UC Grid Portal, which interacts with the Grids and Grid Portals at the ten UC campuses, making available resources that span the ten campuses. At the same time that the UGP architecture presents a uniform appearance to users, it provides for a Grid made up of diverse computing environments (hardware, operating systems, job schedulers) and autonomous administrative domains. Local organizations own and maintain control of the resources involved, and local administrative procedures and security solutions take precedence. UGP makes use entirely of open source software: Globus ToolKit, Tomcat, Java, Gridsphere and MySQL. UGP itself is also open source.

E Other Support of Investigators

Other support of the investigators follow in alphabetical order.

James Amundson – Fermilab

(Effort will be adjusted if pending proposals are funded.)

Current

- **Funding Agency:** DOE
  Project Title: Community Project for Accelerator Science and Simulations
  Total Award: 2.5M
  Person month: 3.6
  Dates: 9/15/07-9/14/12

Pending

None.

David L. Bruhwiler – Tech-X Corporation

(Please note that some of the current support will end around the time that the proposed effort will begin. The levels of effort will be adjusted, if necessary, depending on which pending proposals are funded.)

Current

- **Funding Agency:** DOE
  Project Title: Community Petascale Project for Accelerator Science and Simulations
  Total Award: 1.6M
  Person month: 1.2
  Dates: 9/07-9/12

- **Funding Agency:** DOE
  Project Title: Low-Noise Simulation of 10 GeV electron Bunches in Laser Plasma Accelerators
  Total Award: 1M
  Person month: 0.20
  Dates: 9/11-8/13

- **Funding Agency:** DOE
  Project Title: High-Fidelity Modulator Simulations of Coherent Electron Cooling System
  Total Award: 1M
  Person month: 0.15
  Dates: 8/10-7/12

- **Funding Agency:** DOE
  Project Title: Simulation of Low-Energy Ion Beam Chopping for the SNS
  Total Award: 1M
  Person month: 0.15
  Dates: 8/10-7/12

- **Funding Agency:** DOE
  Project Title: Coherent Electron Cooling Demonstration at RHIC
  Total Award: 460k
  Person month: 0.10
  Dates: 11/10-10/15

- **Funding Agency:** DOE
  Project Title: Innovative hadron accelerator designs to extend the intensity frontier
  Total Award: 150k
  Person month: 0.15
  Dates: 7/11-3/12

- **Funding Agency:** DOE
  Project Title: Design and modeling of tabletop x-ray sources
  Total Award: 150k
  Person month: 0.05
  Dates: 7/11-3/12

Pending

- **Funding Agency:** DOE
  Project Title: Integrated Modeling of Beam Dynamics, Pulse Propagation and Lasing to Design Next-Generation Free Electron Lasers
  Total Award: 150k
  Person month: 0.20
  Dates: 3/12 - 9/12

John R. Cary – Tech-X Corporation

(Effort will be adjusted if pending proposals are funded.)

Current

- **Funding Agency:** DOE
  Project Title: Framework Architecture for Core-Edge Transport Simulations (Tech-X)
  Total Award: 3.495M
  Person month: 3
  Dates: 1/15/07-7/14/12

- **Funding Agency:** DOE
  Project Title: Community Petascale Project for Accelerator Science and Simulations (Tech-X)
  Total Award: 1.6M
  Person month: 1.2
  Dates: 9/15/07-9/14/12

- **Funding Agency:** DOE
  Project Title: Analysis and Direct Numerical Simulation of RF Heating Processes and Advanced Computational Methods For Fusion Applications (U. Colo.)
  Total Award: 300k
  Person month: 0.15
  Dates: 1/1/10-12/31/12

- **Funding Agency:** DOE
  Project Title: Analysis and Direct Numerical Simulation of RF Heating Processes and Advanced Computational Methods For Fusion Applications (U. Colo.)
  Total Award: 605k
  Person month: 0.15
  Dates: 6/1/10-5/31/13

Pending

- **Funding Agency:** DOE/SC
  Project Title: (This proposal) IMMPACTS: Integrated Multiscale Modeling for Plasma Analysis and Control of Tokamak Stability
  Total Award: 4.5M
  Person month: 2.7
  Dates: 1/01/12 - 12/31/16

Estelle Cormier-Michel – Tech-X Corporation

(Effort will be adjusted if the pending proposals are funded.)

Current Support

Project	Sponsor	Period	Effort
Design and modeling of table top x-ray sources	DOE/BES	6/17/11–3/16/12	30%
Rapid Low-Noise Simulation of Ultra-bright 10 GeV Electron Bunches in Laser Plasma Accelerators	DOE/HEP	8/11–8/13	50%

Pending Support

None

Benjamin M. Cowan – Tech-X Corporation

(Effort will be adjusted if pending proposals are funded.)

Current Support

Project	Sponsor	Period	Effort
Design and modeling of tabletop x-ray sources	DOE/BES	6/17/11–3/16/12	25%
Community Petascale Project for Accelerator Science and Simulations	DOE	9/1/07–8/31/2012	15%
Rapid Low-Noise Simulation of Ultra-bright 10 GeV Electron Bunches in Laser Plasma Accelerators	DOE/HEP	2 year duration	20%
Laser-Driven Dielectric Microstructure Based Advanced X-Ray Sources	Stanford University	9/30/2011–9/29/2015	15%

Pending Support

Project	Sponsor	Duration	Effort
Modeling tools and techniques for dielectric laser accelerators	DOE/HEP	9 months	34%

Marc Durant
Software Developer II, Tech-X Corporation

Current Support

Title	Source	Period	Funding	Effort (% FTE)
Visualizing Staggered Vector Fields	DOE SBIR Phase I	06/17/11 - 03/16/12 –	$149,490	25%

Pending Support: None

Miguel Furman – Lawrence Berkeley National Laboratory
(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
ILC Damping Ring R&D effort	DOE	10/1/11 – 9/30/12	50%

Pending Support (None)

Lixin Ge

(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
Community Petascale Project for Accelerator Science and Simulation	DOE	8/1/07 – 7/31/12	50%
LHC Crab Cavity Design	DOE	8/1/11 – 1/31/12	20%
Muon Collider Coiling Cavity Design	DOE	11/1/11 – 4/30/12	30%

Pending Support

Title	Source	Period	Effort
Community Project for Accelerator Science and Simulation	DOE	7/1/12 – 6/30/15	30%
Advanced Simulations for Present and Future Nuclear Science Accelerator Facilities	DOE	7/1/12 – 6/30/17	30%

Cameron G.R. Geddes
(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
Laser-plasma accelerator and detectors for a compact tunable monoenergetic Thomson Gamma Source	DOE NNSA	10/1/11 – 9/30/14	65%
SciDAC Community Petascale Project for Accelerator Science and Simulation (COMPASS)	DOE	6/1/11 – 5/31/12	10%
Berkeley Laser Lab accelerator (BELLA) Advanced Plasma Accelerator Facility	DOE	10/1/11 – ongoing	25%

Pending Support (None)

Daniel T. Graves

(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
SciDAC – FASTMath	DOE	8/1/11 – 7/31/16	70%

Pending Support

Title	Source	Period	Effort
SciDAC-ComPASS	DOE	4/1/12 – 3/31/15	30%

Ki Hwan Lee
(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
Community Petascale Project for Accelerator Science and Simulation	DOE	8/1/07 – 7/31/12	100%

Pending Support

Title	Source	Period	Effort
Community Project for Accelerator Science and Simulation	DOE	7/1/12 – 6/30/15	30%
Advanced Simulations for Present and Future Nuclear Science Accelerator Facilities	DOE	7/1/12 – 6/30/17	30%
SBIR ERL Cavity Design	DOE	2/1/12 – 1/31/13	25%

Current and Pending Support

Xiaoye Li

(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
Community Petascale Project for Accelerator Science and Simulation	DOE	8/1/07 – 7/31/12	20%
Algorithms and Software for Communication Avoidance and Communication Hiding at the Extreme Scale (CACHE Institute)	DOE	2/1/10 – 1/31/13	20%
The Next Generation Computing for X-ray Science	LBNL (LDRD)	10/1/10 – 9/31/13	10%
Fameworks, Algorithms, and Scalable Technologies for Mathematics (FASTMath)	DOE	8/1/11 – 7/31/16	50%

Pending Support

Title	Source	Period	Effort
Advanced Simulations for Present and Future Nuclear Science Accelerator Facilities	DOE proposal	7/1/11 – 6/30/16	20%
Quantum simulations of materials and processes for solar energy conversion	DOE proposal	7/1/11 – 6/30/16	20%
Simulating the generation, evolution and fate of electronic excitations in molecular and nanoscale materials with first principles methods	DOE proposal	7/1/11 – 6/30/16	20%
GAIA: Graphical Advanced Interactive Analysis	DOE proposal	7/1/11 – 6/30/16	25%
This proposal	DOE proposal	7/1/12 – 6/30/15	10%

Zenghai Li
(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
LHC Crab Cavity Desin	DOE	8/1/11 – 1/31/12	40%
Muon Collider Cooling Cavity Design	DOE	10/1/11 – 9/30/12	40%
X-band Accelerator Structure Design	DOE	10/1/11 – 9/31/12	20%

Pending Support

Title	Source	Period	Effort
Community Project for Accelerator Science and Simulation	DOE	7/1/12 – 6/30/15	25%
Advanced Simulations for Present and Future Nuclear Science Accelerator Facilities	DOE	7/1/12 – 6/31/17	15%
APS SPX Cavity Design	DOE	2/1/12 – 1/31/13	30%

Paul Mullowney — Tech-X Corporation

(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Amount Funding	Effort (% FTE)
GPU PETSc	DOE	08/15/2011 – 08/14/2013	$1000K	50%
NL Signal Processing	DOD	06/2011 – 03/2012	$100K	15%
GPU AEM	Subcontract	— – 08/2012	$100K	20%

Pending Support

Title	Source	Period	Amount Funding	Effort (% FTE)
QCD AutoTune	DOE	02/2012 – 11/2012	100K	20%

Todd Munson — Argonne National Laboratory
(The Principal Investigator has multiple funding sources. Should there be an overlap, effort levels will be adjusted accordingly.)

Current Support

Source	Title	Months	Period	Total Award
DOE	Tools for Structured Optimization Problems on High-Performance Architectures: Lagrangians and Complementarity	6.6	10/1/09 – 9/30/12	1.1M
DOE	Next Generation Solvers for Mixed Integer Nonlinear Programs: Structure, Search, and Implementation	3.0	1/1/09 – 12/31/12	1.6M
DOE	Frameworks, Algorithms, and Scalable Technologies for Mathematics (FASTMath) SciDAC Institute	1.2	8/1/11 – 7/31/16	30M
DOE	ExM: System Support for Extreme-Scale, Many-Task Applications	0.6	10/1/10 – 9/30/13	1.0M
NSF	Center on Robust Decision Making Tools for Climate and Energy Policy	0.6	10/1/10 – 9/30/15	6.0M
NSF	Collaborative Research: Next-Generation Solvers for Mixed-Integer Nonlinear Programs: Structure, Search, and Implementation	0.0	10/1/08 – 9/30/12	0.1M

Pending Support

Source	Title	Months	Period	Total Award
DOE	IMMPACTS: Integrated Multiscale Modeling for Plasma Analysis and Control of Tokamak Stability	1.2	1/1/12 – 12/31/16	15.5M
NSF	REU Site: Summer Research Projects in Climate and Energy Policy	0.0	3/1/12 – 2/28/15	0.3M
NSF	RI: Small: Collaborative Research: Scalable Optimization Algorithms for Machine Learning that Exploit Advanced Architectures	0.6	10/1/12 – 9/31/14	0.5M

Cho-Kuen Ng
(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
Community Petascale Project for Accelerator Science and Simulation	DOE	8/1/07 – 7/31/12	30%
Accelerator Science	DOE	10/1/11 – 9/30/12	40%
Dielectric Laser Acceleration	DOE	10/1/11 – 9/30/12	30%

Pending Support

Title	Source	Period	Effort
Community Project for Accelerator Science and Simulation	DOE	7/1/12 – 6/30/15	25%
Advanced Simulations for Present and Future Nuclear Science Accelerator Facilities	DOE	7/1/12 – 6/30/17	10%

Esmond G. Ng

(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
FASTMath SciDAC Institute	DOE	9/1/11 – 8/31/16	50%
Large-scale Eigenvalue Calculations in the Study of Electron Excitation for Photovoltaic Materials	DOE	9/1/10 – 3/31/12	10%
Community Petascale Project for Accelerator Science and Simulation	DOE	8/1/07 – 7/31/12	10%
High Performance Adaptive Algorithms for Ice Sheet Modeling	DOE	9/1/09 – 8/31/12	20%

Pending Support

Title	Source	Period	Effort
Predicting Ice Sheet and Climate Evolution at Extreme Scales	DOE	10/1/11 – 9/30/16	10%
Nuclear Computational Low Energy Initiative	DOE	5/1/12 – 4/30/17	10%

Boyana Norris — Argonne National Laboratory

(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Annual ANL Funding	Effort (% FTE)
SciDAC Institute for Sustained Performance, Energy, and Resilience (SUPER)	DOE	9/11 – 8/16	$325K	15
Scalable Algorithms for Computational Differentiation of Petascale Simulations	DOE	10/10 – 9/11	$398K	25
Combinatorial Scientific Computing and Petascale Simulations Institute	DOE	7/06 – 6/11	$396K	20
Community Petascale Project for Accelerator Science and Simulation	DOE	4/07 – 3/12	$270K	20
Algorithms and Software for Communication Avoidance and Communication Hiding at the Extreme Scale	DOE	9/09 – 8/12	$349K	20
Taxonomy for the Automated Tuning of Matrix Algebra Software	NSF	9/09 – 9/11	$125K	5

Pending Support

Title	Source	Period	Effort (% FTE)
SSI/GEO: Community Model Integration Support	NSF	4/12 – 3/17	16
SciDAC (FES) Integrated Petascale Simulation of Plasma Facing Materials Response to Normal and Transient Fusion Plasmas	DOE	1/12 – 1/17	16
SciDAC (FES) Modeling Microstructural Evolution of Plasma-Facing Materials for Fusion Reactors: Development of Scalable, Data-Driven, Phase Field Models	DOE	1/12 – 1/17	12

Kevin Paul — Tech-X Corporation

(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Annual ANL Funding	Effort (% FTE)
Inverse Cyclotrons for Intense Muon Beams	DOE	8/09 – 8/12	$750k	20
Characterization of the Fast Ion Stopping Cyclotron for NSCL/FRIB	DOE	6/11 – 3/12	$150k	30
GPU Acceleration of Spin Tracking in Colliding Beam Accelerators	DOE	8/11 – 8/13	$1M	16
Rapid Low-Noise Simulation of Ultra-bright 10 GeV Electron Bunches in Laser Plasma Accelerators	DOE	8/11 – 8/13	$1M	30

(No pending support.)

Ernesto E. Prudencio — The University of Texas at Austin

(Efforts will be adjusted if pending proposals are funded.)

Current Support

Title	Source	Period	Annual UT Funding	Effort (% FTE)
Center for Predictive Engineering and Computational Sciences (PECOS)	DOE-NNSA	04/08 – 03/13	$4,000K	16
Bayesian Earthquake Source Validation for Ground Motion Simulations	KAUST	06/10 – 05/12	$145K	40
Bayesian Near Real-Time Earthquake Source Inversion	KAUST	01/12 – 12/14	$165K	42
Quantification of Uncertainty in Extreme Scale Computations (QUEST)	DOE-SC-ASCR	09/11 – 08/16	$150K	2

Pending Support

Title	Source	Period	Annual UT Funding	Effort (% FTE)
Center for UQ in Computational Science and Engineering	KAUST	01/12 – 12/14	$100K	25
Developing Mesh-Free Methods For Atmospheric Process Simulation	DOE-BER-ASCR	06/12 – 05/17	$120K	21
HPC-SI: Software Engineering Support of Computational Science	NSF	07/12 – 06/13	$500K	8
Community Project for Accelerator Science and Simulation (this proposal)	DOE-HEP-ASCR	07/12 – 06/15	$120K	21

Ji Qiang – Lawrence Berkeley National Laboratory
(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
LARP: Large Hadron Collider - LHC	DOE	10/1/11 – 9/30/12	30%
Advanced Modeling of Accelerators for Next Generation Light Sources	DOE	10/1/11 – 9/30/12	10%
Light source Related R&D	DOE	10/1/11 – 9/30/12	20%

Pending Support

Title	Source	Period	Effort
Advanced Simulations for Present and Future Nuclear Science Accelerator Facilities	DOE	7/1/12 – 6/30/17	50%

Peter Schwartz
(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
SciDAC-e: Advanced Simulation of Subsurface Flow and Transport at the Pore Scale	DOE	10/1/11 – 9/30/12	100%

Pending Support

Title	Source	Period	Effort
SciDAC 3 Plasma Edge Computation Center (PEAC)	DOE	4/1/12 – 3/31/17	62%
SciDAC 3 ComPASS	DOE	4/1/12 – 12/31/15	23%

Greg Schussman
(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
Community Petascale Project for Accelerator Science and Simulation	DOE	8/1/07 – 7/31/12	50%
SBIR Large-Scale Visualization	DOE	10/1/10 – 9/30/12	50%

Pending Support

Title	Source	Period	Effort
Community Project for Accelerator Science and Simulation	DOE	7/1/12 – 6/30/15	25%

Panagiotis Spentzouris – Fermilab

(Effort will be adjusted if pending proposals are funded.)

Current

- **Funding Agency:** DOE
  Project Title: Community Project for Accelerator Science and Simulations
  Total Award: 2.5M
  Person month: 3.0
  Dates: 9/15/07-9/14/12
- **Funding Agency:** DOE
  Project Title: GEANT4 Toolkit Evolution and Performance Optimization
  Total Award: 344k
  Person month: 1.0
  Dates: 10/1/11-11/31/12
- **Funding Agency:** DOE
  Project Title: Multi-core capable computational frameworks for offline and online applications
  Total Award: 444k
  Person month: 1.5
  Dates: 10/1/11-11/31/12

Pending

None.

Eric Stern – Fermilab

(Effort will be adjusted if pending proposals are funded.)

Current

- **Funding Agency:** DOE
  Project Title: Community Project for Accelerator Science and Simulations
  Total Award: 2.5M
  Person month: 3.0
  Dates: 9/15/07-9/14/12

Pending

None.

Jean-Luc Vay – Lawrence Berkeley National Laboratory
(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
Heavy Ion Driven Warm Dense Matter	DOE	10/1/11 – 9/30/12	50%
U.S. LHC Accelerator Research Program (Electron Cloud)	DOE	10/1/11 – 9/30/12	20%

Pending Support (None)

Stefan M. Wild — Argonne National Laboratory
(Effort will be adjusted if the pending proposals are funded.)

Current Support

Source	Title	% Effort	Period
DOE	Derivative-Free Optimization Methods for Simulation-Based Complex Systems	80	6/1/10 – 5/31/12
DOE	CACHE Institute: Algorithms and Software for Communication Avoidance and Communication Hiding at the Extreme Scale	5	10/1/10 – 9/30/13
DOE	SUPER: Institute for Sustained Performance, Energy, and Resilience	15	8/1/11 – 7/31/16

Pending Support

Source	Title	% Effort	Period
DOE/NNSA	Nuclear Computational Low Energy Initiative (NUCLEI)	18	5/1/12 – 4/31/17
NSF	Scalable Optimization Algorithms for Machine Learning That Exploit Advance Architectures	10	9/1/12 – 8/31/14

Liling Xiao
(Effort will be adjusted if the pending proposals are funded.)

Current Support

Title	Source	Period	Effort
Project X Main Injector Cavity Design	DOE	12/1/11 – 11/30/12	60%
Accelerator Science	DOE	10/1/11 – 9/30/12	40%

Pending Support

Title	Source	Period	Effort
Community Project for Accelerator Science and Simulation	DOE	7/1/12 – 6/30/15	25%
APS SPX Cavity Design	DOE	2/1/12 – 1/31/13	30%
SBIR ERL Cavity Design	DOE	2/1/12 – 1/31/13	25%

CURRENT & PENDING SUPPORT

CURRENT AND PENDING SUPPORT OF INVESTIGATORS

Key Personnel Name: Chao Yang **Check if no other support** ___

Item # 1 Title of Project: Computational Techniques for Non-crystalline X-ray Imaging

Pending: ___ Active X

Funded by: LBNL LDRD % FTE on project: 30

Period of support: 10/01/2009 – 09/30/2012 Annual funding: $100K

Item # 2 Title of Project: SciDAC FASTmath Insitute

Pending: ___ Active: X

Funded by: DOE % FTE on project: 65

Period of support: 10/01/2011 – 09/30/2016 Annual funding: $6M

Item #_3 Title of Project: _Resources for X-Ray Tomography of Whole Cells

Pending: ___ Active: X

Funded by: NIH % FTE on project: 10

Period of support: 05/06/2004 – 04/30/2015 Annual funding: $500K

Item # 4 Title of Project: _SciDAC NUCLEI__

Pending: X Active: ___

Funded by: DOE % FTE on project: 10

Period of support: 5/01/2012-4/30/2017 Annual funding: $

Item # 5 Title of Project: _SciDAC ComPASS__

Pending: X Active: ___

Funded by: DOE % FTE on project: 10

Period of support: 7/01/2012-6/30/2015 Annual funding: $