Proposal for a Fermilab Working Group on a Hadronic and Electromagnetic package based on the GENIE event generator

A. Mazzacane* G. Perdue†

September 16, 2015

Abstract

Present and future High Intensity experiments at Fermilab have an increasing need to fully understand the effects of hadrons interacting in their detectors. Standalone event generators [1, 2, 3, 4, 5, 6] are available to implement intranuclear transport models simulating the interactions of particles with nuclear matter. However, such models have limited predictive capability because: a) the target is an isolated nucleus; and b) clusterization, de-excitation and evaporation of the final nucleons are rarely implemented. The GENIE simulation package, the MC event generator for every neutrino experiment at Fermilab, implements a unique approach where event generation is aware of the detector geometry and the elementary interaction occurs with a specific nucleus inside the detector. The REDTOP project[7], where a reliable simulation of the hadronic interactions of the beam with the target is crucial to understand the physics background, has successfully demonstrated an initial interface to the standalone hadronic interaction models in GENIE.

In this document, we propose a project to scale these interfaces into a more general simulation package for the Intensity Frontier community. The package, structured as an add-on to GENIE, will allow the user to generate events inside a gdml-root described geometry using an external intra-nuclear transport model as the generation engine. It will further enable neutrino experiments to produce a more accurate simulation of the nuclear remnant and de-excitation products. This is particularly important for experiments using liquid Argon TPCs that are sensitive to soft interactions near the neutrino vertex.

There is a short and a long-term component to this work. The short-term project is to implement and test the interfaces, and validate the performance of the total simulation stack with data that will take less than two years, with some aspects of the project coming online very quickly to help meeting the physics needs of running experiments. This project

*mazzacan@fnal.gov
†perdue@fnal.gov

will be most successful with additional resources in the form of a post-doc and a computing intern. It would be possibile to share the post-doc with the Neutrino Division or the Theory Division to help ensure a good career outcome while still keeping the project on schedule. There is also a long-term project in the form of support for these advancements with the goal of GENIE becoming useful to an entirely new set of users - the hadron scattering community.

1 Executive Summary

Fermilab is establishing itself as the world leader on the Intensity Frontier, making the need for accurately understanding the interactions of the beam with the nuclei in the machine-detector interface and the detector increasingly important. Intense neutrino beams generate hadronic particles in the materials immediately upstream the detector as well as inside the fiducial volume of the latter. Excited nuclei (via weak interactions with the neutrinos) de-excite into nuclear remnants and nucleons which will, consequently, generate a signal in the detector. The situation is even worse for short-baseline neutrino experiments, where even a relatively small contamination of the intense neutrino beam with hadrons will produce undesired hadronic events into the detector. Furthermore, the availability of intense proton beams at Fermilab in the PIP-II era, will likely attract new experimenters and new projects requesting hadron beams (p, K, π, etc.). This is the case, for example, for REDTOP, a project in the design stage that will detect rare eta meson decays produced by the scattering of protons on a Nb target. For such experiments, understanding the secondary particles produced at the target is of paramount importance to properly design the experiment. Other Intensity Frontier experiments and projects at Fermilab will benefit considerably from a more realistic description of the hadronic interactions in their detector such as P-1067.

Several computer-based intranuclear transport models have been implemented in the last few years in order to simulate the scattering of a particle off a nucleus. Given the complexity of the underlying models, those programs are written and maintained mainly by theorists. Several[1, 2, 3, 4, 5, 6] are currently considered as state-of-the-art. Observations from experiments with hadron beams are invariably compared with one or more of them. However, in spite of the extraordinary amount of theoretical physics embedded in those models, from the experimentalist point of view they fall short in at least two respects:

1. The nuclear target is a standalone nucleus surrounded by vacuum;

2. Except for one case[3], nucleons in the final state are listed as free (unaggregated) particles.

As a consequence of 1. the final state particles from the primary interaction are also generated in vacuum. When those particles are propagated throughout the detector during the next step of the simulation (i.e. Geant4), an unrealistic situation occurs, since the matter in the target around the struck nucleus is not taken into account. The immediate consequence is an underestimation of the secondary particles generated inside the target.

As a consequence of 2. the final state nucleons are not condensed into on-shell ions (deuterium, tritium, alpha, etc.) and excited nuclei which can, in turn, de-excite with the production of prompt photons and/or evaporate into smaller and faster nuclei. In both cases, the net effect on the simulation of the experiment is an underestimation of the particles expected into the detector (along with an erroneous kinematics).

One simulation instrument which has correctly addressed the point 1. above is the GENIE Neutrino MC[5]. The approach taken by GENIE, unique among event generators, is, in fact, to select a nucleus and an interaction among those available after a pre-analysis of the nuclei distributed along the path of the beam. Furthermore, GENIE's architecture offers several other tools useful to improve the quality of the simulation; they will be discussed in some details in Sec. 3.

Unfortunately, the physics interactions incorporated into GENIE's official distribution encompass only neutrino physics. The REDTOP project, where the physics models and the correct description of the target and detector geometry are equally important, has made a considerable and successful investment to complement GENIE with the hadronic models considered above as well as to a set of clusterization-evaporation libraries through a set of interfaces. At present, those interfaces are tailored to the needs of the project and some of the features reflects the range of beam energies where the experiment is intended to run. We believe, however, that the work initiated by REDTOP could be made more ample and consolidated into a self-contained add-on to GENIE. In particular, the project so far is a successful demonstrator for REDTOP, but more work is necessary to make it a generally useful hadron-scattering event generator.

Among the Monte Carlo simulation packages presently available, MARS15 provides an interaction engine based on experimental data, a clusterizer and evaporation algorithm finely tuned to the latter and a geometry aware transport mechanism. MARS15 is the de-facto standard package to estimate the particles fluence inside a detector. A useful complement to MARS15 approach would be to employ its superb event generation engine in an event-based (rather than fluence based) framework. A way to do that is to implement an interface between GENIE and MARS15 where the event generation systems of the former request the latter to simulate an interaction between the beam and the target.

The purpose of this proposal is to request from the Scientific Computing Division the resources necessary to establish a new group to scale the already successful demonstrator project developed by REDTOP into a general purpose hadron-scattering event generator, and to make the more sophisticated nuclear codes easily accessible to the neutrino community. There is a short-term component to this task which we may achieve expeditiously with new resources in the form of a post-doc and a computing intern. These individuals will guarantee the project may be completed in a timely fashion to positively impact Fermilab's short-baseline neutrino program. This will also ensure the new functionality is available to REDTOP and other hadron-scattering experiments. This project consists of well-defined steps, and it may be broken into several iterative stages to ensure timely impact on running experiments. Broadly, the steps are:

Short-term research program

1. Creating an add-on to GENIE event generator which interfaces to selected hadronic intranuclear transport models.

2. Complementing the add-on of point 1. with one (or multiple) clusterizer

and evaporation/de-excitation library(s).

3. Creating an add-on to GENIE event generator with an interface to the electromagnetic models of GEANT4[9].

4. Creating an interface to the MARS15 Monte Carlo package[8].

5. Creating a testing suite for validation of the hadronic generators with the experimental data.

Long-term research program

1. Maintaining the above package by re-aligning the interfaces with the newer releases of GENIE and the hadronic generators.

2. Establishing a liaison with the experiments and/or users requesting potential upgrades of the package.

The longer-term component - serving the hadron scattering community - also strongly benefits the neutrino community by making overall validation more meaningful and stringent. We would like to stress that this project will be very valuable for the neutrino community regardless of whether hadron-scattering experiments become a major part of Fermilab's program.

2 Montecarlo simulations for fixed target and neutrino experiments

Among the simulation packages presently available to the experimenter in High Energy and Nuclear Physics, GEANT4[9] is by far the most widely used. However, while its particle transport system of particles throughout the matter is unsurpassed, it is very rarely used as an event generator. Instead, the preferred approach is that of employing a dedicated event generator which will reproduce the physics of interest with a specific model and, in a second step, of requesting GEANT4 to propagate throughout the volumes of the detector the secondary particles previously generated. This is especially true for fixed target and neutrino experiments. There are multiple reasons for that; the two most noteworthy are:

- the step-by-step approach used by GEANT4 to probe the interaction between particles and nuclei is very inefficient at the elementary level when the cross sections are relatively small. For example, the probability of inelastic scattering of a proton with kinetic energy of few GeV off a 1mm thick Nb target is about 0.5%. Therefore, the vast majority of events generated with GEANT4 will represent uninteresting physics (energy loss, elastic scattering, etc.), forcing the user to waste a large amount of computing resources. The situation is even more dramatic when simulating neutrino interactions.

- several physics models implemented in GEANT4 are optimized for reproducing the most realistic detector response, rather than a true primary interaction between the probe and the target nucleus. With this approach, while energy deposition and geometrical position of the secondaries replicate (in most cases) reliably the hits expected in the detector, the kinematics of the primary interaction is rarely modeled in the proper way.

The most simplistic event generation approach taken by GEANT4 is still very useful when the experimenter wants a rough idea of what to expect in his detector and, above all, when the expected (hadronic) background is small. Furthermore, the electromagnetic models found in GEANT4 are considered very reliable by the scientific community. On the other side, when a more realistic description of the primary interaction is required and/or a large number of protons and neutrons are potentially present along with the main physics channel, then one has to resort to a more complete physics model. For example, the two hadronic models implemented in GEANT4 for the scattering of a hadron onto a nucleus, Bertini and BIC (Binary Intranuclear Cascade) limit their final states to protons, neutrons and pions (the latest version of BIC will consider Kaons as well) while completely neglecting other mesons, all barionic resonances and ions (like Deuterium and He3) and, even worse, any excited nuclear remnant which can potentially produce gammas and other barions. The kinematics and the multiplicity of the final state is not well reproduced as well with known limitations especially with neutrons. While the latest version of the models are reproducing the development of hadronic showers in a satisfactory way (through the BERTINI-HP and SHIELDING physics lists) they are not recommended for use as primary event generator of hadronic interactions.

On the other side, a plethora of dedicated packages, whose exclusive intent is to model hadronic interaction, is available to the experimenter. These are commonly adopted by experiments at intermediate energies (i.e., Hades, Wasa, Crystal Ball, etc.) where it is important to have an full understanding of the final state. The physics underneath those models is usually impressive and their development is done by nuclear physics theorists and the applications spans from proton and neutron experiment to heavy ions one. As mentioned in Sec. 1, two features, quite common with all those packages, strongly affect their use when trying to simulate an experimental apparatus:

1. The nuclear target is a standalone and isolated nucleus in a fixed position of the laboratory. This is in stringent contrast to a realistic experimental situation where the nucleus is part of a material volume (for example the target) and were the nuclei on the path of the beam are different, belonging to specific volume of the apparatus (the target, the gas, the beam pipe, the supports, etc.). Even if the secondary particles generated from the interaction have the correct multiplicity and kinematics, their transport to the rest of the detector occurs in vacuum, neglecting the effect on them from the material immediately surrounding the struck nucleus. The latter might have a non-negligible effect on the secondaries, since it

could induce either a tertiary interaction (with production of even more final state particles) and/or a change in the kinematics (for example, via elastic scattering or electromagnetic energy losses.

2. In all cases except INCL++ and MARS15, the nucleons in the target nucleus reappear in the final state as individual, sometimes off-shell, particles (eventually, after a change exchange process) with no attempt to freeze some of them (for example, the spectator nucleons) into a bound, on-shell ion or nuclear remnant. This situation is obviously unrealistic and the subsequent propagation step (usually performed by GEANT4) is fed with the wrong information. In order to completely define a realistic final state, two more algorithms need to be applied to the event generator output:

   (a) a particle clusterizer, whose task is to analyze the kinematics of the available nucleons and to associate some of them into barionic clusters (alpha particle, He ions, Deuteron, etc.) and nuclear remnants (smaller nuclei);

   (b) a nuclear evaporator/de-excitator, whose task is to analyze the excitation energy and the angular momentum of the nuclear remnants and, eventually, of breaking them into smaller clusters with an associated photon (often with an energy of several tens of MeV).

We believe that an event generator cannot be considered reliable for applications in High Intensity experiment unless the two limitations above are overcome.

3 The GENIE event generator

Almost unique among the available event generators, GENIE addresses all points discussed in Sec. 2, in particular in relation to the awareness to the geometry of the apparatus. The latter can be described either with a root TGeo file or via a gdml description. The approach taken by GENIE, is, in fact, as follow:

1. The distribution of nuclei along all possible beam trajectories throughout the detector volume are analyzed prior the starting of the generation process;

2. For all nuclei species found , a list of possible interaction is made, according to a user-defined prescription;

3. Subsequently, during the event generation, GENIE randomly selects a nucleus and an interaction based on the pre-made probability table.

4. A final state with the corresponding kinematics is, finally, generated and returned to the user.

The list of interactions is defined via an xml file; that way, only the physics of interest is considered and the combination of interactions is controlled directly by the user. Consequently, the event generation is very efficient, since it does not require a stepping of each particle trough the detector volumes and only the desired interactions take place. Among the other useful tools offered by GENIE's architecture is the class describing the incoming beam. Such a class allows the user to define a complex beam in several formats:

- using an XML file;
- with a text based file;
- with a root histogram;
- with a root ntuple;
- with a mathematical formula.

Both the energy spectrum and the particle composition can be specified along with the position and the opening angle.

In all respects, the GENIE framework is very well suited to high intensity experiments, being able to efficiently generate events in a realistic geometry and turning on only the desired interactions. As note previously, it falls short in three respects:

1. The physics models and the interactions available in the official distribution only address neutrino physics;
2. Nuclear structure and transport codes are not as sophisticated as what is available in dedicated programs;
3. There are no mechanisms of electromagnetic energy losses or electromagnetic scattering implemented.

4 MARS15

The MARS15 simulation package has few peculiarities that are rarely found in High Energy physics. First of all, rather that event-based, MARS15 has a particle-weight based approach which is especially precious when the experimenter needs to estimate particle fluence in the detector. Secondly, it has a phenomenological and consistent approach to the microscopic interaction between a particle and a nucleus. In fact, not only the intra-nuclear transport code is based on experimental measurements but, furthermore, the package contains also a self-contained clusterizer and an evaporation library which are fully tuned to the main interaction package in order to reproduce the experimental data.

On the other side, sometimes an event-based approach is useful as well, to explore some specific aspects of the signal or of the background. We propose to complement the standalone MARS15 program with an interface between

GENIE and its excellent interaction engine so that MARS15 can be used on an event-based approach. Another important advantage of this proposal is that MARS15 physics models can be directly compared with all the other models contained in the hadronic add-on. Since the generation environment (including the beam and the detector) will be the same for all those generators, only the fundamental models will be probed and exposed.

5 A hadronic and electromagnetic interaction add-on for GENIE

The REDTOP Collaboration is currently exploring the feasibility of a High Intensity experiment using one of Fermilab's low energy proton beams. Given the very large number of simulated events required and the need for a detailed description of the primary interaction (to estimate the background with a good confidence level), none of the available simulation packages satisfy their requirements. Consequently, they wrote some ad-hoc interfaces to use the most popular hadronic interaction generator inside a (slightly modified) GENIE framework. The interaction engine is polled at run time by GENIE's event generation mechanism which request the former to generate a final state corresponding to a specific initial state. The final state is positioned inside the detector volumes according to GENIE's prep-processed interaction probability tables. For each event, a new initial state is passed to the interaction engine which return a new final state. Similarly, REDTOP has realized a family of interfaces between GENIE and the electromagnetic library of GEANT4. The latter provided information on the electromagnetically induced background.

The work initiated by the REDTOP Collaboration, while tightly tailored to the physics and the detector of that experiment., could provide the starting point of a broader and more substantial project which will bring to the scientific community a well maintained add-on to GENIE containing the interface between that framework and a selected number of standalone hadronic and electromagnetic event generators. From a technical point of view, the design of the add-on will go through the following steps:

1. Minor changes need to be applied to GENIE's framework in order to accommodate the expanded physics of the external packages. Most notably, the following information need to be added where necessary:

   (a) The Particle class need to be expanded to include parameters related to nuclear states (i.e., the excitation energy and the angular momentum);

   (b) The geometry has to be accessible in the interaction class, in order to provide information peculiar to the interaction with a particular material (for example, to calculate the energy loss of a charged beam);

(c) The primary event vertex also need to be accessible in the interaction class, to complement the information of point (b);

(d) The beam description class must be able to handle particle of non-zero mass (at present, only neutrinos are allowed);

(e) A more flexible way of registering new software modules need to be implemented.

2. The majority of external event generators considered are standalone application which do not link other packages. This is the case, for example, of GiBUU, Urqmd, PHSD and MARS15. On the other side, GEANT4 is natively available as a shared library while PYTHIA and INCL++ are able to run standalone or linked to other main programs. When that happens, such event generators need to be complemented with an interface in their native language (fortran77 or fortran90 in most cases) and recompiled as a shared library. That interface serves two purposes: a) receiving from GENIE information at run time on the initial state of the event; b) exposing, at the end of the generation process, the internal variables containing the kinematics of the final state. Since an external package is subject to changes/upgrades by the collaborations which owns and maintains it, the corresponding interface requires constant maintenance as well.

3. In order for GENIE to exchange information both-ways with the external generator, a second interface is required for each external package being linked. Such interface must match the one the external package side. Since the latter is changed every time the main library is upgraded, frequent modifications are required to the former in order to keep the two synchronized.

4. As discussed in detail in Sec. 2, many hadronic interaction generators only provide a list of final state nucleons. Clusterizers and evaporation/de-excitation libraries exists and need to be considered in the present proposal if a realistic package has to be implemented. The interface to them follows the same scheme as described in 2. and 3., with a pair of linked interface per each clusterizing and de-exciting model considered.

5. For ease of usability with GENIE and for a most efficient maintenace of the package, the proposed add-on has to be structured in a way that can be easily linked /de-linked to the main program. A separate document will be submitted with the technical details on the architecture.

6. The add-on will be important for several collaborations in the high intensity and in the neutrino fields. In particular, liquid Argon TPCs will be very sensitive to energy around the interaction vertex and this upgrade will address their needs in a very expeditious manner. Appropriate documentation must be created and maintained reflecting the approaches of each scientific community.

7. Create a web site as a front-end to the users.

8. While, in the long term, the list of potential event generators can increase, we will initially concentrate on the following list of event generators, clusterizers and de-excitation libraries:

   Event generators:

   (a) Urqmd;
   (b) PHSD;
   (c) GiBUU;
   (d) INCL++;
   (e) PYTHIA6
   (f) PYTHIA8;
   (g) GEANT4 - electromagnetic library only;

   Clusterizers:

   (a) K. AlWaleed;

   Evaporation/de-excitation libraries:

   (a) ABLA07;
   (b) ABLA++;
   (c) GEMINI++
   (d) K. AlWaleed

6 Proposal to Fermilab Scientific Computing Division

The pourpose of this document is that of encouraging the Fermilab Scientific Computing Division to start a new scientific group with the goal of pursuing the points described in Sec. 5. The advantages to the scientific community from the availability of such an add-on are multiple. First of all, the simulation of a particular apparatus can be studied with events generated by unrelated packages, each one adopting an independent physics model. Comparing the outcome of those simulations will provide a better understanding of the systematic errors related to the physics model adopted. Secondly, the outcome of those packages can be directly compared within the same underlying framework, the latter providing a common experimental environment (beam and experimental apparatus). That comparison could help the authors to get a better insight on their algorithms. Third, the efficient event generation mechanism implemented in GENIE will allow the generation and the reconstruction of a considerably larger sample of events.

Given the large variety of external packages we are considering, each one carrying a different architecture and different parameters, and the large number of tasks to be fulfilled, we estimate that, besides the proponents, two more full time people need to participate into the project:

- a post-doc well acquainted with physics models and event generators. The optimal profile would be that of a nuclear physics or phenomenological theorist. Half of the post-doc's time would be dedicated to GENIE and half to another, releated physics project. Their program would be designed explicitly to provide a clear career path forward with all the requisites for finding permanent employment in the field. The funds for that position could be, eventually, shared with Fermilab's theory division;

- a computer expert intern (with a temporary contract of 1-2 years) capable of assisting into the development and maintenance of the interfaces and with the more technical aspects discussed in Sec. 5.

A. Mazzacane would serve as the supervisor for these individuals, with G. Perdue continuing to coordinate the overall Fermilab GENIE effort. We forecast that the present project will be important to most of Fermilab's neutrino experiments, and particularly to its future long and short-baseline programs. Therefore, intend to fully commit to its success.

References

[1] GiBUU

[2] UrQMD

[3] INCL++

[4] PYTHIA

[5] GENIE

[6] PHSD

[7] Paper in preparation. Invited seminar at University of Chicago.

[8] MARS15

[9] GEANT4