44. Monte Carlo Neutrino Generators

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Monte Carlo neutrino generators are programs or libraries which simulate neutrino interactions with electrons, nucleons and nuclei. In this capacity their usual task is to take an input neutrino and nucleus and produce a set of 4-vectors for particles emerging from the interaction, which are then input to full detector simulations. Since these generators have to simulate not only the initial interaction of neutrinos with target particles, but re-interactions of the generated particles in the nucleus, they contain a wide range of elementary particle and nuclear physics. Viewed more broadly, they are the access point for neutrino experimentalists to the theory inputs needed for analysis. Examples include cross section libraries for event rate calculations and parameter uncertainties and reweighting tools for systematic error evaluation.

Neutrino experiments typically operate in neutrino beams that are neither completely pure nor mono-energetic. Generators are a crucial component in the convolution of beam flux, neutrino interaction physics, and detector response that is necessary to make predictions about observable quantities. Generated events are used to define experimental analyses, like event selection criteria, for efficiency determination and background subtraction. Similarly they are used to relate reconstructed quantities back to true quantities. In these various capacities they are used from the detector design stage through the extraction of physics measurements from reconstructed observable. Monte Carlo neutrino generators play unique and important roles in the experimental study of neutrino interactions and oscillations.

There are several neutrino event generators available, such as ANIS [1], GENIE [2,3], GiBUU [4,5], MARLEY [6], NEGN [7], NEUT [8], NUANCE [9], the FLUKA routines NUNDIS/NUNRES [10,11], and NuWro [12], as well as tools to facilitate cross-generator comparisons, such as NUISANCE [13]. Historically, experiments would develop their own generators. This was often because they were focused on a particular measurement, energy range, or target, and wanted to ensure that the best physics was included for them. These 'home-grown' generators were often tuned primarily or exclusively to the neutrino data most similar to the data that the experiment would be collecting. A major advance in the field was the introduction of conference series devoted to the topic of neutrino interaction physics, NuINT (https://indico.cern.ch/event/703880/) and NuFACT (https://indico.cern.ch/event/855372/) in particular. Event generator comparisons have been a regular staple of the NuINT conference series from its inception, and a great deal of information on this topic can be found in the Proceedings of these meetings. These meetings have facilitated experiment-theory discussions leading to the first generator developed by a theory group (NuWro) [12], the extension of established nuclear interaction codes (FLUKA and GiBUU) to include neutrino-nuclear processes [4,5,10,11], and inclusion of theorists in existing generator development teams.

These activities have led to more careful scrutiny of the crucial hadron and nuclear theory inputs to these generators, which is evaluated in particular through comparisons to electron-scattering data. At this point in time all simulation codes face challenges in describing the full extent of the lepton scattering data, and the tension between incorporating the best available theory versus obtaining the best agreement with the data plays out in a variety of ways within the field. For the field to make progress, inclusion of state of the art theory needs to be coupled to global analyses that correctly incorporate correlations between measurements. Given the rapid pace of new data and the complexity of analyses, this is a significant challenge for the field in the coming years.

There are many neutrino experiments which use various sources of neutrinos, from reactors, accelerators, the atmosphere, and astrophysical sources, thereby covering a range of energies from MeV to TeV. Much of the emphasis has been on the few-GeV region in the generators, as this is the relevant energy range for short- and long-baseline neutrino oscillation experiments. These generators use the impulse approximation, which treats the nucleus as a collection of independent nucleons and the primary interaction occurs between the probe and a single nucleon, for most of the initial interaction, and subsequently simulates the interactions of secondary particles in the nucleus in semi-classical ways. Semi-classical hadron transport approaches are commonly used as they are able simulate a variety of nuclei in a single model, fully describe complex multi-particle final states, and for practical considerations as these approaches are fast. However, there are several challenges facing these simulations coming mainly from the complexity of the nuclear physics, and the need to avoid double counting in combining perturbative and non-perturbative models for the neutrino-nucleon scattering processes. The overall validity of this impulse approximation-based scheme, and in particular the importance of scattering channels that involve more than one nucleon, is a crucial question that is the topic of much current work. While generators share many common ingredients, differences in implementation, parameter values, and approaches to avoid double counting can yield dramatically different predictions [14]. In the following sections, interaction models and their implementations, including final-state interactions of hadrons produced in the nuclei, are described.

In order to assure their validity, neutrino event generators are tuned and validated against a wide variety of data. This means that the quality of the outputs from generators is limited by the quality of experimental data. The existing neutrino-nucleon and neutrino-nucleus scattering data sets are not restrictive enough to eliminate many approaches. On the other hand, there are various precise data sets, which use photon, charged lepton, and hadron probes. These data sets are extensively used to validate the generators. The results from these external data tuning exercises are important for experiments as they quantify the uncertainty on model parameters, needed by experiments in the evaluation of generator-related systematic errors. Electron scattering data plays an important role in determining the vector contribution to the form-factors and structure functions, as well as in evaluating specific aspects of the nuclear model [15, 16]. Hadron scattering data is used in validating the nuclear model, in particular of interactions between hadrons produced in the primary interaction and the residual target nucleus (final state interactions). As mentioned, tuning of neutrino-nucleon scattering and hadronization models relies heavily on the previous generation of high energy neutrino scattering and hydrogen and deuterium bubble chamber experiments. More recent data from the K2K, MiniBooNE, NOMAD, SciBooNE, MINOS, T2K, ArgoNEUT, MINERvA, NOvA, MicroBooNE, ICARUS, SBND and Ninja experiments has been, or will be, used for this purpose, although caution is advisable due to possible biases that mismodeled nuclear effects might introduce. In practice, there are often choices to be made about which models to include in an overall simulation, and which data sets to use for tuning. The process of developing a comprehensive tune in GENIE is discussed in Ref. [3].

However, all the recent experiments use nuclear targets and it is challenging to disentangle the neutrino-nucleon interaction from the effects of the nuclear environment. For example, it is difficult to separate charged current quasi-elastic scattering from the multi-nucleon quasi-elastic like scattering or single pion production, in which a pion is absorbed in the nucleus. Sometimes, there are tensions between the data sets from different experiments. Data on multi-pion and meson production are limited, but are anticipated to be measured in the near future experiments. Next generation experiments are expected to provide better detection capabilities with higher statistics and these data will help in evaluating and validating the models implemented in the generators.

44.1 Neutrino-Nucleon Scattering

Event generators typically begin with free-nucleon cross sections which are then embedded into a nuclear physics model. The most important processes are quasi-elastic (elastic for neutral current (NC)) scattering, resonance production, and non-resonant inelastic scattering, which make comparable contributions for few-GeV interactions. The neutrino cross sections in this energy range can be seen in Figure 52.1 of this *Review.*

44.1.1 *Quasi-Elastic Scattering*

The cross section for the neutrino nucleon charged current quasi-elastic scattering is described in terms of the leptonic and hadronic weak currents, where dominant contributions to the hadronic current come from the vector (V) and axial-vector (A) form factors. Contributions from the pseudoscalar form factor (P) are typically small for muon and electron neutrinos and are related to the axial form factor (A) assuming partially conserved axial currents (PCAC). Owing to isospin symmetry, the vector form factors are related to those measured by precise electron scattering experiments [17]. Therefore, most of the generators use parametrizations of these form factors taken directly from the data. For the axial form factor there is no such precise experiment, and most of the generators use a dipole form [18]. Generally, the value of axial form factor at $q^2 = 0$ (q is the four-momentum transfer) is extracted from the polarized nucleon beta decay experiment. However, the selection of the axial vector mass parameter depends on each generator, with values typically around 1.00 GeV/c^2. Recently, there are several attempts to use the other functions for the axial form factors [19,20] and some generators have already implemented these form factors [8,21].

44.1.2 *Inelastic Production*

Most generators use the prescriptions of Rein-Sehgal [22] to simulate neutrino-induced single pion production, or updated versions that incorporate lepton mass terms and pion pole contributions [23,24]. To obtain the cross section for a particular channel, they calculate the amplitude for the production of each resonance multiplied by the probability for the decay of that resonance into that particular channel. Implementation differences include the number of resonances included, whether the amplitudes are added coherently or incoherently, the invariant mass range over which the model is used, how non-resonant backgrounds are included, inclusion of lepton mass terms, and the model parameter values (in particular the axial mass). In this model it is also possible to calculate the cross-sections of single photon, and η production by changing the decay probability of the resonances, which are included in some of the programs. However, it is known that discrepancies exist between the recent pion electro/photoproduction data and the results from the simulation data with the same framework, i.e. vector part of this model. There are several attempts to overcome this issue [25] and some of the generators started using more appropriate form factors. Recently, there are approaches that improve the theoretical description of non-resonant contributions in the resonance region, [26–28], and which account for interference between resonant and non-resonant amplitudes. This work is expected to be implemented in the generators soon. GiBUU and NuWro generators do not use the Rein-Sehgal model, and instead rely directly on electro-production data for the vector contribution and fit bubble chamber data to determine the remaining parameters for the axial contribution [29–32]. The dynamical coupled-channel model, which has been developed to simulate various electro- and photo-meson productions, was extended to simulate the neutrino single pion production [33]. In this approach pion-nucleon scattering is used to fix the form of the axial current at $q^2 = 0$. This model is also being implemented and expected to be available in some of the generators in future.

44.1.3 *Deep and Shallow Inelastic Scattering*

For this process the fundamental target shifts from the nucleon to its quark constituents. Therefore, the generators construct the nucleon structure functions F_2 and xF_3 from parton distributions for high Q^2 (the DIS regime: W$\gtrsim$ 2 GeV/c^2 and $Q^2 \gtrsim 1$ GeV^2) to calculate the direction and momentum of the lepton. The first challenge is in extending this picture to the lower values of Q^2 and W that dominate the available phase space for few-GeV interactions (the so-called 'shallow inelastic scattering', or SIS regime). GRV98LO parton distribution functions [34] with the corrections proposed in [35, 36] are widely used, while others [10] implement their own modifications to the parton distributions at low Q^2. Both DIS and SIS generate hadrons but their production depends on each generator's implementation of a hadronization model as described in the next section. There are various difficulties not only in the actual hadronization but the relation with the single meson production. It is necessary to avoid double counting between the resonance and SIS/DIS models, and all generators are different in this regard. The scheme chosen can have a significant impact on the results of simulations at a few-GeV neutrino energies. For simulating ultra-high energy interactions currently being studied with neutrino telescopes, fully partonic descriptions, which utilize beyond-leading-order pQCD calculations [37, 38] are the norm [39].

44.2 Hadronization Models

For hadrons produced via baryonic resonances, the underlying model amplitudes and resonance branching fractions can be used to fully characterize the hadronic system. For shallow- and deep-inelastic scattering, a hadronization model is required. Most generators use PYTHIA [40] for this purpose, although some with modified parameters. In addition some implement their own models to handle invariant masses that are too low for PYTHIA, typically somewhere around 2.0 GeV/c^2. Such models rely heavily on measurements of neutrino hadro-production in high-resolution devices, such as bubble chambers and the CHORUS [41] and NOMAD experiments [42], to construct empirical parametrizations that reproduce the key features of the data [43, 44]. The basic ingredients are the empirical observations that average charged particle multiplicities increase logarithmically with the invariant mass of the hadronic system, and that the distribution of charged particle multiplicities about this average are described by a single function (an observation known as KNO scaling [45]). The multiplicity of the neutral particles are usually obtained by scaling the charged particle multiplicity. Simple parametrizations to more accurately reproduce differences observed in the forward/backward hemispheres of hadronic systems are included in GENIE, NEUT, and NuWro.

44.3 Nuclear Physics

The nuclear physics relevant to neutrino-nucleus scattering at few-GeV energies is complicated, involving Fermi motion, nuclear binding, Pauli blocking, in-medium modifications of form factors and hadronization, intranuclear rescattering of hadrons, and many-body scattering mechanisms including long- and short-range nucleon-nucleon correlations.

44.3.1 *Treatment of nuclear effects*

In order to obtain the cross-section off nucleons in the nucleus, it is necessary to take into account various in-medium effects. Most of the models used for neutrino-nuclear scattering kinematics were developed in the context of few-GeV inclusive electron scattering, by experiments going back nearly 50 years. The basic models employed in event generators rely on impulse approximation schemes, the most simple of which is the Relativistic Fermi Gas Model. The most common implementations have been the Smith-Moniz [46] and Bodek-Ritchie [47] models. However, the results from neutrino-nucleus scattering experiments in 2000 and afterwards, beginning with K2K, MiniBooNE have shown large discrepancies from the naive expectation from the models. Most striking differences are a suppression of forward going muons (low Q^2), a high Q^2 enhancement in the event rate, and an overall larger than expected number of observed events. In order to reproduce the data, the quasi-elastic axial mass was used as the effective parameter and increased by roughly 20% from the nominal values obtained by an earlier generation of bubble chamber experiments using hydrogen or deuterium [18]. This inconsistency between nucleon and nucleus targets suggests that the simple nuclear model is not appropriate in describing the data. Moreover, these simple Fermi-Gas models are not expected to describe the kinematical distributions of final state nucleons. Therefore, several generators have to implement better models, such as local Fermi-Gas model or more sophisticated models. Within the electron scattering community, the analogous calculations have for decades relied on spectral functions, which incorporate information about nucleon momenta and binding energies in the impulse approximation scheme [15]. Therefore, most of the generators have implemented the realistic spectral functions in their latest releases.

Actually, the discrepancies in small q^2 could not be solved alone by just introducing the local Fermi-gas model nor spectral function models. This implies that the additional medium correction effects are needed to be taken into account. One of the implemented solutions is the local Fermi-Gas model with medium correction calculated using the random phase approximation, which is known to give large suppression in small q^2 [48,49]. Although, the fundamental parts of the models are same, actual implementations are quite different between the generators. Especially, the constructions of the final state hadron kinematics are quite different. Especially for the quasi-elastic scattering case, treatment of the nucleon masses in the nucleus, the binding and the separation energies are sometimes quite different [50]. Recently, Super-Scaling model with relativistic mean field theory effects (SuSAv2) [51,52] is implemented in some of the generators. Indications of the suppression in small q^2 in the single pion productions were also observed in K2K and MiniBooNE and it is clearly observed at the MINERνA and NOνA experiments. However, the models to explain the suppression have not been implemented, other than the phenomenological ones. Also, q^2 dependence of the cross-section is largely model and parameter dependent. Further studies of newly implemented single pion models may give new insights. The cause of the discrepancy of small q^2 seems to be identified but the issue of the observed interaction rates are not solved. This implies that there must be some interaction channels which are missing and not considered in the generators.

These led to a revisitation of the role played by excitation of multiple particle-hole states in the nucleus, and the experimental study of these scattering channels is an area of intense experimental interest [53]. The contribution of these scattering processes is an extremely active area of theoretical research as well, with significant implications for generators and analyses [54]. Several approaches, ranging from strictly phenomenological descriptions to full theoretical calculations, have recently been incorporated into generators [55–57]. One example of a phenomenological approach utilizes an Effective Spectral Function [58] and a Transverse Enhancement Model [59], which together encapsulate information derived from electron scattering experiments at relevant kinematics. The microscopic model of Nieves and collaborators is now available in GENIE and NEUT [60, 61]. SuSAv2 model [52] also has capability to simulate this multi-nucleon quasi-elastic like interaction and is also implemented in GENIE.

One of the challenges in incorporating full theoretical models of these processes is that they are typically slow, so generators have developed new approaches whereby much of the computation is done offline, and the generators simply read in the hadronic tensor components. This allows for a full prediction of the lepton kinematics, however the ability to simulate the hadronic component of these multinucleon states then relies on separate models. The other challenge is that the theoretical models are not designed to describe exclusive final states. These approaches, while making simulations computationally tractable, neglect correlations between the lepton and hadron kinematics. Also, there are limitations of the model itself to describe some of the kinematic regions. However, the generators need to simulate final all the state particles and thus, several assumptions are made by authors of the generators from time to time.

Also, it is known from photo and electro-nuclear scattering that the Delta width is affected by Pauli blocking and collisional broadening. These effects are included in some, but not all generators.

The remnant nucleus after the scattering is usually in an excited state. Therefore, the remnant may emit gamma-rays, additional nucleons or an alpha particle during the de-excitation process. This de-excitation gamma-ray is used in searching for proton decay in water Cherenkov detectors. Some generators have implemented this process. NEUT implemented the de-excitation process but only for Oxygen. Recently, GENIE has de-excitation processes for various nuclei.

When scattering from a nucleus, coherent scattering of various kinds is possible. Most simulations incorporate, at least, coherent neutral and charged single pion production. While the interaction rate for these interactions is typically around a percent of the total yield, the unique kinematic features of these events can make them potential backgrounds for oscillation searches. Implemented in Monte Carlo are several PCAC-based methods [62,63]. Microscopic models, valid at lower neutrino energies [64–67], have also been implemented in several generators. One commonly used model by Rein and Sehgal [62] predicts a cross section for charged-current coherent pion production that is much larger than what is observed by K2K, MINERvA and T2K. However, the cross-section is sensitive to the pion cross-section used in the model as parameters and improved models with lepton mass correction [63] give better agreement with the recent data. This improved model is implemented in most of the generators. In addition to coherent pion production, some generators can simulate coherent single photon production [68] and coherent elastic neutrino-nucleus scattering.

44.3.2 *Hadron Production in Nuclei*

Neutrino pion production is one of the dominant neutrino scattering mechanisms in the few-GeV region and the pions produced in the nucleus have quite large interaction cross sections. Therefore, pion intranuclear scattering can have sizable effects on the results of simulations at these energies. Also, recent neutrino oscillation experiments use the observed information of protons and pions more extensively, in addition to the charged leptons. Therefore, most generators implement this physics through an intranuclear cascade simulation. In generators which utilize cascade models, a hadron, which has been formed in the nucleus, is moved step by step until it interacts with a nucleon or escapes from the nucleus. The probabilities of each interaction in nucleus are usually given as the mean free paths and used to determine whether the hadron has interacted or not. If the hadron is found to have interacted, appropriate final states are selected. Usually, absorption, elastic, charge exchange, and inelastic scatterings including particle productions are simulated as intranuclear interactions. The determination method of the kinematics for the final state particles heavily depends on the generators but most of them use experimentally validated models to simulate hadron interactions in nucleus. No two intranuclear cascade simulations implemented in neutrino event generators are the same [69]. In all cases hadrons propagate from an interaction vertex chosen based on the density distribution of the target nucleus. In determining the generated position of the hadrons in nucleus, the concept of the formation length is sometimes employed. Based on this idea, the hadronization process is not instantaneous and it takes some time before generating the hadrons [12]. The basis for formation times are measurements at relatively high energy and Q^2, and most generators that employ the concept do not apply them to resonance interactions.

GiBUU does not employ an intranuclear cascade simulation, instead, it utilizes a semi-classical transport model in coupled channels that describes the space-time evolution of a many body system in the presence of potentials and a collision term [4]. This approach assures consistency between nuclear effects in the initial state, such as Fermi motion, Pauli blocking, hadron self-energies [70], and modified cross sections, and the final state, such as particle re-interactions, since the two are derived from the same model. This model has been previously used to describe a wide variety of nuclear interaction data. Similarly, the hadronic simulation of the NUNDIS/NUNRES programs are handled by the well-established FLUKA hadronic simulation package [10]. Recently, GENIE included the interface to the external hadronic simulation package INCL++ [71].

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