Generator `R-3_00_04` bug-fix release

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The Nieves quasielastic model was published by Nieves, Ruiz-Simo, and Vicente-Vacas [1] and implemented in GENIE by Joe Johnston (Pittsburgh) with significant help from Juan Nieves. The goal was to have code as close to the publication as possible consistent with the structure of GENIE. It was tested and documented by Joe (see Genie-doc-90). A key feature was comparing GENIE results with the Fortran code used for the publication. To use the model fully, he had to use the new event generator developed for T2K by Jan Sobczyk (Wroclaw) and others, then adapted to GENIE by Andy Furmanski (Warwick). This event generator fixed a bug in the original implementation and provided a broader cross section definition that can be used in spectral function approaches. Documentation for this is Genie-doc-89. Both authors are still in research, Andy is aware of the changes to his model and Steve supplied Joe's original work.

While validating the LArSoft interface to Generator `R-3_00_02` in preparation for their next Monte Carlo production campaign ("MCC9"), MicroBooNE collaborators discovered a number of issues in the implementation of the `QELEventGenerator` class and in the CCQE differential cross section algorithms that are compatible with it (`LwlynSmithQELCCPXSec` and `NievesQELCCPXSec`).

Two small physics changes were also added for resonant and DIS interactions. The major fix was in the pion angular distribution associated with $\Delta(1232)$ decay.

A new bug-fix release of the GENIE Generator product ("R-3_00_04") has been produced to resolve these problems, which are described in section 3.

1 Quasielastic event generation in Generator v2

Prior to Generator v3, the default GENIE configuration generated CCQE events using the free nucleon differential cross section, which may be written in the form

$$\frac{d\sigma}{dQ^2} = \frac{G_F^2 \cos^2\theta_C}{64\,\pi\,|\mathbf{k}_0|^2\,s}\,L_{\mu\nu}A^{\mu\nu}. \tag{1}$$

Here $Q^2 \equiv -q^2$ is the negative square of the 4-momentum transfer, G_F is the Fermi constant, θ_C is the Cabibbo angle, $\mathbf{k}_0$ is the neutrino 3-momentum in the center-of-momentum (CM) frame, $L_{\mu\nu}$ is the leptonic tensor, $A^{\mu\nu}$ is the nucleon's hadronic tensor, and Mandelstam $s = (k+p)^2$, where k (p) is the

4-momentum of the neutrino (initial struck nucleon). The effects of binding energy were taken into account in an approximate way in two stages. First, the time component of p (the hit nucleon total energy) was set to an off-shell value by `FermiMover`, which also sampled an initial nucleon 3-momentum $\mathbf{p}$ according to the relativistic Fermi gas model. Second, a constant binding energy correction was subtracted from the kinetic energy of each final-state nucleon by `BindingEnergyAggregator`. Pauli blocking was similarly accounted for in two stages. First, a Pauli suppression factor, calculated analytically for the Fermi gas model, was applied when integrating total cross section splines. Second, quasielastic events involving the production of a final nucleon that would be Pauli blocked were vetoed and forced to be resampled by `PauliBlocker`.

While this approach to producing CCQE events was used successfully in GENIE for many years, it has a number of limitations. The binding energy correction was not propagated properly into the rest of the interaction. In particular, FSI could generate another nucleon which also had the correction applied. In addition, we discovered that the muon-recoil nucleon phase space was incorrect at the kinematic boundaries. Finally, generating the lepton kinematics (sampling a value of Q^2 using eq. (1)) separately from the initial nucleon 3-momentum ignores the correlations between the two, e.g., the cross section will be larger for some nucleons (with a particular 3-momentum and binding energy) than for others. Overcoming these limitations is what prompted the development of the `QELEventGenerator` class, which became part of the default event generation chain for CCQE events in Generator v3.

2 Event generation in QELEventGenerator

In QELEventGenerator, the `kPSQELEvGen` phase space, which corresponds to the differential cross section

$$d\sigma = \frac{G_F^2 \cos^2\theta_C}{8\,\pi^2\,E_{\mathbf{k}}\,E_{\mathbf{p}}\,E_{\mathbf{k}'}\,E_{\mathbf{p}'}}\,L_{\mu\nu}\,\tilde{A}^{\mu\nu}\,P(\mathbf{p},E)\,\frac{\sqrt{1+(1-\cos^2\theta_0)(\gamma^2-1)}}{|\mathbf{v}_{\mathbf{k}'}-\mathbf{v}_{\mathbf{p}'}|}\,|\mathbf{k}_0'|^2\;d\cos\theta_0\,d\phi_0\,dE\,d^3\mathbf{p}. \tag{2}$$

is used to sample kinematics for each event. This expression is much more complicated but also much more general than the original treatment.

In eq. (2), $\mathbf{k}$ ($\mathbf{k}'$) is the 3-momentum of the initial (final) lepton, $\mathbf{p}$ ($\mathbf{p}'$) is the 3-momentum of the initial (final) nucleon, $E_{\mathbf{p}}$ is the on-shell total energy for the particle with 3-momentum $\mathbf{p}$, $P(\mathbf{p},E)$ is the spectral function (probability density for sampling the initial nucleon 3-momentum and removal energy E), $\mathbf{k}_0'$ is the outgoing lepton's 3-momentum in the CM frame,[1] γ is the Lorentz factor for boosts between the lab and CM frame, and $\mathbf{v}_{\mathbf{k}'}$ ($\mathbf{v}_{\mathbf{p}'}$) is the lab-frame velocity of the final lepton (final nucleon). The nucleon's hadronic tensor $\tilde{A}^{\mu\nu}$ is corrected (via the de Forest prescription[2]) for the effects of its removal energy

[1] This is the CM frame of the neutrino and initial struck nucleon system, not the neutrino-nucleus CM frame.

[2] Under the de Forest prescription, the nucleon tensor $\tilde{A}^{\mu\nu} = \tilde{A}^{\mu\nu}(p,\tilde{q})$ is evaluated using

and (possibly) the Coulomb potential. As written above, the removal energy E is given by

$$E = E_B + T_f \tag{4}$$

where T_f is the kinetic energy of the recoiling final-state nucleus and the binding energy

$$E_B = M_f + m_{N_i} - M_i. \tag{5}$$

Here, M_f is the mass of the recoiling final-state nucleus, m_{N_i} is the (on-shell) mass of the initial struck nucleon, and M_i is the mass of the target nucleus. One may also define

$$\epsilon_B = E_{\mathbf{p}} - E_{N_i}, \tag{6}$$

the energy needed to put the initial nucleon on the mass shell. Here $E_{\mathbf{p}} = \sqrt{m_{N_i}^2 + |\mathbf{p}|^2}$ and $E_{N_i} = m_{N_i} - E$ is the off-shell energy of the initial nucleon.

It should be noted that, in eq. (2), the angles θ_0 and ϕ_0 are measured between $\mathbf{k}'_0$ and $\mathbf{v}$, the velocity of the CM frame as measured in the lab frame:

$$\mathbf{v} = \frac{\mathbf{k} + \mathbf{p}}{E_{\mathbf{k}} + m_{N_i} - E} = \frac{\mathbf{k}' + \mathbf{p}'}{E_{\mathbf{k}'} + E_{\mathbf{p}'}}. \tag{7}$$

It should also be noted that Mandelstam s (the square of the CM frame total energy) should be computed using the off-shell nucleon 4-momentum p:

$$s = (k + p)^2 = (k' + p')^2 \tag{8}$$

where $p^0 = m_{N_i} - E$.

In `QELEventGenerator`, the differential cross section given in eq. (2) is used in the accept/reject loop to select kinematic variables, with θ_0 and ϕ_0 being sampled from uniform distributions and the initial nucleon variables being sampled from the initial state nuclear model.

3 Bugs fixed in Generator R-3_00_04

Several problems of varying severity have been found in the implementation of CCQE event generation in Generator R-3_00_02. They are briefly described one by one in the following subsections. This is followed by discussion of the RES and DIS changes.

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an on-shell 4-momentum for the initial struck nucleon ($p_{\text{on shell}} = p|_{p^0=E_{\mathbf{p}}}$) and an effective value of the 4-momentum transfer $q \to \tilde{q}$, where

$$\tilde{q} = p' - p_{\text{on shell}} = q - (\epsilon_B, \mathbf{0}), \tag{3}$$

where ϵ_B is defined as in eq. (6).

3.1 Hit nucleon always forced on-shell

Regardless of the removal energy sampled by the initial state nuclear model, the current implementation of `QELEventGenerator` always forces the struck nucleon to be on the mass shell. Internal testing by MicroBooNE revealed that this approximation leads to a significant (tens-of-percent) bias in the distribution of Bjorken x, where

$$x = \frac{Q^2}{2\,M\,\nu}, \tag{9}$$

M is the nucleon mass, and $\nu = E_\nu - E_\mu$ is the energy transfer in the lab frame. An obvious effect can also be seen in plots of ν.

The default CCQE event generation chain in version 2 of the Generator product employed the `FermiMover` event record visitor to assign an off-shell 4-momentum to the struck nucleon. On the other hand, `QELEventGenerator` in `R-3_00_02` ignores the nucleon removal energy entirely and puts it on-shell. This behavior has been corrected in `R-3_00_04`. Additionally, the functions used to calculate differential cross sections for `QELEventGenerator` have been updated to correctly handle the off-shell hit nucleon.

3.2 Incorrect reference frame used to compute Nieves model tensor contraction

In the original calculation by Nieves, Amaro, and Valverde [2, 3], the nuclear hadronic tensor $W^{\mu\nu}$ is computed in the lab frame (i.e., the rest frame of the target nucleus, see commentary below their eq. 8), but with the coordinates chosen so that the 3-momentum transfer $\mathbf{q}$ points along the positive z axis. As shown in their eq. 47, the nuclear tensor $W^{\mu\nu}$ may be expressed in terms of a single-nucleon response tensor $A^{\mu\nu}$. In the existing implementation of `QELEventGenerator`, the contraction of $A^{\mu\nu}$ with the leptonic tensor is calculated in the hit nucleon rest frame instead of the lab frame. While in principle this should not matter, since the tensor contraction itself is Lorentz-invariant, the code makes use of the expressions for elements of $A^{\mu\nu}$ given in appendix A of ref. [2], which assume the same frame of reference (the lab frame) as that used for $W^{\mu\nu}$.

We verified that the lab frame (rather than the hit nucleon rest frame) was used by Nieves et al. both via private communication with J. Nieves and by checks of the original Fortran code.

3.3 Nieves Coulomb correction is not applied to 3-momentum transfer

In the Valencia model, Coulomb effects are incorporated into the differential cross section calculation via two approximate corrections:

- An overall factor of $\frac{|\mathbf{k}_\ell^{\mathrm{eff}}|\,E_\ell^{\mathrm{eff}}}{|\mathbf{k}_\ell|\,E_\ell}$ is applied to the differential cross section, where $\mathbf{k}_\ell$ and E_ℓ are the uncorrected 3-momentum and total energy of the outgoing lepton, and "eff" denotes the corrected versions.

- The 3-momentum transfer $\mathbf{q} \to \mathbf{q}^{\text{eff}}$ should be calculated using the Coulomb-corrected lepton 3-momentum: $\mathbf{q}^{\text{eff}} = \mathbf{k}_\nu - \mathbf{k}_\ell^{\text{eff}}$.

In the current implementation, only the first correction is applied. It should be noted that the calculation of $\mathbf{q}^{\text{eff}}$ should be performed before coordinates are rotated to place $\mathbf{q}^{\text{eff}}$ along the z axis for the hadronic tensor calculation.

3.4 Miscalculation of $\mathbf{Q^2}$

On line 783 of `QELEventGenerator.cxx` as it appeared in `R-3_00_02`, the neutrino 4-momentum was retrieved via a call to `InitialState::GetProbeP4()`. This function defaults to returning the probe 4-momentum in the rest frame of the hit nucleon. However, in the context of the function call (the calculation of Q^2 using the lepton and neutrino 4-momenta), what was intended is to retrieve the lab-frame neutrino 4-momentum. This discrepancy was corrected by specifying the correct frame (`kRfLab`) in the call to `GetProbeP4()`.

3.5 $\mathbf{R_{max}}$ problem

The Coulomb correction is based on an integral over the nuclear volume that is done once for each nucleus. Nuclear sizes grow as $A^{\frac{1}{3}}$ but the original code didn't account for this. As a result, the correction was too small for heavy nuclei. The integration limit was changed to have the right A dependence.

3.6 Spline generation problem

With all of the fixes for the previous issues applied, `gmkspl` gets "stuck" while integrating the cross section at the knot just above threshold. To resolve this issue and achieve consistency with the differential cross section used in event generation, a new spline integrator, `NewQELXSec`, was implemented for this release. The differential cross section in the `kPSQELEvGen` phase space (as shown in eq. (2)) is now directly integrated during spline production.

3.7 Pauli blocking in CCQE

Applying the above changes, it became clear that application of Pauli blocking could be done in a more standard way. The code for analytically calculating the cross section suppression was replaced by a specific cut on the outgoing nucleon momentum. This allows new momentum distributions to be applied more readily.

In Generator `R-3_00_02`, `PauliBlocker` was erroneously included in the event generation chain for Charm-CCQE events. It has been removed in this release.

3.8 Fermi motion applied to free nucleon targets

In R-3_00_02, QELEventGenerator sampled a 3-momentum for the initial struck nucleon unconditionally, even for a free nucleon target, which should be at rest in the lab frame. This behavior was corrected for this release, with bound nucleons treated in the usual way and free nucleons chosen to be at initially at rest.

3.9 Rotation edge case in Nieves CCQE model

The Nieves CCQE model implementation in GENIE uses explicit forms for the hadronic tensor that should be evaluated in the lab frame with coordinates rotated so that the Coulomb-corrected 3-momentum transfer $\mathbf{q}^{\mathrm{eff}}$ points along the positive z direction. While this rotation was carried out correctly in most cases in R-3_00_02, no correction was applied when the unrotated $\mathbf{q}^{\mathrm{eff}}$ pointed along the negative z direction. Code to handle this edge case has been added to the NievesQELCCPXSec class in this release.

3.10 Delta decay

In GENIE the Delta resonance decay is not isotropic. Specifically, in the Delta reference frame, the pion coming from the decay has an angular distribution due to the polarization of the exchanged meson. This effect was measured by a number of different experiments for both neutrinos and electron scattering. The definitions of the angles used in the parameterization of this effect can be seen in Figure 1 (taken from Raskin and Donnelly [4]). As a default, GENIE is using an angle distribution provided by Miniboone, which has just a θ^* dependency.

In previous versions the definition of θ^* was wrong. The fix required a tweak in some interfaces so that the information related to transferred momentum and lepton directions were available at the decay stage. This is consistent with a new interface under development to give a more relaxed dependency on PYTHIA 6 libraries. Since testing on these changes was completed, it has been fully deployed in this version.

The new release also provides part of the functionality to support the angular dependencies measured by ANL and BNL, which have a ϕ^* dependency. This functionality needs some optimization and is not ready to be used for physics production.

3.11 Changes in the Inelastic W Limits

In upgrading the code to do $\Delta \to N\gamma$ more accurately in GENIE v2, the kinematic lower limit was decreased for resonance processes. This unfortunately was also applied to DIS interactions. A few lines of that code have been revisited: to be sure only RES interactions can have an W lower than pion mass + nucleon mass. This has a small effect on output events.

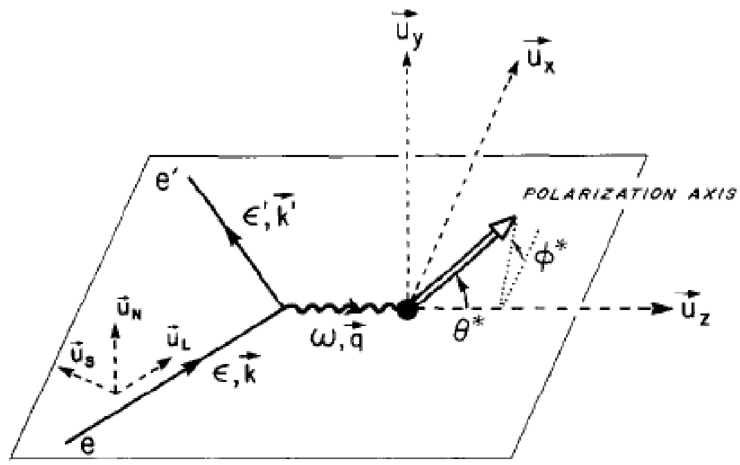

Figure 1: Kinematics and coordinate system for the scattering of polarized electrons from polarized nuclear targets [4].

4 Validation Process

As part of our validation process, we carried out comparisons involving both electrons (figure 2) and neutrinos (figure 3), before and after the introduction of fixes for this release. The left side of Figure 2 shows the importance of binding energy correction in shifting the peak; this provides important verification that the size of correction is right (impossible in neutrino data). Figure 3 shows the effect of adding the effects one at a time; the largest change comes from adding the correct binding energy.

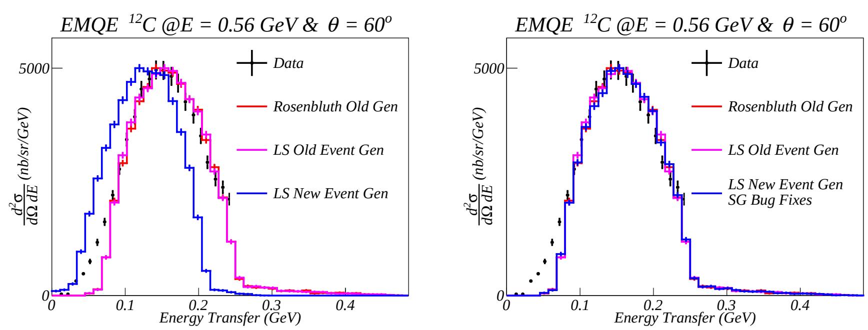

Figure 2: Comparisons for electrons before (left) and after (right) the implementation of the changes for `R-3_00_04`.

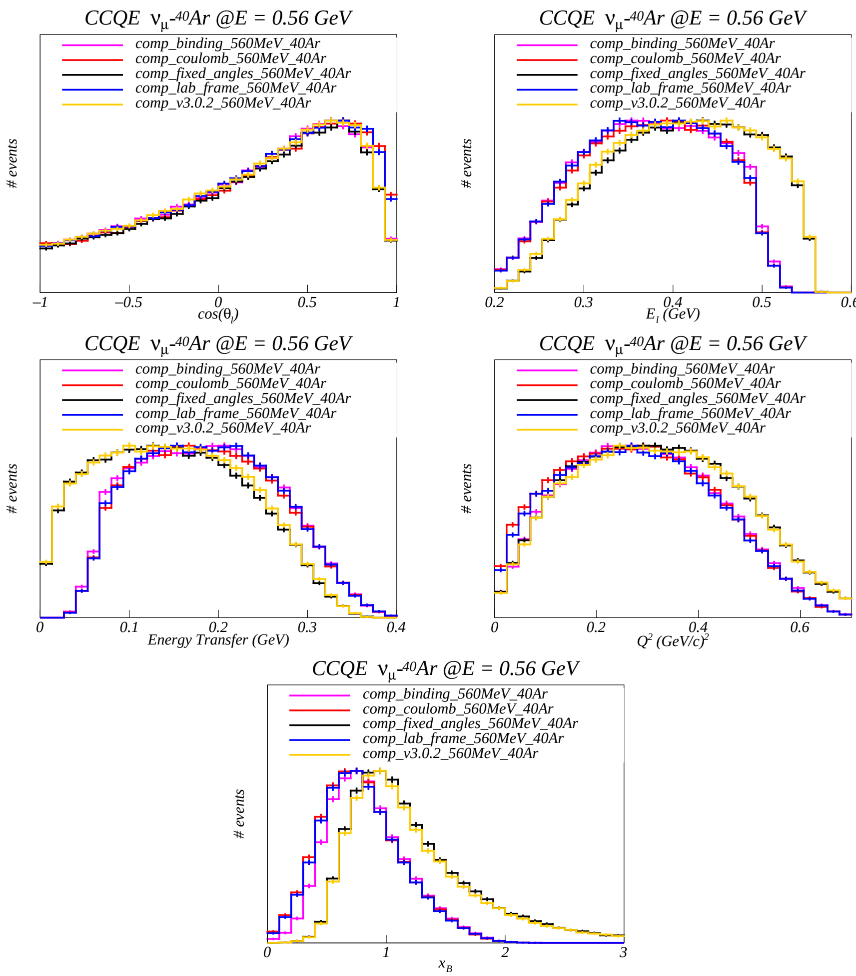

Figure 3: Comparisons for neutrinos studying the impact of each one of the the bug fixes. Effects were applied in perceived order of importance - fixed angles, binding, interaction frame, and Coulomb.

References

[1] J. Nieves, I. R. Simo and M. J. V. Vacas, Phys. Rev. C **83** (2004).

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[4] A. S. Raskin and T. W. Donnelly, Annals Phys. **191**, 78 (1989), [Erratum: Annals Phys.197,202(1990)].