Status of the BooNE Geant4 Beamline simulation, May 2015

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Abstract

This informal note summarized the upgrades made to the BooNE beamline Geant4 package. At a neutrino energy of 0.9 GeV, the ν_μ flux is found to be about 9% lower than previously estimated. The difference at lower energies (≈ 250 MeV) and, to a lesser extend at higher energy are larger, of the order of 20%. The code has been instrumented with more diagnostics. The π^+ flux measured at the downstream end of the collimator have characterized, and compared to those obtained running the existing BooNE beamline G4, production version, which is based on an earlier version of Geant4.

1 Motivation and Scope for this Software Upgrade

The existing version of the BooNE Geant4 Beamline simulation package ("BooNE") has been extensively used to predict the neutrino flux at MiniBoone[1], and, more recently, to redesign the BNB Horn to increase this neutrino flux. Unfortunately, this package does not run on the Fermilab Grid system[5], because of the use of antiquated packages. We'd like to be able to access the large CPU resources available on the Grid, as we'd like to improve the neutrino flux prediction's. More importantly, significant progress have been made in the Geant4 hadronic packages.

A new Geant4 simulation of this short range neutrino beamline has been written, solely based on the use of Geant4, version 4.9.6.p04. The goal was to investigate possible upgrade of the BNB instrumentation systems. However, this package did not use the HARP[2] data, and therefore would not be trustworthy. Thus, the right thing to do is to start from the existing package, upgrade to a more recent version of Geant4. In a second step, the geometry package will be upgraded, using native Geant4 construction methods, allowing a much more detailed rendering of the geometry, to include, for instance the layer of water on the horn and a more precise shape of its inner conductor. [1]

This note describes only the first step in this upgrade plan, which consists of:

- Code clean-up, such as fixing a few uninitialized variables.
- Upgrade to the version of 4.9.6.p04 of Geant4.
- Reorganization of the G4 User Interface Messenger classes and G4 Run initialization sequences, such that the package can accept a simple "default" set of parameters, without having to declare all the parameters (hundreds of them) in a user macros file. The motivation here is to avoid having to keep the near-complete set of parameters setting in the input G4

[1] In the case of Minerva, a change of 5 to 10 % in the predicted flux has been observed when similar upgrades have been implemented. Note that the thickness of the inner conductor was $\approx 2mm$, while it is 3 mm for the BNB horns.

macro file for all runs. This could cause an accidental or unwanted modification of a parameter while editing such an input file, and becomes quickly a file management headache if a default value for a given "adopted" parameter has to change. Default values of parameters are best set in the code itself, and thereby "hidden", following the usual Object Oriented methodology.

- Evidently, the BooNE hadroproduction model, based on the HARP data, is preserved and will be maintained. However, it might be quite useful to be able to run the native Geant4 hadro-production models as well, for comparison. Thus, the BooNE G4PhysicsList has been upgraded to allow for the use of the low energy hadronic model, "QGSP_BERT".
- Use of the GDML file to upload the default geometry. (Hopefully, this will be temporary, to be removed in the next round of upgrades.).
- Implementation of a Dk2nu[4] interface, allowing for a versatile study of neutrino fluxes for different experiments.
- Implement a set of simple ASCII Ntuples for debugging and analysis.
- Validation support code to produce plots of neutrino fluxes, meson distribution, etc.

2 Methods

The existing code has been uploaded in a Fermilab RedMine project[6] by Zarko Pavlovic. The code repository is maintained with git.[8]. Details of the implementation, bug fixing, etc can be found on the corresponding wiki page[7] Also uploaded was a GDML geometry file, created on a MiniBoone machine where the existing code runs. Our first step was to upload this geometry in our new BooNE and link it to Geant4 v 4.9.6.p02, and make necessary changes in the code. Our second step was to perform a first order check of the resulting code with Valgrind[9], looking for uninitialized variables.

This led us to a comprehensive study of the initialization sequences of the G4 hadronic processes. This is - by far - the most complex part of the BooNE code, as, in the same application, one incorporates a very specific hadron production model (based on the Sanford-Wang parameterization of the HARP data) for the first inelastic collision proton-Beryllium, and, for the other hadronic interactions, use the default Geant4 hadro-production models. In addition, scale factors for the inelastic and/or total cross-section have been introduced by various authors, allowing to study the sensitivity of the neutrino flux to such basic assumptions.

While all the options (defined via G4UIMessenger instances) have been kept in this upgrades, few have been tested, as the validation of such changes is difficult to assess, and time consuming. However, it has been verified that change in the p-Be Sanford-Wang parameterization via the existing G4UIMessenger data cards works, in the sense that the new values for the parameters are correctly transfer to the private method that generate the hadron momentum vectors, upon the generation of a G4Vertex.

This initialization occurs in multiple phases: The constructor for the relevant Hadronic classes (about 9 of them, not counting the associated messenger classes) in some cases does the the initialization (explicitly, or via call to the messenger), but not always: the initialization has to be postponed until other classes have been initialized. Thus, new methods have been introduced to some of BooNE hadronic classes to allow for the adhoc, selected estimate of parameters, based on the knowledge acquired thus far.

Furthermore, some private members of the BooNE hadronic classes are re-initialized upon the invocation of the simulation of the first collision. This caused the introduction of a weight associated to the outgoing track. After the re-organization of the formal initialization, these constants are now equal to unity, and the BooNE event generator is no longer a weighted Monte-Carlo. This simplifies the analysis of the data generated by BooNE.

Yet, the initialization of this mixed (Native G4 and Sanford-Wang) G4HadronicProcess is far from perfect, and is expected to cause headaches for future releases of Geant4, v4.10.x. This is because specific hadronic sub-process have to be re-defined when the corresponding cross-section section changes via the G4UIMessenger.

Finally, BooNE has now the capability to generate a set of ASCII files, simple row/column "NTuple" format, such that the hadronic fluxes can be determined without having to rely on HBOOK or ROOT analysis system. The figures shown below have been obtained using the R statistical package[10].

3 Results

The neutrino flux at the MiniBoone has been estimated based on the Dk2Nu ROOT Tree obtained by running the new BooNE package, and directly compared to the flux tables obtained from the MiniBoone machine[3][2] As the MiniBoone detector is relatively close to the BNB target hall(by NuMI standard), the MiniBoone detectors sees a line source, not a point source. Thus, to provide an average flux, the Dk2Nu neutrino are "smeared" over the finite surface of the MiniBoone detector, in the post-processing phase of the data obtained by running BooNE.

Again, BooNE now runs on the Fermilab Grid, using the "Larsoft"[11] installed versions of Geant4, Root and Dk2nu. Therefore, access to sufficient compute power and scratch disk space/tape is not the problem[3]

3.1 ν_μ flux at MiniBoone

The MiniBoone horns runs a "forward" current, focusing the π^+. The normalized difference between the PRD flux[3] and the upgraded BooNE is shown on figure 1. The upgraded BooNE underestimates the flux by $\approx 9.0\%$ at the peak ($\approx 1.$ to ≈ 1.5 GeV) with respect to the PRD flux, and by almost $\approx$ 50 % at very low energy. It also possible that the PRD flux was not smeared over the MiniBoone detector, as the high energy components of the upgraded BooNE flux, not smeared, seems to agree better.

3.2 $\bar{\nu}_\mu$ flux at MiniBoone

The MiniBoone horns runs a "backward" current, focusing the π^-. The normalized difference between the PRD flux[3] and the upgraded BooNE is shown on figure 2. As for ν_μ flux, the upgrade BooNE package underestimate the flux by a slightly (but statistically significantly!) bigger amount ($\approx 14.0\%$).

[2]Note that a change of unit had to be made: Dk2Nu gives a flux as the number of neutrino, per proton on target (PoT), for a virtual detector of a radius of one meter, while the MiniBoone units are more conventional, number of neutrino per PoT per cm^2.

[3]Dedicated help from the Fermi Grid team is truly acknowledged.

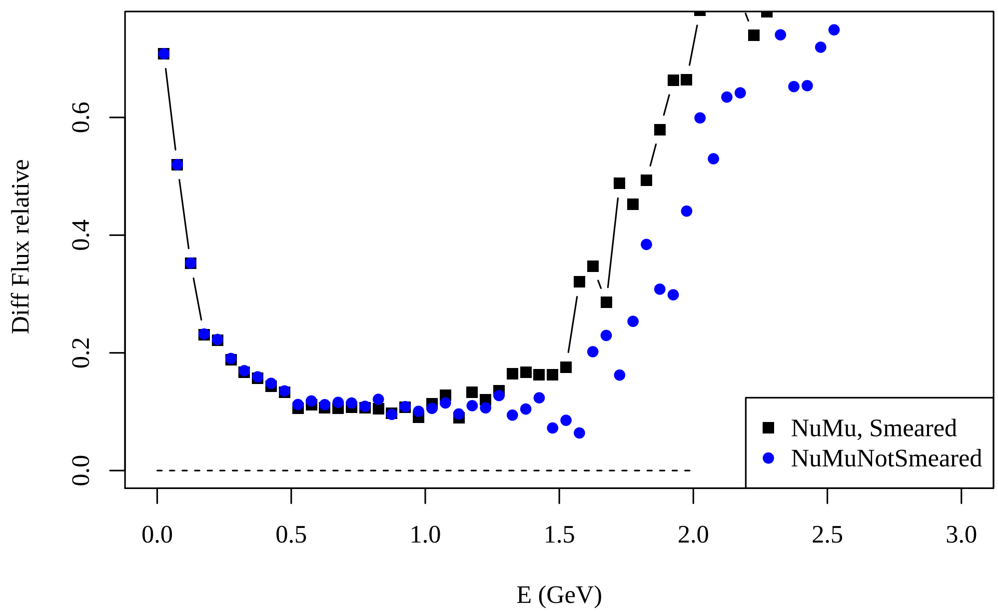

Figure 1: The relative difference between the PRD[3] and upgraded BooNE ((PRD - BooNE)/PRD) of the ν_μ flux measured at the MiniBoone detector.

3.3 ν_μ flux at MiniBoone, Native Geant4

The MiniBoone horns runs a "forward" current, focusing the π^+, the hadronic physics list is based on the so-called QGSP_BERT model. The result are shown on figure 3. A bigger discrepancy is observed.

3.4 Validation Studies

Where do these differences in the neutrino flux come from? Note that a simple rescaling of the total cross-section proton on Beryllium will not fix the problem, as the change in flux are strongly energy dependent. Numerous changes to the code has been made. A formal code review of these changes has not been conducted. However, a comprehensive set of systematic analysis of intermediate results has been made.

3.4.1 Commissioning of the BooNE geometry based on the GDML file

Geantino and related simple row/column NTuples were used to check the location and extend of the components of the BNB beamline. Intersections of Geantino tracks with relevant volumes were compared to the the corresponding entries in the GDML file. For such a simple geometry, no errors were found in the GDML to Geant4 interface.

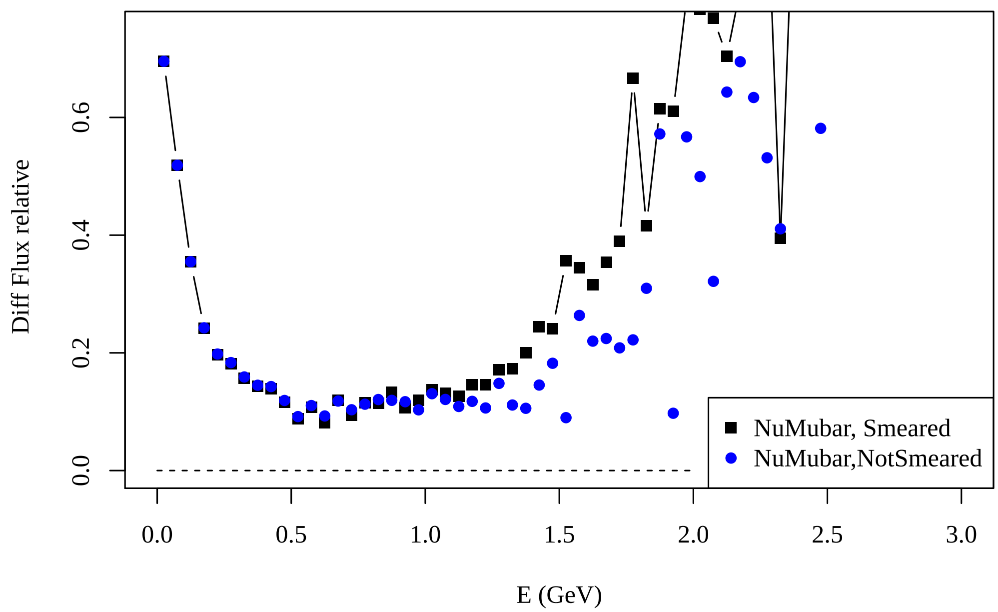

Figure 2: The relative difference between the PRD[3] and upgraded BooNE ((PRD - BooNE)/PRD) of the $\bar{\nu}_\mu$ flux measured at the MiniBoone detector.

3.4.2 The HARP, Sanford-Wang parameterization, hadronic flux at the first proton-Be interaction

A simple row/column NTuple has been generated by the upgrade BooNE package (method *BooNEOutput::RecordpBeInteraction*, invoked from the class *BooNEpBeInteraction*) for each proton on target that does interact in the Beryllium target. The average pion, kaon and nucleon multiplicity from our upgraded BooNE has been directly compared to those found on Table X of the reference paper [1]. The average production angle and momenta have also been compared. Good agreement, within statistics, has been found, except for the π^-. It turns out that the fit to the HARP data published in reference [1] has been refined as that paper was in the late stage of publication, and slightly different values for the eight Sanford-Wang parameters have to be used. The values quoted in reference [1] (Table VI) are:

```
213.66 0.93785 5.4537 1.2096 1.2836 4.7807 0.073383 8.3294
```

The values that give the Table X results are:

```
237.2  0.8986  4.521  1.154  1.105  4.224  0.06613  9.961
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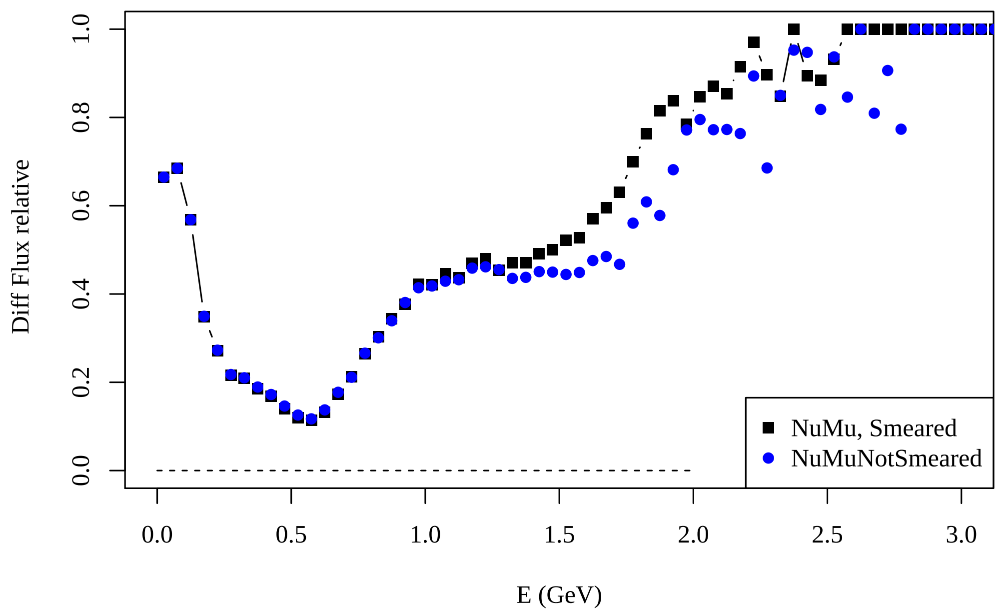


Figure 3: The relative difference between the ν_μ fluxes, PRD[3] and upgraded BooNE running the Native Geant4 QGSP_BERT physics list.

3.4.3 A quick comparison of the QGSP_BERT generator and Sanford-Wang parameterization of the HARP data.

This comparison seems irrelevant, as we plan to use the Sanford-Wang parameterization for the primary (8 GeV beam) proton-Beryllium interactions. However, the maintenance of this interface in future release of Geant4 will be difficult, given the complexity of the multi-step initialization of numerous parameters. So, it is fair to ask how big of a "mistake" when make using the default hadronic generator of Geant4, instead of our BooNE hadronic model.

The comparison of the momentum distribution for π^+ emitted at the primary proton-Beryllium interaction, in forward cone, with a kinetic energy above 50 MeV[4] is shown on figure 4. In the momentum range where HARP has good sensitivity and good statistics (above 0.75 GeV, and below 2.5 GeV), the disagreement between the two models is at the level of a few percent, well within the overall statistical + systematic uncertainty of $\approx 9\%$ quoted by the HARP collaboration [2]. Therefore, the statement that the BooNE package is more accurate than the native Geant4 because it uses the HARP data is a bit unfair, as, most likely, the recent modification to the QGSP_BERT model also use the same data. [5]

[4]The default minimum kinetic energy considered in tracking hadrons in BooNE. Very low energy ($\approx$ 20 MeV neutrinos are of no concern for the Booster Neutrino program. This particular analysis has been done at the Geant4 pre-tracking stage (method *BooNETrackingAction::PreUserTrackingAction* and *BooNEOutput::RecordBeginOfTrack*

[5]In all fairness to MiniBoone, progress has also been made in the accuracy of the estimate of the double differential cross-section p-Be at 8 GeV by fitting directly the HARP data with splines. Since the Sanford-Wang functional form does not exactly fit the data, better precision is obtained by using the data more directly. But it is worth noting that, of course, the range of validity of such spline fit is strictly limited to the range covered by the data.

However at low energy ($\approx$ 0.5 GeV) the Sanford-Wang parameterization disagrees with the QGSP_BERT model, by a large factor. It seems that the implementation of the $\Delta\,1232$ resonance differs notably.

3.4.4 Energy/Momentum conservation at the first proton-Beryllium interaction

The BooNE implementation of the Sanford-Wang model is explicit, in the sense that, should an inelastic, 8 GeV, primary proton on Beryllium interaction occur, than, a set of secondary particle is generated according to the estimate of the double differential cross-sections, (angle, momentum), for each relevant hadron species (charge pions, kaons and nucleon), following the Poisson law, straightforwardly. Each set of such particles is generated independently of the other set. Consequently, total energy and momentum are not conserved. This is shown on figure 5, where the total energy found in the Geant4 stack of secondaries from that primary p-Be interaction is histogrammed. Often, energy is missing, this mean that the number of tertiaries could be underestimated if the "BooNE" physics list is used. Occasionally, energy is created, in which case the number of tertiary could be overestimated. The overall impact is hard to quantify at this stage.

The QGSP_BERT model works a differently: the underlying hadronic model(s) are more realistic. Energy conservation is paramount for hadron calorimetry, which remains to this date one of most popular use of Geant4. As a result, the QGSP_BERT model gives back the 8.9 GeV from the incident Booster beam, plus an occasional nucleon liberated from the Beryllium nucleus, as it should be.

3.4.5 Study of absorption

We still do not have a clear account for the differences in neutrino fluxes using the "BooNE" physics list, Geant4 version 4.8 versus 4.9.6.p04. (See first few figures in this note). Beside different hadronic models for the production of tertiary pions, one should expect yet an other difference: the hadronic models for pion scattering on Beryllium, Aluminum air and iron have also been updated. The absorption of charge pion is very significant. To see this we have restored and regenerated[6] the NTuples of hadrons observed just downstream of critical element. For sake of brevity, let us focus on the π^+ flux observed just downstream of the collimator[7]. A statistics of 1.39 (5.0) millions PoT has been collected from run on the MiniBoone (Fermilab grid) systems, for the MiniBooNE (G4 v4.8) and upgraded BooNE package, respectively. Both were running in neutrino mode ("forward" Horn current). Both were using the "BooNE" physics list, i.e., the HARP model for the first p-Be interaction.

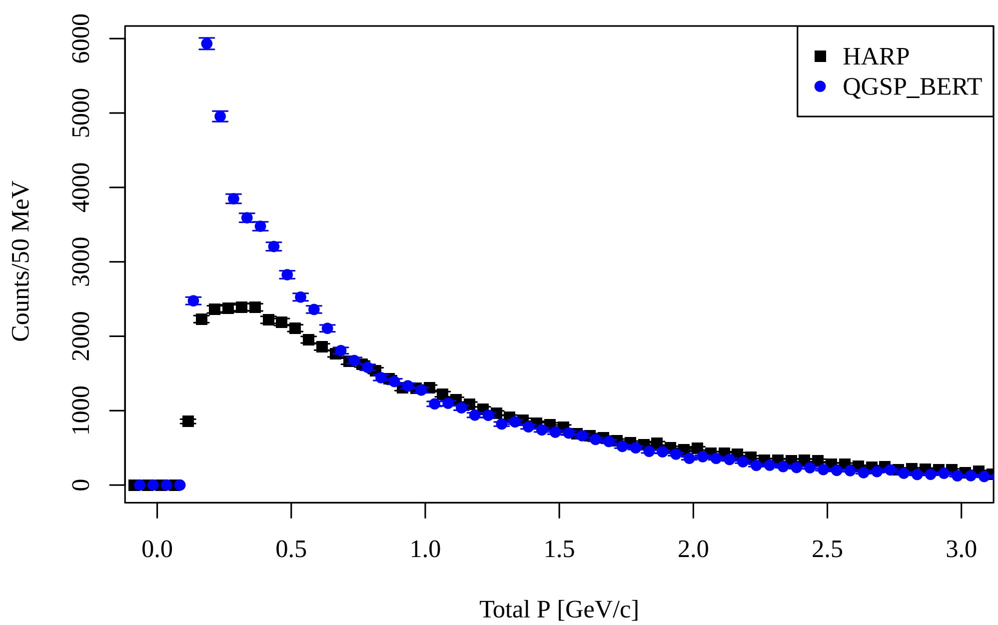
Different cross-checks can be made:

1. The momentum distribution distribution of π^+ after the collimator is shown on figure 6 for the MiniBooNE (noted "Old HARP" on the plot) and for the upgraded BooNE package. Only the secondary π^+ are selected. (Their parents must be the incident beam protons). Also shown on figure 7 is the angular distribution. The pion flux decreased by $\approx$ 4% at 0.9 GeV, $\approx$ 9% at 20 degrees of axis.

2. Geant4 provides additional capabilities for characterizing particle loss, such as the *UserSteppingAction* class. This method has been upgraded to generate a new Ntuple that records where mesons are lost, by selecting Geant4 processes that are not transport, ionization, or decay. Let us further select only secondary pions, to characterize absorption of pions created

[6]This work has been done by Zarko Pavlovic

[7]Ntuple 104 in the class BooNEOutput, and it's ASCII version in the upgraded BooNE package



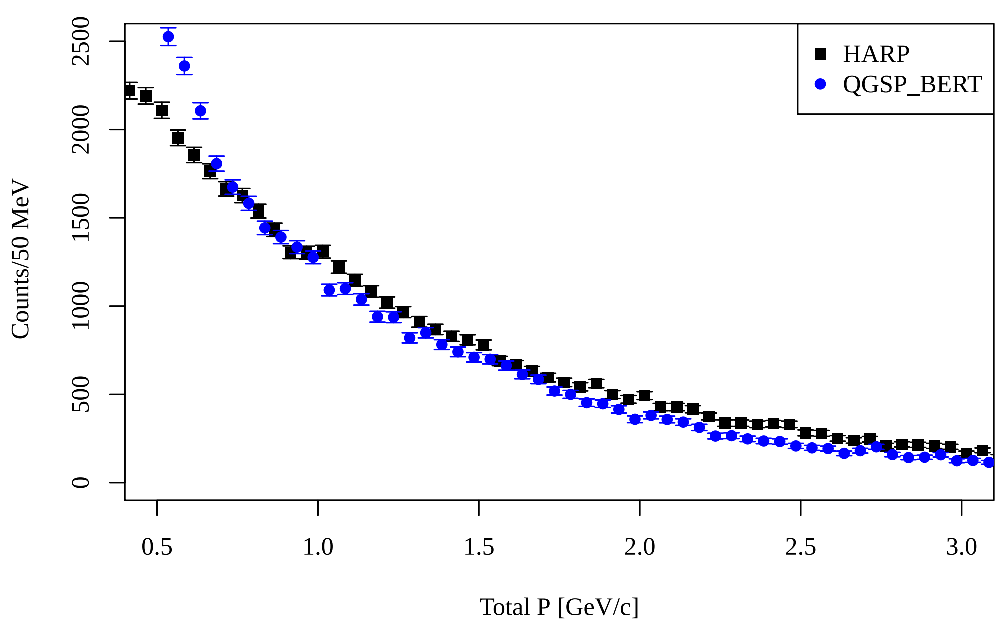


Figure 4: The momentum spectrum of π^+ emitted in proton-Beryllium inelastic interactions at 8 GeV, based on the Sanford-Wang parameterization of the HARP data and based on the QGSP_BERT model from Geant4, version 4.9.6.p04 Top and bottom are based on the same Monte Carlo runs, just different scales. Errors shown here are statistical only.

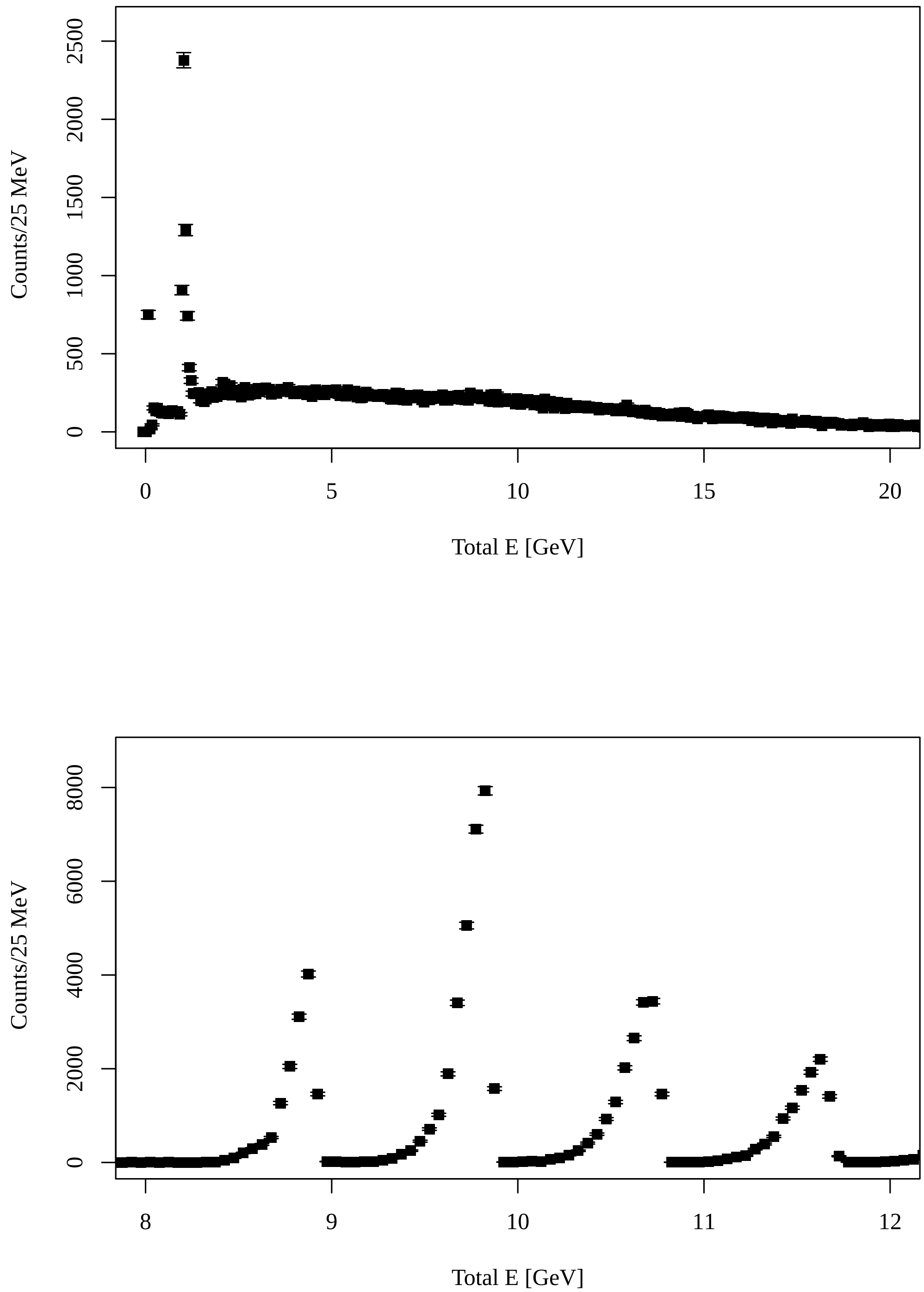


Figure 5: Histogram of the total energy liberated in a p-Be primary interaction. Top is for the "BooNE" physics list, bottom for the "QGSP_BERT", using Geant4.9.6.p04

by the Sanford-Wang model. Such pions are indeed lost where we expect them to be lost, as shown on figure 8 Table 1 summarizes some relevant findings. The loss rate is significant, should the target and the horn made of thin air, we would gain about a factor two in pion flux entering the decay pipe. A change in the pion scattering cross section of ten to twenty percent in G4Hadronic codes are commensurate with the change seen in neutrino flux in the decay pipe. Note that the edge of the hadron collimator also plays a non trivial role, this means that our results are also sensitive to the charged meson - Iron cross sections.

3. We have yet an other way to characterize the relevant pion losses in the horn. The tests above give pion yields that are integrated over all emission angles in the forward hemisphere, and all kinetic energies above 50 MeV. The following test addresses what we are really after, namely the ν_μ flux. To give us an corroborating idea of the importance of the absorption in the horn, let us simply reduce the density of the Aluminum by three orders of magnitude, leaving all other parameters identical, and tally the ν_μ from the Dk2Nu files. The integrated ν_μ flux, appropriately weighted for the MiniBoone detector, for neutrino above 100 MeV, is 24 % higher should Aluminum be of negligible density. The weighted Z distribution for neutrino coming from secondary pions is shown on figure 9. A rough estimate of the probability for absorption based on the p-Be cross section assumed in the BooNE package and these Z-distributions is consistent with a total (target + horn) relative absorption rate of $\approx 30\%$.

Table 1: A characterization of various π^+ production yields and possible loss rates, normalized to one proton on target.

Condition/cuts	Secondary π^+ yield per PoT
Produced in the target from p-BE, forward, $E > 50$ MeV	0.594
Hadronic interaction in the Target ($r < 2.0$ cm)	0.0606
Hadronic interaction in the Inner Conductor ($2.0 < r < 28.$ cm)	0.0621
Hadronic interaction in the Outer Conductor ($r > 28.$ cm)	0.0759
Detected after the collimator	0.13
Detected after the collimator, $r > 30$ cm	0.0242
	All π^+, yield per PoT
Detected after the collimator	0.159

3.4.6 Study of tertiaries

Because 93% of the weighted flux at the MiniBoone detector originates from secondary pions, as opposed to tertiary pions, uncertainties in the hadronic models that describe the kinematics of tertiaries matter less. Yet, there are differences between QGSP_BERT, version Geant4 4.8 and 4.9.6.p04 in the pion yield observed after the collimator, as shown on figure 10. For sake of completeness, figure 11 shows the Z-distribution of the creation point of tertiary pions yielding ν_μ with an energy above 100 MeV, compared to the same Z-distribution for secondary pions.

4 Conclusions

The upgraded MiniBoone Geant4 beam simulation package has been upgraded to Geant4.9.6.p04 and can be installed on any machine running Scientific Linux6, including the Fermi-Grid sys-

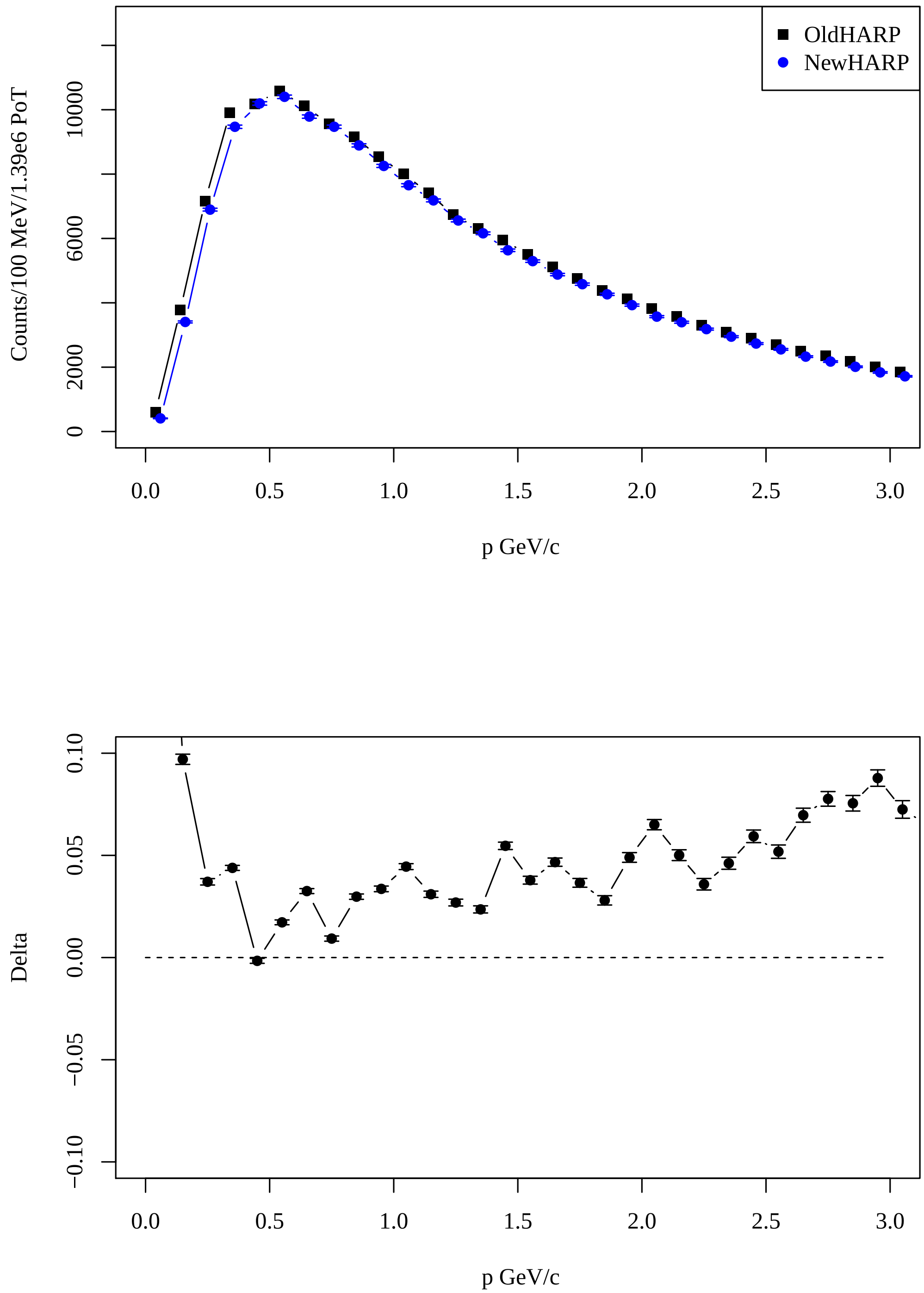


Figure 6: Top: Histogram the π^+ momentum distribution observed after the collimator. Only pions generated at the first p-Be interaction are selected. "Old HARP" refers to the data obtained from a dedicated run on the MiniBoone system, using Geant4 v4.8. "New HARP" refers to this "BooNE" package. Bottom: the relative difference between the above curves.

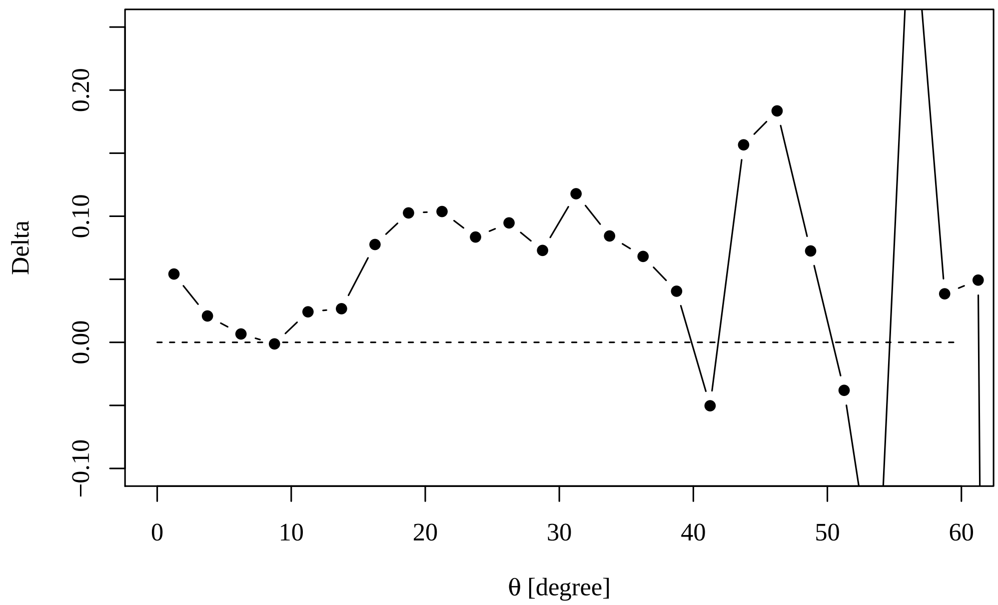


Figure 7: The relative difference between the angular distribution, “Old” vs “New” HARP samples shown on the previous figures. above curves.

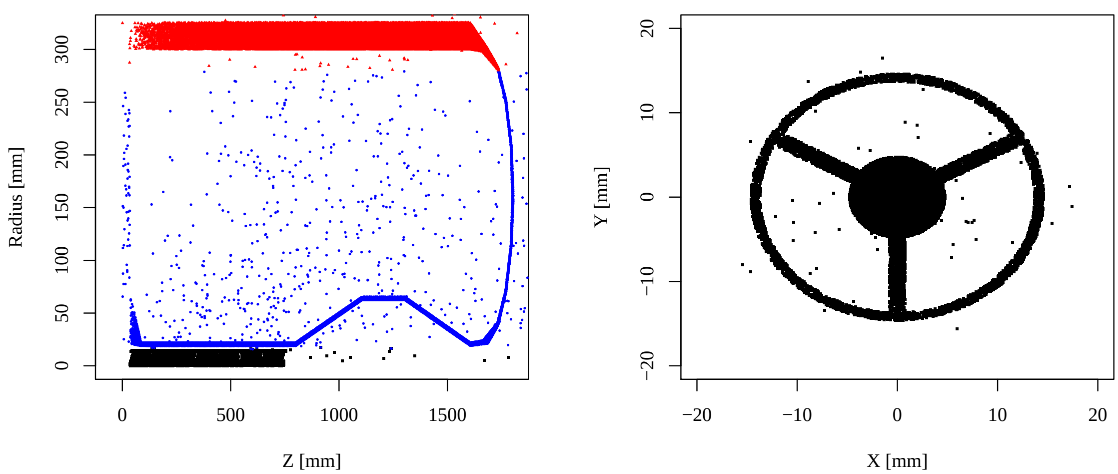


Figure 8: Scatter plot of the position where pions are undergoing hadronic scattering. The color on the left hand side are simply match to the radius. Right: same data, transverse view of the target region.

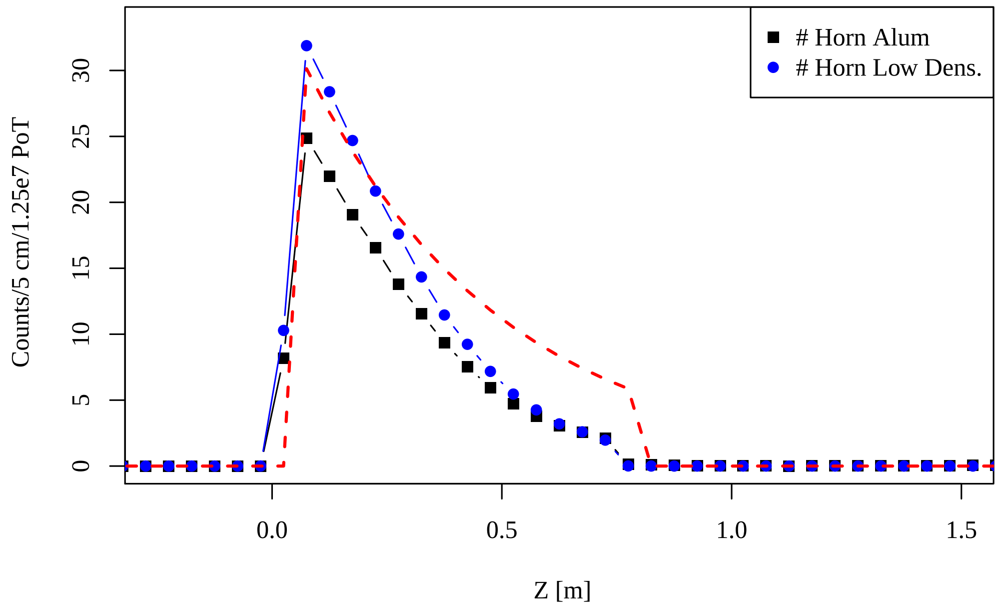


Figure 9: Histograms of z position where pions are created, for such pions yielding a neutrino in the decay pipe. Only neutrinos from secondary pions are selected. The red- dashed curve is obtained by assuming no hadronic re-interaction and the p-Be total cross-section used in the BooNE package.

tems. The implementation of the Sanford-Wang parameterization of the HARP data has been re-commissioned and verified against distribution obtained with the existing MiniBooNE version. Additional debugging code has been written, and the neutrino Ntuple are now available in the standard form, i.e., using the Dk2Nu Fermilab package.

Due to significant changes in the scattering cross-sections for mesons on Beryllium, Aluminum, Iron, etc.., Geant4 version 4.8 version Geant4.9.6., we observed a significant decrease in the ν_μ flux at the MiniBoone of about 9% at the peak of the spectrum, worse at lower momentum.

References

[1] A.A. Aguilar-Arevalo et al, arXiv:0806.1449 [hep-ex], Phys. Rev. D. 79, 072002 (2009)

[2] M. G. Catanesi et al., Eur. Phys. J. C52, 29 (2007), (Note: The HARP data used in the MiniBooNE analysis result from a preliminary analysis of the data prior to publication. The cross sections therefore differ slightly from those reported in this publication, hep-ex/0702024.)

[3] http://www-boone.fnal.gov/for_physicists/data_release/flux/

[4] R. Hatcher Private Communications regarding the use of the Fermilab/ND Dk2Nu package.

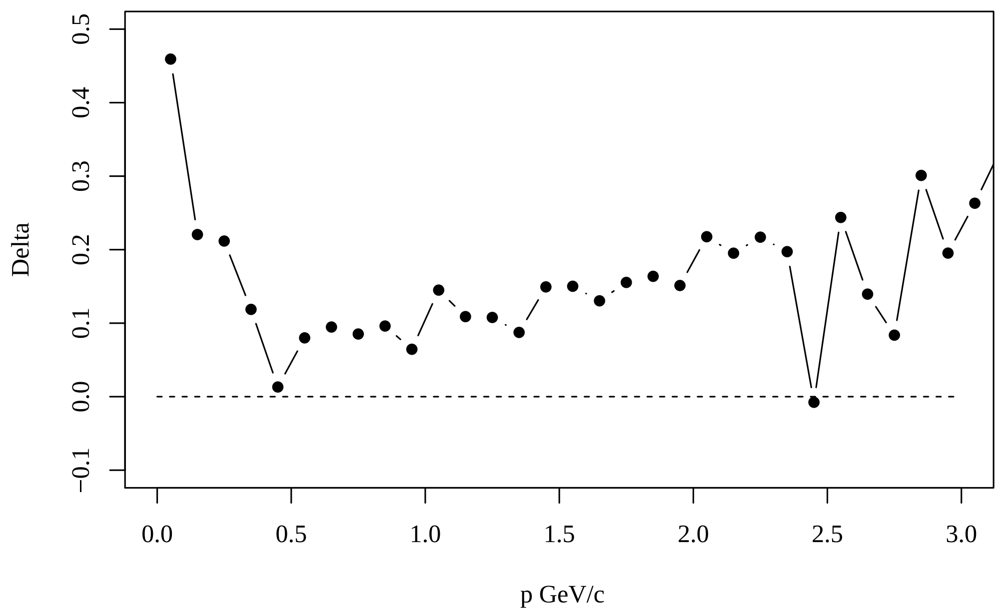


Figure 10: Relative difference in the tertiary pion momentum spectrum observed after the collimator, MiniBoone run vs this upgraded BooNE package.

[5] Computing.fnal.gov/xms/About/Cutting_Edge_Computing/Grid_Computing

[6] http://cdcvs.fnal.gov/redmine/projects/booster-neutrino-beamline/wiki

[7] http://cdcvs.fnal.gov/redmine/projects/booster-neutrino-beamline /wiki/Status_of_Commisioning

[8] https://cdcvs.fnal.gov/redmine/projects/fermi-redmine/wiki/Git

[9] See Valgrind.org

[10] http://www.r-project.org/

[11] https://cdcvs.fnal.gov/redmine/projects/larsoftsvn/wiki

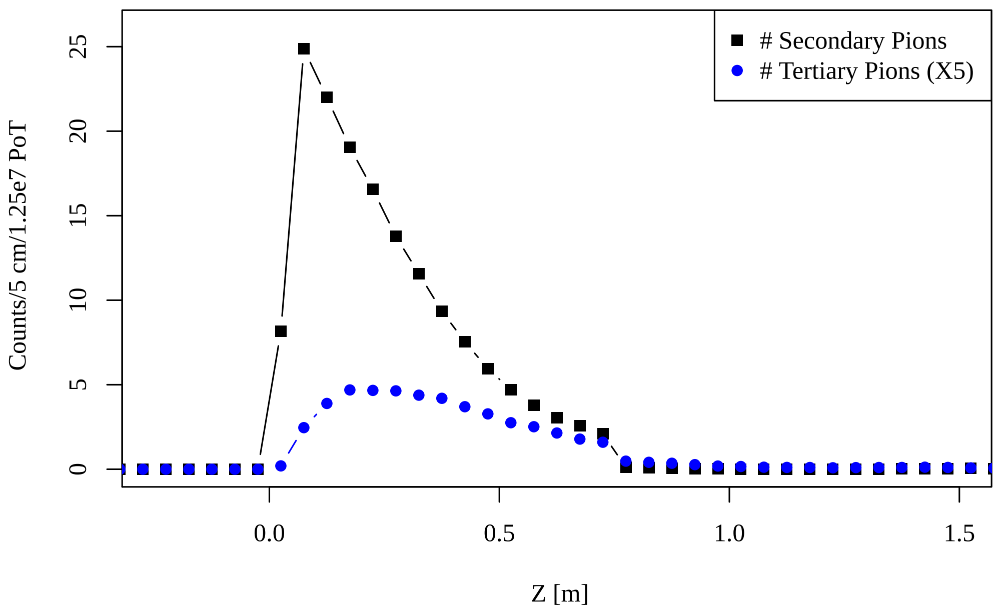


Figure 11: Histograms of z position where pions are created, tertiary versus secondary, for pions yielding a neutrino in the decay pipe.