


Validation of the GENIE *AtharSingleKaon* branch

(1) Introduction

To add single kaon production to the GENIE framework, we decided to use the article “Weak kaon production off the nucleon” (Alam et al., PRD 82, 033001, 2010) as a theoretical basis. The authors were happy to hear of our efforts, and provided us with code as well as a document (notes.pdf) that explains in detail the coordinate frame and calculations used to calculate the differential cross-section. We strongly recommend reading the [publication](#) as well as the authors notes before changing any code!

(2) Code

The original code was written in Fortran by the authors of the theory paper that is the basis of this branch. It was translated to C++  to calculate a 4D differential cross-section for the various possible modes of single kaon production. The code was validated by checking the output manually. It was shown that the cross-section splines calculated matched the Fortran output up to 14 digits. This code was then added to GENIE to perform the cross-section calculation.

singlekaon_xsec.cxx / singlekaon_xsec.h


Within this class, the calculation can be initialised by with

```
void init(double Etot, int type, int reac)
```

where a neutrino energy **Enu**, a neutrino flavour **type** (1=e, 2=mu, 3=tau) and a reaction type **reac** (1=NN, 2=NP, 3=PP) must be specified.* Once set up, the differential cross section can be calculated:

```
double diffxsec(double Tlep, double Tkaon, double theta, double phikq)
```

where the lepton kinetic energy **Tlep** [GeV], the kaon kinetic energy **Tkaon** [GeV], the polar lepton angle **theta** [rad] and the azimuthal kaon angle with respect to the momentum transfer to the hadronic system **phikq** [rad] must be given as inputs. The 4D differential cross section is then returned in $\text{cm}^2/\text{GeV}^2/\text{rad}^2$. A conversion factor $\text{GeV}^2/\text{cm}^2/2\pi$ is multiplied at the end of the calculation – this is not done in GENIE since the software takes care of such unit conversions elsewhere.

Additional standalone code was then developed in ROOT to independently validate the GENIE  output. The programs were usually compiled with ACLiC in debugging mode: e.g. to run example.C, execute

```
$ root -l -b -q example.C+g
```

*Note that the interactions for nu_tau have a threshold of ~5 GeV and have only been added for completeness. The authors published their work up to 2 GeV. While their code goes up to 3 GeV, they recommend not using it at higher energies, as additional effects would come into play that haven't been taken into account in their calculations.

The following programs perform integrations of the differential cross sections, save the differential cross sections, or plot them respectively.

d4sigma_calc.C

This program integrates the 4D differential cross-section to calculate the total cross-section for various energies. The energy range goes from the threshold for the specified interaction to 3.1 GeV, making the output comparable to GENIE splines. When executed, the user is prompted to enter a time complexity **COMP**. This indirectly specifies the number of bins for all integration variables. Since the integration is performed over four dimensions, the time complexity scales with $O(n^4)$. If not otherwise stated, the complexity is set to 10 by default in later calculations. Other steering parameters have been hard-coded:

verbosity	specify amount of output (default is 0)
pLeptonIsUsed	bin over lepton momentum instead of kinetic energy (default is 1)
thetaIsUsed	bin over lepton polar angle instead of its cosine (default is 1)
type	specify the neutrino flavour (see above, default is 2)
reac	specify the reaction type (see above, default is 3)

The output is written into a text file and contains two columns for energy and total cross-section.

d3sigma_calc.C

Similar to the code above, this program performs the integrations in just three dimensions to save time. Since the variable ϕ_{kq} has the smallest effect on the cross section, its integration can be approximated by choosing an average value (e.g. $0.5 \cdot \pi$) and multiplying the differential cross-section by an additional factor of $2 \cdot \pi$ (since this is the integration range for this variable). Note that the cross section is maximal for $\phi_{kq} = \pi$ and minimal for $\phi_{kq} = 0$. It was shown that the best approximation is to choose an energy dependant value for ϕ_{kq} , that runs linearly from $0.50 \cdot \pi$ (at E_{min}) to $0.55 \cdot \pi$ (at E_{max}). The discrepancy with respect to the 4D-integration is less than 1%, which is why the same trick is used in the GENIE integrations. The time complexity is hard-coded and set to 10, otherwise the same steering parameters described above are used. However, an additional parameter is used here:

varPhiKqIsUsed	specify whether a variable ϕ_{kq} should be used (default is 1)
----------------	--

If this parameter is set to 0, the user is prompted to enter a value (as a fraction of π) upon execution.

d4sigma_hist.C

Very similar to `d4_sigma_calc.C`, only that instead of performing integrations to produce a spline file of the total cross section, the differential cross-sections are saved in a histogram. Since this is computationally intensive, separate output files are generated for each neutrino energy. Upon execution, the user is prompted to enter the neutrino energy in GeV. Other parameters are hard-coded

as usual, only that the binning is done for Tlep (not plep) and costheta (not theta), since these are the variables we want to eventually plot. (Discrepancies for various permutations were observed to be of the order of $\sim 1\%$.) Since ROOT doesn't support 4D histograms, the output is saved in a 1-dimensional array of TH3D histograms. This array is then written into a ROOT file in ./data/ called d4sigma_hist_xxxGeV.root, where xxx is the specified neutrino energy.

d4sigma_plot.C

Since generating aforementioned histograms takes a lot of time, this program is used separately to integrate and plot the differential cross sections. Upon execution, the user is prompted to enter the neutrino energy in GeV. The program then looks for the pre-generated ROOT file for the specified energy in the data directory . If it cannot find such a file, it terminates with an error. In this case, you must first run d4sigma_hist.C for the desired energy! If the file is found, integration over 3 of the 4 variables is performed, thereby calculating the 1-dimensional differential cross-section over the fourth variable. These 1D histograms are then plotted (a PNG image is created in ./images/) and written into a ROOT file in ./data/ called d4sigma_plot_xxxGeV.root, where xxx is the specified neutrino energy.

The following programs calculate the kinematics of outgoing final state particles, and generate many events to produce histograms of the relevant variables.

kinematics.C

This program randomly generates the four kinematic variables needed for the 4D differential cross-section. If this set is outside the allowed phase space for the specified reaction (hard-coded), the differential cross-section is zero and a new set is generated, until a positive cross-section is found. Using these variables as input, kinematics of the outgoing final state particles are calculated.** The 3-vector momenta px, py, pz, the total energy E and the mass m of the initial and final state particles are then printed as an ASCII table to the screen. The program checks for conservation of momentum and energy (differences must be smaller than 1 keV), and issues a warning if this is not the case.

To validate the kinematics calculated by GENIE, we manually compared 10 events with identical inputs. The output agreed within 3 digits for all variables (discrepancy < 1 MeV), leaving us confident that the GENIE kinematics generator works correctly for this new branch.

validation.C

This program essentially does the same calculations as kinematics.C, only for many events. Steering parameters are hard-coded as usual, where the default is to generate 10^6 events for muon neutrinos interacting with a proton. Upon execution, the user is prompted to enter the neutrino energy in GeV.

**One intermediate variable that is tricky to calculate is the polar angle of the kaon with respect to the momentum transfer to the hadronic system: theta_Kq. This calculation is luckily given by the authors in equation (17) of the notes they sent us.

The program then looks for the pre-generated ROOT file for the specified energy in the data directory. If it cannot find such a file, it terminates with an error. In this case, you must first run `d4sigma_hist.C` for the desired energy! If the file is found, kinematics for the specified number of events are calculated, these events are then weighted by the corresponding 4D differential cross-section and filled into 1D histograms. These histograms are then compared to the output produced by `d4sigma_hist.C` by normalising their area to the total cross-section for the selected energy. Two canvases with four plots each are created (PNG images are produced in `./images/`). The first canvas contains the histograms of the four input variables used for the cross-section calculation: T_{lep} , T_k , $\cos\theta$, and ϕ_{Kq} . The second canvas includes histograms of all three final state particles for experimentally observable variables: the momentum transfer to the nucleon Q^2 , the kinetic energy T , the polar angle w.r.t. the neutrino $\cos(\theta)$, and the azimuthal angle w.r.t. the neutrino (z-axis) and lepton (x-axis) ϕ . Since the last variable is the difference between the azimuthal angles of the lepton and another final state particle in the lab frame, the value for the lepton itself should always be zero by definition. For comparison to the output of the GENIE kinematics generator, all histograms are saved to a ROOT output file whose name contains the selected neutrino energy. The latest comparisons show excellent agreement at various energies ranging from the reaction threshold (0.8 GeV for ν_μ PP) to higher values (3.0 GeV). **(HAS THE DISCREPANCY FOR THE PHI ANGLE BEEN RESOLVED!?)**

(3) Results

In this section, some results of the standalone C++ code are discussed. If not otherwise noted, plots are valid for the ν_μ PP interaction.

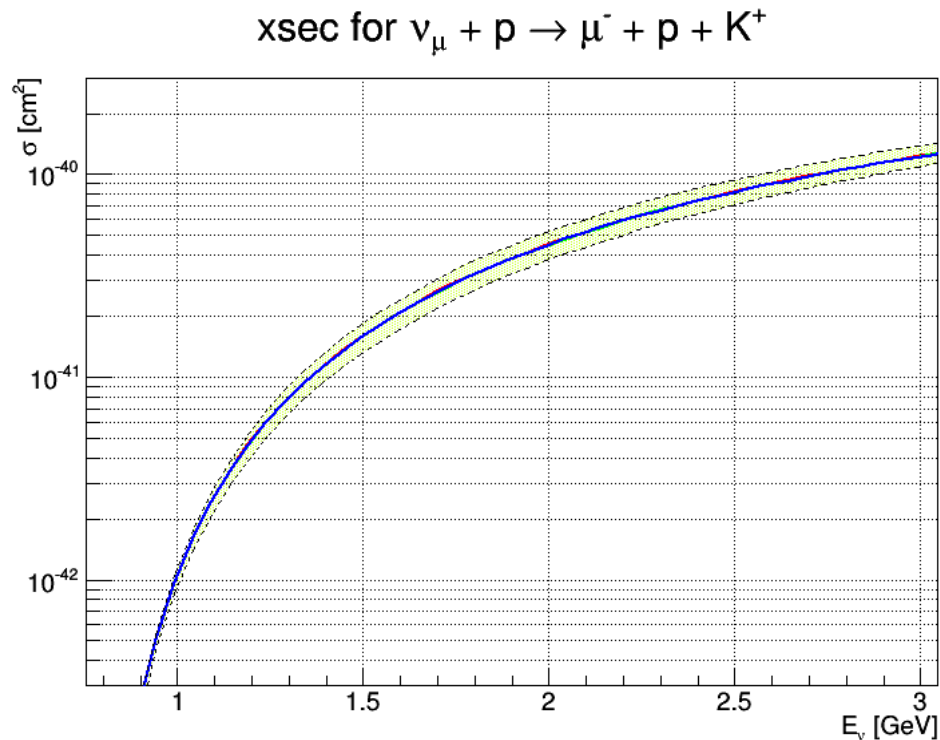


Figure 1: Total cross section as a function of the neutrino energy. The shaded green band shows the effect of using the 3D integration with fixed values of ϕ_{kq} . The difference to the 4D integration is less than 20% for all values, showing that this parameter has the smallest effect on the total xsec.

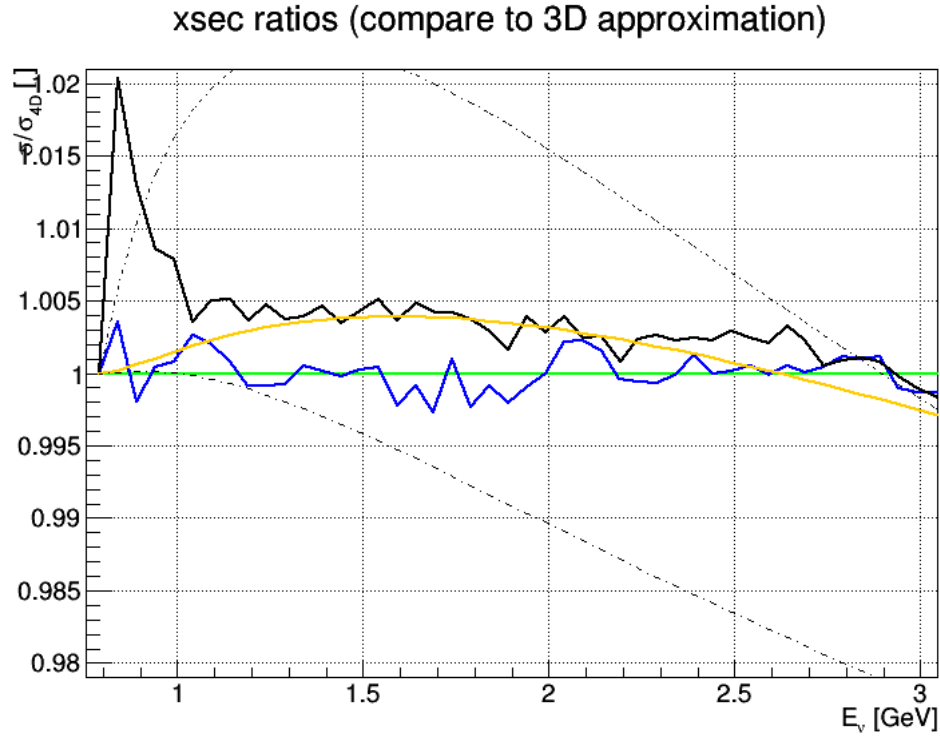


Figure 2: Relative total cross-sections compared to the full 4D integration (green). The original Fortran output (blue) as well as the 3D approximation using a variable ϕ_{kq} (yellow) agree within 0.5%. The dashed-dotted lines are valid for a fixed ϕ_{kq} value of $0.50 \cdot \pi$ (below) and $0.55 \cdot \pi$ (above). A spline generated in GENIE (black) also shows good agreement, except at low energies (< 1 GeV). This is a threshold effect that is not fully understood, but is further investigated below.

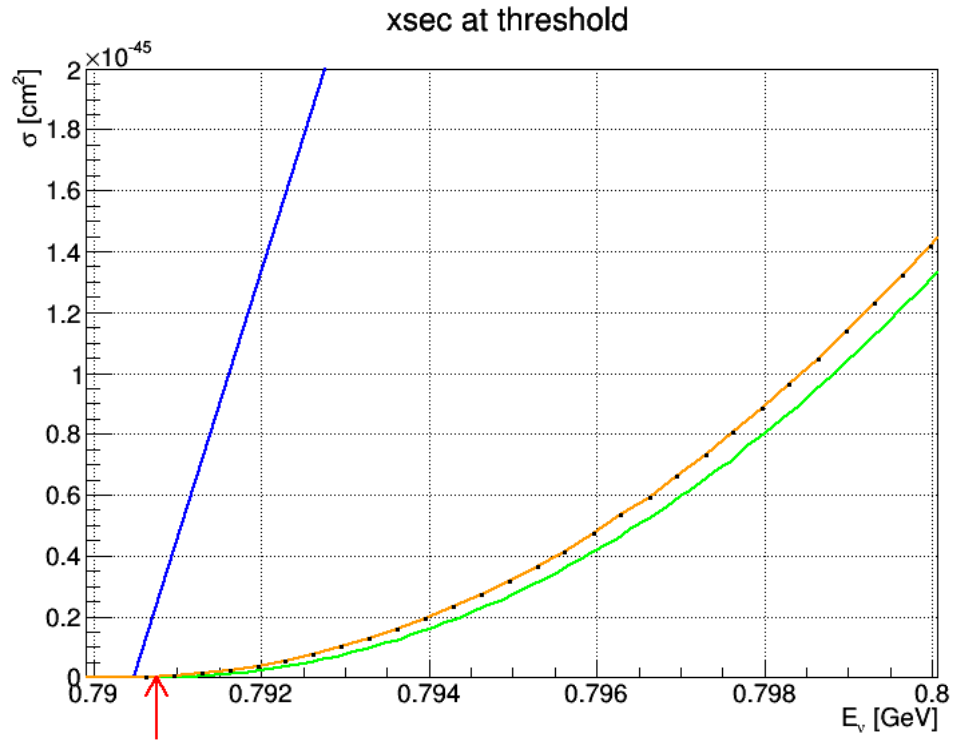


Figure 3: Total cross-section calculated with small step sizes very close to the threshold. The GENIE spline (orange, black dots indicate knots) is slightly higher than the 4D integration from the standalone tool (green), but has the same shape. Fortran code (blue) has a seemingly large discrepancy which is due to the much lower number of knots. A red arrow indicates the threshold energy of 0.790 GeV.

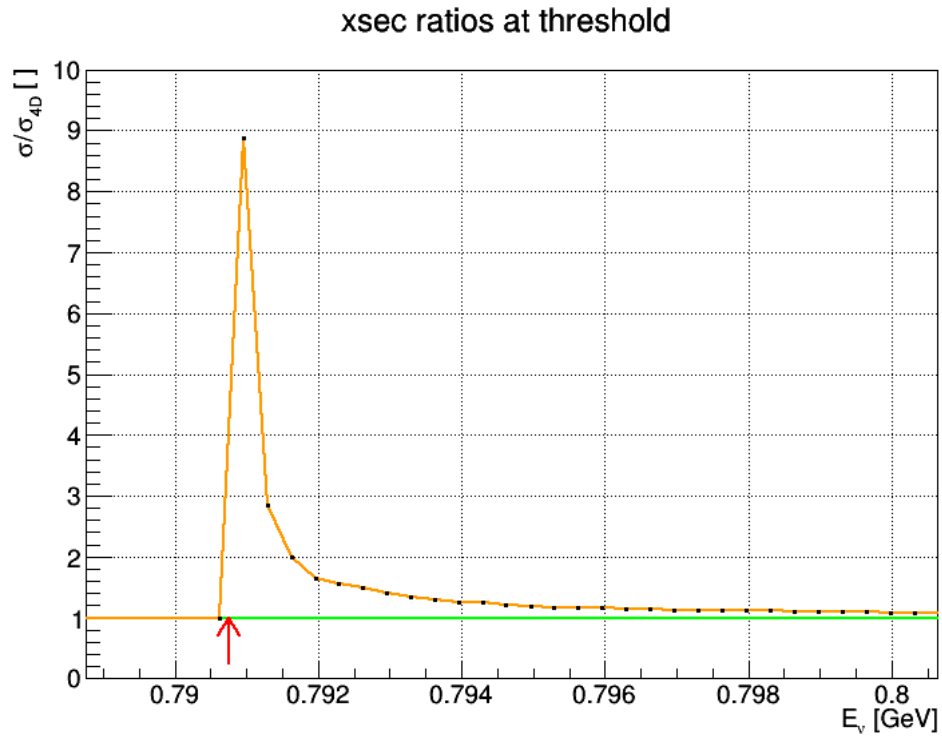


Figure 4: Relative total cross-section compared to the full 4D integration (green), plotted very near the

threshold energy for this reaction (red arrow). The GENIE spline (orange, black dots indicate knots) shows exponentially increasing disagreement when approaching the threshold. This behaviour is not fully understood and may have to do with the “gmkspl” utility. However, since the total cross-section is extremely low ($< 10^{-45} \text{ cm}^2$) at near-threshold energies ($< 0.8 \text{ GeV}$), we can safely neglect this effect.

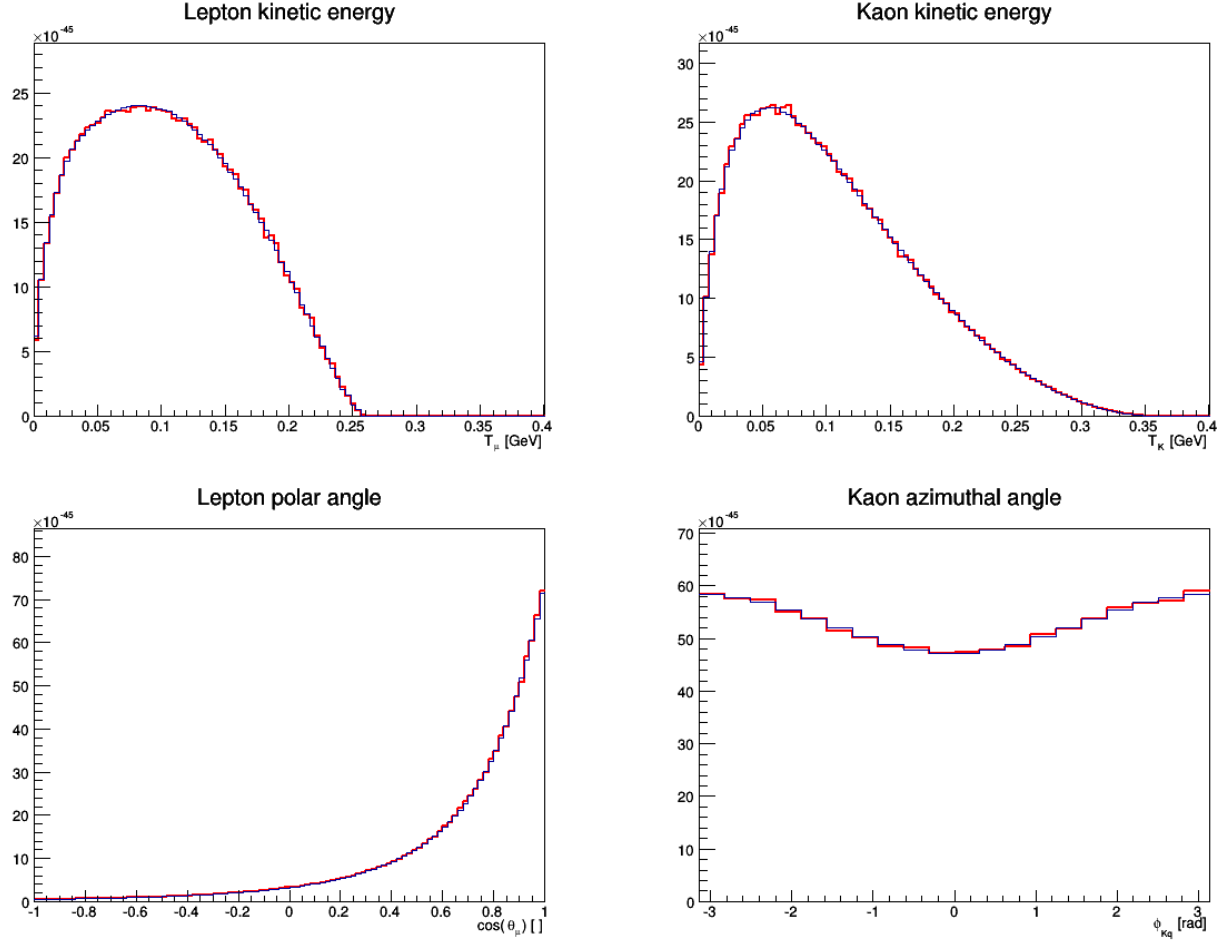



Figure 5: Differential cross-sections for a neutrino energy of 1 GeV, plotted for the four variables used as input to the calculations. The blue histogram is obtained by integrating the 4D differential cross-sections using `d4sigma_plot.C`. The red histogram is obtained by generating 10^6 randomised sets of input variables (“events”) and weighting each entry by its respective differential cross-section with the program validation.C (see above). The histograms show excellent agreement 

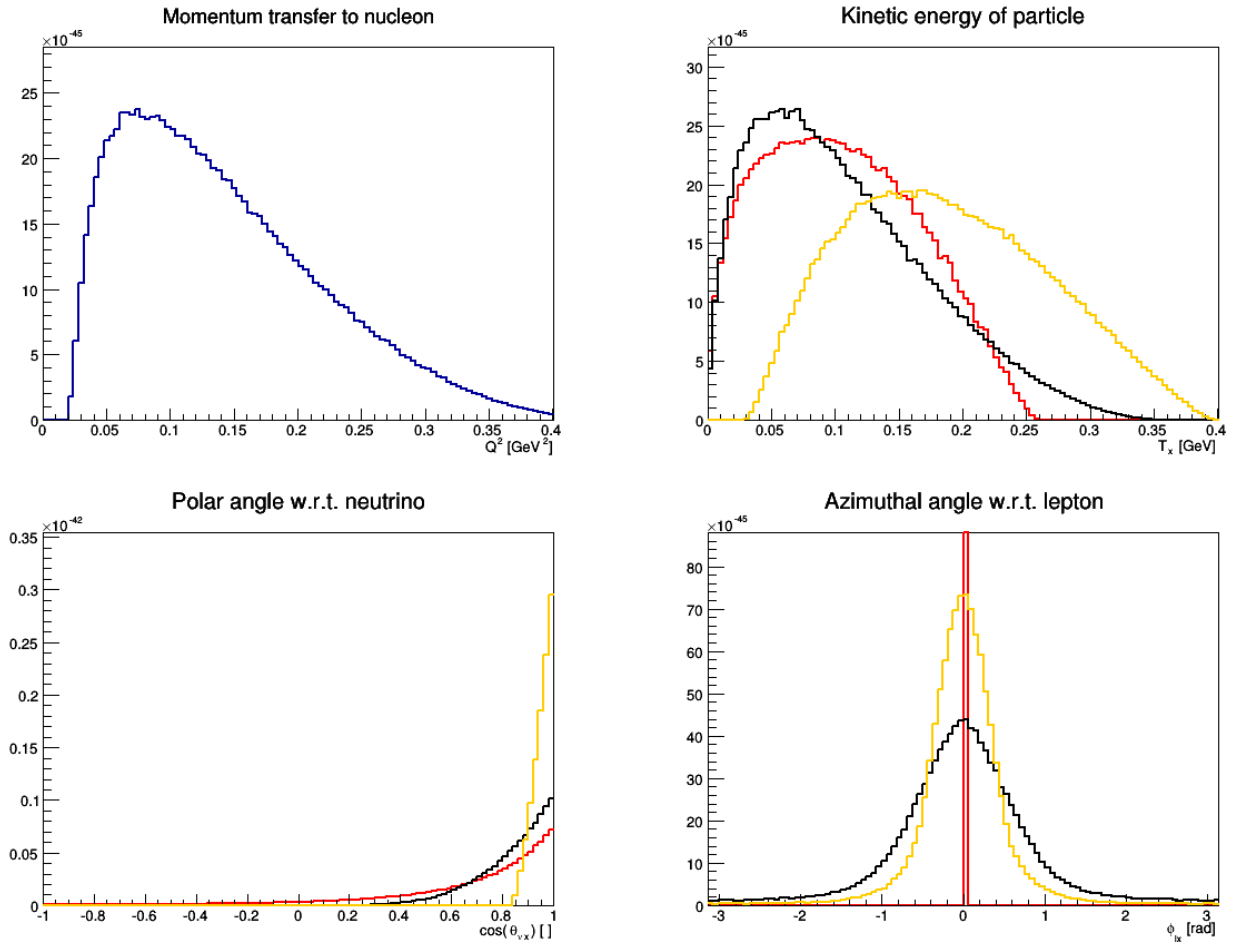


Figure 6: Kinematic distributions for a neutrino energy of 1 GeV. Coloured histograms show the distributions of muons (red), protons (yellow) and kaons (black). Where applicable, the plots are valid in the lab frame, where the z-axis denotes the direction of the incoming neutrino.

(4) Correspondence

For completeness, here is the complete correspondence (that I am aware of) between the authors of the theory paper and members of the GENIE collaboration.

Costas Andreopoulos, 4th Oct 2013

Dear colleagues.

We would like to make an effort to include your Kaon production model (described in arXiv:1004.5484) in the next production version of GENIE. Hugh Gallagher and I are in contact with PhD students from MINERvA and T2K who would like to measure Kaon production in these experiments. Inclusion of such a model is now a relatively high priority for GENIE.

We were wondering whether there is any code (in any language) that you may be able

to contribute as a starting point for this work, or whether you are able to give us a differential single Kaon production cross-section formula in a more convenient form (than the one shown in the paper) for inclusion in a MC generator.

I am available to discuss further if you want and we would very much welcome your guidance on how to best include this model in GENIE.

best regards
Costas

Sajjad Athar, 7th Oct 2013

Dear Dr. Constantinos Andreopoulos

I am presently out of station I will let you know about it by this week end.

(...)

I am back to work. May I know precisely what you would like to have from us, the results for the total scattering cross section, Q^2 distribution and Kaon energy distribution?

Do you require it for both neutrinos and antineutrinos?

OR you would like to have FORTRAN code from us?

I am sorry for being late.

best wishes
Sajjad Athar

Costas Andreopoulos, 21st Oct 2013

Dear Sajjad, all

Thank you for your reply.

We are generating MC events and we need to simulate all final state particles appearing in the reaction $\nu + N \rightarrow l + K + N'$.

Typically, we use a differential cross-section as probability density function (pdf) to generate kinematical variables (for example, in CCQE, we sample $d\sigma/dQ^2(E_\nu, Q^2)$ to generate Q^2 values for a particular neutrino energy E_ν).

What we would need, is a differential cross-section $d^N \sigma / dx_1 dx_2 \dots dx_N$, where the variables x_1, x_2, \dots, x_N can fully characterise the final state kinematics of $\nu + N \rightarrow l + K + N'$.

$d\sigma/dQ^2$ may not be sufficient: It lacks information on the $K+N'$ system

invariant mass (W) distribution.

$d^2\sigma/dQ^2 dW$ may not be sufficient either: It will leave some ambiguity over how to generate the Kaon direction distribution, in the "decay" of a $K+N'$ system of invariant mass W . But it may be sufficient, if you think that a phase space decay of the $K+N'$ is a good approximation.

Perhaps something like $d^3\sigma/dQ^2 dW d\cos\theta$ (where θ is the angle between the K and the N' , in the $K + N'$ rest frame) would be ideal for us? (What do you think Hugh?)

In your paper, you calculate the spin-averaged invariant amplitude $|M|^2$. Together with the flux factor and phase space factor this gives you $d^9\sigma$ (page 4). If you give us a code to calculate $|M|^2$, then we can turn that (numerically) into any differential cross-section we like, using the trick shown in the attached pdf. I know that MCs for the collider physics community use that trick routinely. This may have its advantages, since $|M|^2$ is the fundamental object you computed. But this approach may not be very efficient (computationally) for our purposes. So, if you can do some of the integrations analytically, then this would be our preferred option.

We do not need the total scattering cross-section for MC generation, as we integrate (numerically) the differential cross-section you provide. Of course, we will use your total scattering cross-section during validation, to make sure that the differential cross-section and the numerical integration were implemented correctly, and that are getting the answer that we were meant to get.

Yes, we need this both for neutrinos and anti-neutrinos.

Formulas in paper (describing the full calculation we need to do) or fortran code would be fine. Both, if possible, would be even better.

I hope this is clear.

Many thanks for your help.

Best regards
Costas

Sajjad Athar, 6th Nov 2013

Dear Dr. Constantinos Andreopoulos & Dr. Hugh Gallagher
Greetings

I am enclosing the kaon code along with a pdf file explaining the kinematics.

This is for Neutrino induced process. If you are OK with this format then we will send the Antikaon code in a few days.

Feel free to suggest any change/format.

best wishes
Sajjad

Martti Nirkko, 13th Apr 2014

Dear Prof. Sajjad Athar,

In the name of the GENIE collaboration, I would like to thank your group for the valuable help you have provided us with to facilitate the implementation of your model for weak kaon production (arXiv:1004.5484). Especially the code for calculating the cross-section was extremely useful to us. Last month, we had a GENIE developers workshop, in which a small group had the task of writing a package in GENIE to incorporate this model. In just one week, we set up a framework for the generator to produce this reaction, and included the cross-section code. This will potentially be used by both MINERvA and T2K. To better understand the model and clarify a few points, we would like to ask you a few questions:

(1) We don't fully understand the effect of the parameter ϕ_{kq} on the cross-section calculation. It seems that whatever value one sets in the code, the output does not change. Can the value be chosen at random? If yes, why is it one of the remaining parameters at the end of the notes? We realise that when $\phi_{\nu l}$ is chosen (any value since the distribution is isotropic), this has an effect on the possible phase space for ϕ_{kq} (the kaon is less likely to move in the "same" direction as the lepton). However, when one integrates over all $\phi_{\nu l}$ ($0..2\pi$), these effects cancel each other and we get a factor 2π for both integrations. Is this the correct interpretation? Can you elaborate on the effect of this parameter?

(2) In your paper, the model for single kaon production runs up to a neutrino energy of 2 GeV. Is the reason you don't go to higher energies simply because associated production becomes dominant in that region, or is there a different reason? We would like to extrapolate the models to higher energies to estimate the event rates (important especially for MINERvA), how far would you say is it safe to go? (Also, for 5 GeV and above, we could add the tau neutrino for completeness...)

(3) Concerning the reaction types in neutrino interactions, it is important to use understandable naming conventions in order to have clarity in discussions between different groups of experimentalists and theorists. What description would you apply to single kaon production? It's not a resonance, definitely not quasi-elastic, not really deep-inelastic...

I am happy to elaborate further if anything is unclear, and we would welcome any

further guidance you can give us on this matter.

Best regards,
M. Nirkko

Sajjad Athar, 17th Apr 2014

Dear all

Thank you for incorporating single kaon production in the GENIE MC.

(1) Let me point out that ϕ_{kq} is not a parameter. If you see (the notes which we sent) the expression of the differential cross section ϕ_{kq} has to be integrated over 0 to 2π

$\phi_{n\ell}$ is just integrated out and gives 2π as there is no azimuthal dependence on n_{ℓ}

(2) Yes we have gone up to 2GeV because of the limitation of the model and at high energies many new terms and different mechanisms will become dominant and they are not included in our model. At the same time **at high energies we have the dominance of associated production (not Cabbibo suppressed)**.

(3) This is an inelastic reaction and you may call it Inelastic Single-Kaon Production

Let me also tell you that we have done antineutrino induced single hyperon production (PRD 88 077301 2013) where we have shown the contribution of pions coming from the hyperons are very important at $\sim 1\text{GeV}$. What is the present status of this contribution in GENIE?

we will be happy to reply to any further query.

regards

Martti Nirkko, 13th Oct 2014

Dear Prof. Athar,

While studying a few problems in the GENIE code as well as our standalone tool translated from your Fortran code, we discovered that there is a value "nucleon mass" that is always set to the mass of the neutron. It seems to us that this is the struck nucleon mass, which is not always a neutron (see PP reaction). We noticed this due to some numerical issues we were getting at the edges of the allowed phase space.

E.g. in your code "xsec.f" on line 16, we have:

```
am=0.939565346d0          // neutron mass [GeV]
```

We are getting less of these issues since we have set this to the mass of the

struck nucleon, but we are not sure if this is entirely correct.

Additionally for the NP case, we have a neutron being struck (initial state) and a proton being ejected (final state) - which mass should be used here? For final state kinematics this is obvious, but for the cross-section calculation we wanted to check with you before changing anything.

This parameter is used many times in the code, to calculate the threshold as well as the differential cross-section. We would appreciate some clarification on this matter.

Best regards,
M. Nirkko

Rafi Alam, 14th Oct 2014

Dear M. Nirkko,

As I understand you are worried about the difference between neutron and proton mass and its consequence in the numerical results.

We took the same mass for proton and neutron as the mass difference is about 1.3 MeV, and we have found that the difference in the result is hardly any.

I think this clarify your confusion.

Fell free to ask any other question/clarification.

Regards
Rafi

- Martti Nirkko, 28th November 2014