Optimizing Geant4 Hadronic Model Parameters

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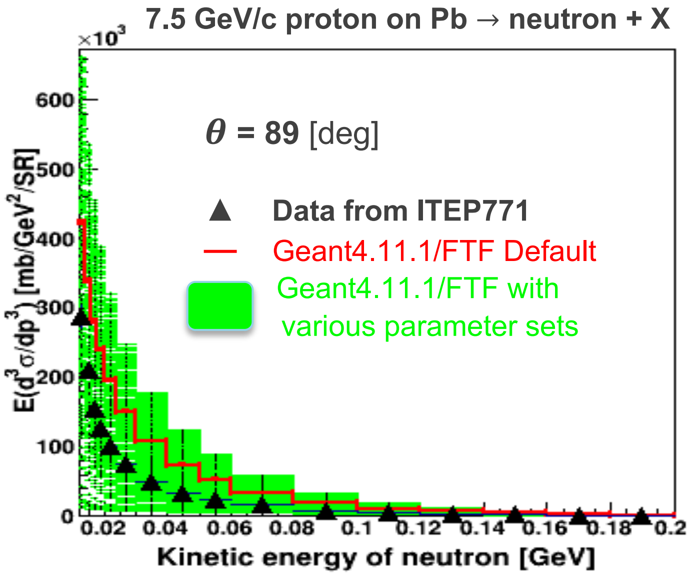
General Information (I)

- Geant4 employs a set of physics models to simulate interactions of particles with matter across a wide range of interaction energies
- These models rely largely on physically motivated parameters; but they generally aim to cover a wide range of possible simulation tasks and may not be optimized for a given process or material
- Critical questions: how sensitive are Geant4 predictions to the variations of model parameters, and how does it translate into simulation of a detector design and experimental observables
- Making parameters configurable opens a possibility to
  - Explore how much the simulated observables would change with variations of parameters
  - Fit simulated distributions to experimental datasets and extract optimal values of the model parameters and the associated uncertainties



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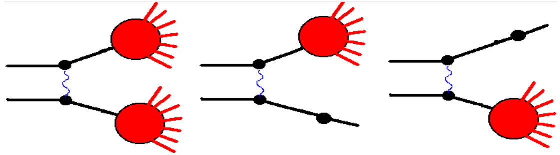
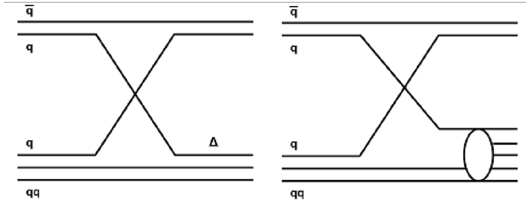
General Information (II)

- Findings from earlier study of varying the **initial** set of configurable parameters available among such key hadronic models as Fritiof (FTF), Bertini Cascade, and PreCompound
  - Varying/optimizing parameters of the Geant4 models generally leads to better agreement with some data
  - The number of configurable parameters available at the time, per model, were too few in order to reach a better agreement across the board
- Currently the focus is on **FTF**
  - Very popular model with the wide validity range from 3 GeV to TeV scale; in active development
  - Based on non-diffractive and diffractive quark-gluon string reactions and LUND string fragmentation
  - Modeling of string formation involves various processes, including but not limited to
    - Quark exchange with or without excitation of participants
    - Nuclear target destruction





Datasets Used in the Study (so far)

Experiment	Projectile	Target	Final State	Observable
ITEP771	7.5 GeV/c proton 5 GeV/c $\pi^{\pm}$	C, Cu, Pb	pX, nX (data for $\pi^{\pm}$ beam exist at θ>60deg)	$Ed^3\sigma/dp^3$
K.Ishibashi et al., J.Nucl.Sci.Tech. Vol.34 N.6 1997	3 GeV/c proton	C, Fe, Pb	nX	$d^2\sigma/d\theta dE$
HARP	3-12 GeV/c proton 3-12 GeV/c $\pi^{\pm}$	C, Cu, Ta, Pb	$\pi^{\pm}$X, pX	$d^2\sigma/d\theta dp$
NA61/SHINE	31 GeV/c proton 60 GeV/c π^{+}	C (data for $\pi^{\pm}$ beam on Be will be added shortly)	$\pi^{\pm}$X (more data exit; will be added shortly)	$d^2\sigma/d\theta dp$

Additional details are available in backup slides

Fitting Package : Professor Toolkit

- http://professor.hepforge.org
  - "Fundamentally, the idea of Professor is to reduce the exponentially expensive process of brute-force tuning to a scaling closer to a power law in the number of parameters, while allowing for massive parallelization and systematically improving the scan results by use of a deterministic parameterization of the generator's response to changes in the steering parameters." – from Professor's web site
  - A set of parameters Pi={xi , yi , zi ,…} is a "point" in the multi-parameter space
    - Randomly sample points the multi-parameter space (within physically meaningful range of values)
    - For **each Pi** simulate data combinatorics: beam ✕ energy ✕ target …
    - Derived quantities are histograms
  - Bin-wise approximation of Monte Carlo results with a polynomial $f(P_i)$ (default is 3rd order)
  - Fit experimental data with $f(P_i)$ to explore sensitivity and coupling of parameters
    - Construct overall $\chi^2 = \Sigma_{bin}$ (interpolation-data)^2 / error^2
    - Numerically minimize (pyMinuit, SciPy)

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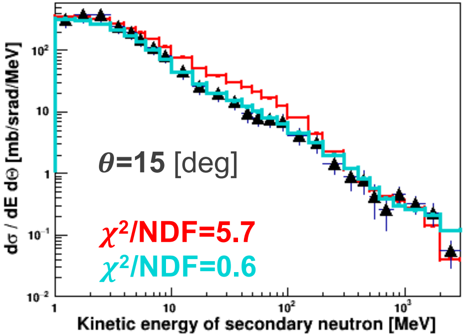
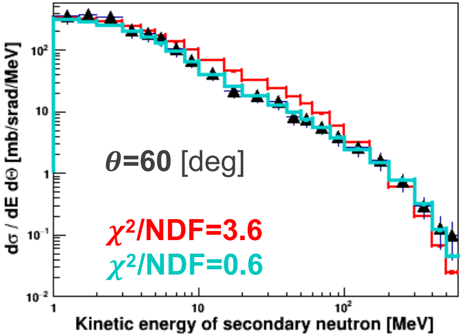
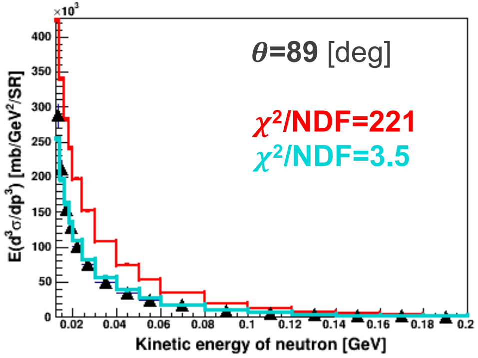
Simulation of neutron production in proton-Pb interactions

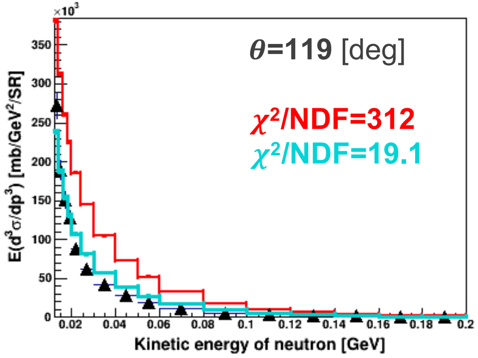
3 GeV proton on Pb → neutron + X





7.5 GeV/c proton on Pb → neutron + X





▲ Data

- **3 GeV** - K.Ishibashi et al., J.Nucl.Sci.Tech. Vol.34 N.6 1997
- **7.5 GeV/c** - Yu. D. Bayukov et al., Preprints ITEP-148-1983; ITEP-172-1983; Sov.J.Nucl.Phys. 42 116, 1985 (ITEP771)

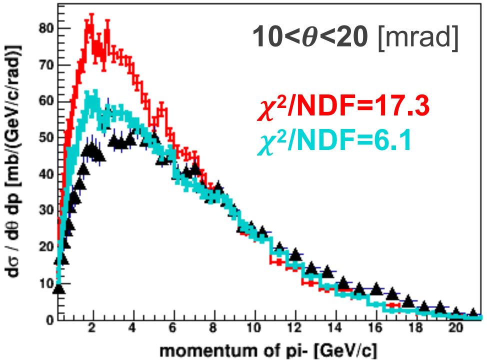
— Geant4.11.1/FTF Default

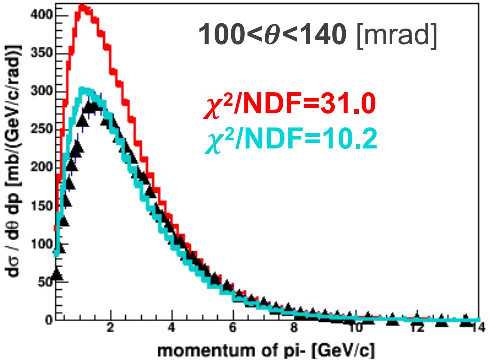
— Geant4.11.1/FTF with Best Fit Parameters

Best fit values of the FTF parameters for the nuclear target destruction process for the baryon (proton) projectile have been obtained through global fit to a collection of experimental thin target data, including correlation of parameters.

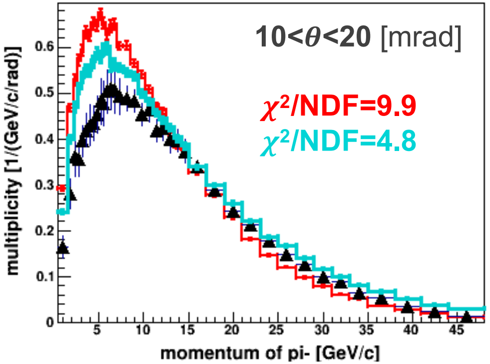
Simulation of π^- production in proton-C or π^+-C interactions

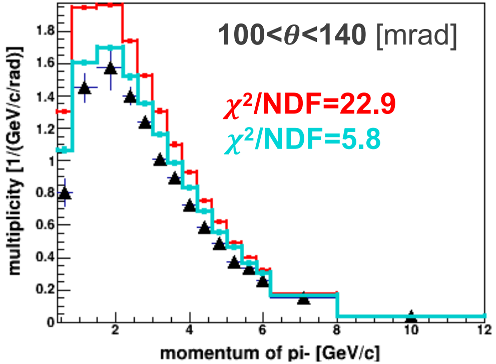
31 GeV/c proton on C → π^- + X





60 GeV/c π^+ on C → π^- + X





▲ Data (all from NA61/SHINE)

- **proton** - N. Abgrall et al. , Eur.Phys.J.C 76, 2016
- π^+ - A. Aduszkiewicz et al. , Phys.Rev.D100 112004, 2019

— Geant4.11.1/FTF Default

— Geant4.11.1/FTF with Best Fit Parameters

Best fit values of the FTF parameters for the quark exchange process have been obtained through global fit to a collection of experimental thin target data, including correlation of parameters.
Best fit parameters have been obtained separately for the proton or pion projectile; this reflects the physics of the interactions.

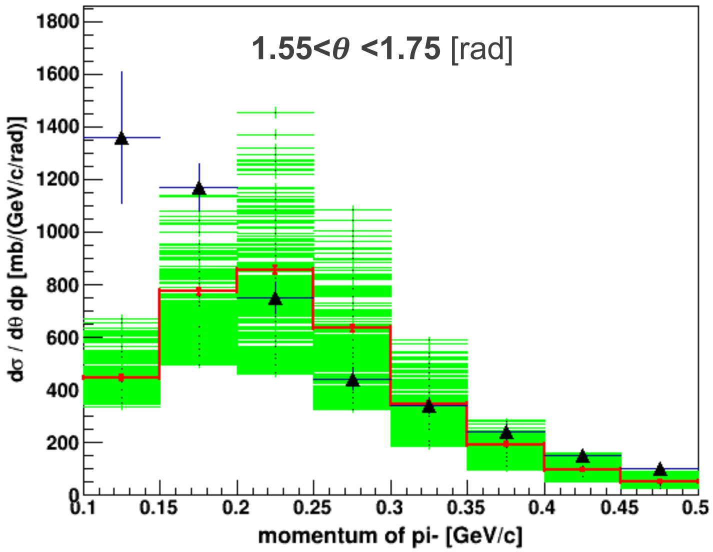
The Idea of Introducing Tunes in Geant4

- Although the work remains largely in progress, we have decided to introduce a possibility to set alternative (as compared to defaults) group of selected parameters, aka tunes
- **Preliminary** tunes for FTF become available in release 11.1 and reflect the two ongoing study cases, for baryon or pion projectile
  - In the future - for kaons, hyperons, etc.
  - In the future – maybe also tunes for different energy ranges
- At present
  - The feature is meant for internal tests and further study/development
  - The required infrastructure is in the early phase of development
- In the future
  - Similar tunes can be introduced for other Geant4 Hadronic models
  - When properly mature, tunes may be offered to users for certain applications

Future Plans

- Continue study of the FTF parameters, with the focus on the cases where varying available parameters does not yet bring the simulation closer to the data
  - E.g. focus on the cases where the shapes of the simulated distributions are significantly different from the experimental ones, etc.
- Expand collection of experimental data in the study, including recent and/or upcoming results, e.g. from NA61/SHINE (CERN) and/or EMPHATIC (Fermilab)
- Expand work towards other Geant4 models
- Explore new tuning packages that become available
  - E.g. Apprentice package and/or AI based fitting tools

5 GeV/c proton on Pb → π^- + X



▲ Data (from HARP)
— Geant4.11.1/FTF Default
Geant4.11.1/FTF with various parameter sets

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Summary

- Developing and expanding a configuration interface to the Geant4 models allows to fit simulated distributions to experimental datasets and to extract optimal values of the model parameters
- We have preliminarily explored such avenue with regards to such Hadronic models as PreCompound, Bertini cascade, and Fritiof (FTF)
- We are currently concentrating on the FTF model, and have demonstrated that certain model parameters can be optimized, through fitting techniques, to bring the MonteCarlo results closer to experimental thin target data
- We plan to continue the study of the FTF parameters, with the focus on further improving the agreement between the simulated results and the experimental data
- We also plan to gradually expand the efforts to other Geant4 Hadronic models
- In the future, when properly tested and mature, we consider offering alternative tunes for FTF and other models, for certain study cases

BACKUP SLIDES

Additional Information on the Datasets

- From the IAEA DB – 3 GeV proton on C, Fe, Pb

  K.Ishibashi et al., J.Nucl.Sci.Tech. Vol.34 N.6 1997

- HARP -- 3-12 GeV/c proton or pion on various nuclear targets

  M. Apollonio et al., Nucl. Phys. A821 118, 2009; Phys.Rev.C80 065207, 2009;

  Phys.Rev.C80 035208, 2009; Phys.Rev.C82 045208, 2010

  M.G. Catanesi et al., Phys.Rev.C77 055207, 2008

- ITEP771 – 5-7.5 GeV/c proton or 5 GeV/c pion on various nuclear targets

  Yu. D. Bayukov et al., Preprints ITEP-148-1983; ITEP-172-1983; Sov.J.Nucl.Phys. 42 116, 1985

- NA61 – 31 GeV/c proton or 60 GeV/c pi+ on Be, C

  N. Abgrall et al. , Eur.Phys.J.C 76, 2016 (proton beam)

  A. Aduszkiewicz et al. , Phys.Rev.D100 112004, 2019 (pion beam, only data on C used so far)

- SAS M6E – 100 GeV/c proton or pi+ on C, Cu, Pb (at present, not used in fits but is used in validation)

  D.S. Barton et al., Phys. Rev. D27, 2580 (1983)

- NA49 – 158 GeV/c on C (at present, not used in fits but is used in validation)

  http://spshadrons.web.cern.ch/spshadrons/

FTF: Nuclear Destruction (from the Geant4 documentation)

The GEANT4 FTF model uses reggeon cascade in the impact parameter space to simulate production of fast nucleons in the hadron-nucleus interactions. After the projectile particle interacts with one of the nucleons in the target nucleus, this "wounded" nucleon may involve another nucleon in the cascade with the probability that is given as follows:

$$P(|\vec{s}_i - \vec{s}_j|) = C_{nd}\ exp[-(\vec{s}_i - \vec{s}_j)^2/R_c^2]$$

In this formula $\vec{s}_i$ and $\vec{s}_j$ are projections of the radii of *i*-th and *j*-th nucleons on the impact parameter plane, $R_c^2 = 1.5(fm)^2$, and the coefficient C_{nd} is defined as follows:

This is fixed (D) for baryons but not for pions/mesons

$$C_{nd} = P_1\ e^{P_2\ (y-P_3)}/[1 + e^{P_2\ (y-P_3)}]$$

where y is the projectile rapidity. The parameter P_1 in the above formula can be a fixed value (DEFAULT), or it can be expressed as a function of

- baryon number of the projectile in the case of the projectile destruction
- number of nucleons in the target nucleus in case of the target destruction

Modeling of momentum distributions of the nucleons involved in the cascade is described in greater details later in this document; however, one of the characteristics we would like to mention here is the average transverse momentum squared which can be expressed in a parametric way:

$$\langle P_T^2 \rangle = C_1 + C_2 \frac{e^{C_3\ (y_l ab - C_4)}}{1. + e^{C_3\ (y_l ab - C_4)}} \quad [(GeV/c)^2]$$

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FTF: Quark Exchange (from the Geant4 documentation)

The original Fritiof model contains only the pomeron exchange process shown in Fig. 44*(d)*. It would be useful to extend the model by adding the exchange processes shown in Fig. 44*(b)* and Fig. 44*(c)*, and the annihilation process of Fig. 44*(a)*. This could probably be done by introducing a restricted set of mesonic and baryonic resonances and a corresponding set of parameters. This procedure was employed in the binary cascade model of GEANT4 (BIC) [BIC] and in the Ultra-Relativistic-Quantum-Molecular-Dynamic model (UrQMD) [UrQMD1], [UrQMD2]. However, it is complicated to use this solution for the simulation of hadron-nucleus and nucleus-nucleus interactions. The problem is that one has to consider resonance propagation in the nuclear medium and take into account their possible decays which enormously increases computing time. Thus, in the current version of the FTF model only quark exchange processes have been added to account for meson and baryon interactions with nucleons, without considering resonance propagation and decay. This is a reasonable hypothesis at sufficiently high energies.

For each projectile hadrons the following probabilities are set up:

- Probability of quark exchange process without excitation of participants (Fig. 44*(b)*); *(Proc# 0)*
- Probability of quark exchange process with excitation of participants (Fig. 44*(c)*); *(Proc# 1)*
- Probability of projectile diffraction dissociation; *(Proc# 2)*
- Probability of target diffraction dissociation. *(Proc# 3)*

All these probabilities have the same functional form:

$$P_p = A_1\, e^{-B_1\, y} \; + \; A_2\, e^{-B_2\, y} \; + A_3,$$

where y is the projectile rapidity in the target rest frame.

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