Introducing Tunes in Geant4 Hadronic Models

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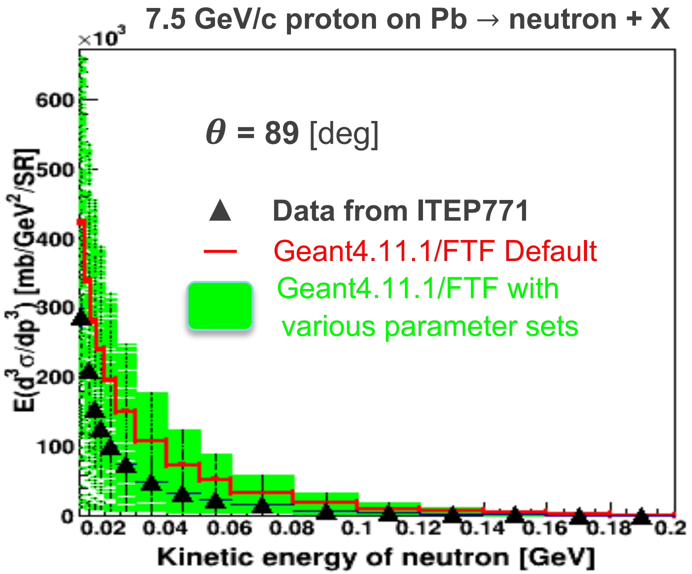
General Information (I)

- Geant4 hadronic models rely largely on physically motivated parameters; but they 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 ?
- From release 10.4, Geant4 is introducing configurable parameters which opens a possibility to
  - Explore how much the simulated observables would change with variations of parameters
  - Fit simulated distributions to experimental data and extract optimal values of the model parameters and the associated uncertainties
- The tuning activity started as a confluence of
  - Hadronic Physics Validation (benchmark vs thin target data)
  - Request from the user community for making Geant4 parameters run time configurable so that one could explore the effect of varying such parameters on the simulated observables



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General Information (II)

- Findings from earlier study of varying the **initial** set of configurable parameters available (at the time) 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
  - V. Elvira et al., JINST 15 02025 (2020)
- Currently the focus is on **FTF**
  - Popular model with the wide validity range from 3 GeV to TeV scale; in active development
  - Based on quark-gluon string formation, with subsequent LUND string fragmentation
  - Modeling of string formation involves various processes, including but not limited to
    - Nuclear target destruction
    - Quark exchange with or without excitation of participants
    - Non-diffractive or diffractive interactions

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

Best Fit Values of Selected Geant4 FTF Parameters (as of 11.1)

BARYON_EXCI_E_PER_WNDNUCLN = 26.1 +/- 0.4 (D=40)

BARYON_NUCDESTR_P1_TGT = 0.00173 +/- 0.00004 (D=1)

USE_BARYON_NUCDESTR_P1_ADEP_TGT = true (D=false)

BARYON_PROC1_A1 = 23..6 +/- 0.8 (D=25)

BARYON_PROC1_A2 = -99.3 +/- 0.4 (D=-50.34)

BARYON_PROC1_B1 = 0.815 +/- 0.007 (D=1)

BARYON_PROC1_B2 = 1.98 +/- 0.03 (D=1.5)

Details:

https://indico.cern.ch/event/1158833/contributions/4880823/attachments/2446731/4192593/G4HAD-VMP-May18-2022.pdf

MESON_EXCI_E_PER_WNDNUCLN = 58.1 +/- 0.7 (D=40)

MESON_NUCDESTR_P1_TGT = 0.001026 +/- 0.00003 (D=0.0048)

USE_MESON_NUCDESTR_P1_ADEP_TGT = true (D=true)

PION_PROC1_A1 = 5..84 +/- 0.12 (D=5.77)

PION_PROC1_A2 = -7.57 +/- 0.08 (D=-5.77)

PION_PROC1_B1 = 0.337 +/- 0.006 (D=0.6)

PION_PROC1_B2 = 0.44 +/- 0.008 (D=0.8)

Details:

https://indico.cern.ch/event/1156193/contributions/5051173/attachments/2515999/4325623/G4CM-FTFParams-2022_v2.pdf

The values have been obtained though **global fits** to thin target data, using **Professor tuning toolkit** (details in backup)

Snapshots from the Geant4 FTF documentation explaining the parameters in question are in backup

Complete Geant4 documentation on the matter : https://geant4-userdoc.web.cern.ch/UsersGuides/ForToolkitDeveloper/html/GuideToExtendFunctionality/HadronicPhysics/hadronics.html#changing-internal-parameters-of-an-existing-hadronic-model

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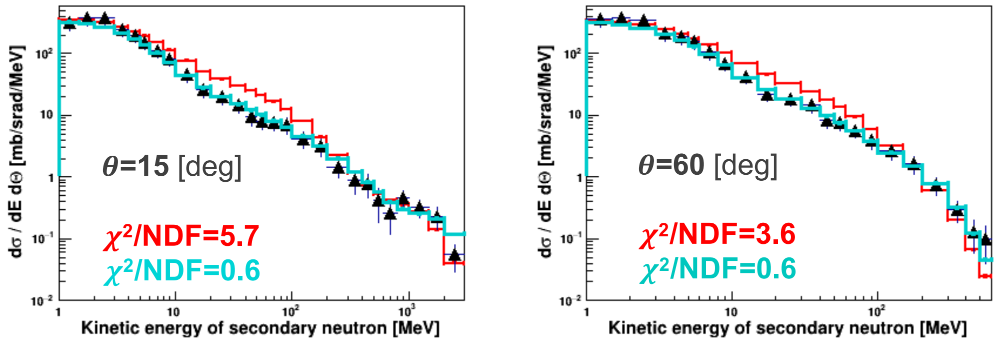
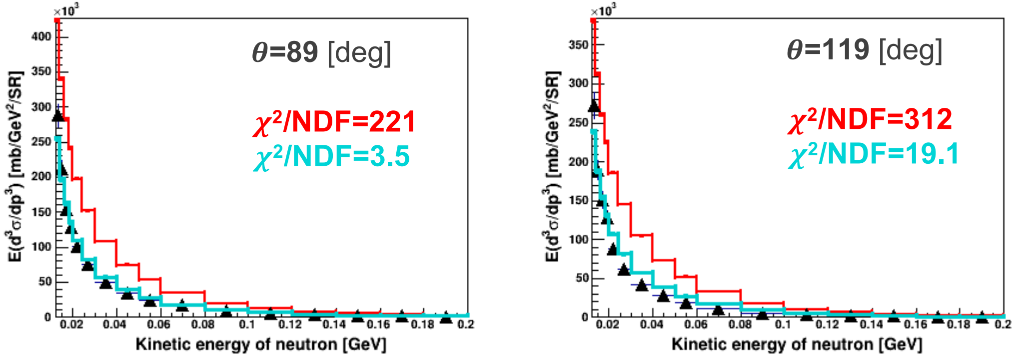
Simulation of neutron production in proton-Pb interactions

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.

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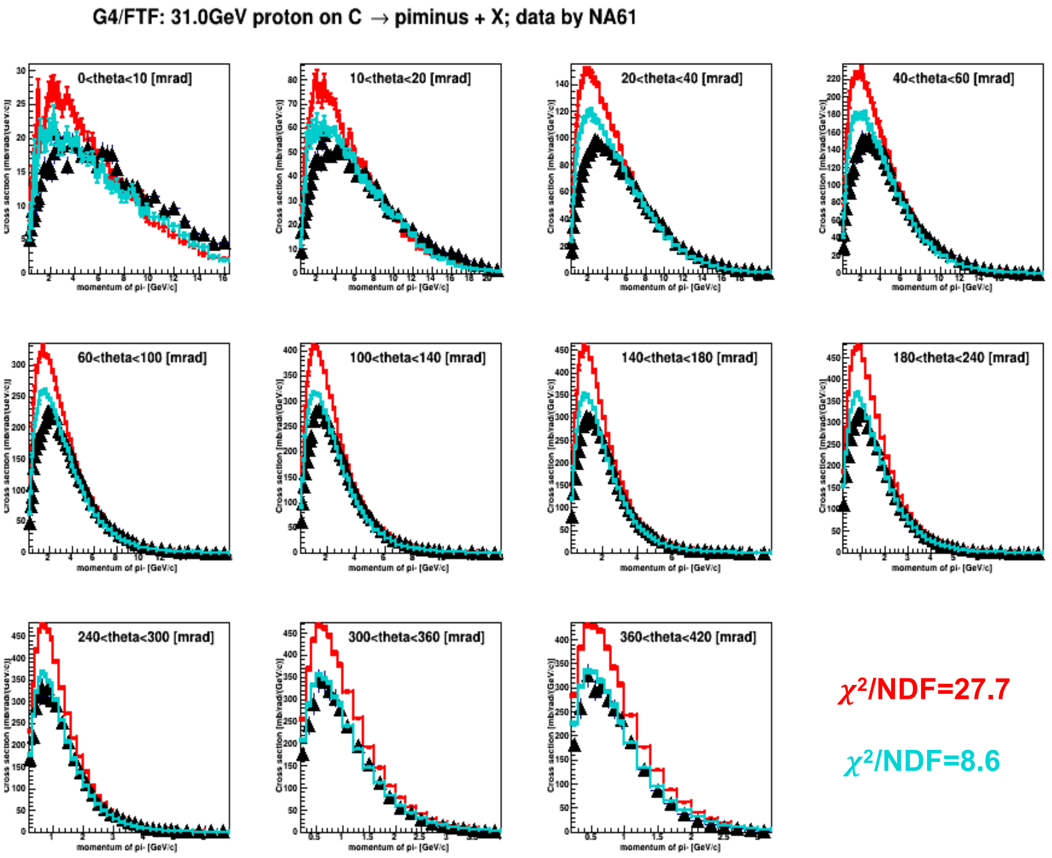
Simulation of π^- production in 31 GeV/c proton-C interactions



▲ Data (all from NA61/SHINE)

- N. Abgrall et al. , Eur.Phys.J.C 76, 2016

— Geant4.11.1/FTF Default

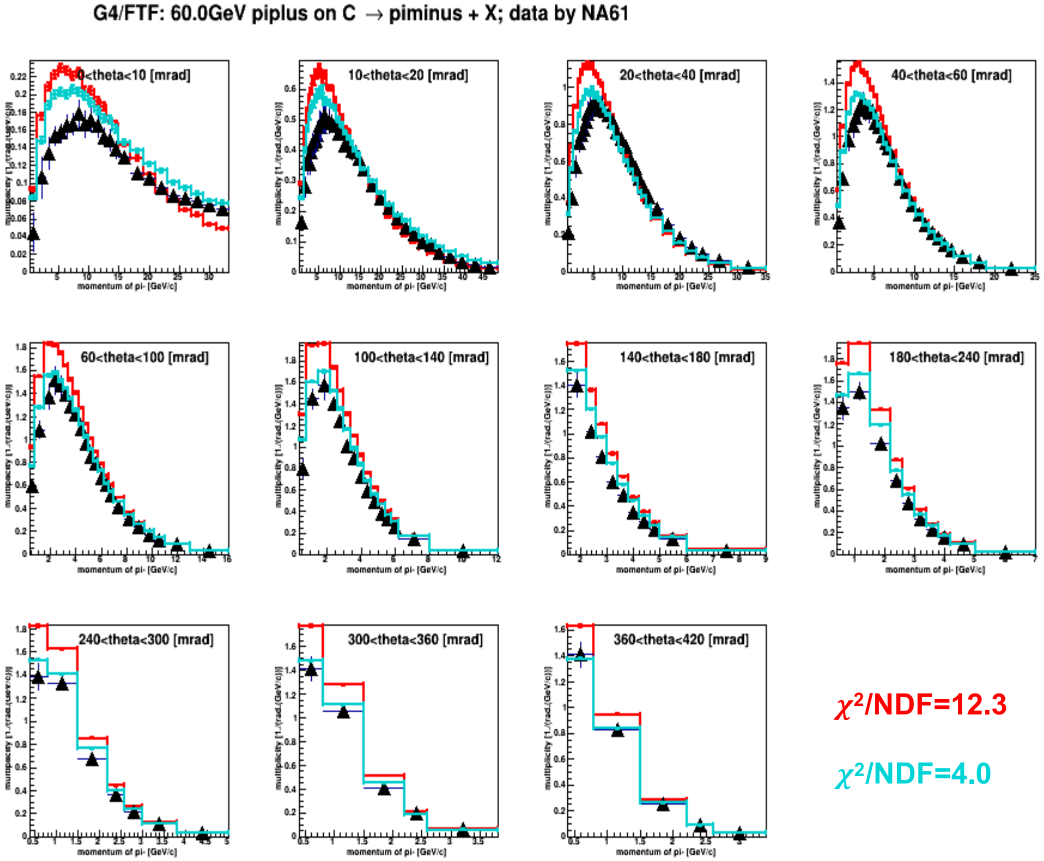
— Geant4.11.1/FTF with Best Fit Parameters

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.

χ^2/NDF=27.7

χ^2/NDF=8.6

Simulation of π^- production in 60 GeV/c π^+-C interactions



▲ Data (all from NA61/SHINE)

- 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.

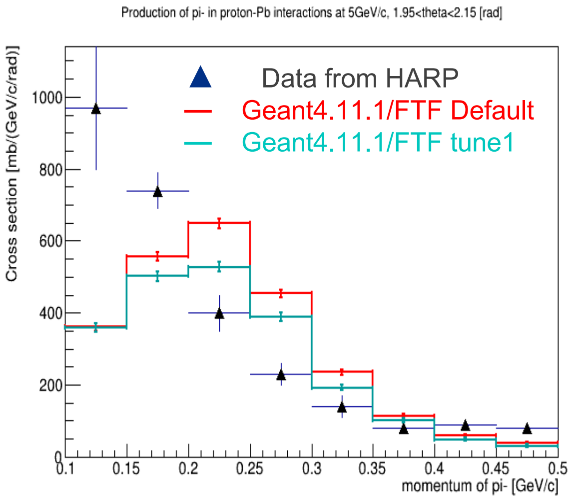
χ^2/NDF=12.3

χ^2/NDF=4.0

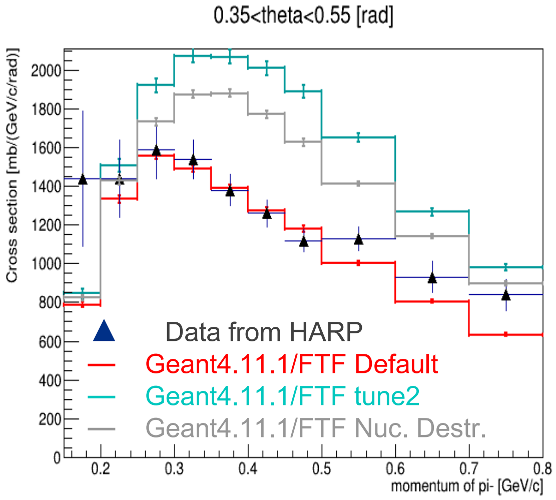
The Idea of Introducing Tunes in Geant4

- Although the work remains largely in progress, we have decided to introduce a possibility to select at run time alternative (as compared to defaults) groups of selected parameters, aka tunes
- **Preliminary** tunes for FTF become available in release 11.1 and reflect the two ongoing study
  - tune1 – baryon projectile (see slide5)
  - tune2 – pion projectile (see slide 5)
  - tune3 – tune1+tune2; introduced because at the time the infrastructure allowed to select only one at a time
- 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
  - Maybe similar tunes for other projectiles (kaons, hyperons, etc.)
  - Maybe tunes for different energy ranges
  - Similar tunes can be introduced for other Geant4 Hadronic models
  - When mature and properly tested, tunes maybe offered to users for certain studies

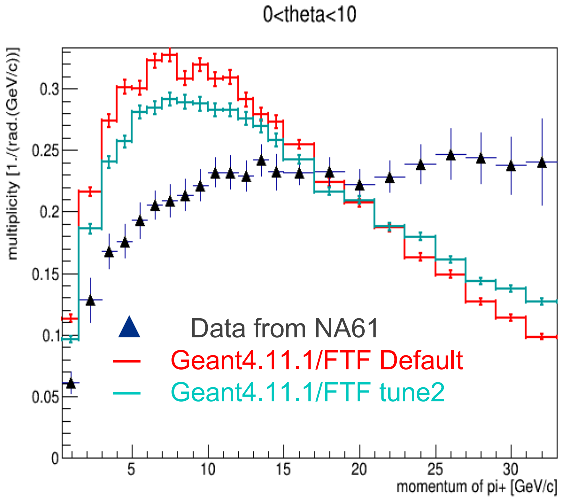
Some examples of concerns with tune1 and tune2



5GeV/c proton on Pb → π^-
For π^- production in the backward hemisphere, can we get the shape of the simulated spectrum right ?



5GeV/c π^+ on Pb → π^-
Increase in π^- production in the forward hemisphere is an artefact of using best fit parameters for the nuclear destruction (grey curve).
Can we compensate ?



60GeV/c π^+ on C → π^+
Can we get the shape of the simulated spectrum right ?

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 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
- Following initial progress, we have introduced a possibility to select alternative (as compared to default) groups of FTF parameter values, aka tunes, obtained through fits vs thin target data
  - The tunes are preliminary, and at present are mainly meant to facilitate internal validation and further work
  - However, when they are mature and properly tested, we may consider offering this option for certain studies
- We continue efforts to further optimize FTF parameters
- We also plan to gradually expand (and/or resume) the efforts to other Geant4 Hadronic models

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/

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)

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:

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

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.