FERMILAB-SLIDES-23-305-CSAID

Update on Tuning Geant4 FTF Parameters

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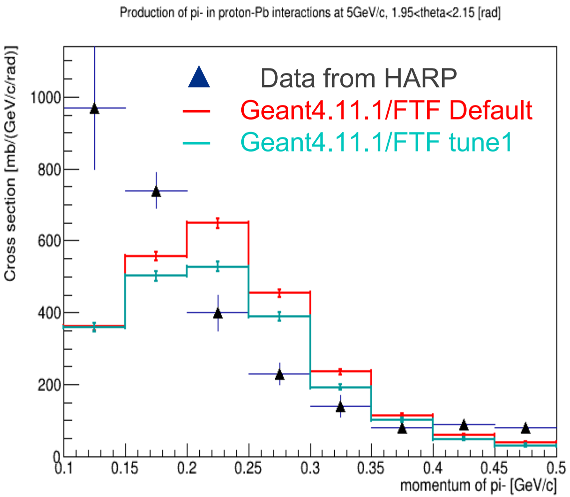
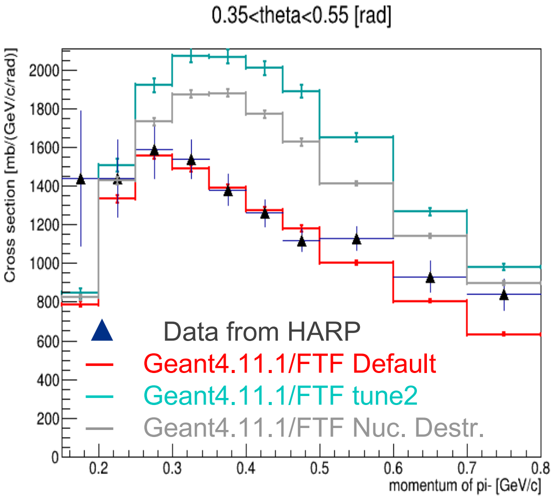
General Information

- General introduction to the activity is given in Plenary
- Currently the focus is on **FTF** modeling of the quark-gluon string formation, specifically on the following (sub)processes
  - Nuclear target destruction
  - Quark exchange with excitation of participants (QEX w/o excitation is kept as-is)
  - Since the probability of non-diffractive interactions is calculated as (1. – sum probability of other processes), this part of FTF workflow is also affected
- We have demonstrated that certain model parameters can be optimized, through fitting techniques, to bring the MonteCarlo results closer to experimental thin target data
- Starting release 11.1 we have introduced a possibility to select at run time alternative (as compared to defaults) group of selected parameters, aka tunes; the tunes are groups of FTF parameters **collectively** obtained through fits to thin target data, and should be used as such
- However, one should confess that there still remain certain areas where further improvement is needed
  - Use of tunes may induce some side effects
  - The MonteCarlo does not match the data “shapewise”, no matter what

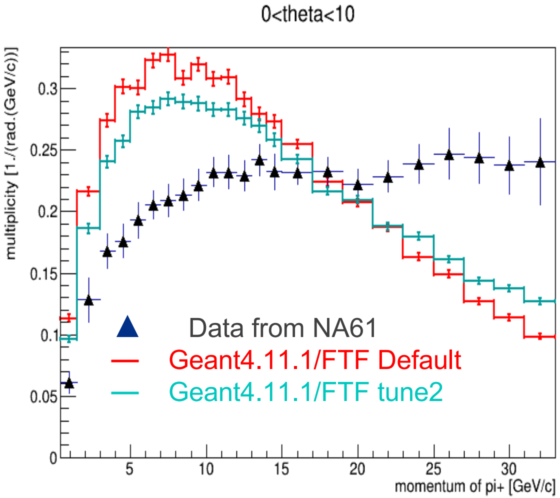
Some examples of concerns with tune1 and tune2


Production of pi- in proton-Pb interactions at 5GeV/c, 1.95<theta<2.15 [rad]

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


0.35<theta<0.55 [rad]

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 ?


0<theta<10

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

Adding More FTF Parameters to the Study

BARYON_AVRG_PT2	**D=0.3 GeV^2 , range 0.08 - 1**
BARYON_DIFF_M_TGT	**D=1.16 GeV, range 1.16 - 3**
BARYON_NONDIFF_M_TGT	**D=1.16 GeV, range 1.16 - 3**

NOTE: initially explored within Geant4.10.4, see https://g4cpt.fnal.gov/g4vmp.html

PION_AVRG_PT2	**D=0.3 GeV2 , range 0.08 - 1**
PION_DIFF_M_TGT	**D=1.16 GeV, range 1.16 - 3**
PION_NONDIFF_M_TGT	**D=1.16 GeV, range 1.16 - 3**

NOTE: none of the configurable parameters were available for the pion projectile in 10.4

Screenshots of Geant4 FTF documentation fragments are in backup slides

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

In short, the 1st parameter is involved in modeling non-diffractive interactions, and its change can affect behavior of particle distributions at large xF.

The 2nd and the 3rd define the string mass sampling thresholds

Changing the 3rd parameter can produce a significant effect e.g. on the simulated yield of secondary pions (reduction in the yield); in bare eye inspection the effect is larger in the forward direction, and is relatively mild in the backward hemisphere

Varying and fitting selected FTF parameters

- **Adopted from tune1 :**

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)

- **Varied :**

BARYON_PROC1_A1	**from 12.5 to 50**
BARYON_PROC1_A2	**from -100 to 0**
BARYON_PROC1_B1	**from 0.5 to 1.2**
BARYON_PROC1_B2	**from 1 to 5**
BARYON_AVRG_PT2	**from 0.08 to 1**
BARYON_DIFF_M_TGT	**from 1.16 to 3**
BARYON_NONDIFF_M_TGT	**from 1.16 to 3**

- **Simulation :** 5 or 12 GeV/c proton on C or Pb, 8 GeV/c proton on Ta, 31 GeV/c proton on C

- **Adopted from tune2 :**

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)

- **Varied :**

PION_PROC1_A1	**from 3 to 10**
PION_PROC1_A2	**from -9 to -1**
PION_PROC1_B1	**from 0.3 to 0.9**
PION_PROC1_B2	**from 0.4 to 1.2**
PION_AVRG_PT2	**from 0.08 to 1**
PION_DIFF_M_TGT	**from 1.16 to 3**
PION_NONDIFF_M_TGT	**from 1.16 to 3**

- **Simulation :** 5 or 12 GeV/c π^{+}/π^{-} on C or Pb, 60 GeV/c $\pi^{+.}$ on C

- 200 points in the multiparameter space (good for Professor parametrization with 3rd order polynomial)
- Fits : Professor 2.4.0 (April 2023); compatible with Python 3.9.X and gcc-12.1.0; iMinuit 2.22.0

Best fit values of selected FTF parameters

- **Adopted from tune1 :**

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)

- **Best fit values :**

BARYON_PROC1_A1 = 44..9 +/- 0.6 (D=25)

BARYON_PROC1_A2 = -57.9 +/- 2.4 (D=-50.34)

BARYON_PROC1_B1 = 0.864 +/- 0.007 (D=1)

BARYON_PROC1_B2 = 1.17 +/- 0.05 (D=1.5)

BARYON_AVRG_PT2 = 0.73 +/- 0.01 (D=0.3 GeV^2)

BARYON_DIFF_M_TGT = 2.07 +/- 0.05 (D=1.16 GeV)

BARYON_NONDIFF_M_TGT = 2.046 +/- 0.05 (D=1.16 GeV)

BARYON_PROC1_YMIN - recalculates from 1.4 to 1.03

BARYON_PROC4_YMIN - same as above

- **Adopted from tune2 :**

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)

- **Best fit values :**

PION_PROC1_A1 = 3..7 +/- 0.04 (D=5.77)

PION_PROC1_A2 = -7.28 +/- 0.05 (D=-5.77)

PION_PROC1_B1 = 0.366 +/- 0.002 (D=0.6)

PION_PROC1_B2 = 0.662 +/- 0.005 (D=0.8)

PION_AVRG_PT2 = 0.33 +/- 0.007 (D=0.3 GeV^2)

PION_DIFF_M_TGT = 2.14 +/- 0.02 (D=1.16 GeV)

PION_NONDIFF_M_TGT = 1.226 +/- 0.004 (D=1.16 GeV)

NOTE: Given that we have only tried 3rd order polynomial in Professor parametrization, these results should be considered as “pilot”

χ^2/NDF– baryon projectile (proton)

		5 GeV/c proton						12 GeV/c proton					
		C			Pb			C			Pb		
		11.1.r7	tune1	BestFit	11.1.r7	tune1	BestFit	11.1.r7	tune1	BestFit	11.1.r7	tune1	BestFit
π^-	FW	6.53	3.59	2.63	2.29	1.71	1.52	8.2	5.62	5.45	8.38	2.3	4.32
	LA	8.45	3.56	3.57	20.66	14.04	12.48	22.06	2.85	2.78	67.84	10.48	11.0
π^+	FW	9.31	7.76	7.78	3.54	2.51	2.44	19.26	10.35	12.88	14.90	6.89	8.33
	LA	7.83	6.59	7.4	8.82	5.81	11.01	7.66	7.81	3.99	22.59	12.37	7.71

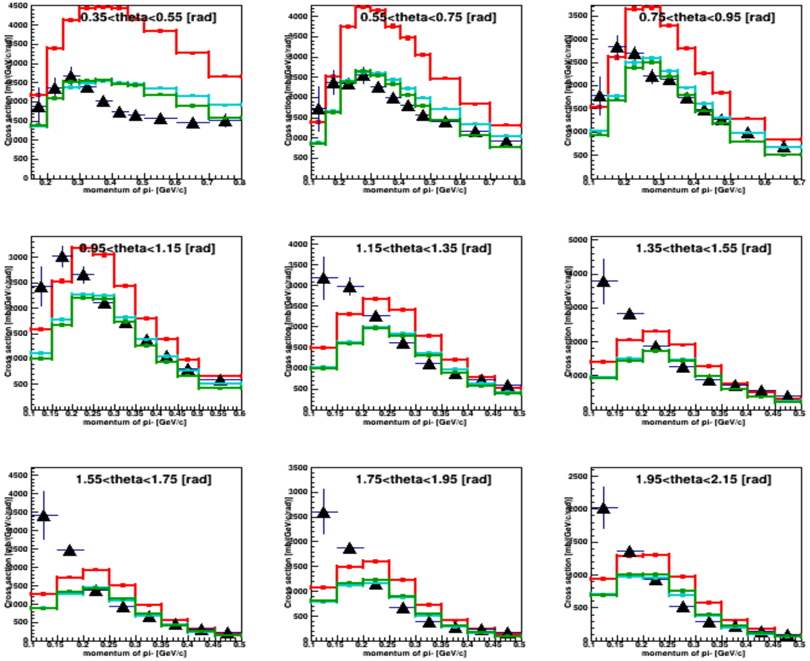
	31 GeV/c proton on C		
	11.1.r7	tune1	BestFit
π^-	27.68	8.65	12.76
π^+	37.29	16.58	16.69

In general, using tuned (best fit) parameters for the baryon projectile improves agreement between MC and thin target data, except for some discrepancies in the backward hemisphere.

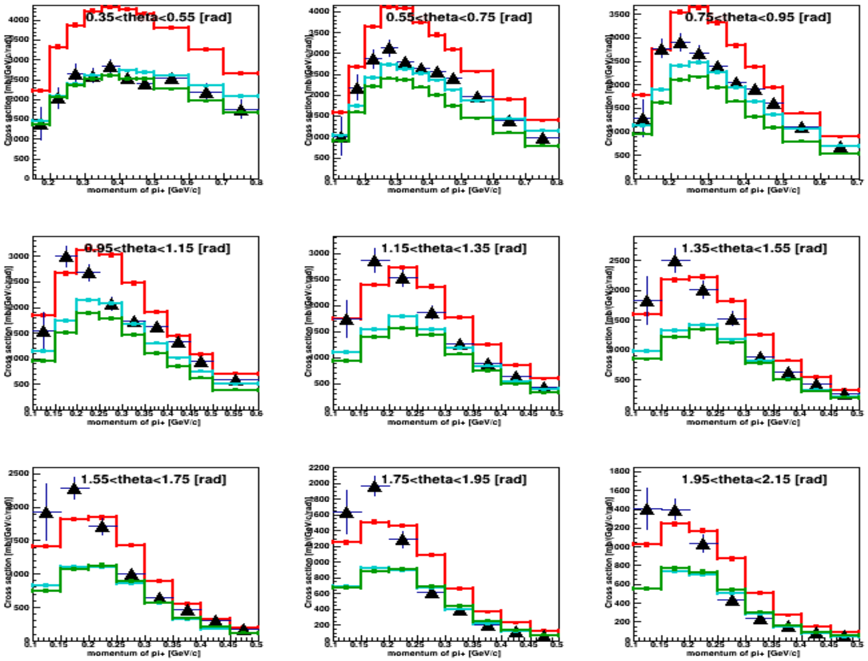
However, changing thresholds in the string mass sampling does not bring any sizeable benefits.

12 GeV/c proton on Pb (LA production of pions)

G4/FTF: 12.0GeV proton on Pb → piminus + X; data by HARP



G4/FTF: 12.0GeV proton on Pb → piplus + X; data by HARP



G4/FTF Default χ^2/NDF = 67.84

G4/FTF tune1 χ^2/NDF = 10.48

G4/FTF BestFit χ^2/NDF = 11.0

G4/FTF Default χ^2/NDF = 22.59

G4/FTF tune1 χ^2/NDF = 12.37

G4/FTF BestFit χ^2/NDF = 7.71

Example contributions of underlying algorithms (I)

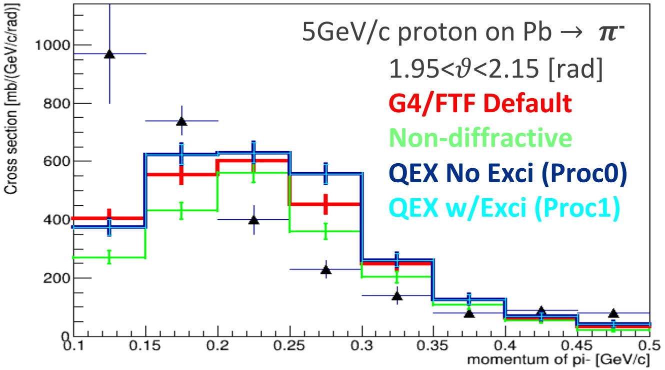
As of 11.1, **3** (sub)processes are involved at the step leading to quark-gluon string creation, i.e. non-diffractive interactions and quark exchange (QEX) with or without excitation

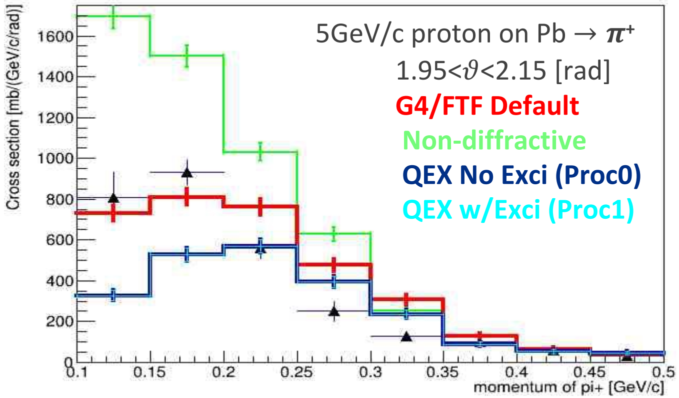
The probability of non-diffractive interaction is defined as 1.- Probability(both QEX)

Thus changing parameters that define contribution of either QEX process (or both) automatically changes the probability of non-diffractive interactions

Via configurable parameters one can turn ON one of them and completely switch OFF the other two

As for **backward production of π^-** by a proton beam on heavy target (e.g. Pb), none of the underlying (sub)processes gives the momentum distribution matching the experimental thin target data





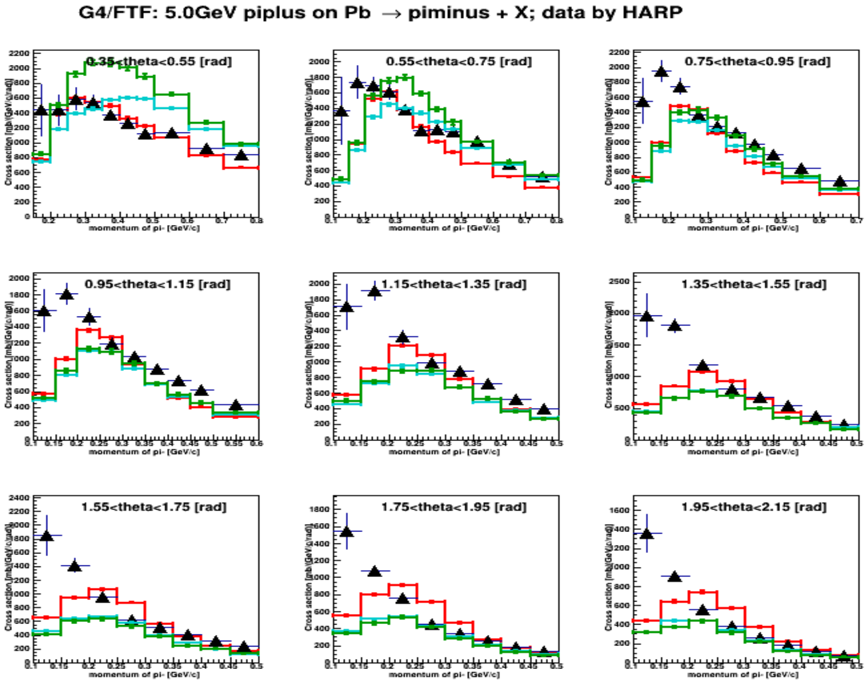
χ^2/NDF - π^+ projectile

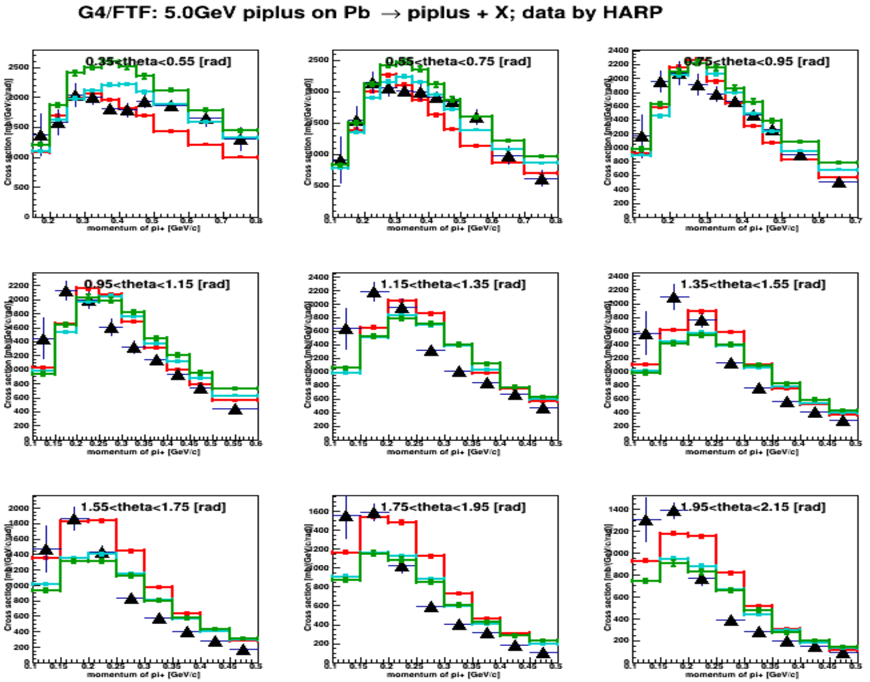
		5 GeV/c pi+						12 GeV/c pi+					
		C			Pb			C			Pb		
		11.1.r7	tune2	BestFit	11.1.r7	tune2	BestFit	11.1.r7	tune2	BestFit	11.1.r7	tune2	BestFit
π^-	FW	19.19	18.09	19.82	8.78	9.73	9.46	1.37	1.43	1.08	31.99	36.39	31.96
	LA	31.88	34.1	28.55	12.23	20.28	16.79	4.16	3.73	3.88	6.27	5.52	4.33
π^+	FW	35.3	37.82	34.42	9.97	19.41	16.59	4.0	3.64	2.84	8.94	9.15	7.58
	LA	4.88	4.77	5.41	15.36	12.2	10.11	1.59	2.0	2.4	4.27	3.04	2.29

	60 GeV/c pi+ on C		
	11.1.r7	tune2	BestFit
π^-	10.42	4.0	6.35
π^+	21.88	11.88	11.94

In general, using tune2 or recent best fit parameters for the pion projectile improves agreement between MonteCarlo and thin target data. However, tune2 may induce side effect of increased pion production by a several-GeV beam on heavy targets. The effect could be somewhat compensated by increasing thresholds in the string mass sampling. However, the nature of the effects still needs to ne better understood, as well as several other effects.

5 GeV/c π^+ on Pb (LA pion production)

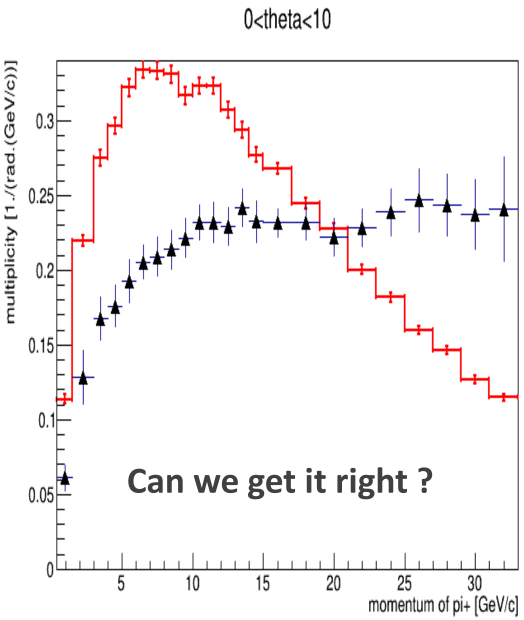




G4/FTF Default χ^2/NDF = 12.23
G4/FTF tune2 χ^2/NDF = 20.28
G4/FTF BestFit χ^2/NDF = 16.79

G4/FTF Default χ^2/NDF = 15.36
G4/FTF tune2 χ^2/NDF = 12.2
G4/FTF BestFit χ^2/NDF = 10.11

Modeling very forward 60GeV/c π^+ on C $\rightarrow \pi^+$

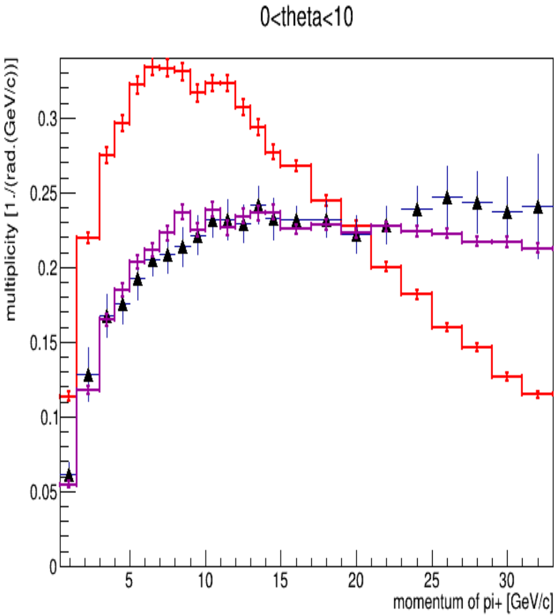


Can we get it right ?

These are not fit results but one of the points out of 200 in the multiparameter space, selected by the closest match for this particular spectrum (point #120) :

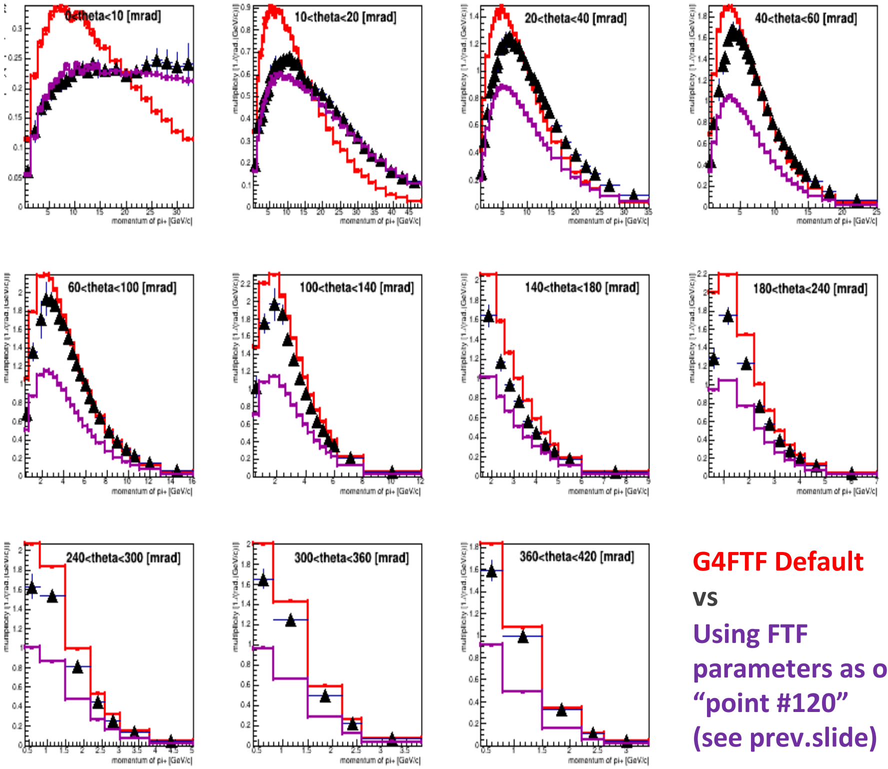
MESON_EXCI_E_PER_WNDNUCLN=58.1
MESON_NUCDESTR_P1_TGT=0.001026
PION_AVRG_PT2=0.395471
PION_DIFF_M_TGT=2.82167
PION_NONDIFF_M_TGT=2.8675
PION_PROC1_A1=4.90664
PION_PROC1_A2=-6.61704
PION_PROC1_B1=0.323679
PION_PROC1_B2=0.899831
USE_MESON_NUCDESTR_P1_ADEP_TGT=1

But then one needs to see what happens to other spectra of the secondary pi+ (see next slide)



Example contributions from different algorithms (II)

G4/FTF: 60 GeV piplus on C → piplus + X; data by NA61

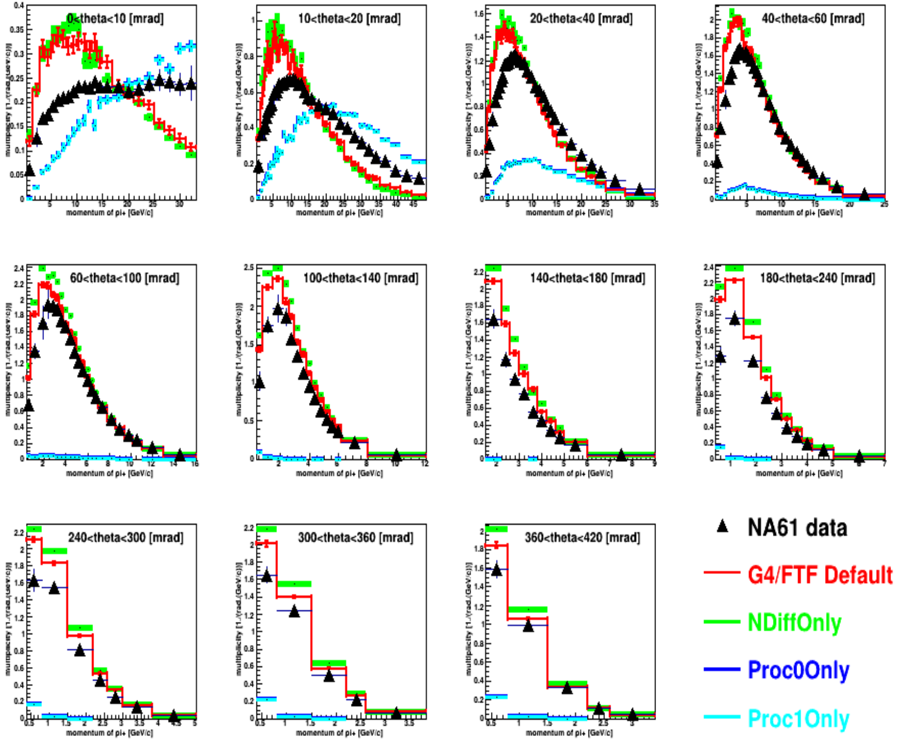


G4FTF Default

vs

Using FTF parameters as of "point #120" (see prev.slide)

G4/FTF: 60GeV piplus on C → piplus + X; data by NA61



Summary

- In general, using tuned (best fit) FTF parameters improves agreement between MC and thin target data, for both baryon (proton) or pion projectiles
- For the baryon projectile it includes FTF parameters involved in modeling nuclear target destruction and those that define contribution from quark exchange
  - Fitting/changing thresholds of the string mass sampling in the string formation does not bring sizeable benefits (although these parameters can produce non-negligible impact if varied individually)
  - Discrepancies between FTF results and thin target data for pions produced in the backward hemisphere by proton projectile on heavy nuclei are due to the underlying algorithms rather than currently available configurable parameters
- For the pion projectile, using FTF best fit parameters related to nuclear target destruction and quark exchange generally improves agreement between FTF results and thin target data but changing parameters of nuclear destruction may induce undesired increase in pion production on heavy targets
  - Perhaps the effect needs to be revisited/explored some more
  - The effect might be somewhat compensated by adjusting thresholds in string mass sampling
  - Some discrepancies between FTF results and experimental data, e.g. on pion production in the very forward direction by higher momentum beam (e.g. 60 GeV/c) are likely to be due to underlying mechanisms and not only the combination of FTF parameters defining contribution(s) from quark exchange (vs non-diffractive interactions)

BACKUP SLIDES

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)

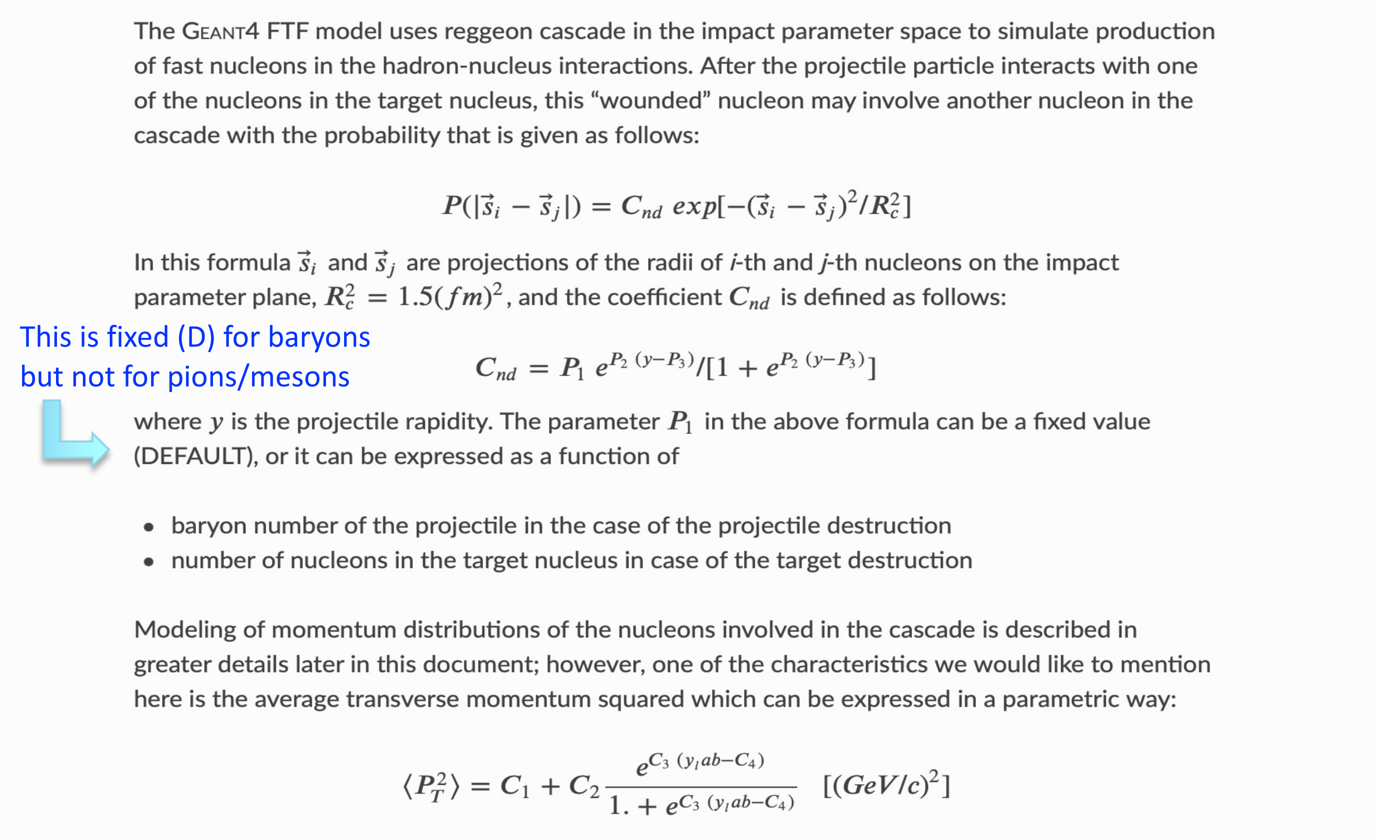
- NA49 – 158 GeV/c on C (at present, not used in fits but is used in validation)

  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 $\chi^2 = \Sigma_{\text{bin}}$ (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

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

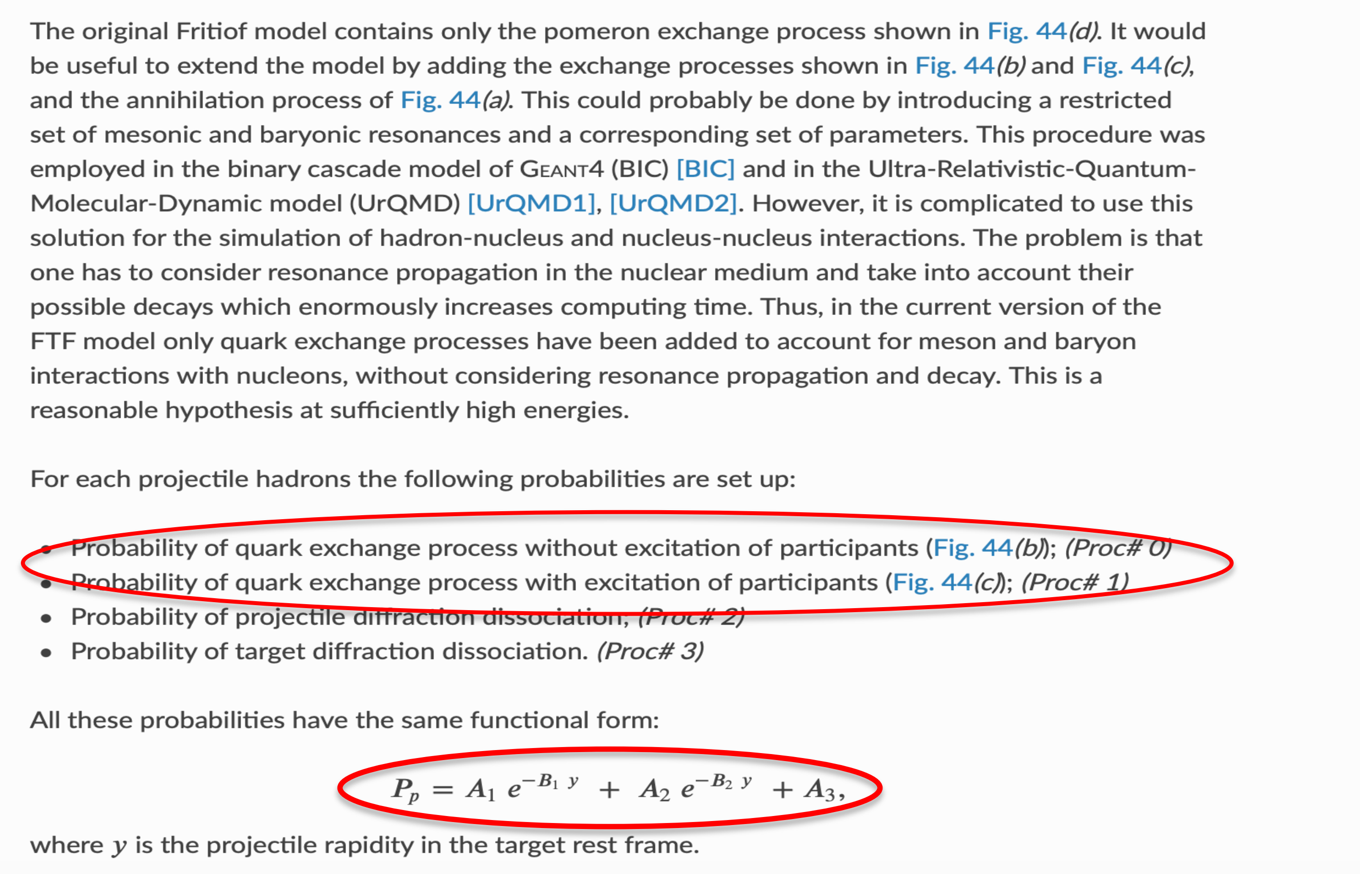
where y is the projectile rapidity. The parameter P_1 in the above formula can be a fixed value (DEFAULT), or it can be expressed as a function of

- 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:

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

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:

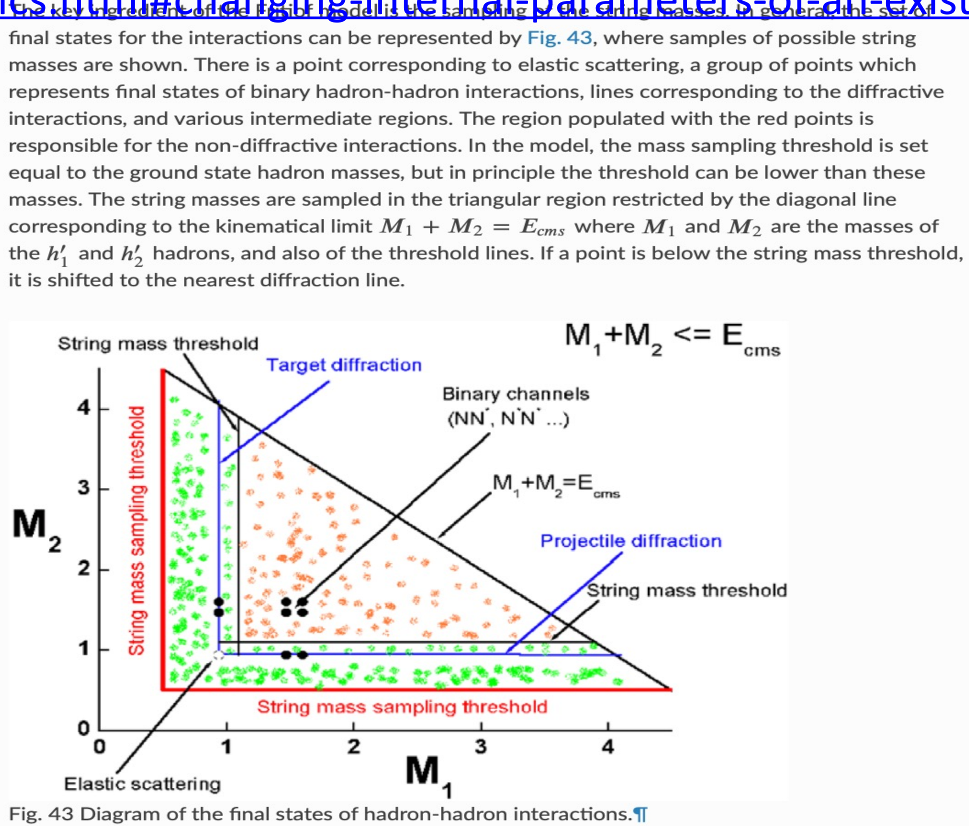
- Probability of quark exchange process without excitation of participants (Fig. 44*(b)*); *(Proc# 0)*
- Probability of quark exchange process with excitation of participants (Fig. 44*(c)*); *(Proc# 1)*
- Probability of projectile diffraction dissociation; *(Proc# 2)*
- Probability of target diffraction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

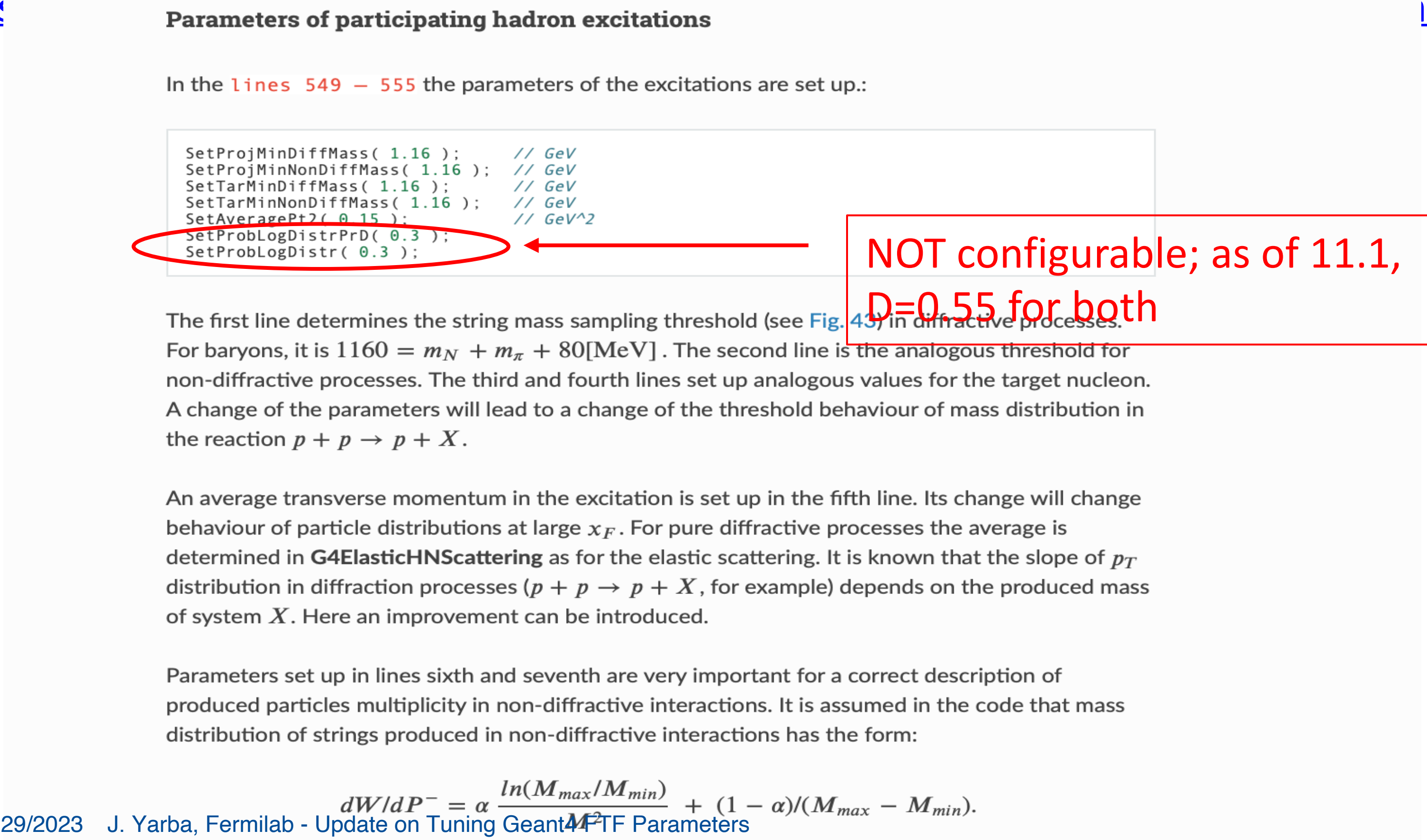
From the Geant4 Documentation : https://geant4-userdoc.web.cern.ch/UsersGuides/ForToolkitDeveloper/html/GuideToExtendFunctionality/HadronicPhysics/hadronics.html#changing-internal-parameters-of-an-existing-hadronic-model



The key ingredient of the Fritiof model is the sampling of the string masses. In general, the set of final states for the interactions can be represented by Fig. 43, where samples of possible string masses are shown. There is a point corresponding to elastic scattering, a group of points which represents final states of binary hadron-hadron interactions, lines corresponding to the diffractive interactions, and various intermediate regions. The region populated with the red points is responsible for the non-diffractive interactions. In the model, the mass sampling threshold is set equal to the ground state hadron masses, but in principle the threshold can be lower than these masses. The string masses are sampled in the triangular region restricted by the diagonal line corresponding to the kinematical limit $M_1 + M_2 = E_{cms}$ where M_1 and M_2 are the masses of the h_1' and h_2' hadrons, and also of the threshold lines. If a point is below the string mass threshold, it is shifted to the nearest diffraction line.

Fig. 43 Diagram of the final states of hadron-hadron interactions.¶

From the Geant4 Documentation : https://geant4-userdoc.web.cern.ch/UsersGuides/ForToolkitDeveloper/html/GuideToExtendFunctionality/HadronicPhys odel



Parameters of participating hadron excitations

In the `lines 549 – 555` the parameters of the excitations are set up.:

```
SetProjMinDiffMass( 1.16 );      // GeV
SetProjMinNonDiffMass( 1.16 );   // GeV
SetTarMinDiffMass( 1.16 );       // GeV
SetTarMinNonDiffMass( 1.16 );    // GeV
SetAveragePt2( 0.15 );           // GeV^2
SetProbLogDistrPrD( 0.3 );
SetProbLogDistr( 0.3 );
```

The first line determines the string mass sampling threshold (see Fig. 43) in diffractive processes. For baryons, it is $1160 = m_N + m_\pi + 80[\mathrm{MeV}]$. The second line is the analogous threshold for non-diffractive processes. The third and fourth lines set up analogous values for the target nucleon. A change of the parameters will lead to a change of the threshold behaviour of mass distribution in the reaction $p + p \rightarrow p + X$.

An average transverse momentum in the excitation is set up in the fifth line. Its change will change behaviour of particle distributions at large x_F. For pure diffractive processes the average is determined in **G4ElasticHNScattering** as for the elastic scattering. It is known that the slope of p_T distribution in diffraction processes ($p + p \rightarrow p + X$, for example) depends on the produced mass of system X. Here an improvement can be introduced.

Parameters set up in lines sixth and seventh are very important for a correct description of produced particles multiplicity in non-diffractive interactions. It is assumed in the code that mass distribution of strings produced in non-diffractive interactions has the form:

$$dW/dP^- = \alpha \frac{ln(M_{max}/M_{min})}{M^2} + (1-\alpha)/(M_{max} - M_{min}).$$

NOT configurable; as of 11.1, D=0.55 for both