Summary of Hadronic Parallel Session 3A

Alberto Ribon
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Geant4 Collaboration meeting, Sapporo, 29 September 2023

Parallel Session 3A : Hadronic Physics **1**

- Yoshihide Sato “*Development and implementation of a new Geant4 QMD model and its validation*”

- Lorenzo Arsini “*Graph Neural Networks for fast emulation of nuclear interaction models*“

- Julia Yarba “*Update on tuning of hadronic model parameters*“

Yoshihide Sato

“*Development and implementation of a new Geant4 QMD model and its validation*”

Yoshihide Sato,
Graduate School of Health Science, Tokushima University

Development of more accurate QMD model for hadron therapy

Introduction


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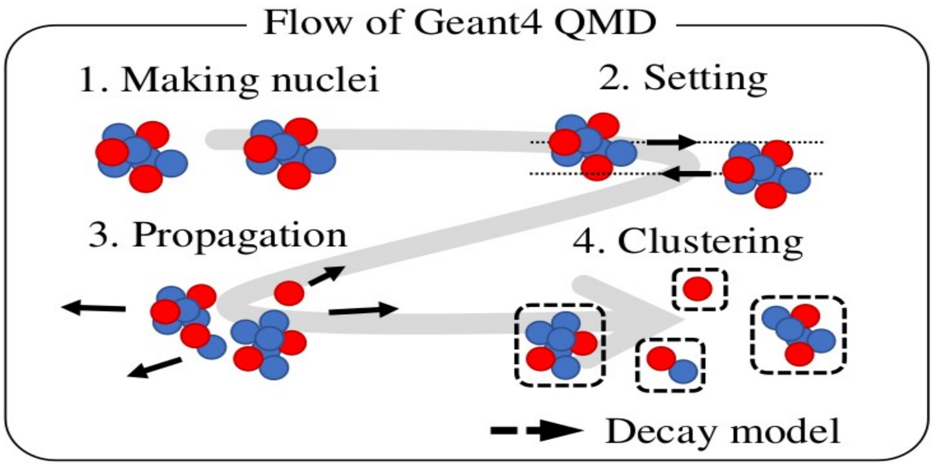
PAPER

Development of a more accurate Geant4 quantum molecular dynamics model for hadron therapy

Yoshi-hide Sato[1], Dousatsu Sakata[2,3,*], David Bolst[4], Edward C Simpson[5], Susanna Guatelli[4] and Akihiro Haga[1,*]

Sato, Y.-H. *et al*. Development of a more accurate Geant4 quantum molecular dynamics model for hadron therapy. *Phys. Med. Biol.* **67**, (2022)

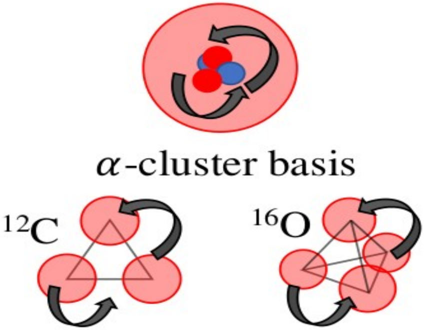


Three improvements

1. Modern interaction

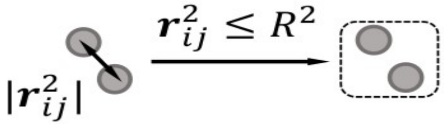
	JQMD[b] (G4QMD)	SLy4[c]	SkM*[c]	SIII[c]
A [MeV]	−219.4	−297.82	−318	−122.921
B [MeV]	165.3	219.21	249.5	55.343
g_0 [MeV fm^2]	—	24.569	21.86	18.286
g_τ [MeV]	—	9.70	5.9357	6.439
C_s [MeV]	25	32	32	32
κ_s [fm^2]	—	0.08	0.08	0.08
γ	4/3	7/6	7/6	2
η[a]	—	5/3	5/3	5/3
ρ_0 [fm^{-3}][a]	0.168	0.160	0.165	0.1452
BE [MeV][a]	−16.00	−15.97	−15.77	−15.83
K_0 [MeV][a]	237.8	230.2	216.8	355.9

2. α-cluster structure



3. QMD model Parameter optimization

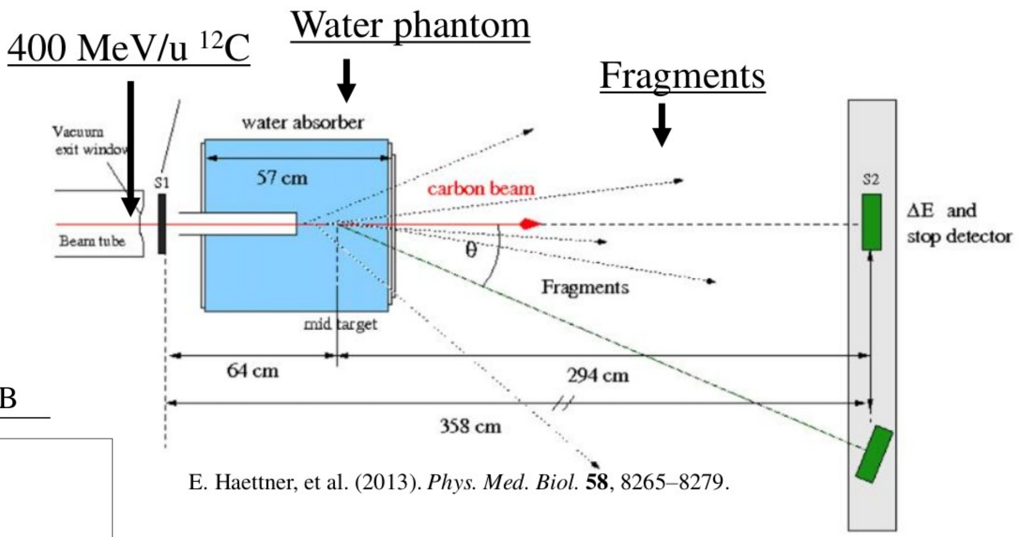
$$\varphi_i(\boldsymbol{r}) \equiv \frac{1}{(2\pi L)^{3/4}} \exp\left(-\frac{(\boldsymbol{r}-\boldsymbol{r}_i)^2}{4L} + \frac{i}{\hbar}\boldsymbol{r}\cdot\boldsymbol{p}_i\right)$$



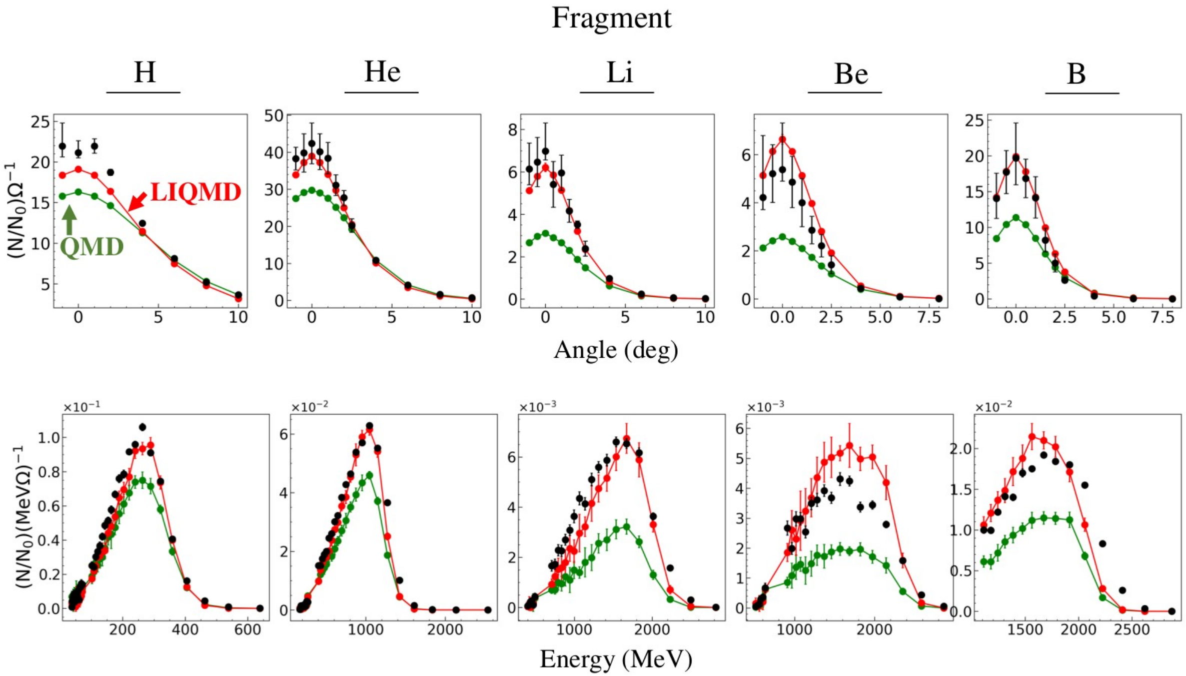
Development and implementation of new Geant4 QMD model and its validation

Yoshihide Sato,
Graduate School of Health Science, Tokushima University

Recommended energy range: 30 – 500 MeV/u



E. Haettner, et al. (2013). *Phys. Med. Biol.* **58**, 8265–8279.



Development and implementation of new Geant4 QMD model and its validation

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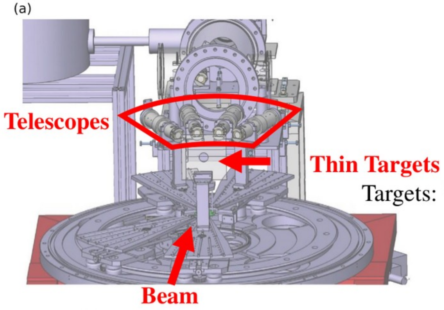
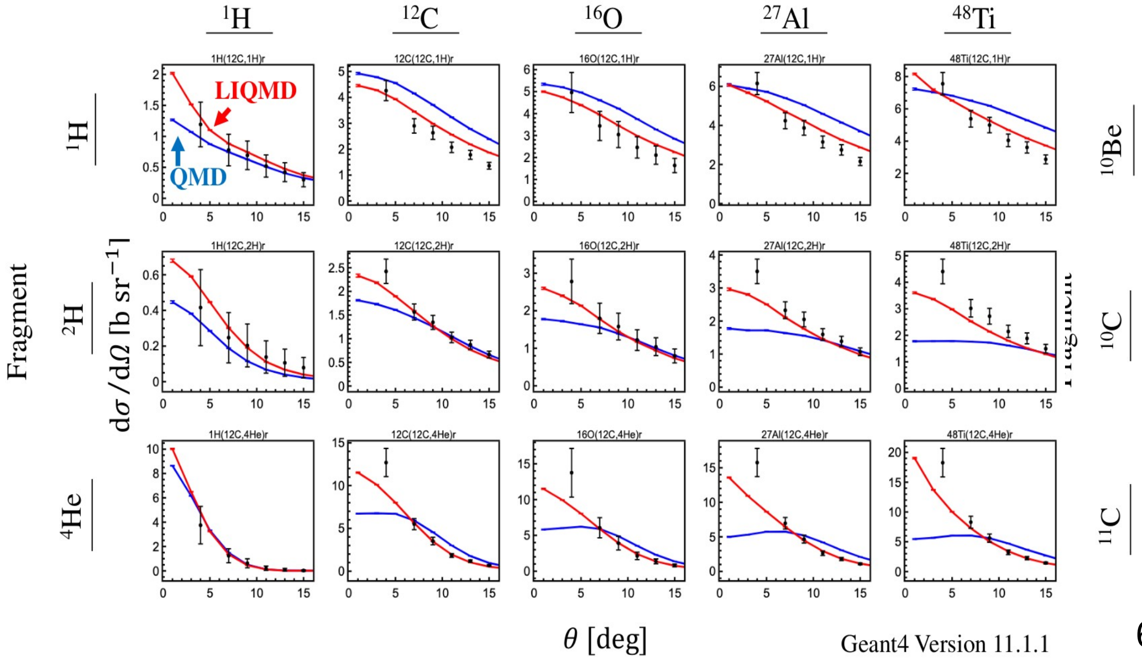
Recommended energy range: 30 – 500 MeV/u

Fragments: ^{1,2,3}H, ^{3,4,6}He, ^{6,7}Li, ^{7,9,10}Be, ^{8,10,11}B, ^{10,11,12}C

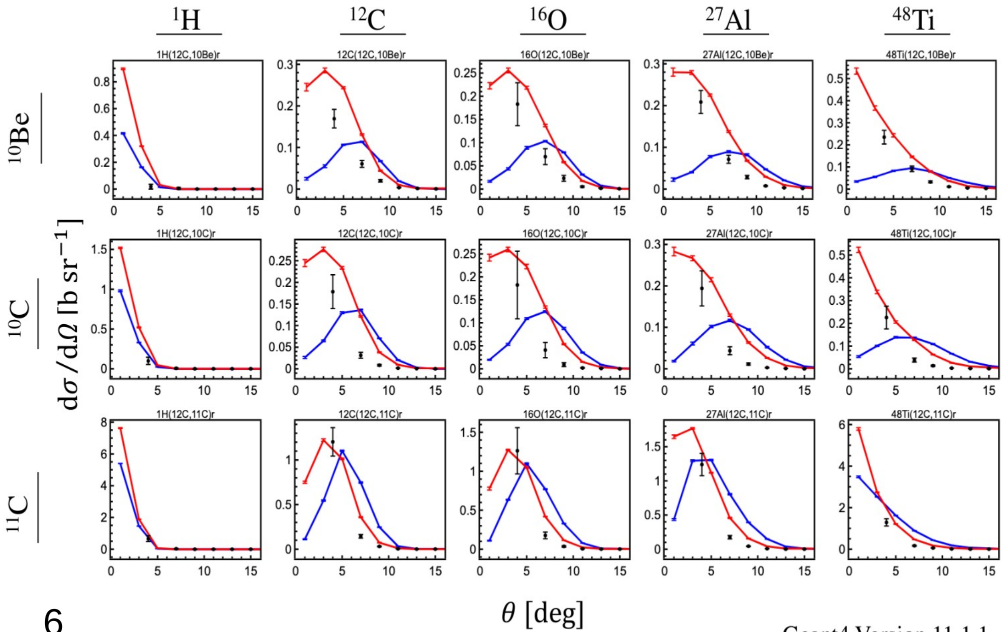


Targets: ^{1}H, ^{12}C, ^{16}O, ^{27}Al, ^{48}Ti

Beam: ^{12}C, 94.6±0.09 MeV/A



Geant4 Version 11.1.1



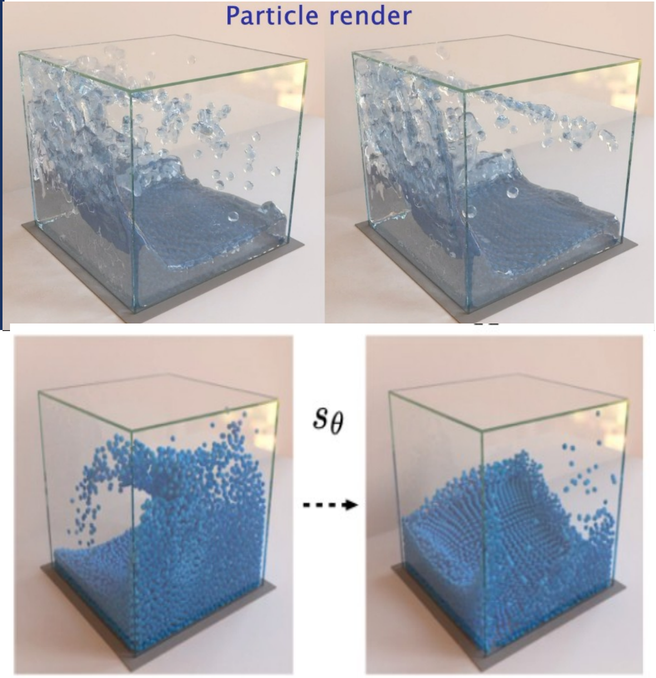
Geant4 Version 11.1.1

Lorenzo Arsini

“*Graph Neural Networks for fast emulation of nuclear interaction models* ”

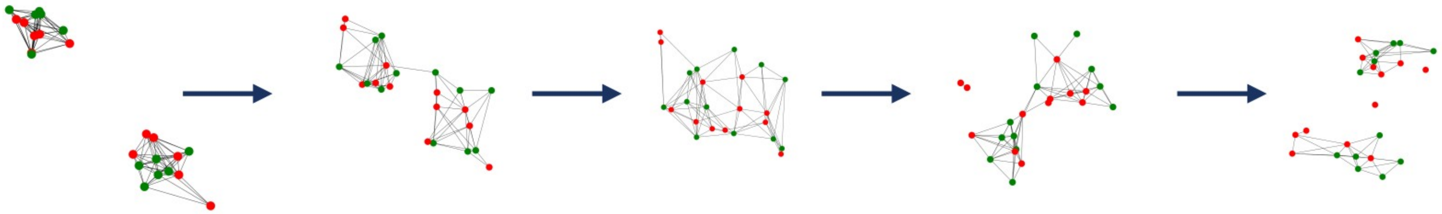
Graph Neural Networks for fast emulation of nuclear interaction models

L. Arsini[1,2], B. Caccia[3], A. Ciardiello[1], M. Colonna[4], S. Giagu[1,2], C. Mancini Terracciano[1,2]



GNN approach

Emulating the dynamics of **QMD** in **^{12}C on ^{12}C** reaction at **12 MeV/u**

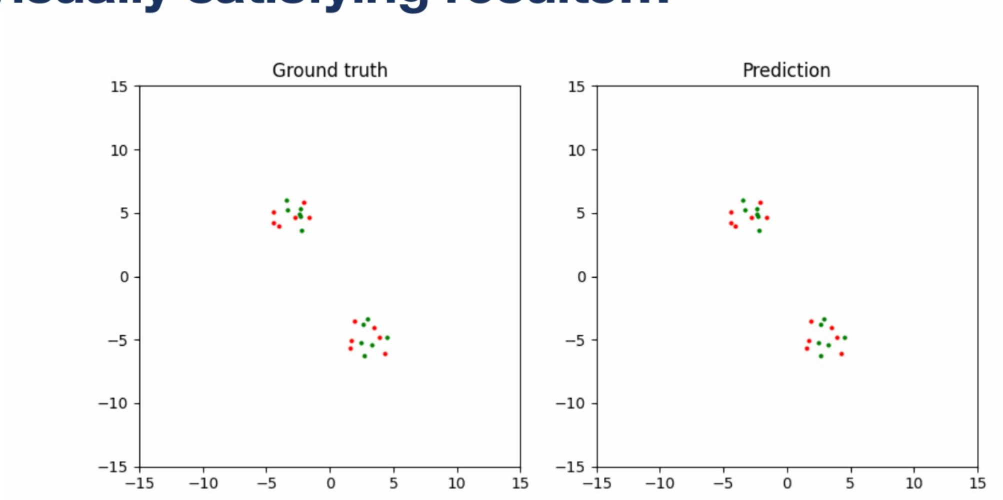


Each nucleon is a node of the graph

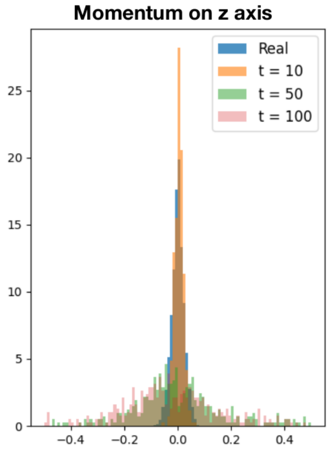
Graph Neural Networks for fast emulation of nuclear interaction models

L. Arsini[1,2], B. Caccia[3], A. Ciardiello[1], M. Colonna[4], S. Giagu[1,2], C. Mancini Terracciano[1,2]

Visually satisfying results…



… which are not Physical



In the **best case scenario**:

> Quantities are conserved on average
>
> Variance explodes increasing time steps

Cannot be used to infer physical quantities at the end of the reaction

Differences in the Physics

QMD, BLOB	Liquid simulations
Long range interactions Collisions	Short range interactions Gravity

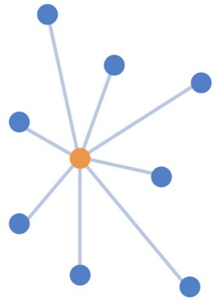
→ Building **fully connected** graphs

Graph Neural Networks for fast emulation of nuclear interaction models

L. Arsini[1,2], B. Caccia[3], A. Ciardiello[1], M. Colonna[4], S. Giagu[1,2], C. Mancini Terracciano[1,2]

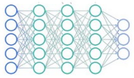
Learning the Potential: DL model

Particle-wise MLP for Potential Prediction



$$V_i = \sum V_{ij} = \sum f\left(q_i, q_j, p_i, p_j, c_i, c_j\right)$$

/ =



Embed particle exchange symmetry

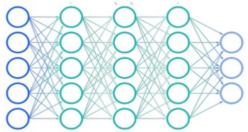
Why the Potential

Get more control on the Physics

No blackbox AI solution

DL computes a **known**, but complex function

$\{q, p\} \longrightarrow$



$\longrightarrow V_i$

Enforce physical **conservation laws** in the model

Once you've learned the Potential

Mixing Deep Learning with standard methods

Hybrid Models

Get F_i **automatically differentiating** V_i → **Integrate** the equation of motion with standard methods

Export the DL model as a function → Integrate it into existing code, **replacing** potential computation

GetPotential() method in QMD

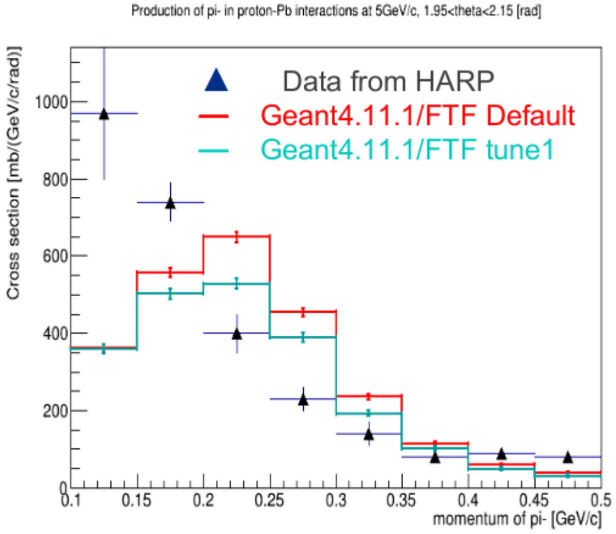
Julia Yarba

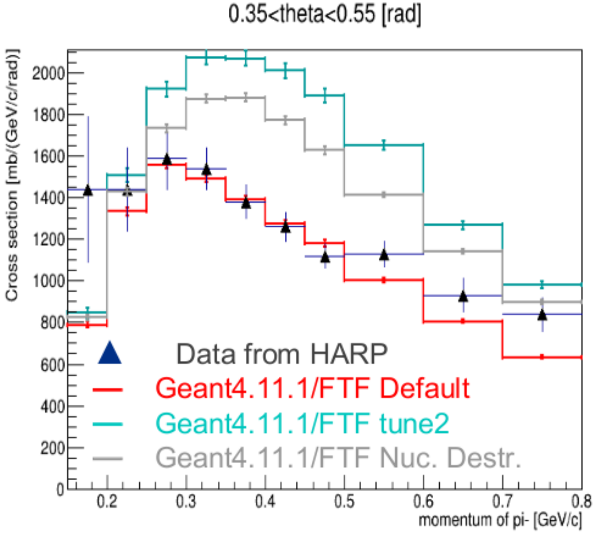
“*Update on tuning of hadronic model parameters*”

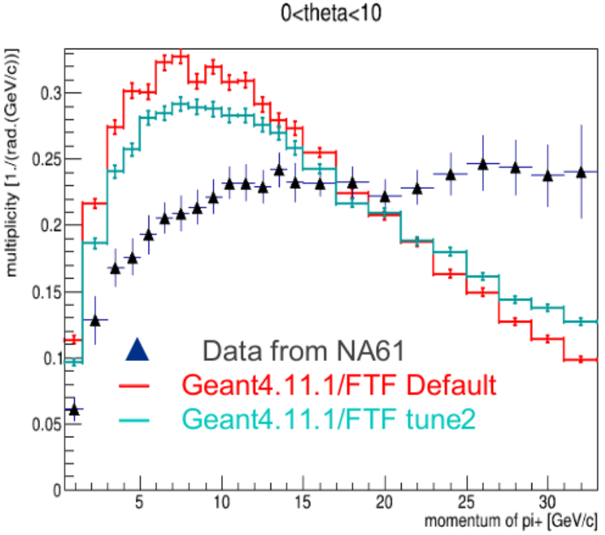
Update on Tuning Geant4 FTF Parameters

Julia Yarba, Fermilab

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 ?

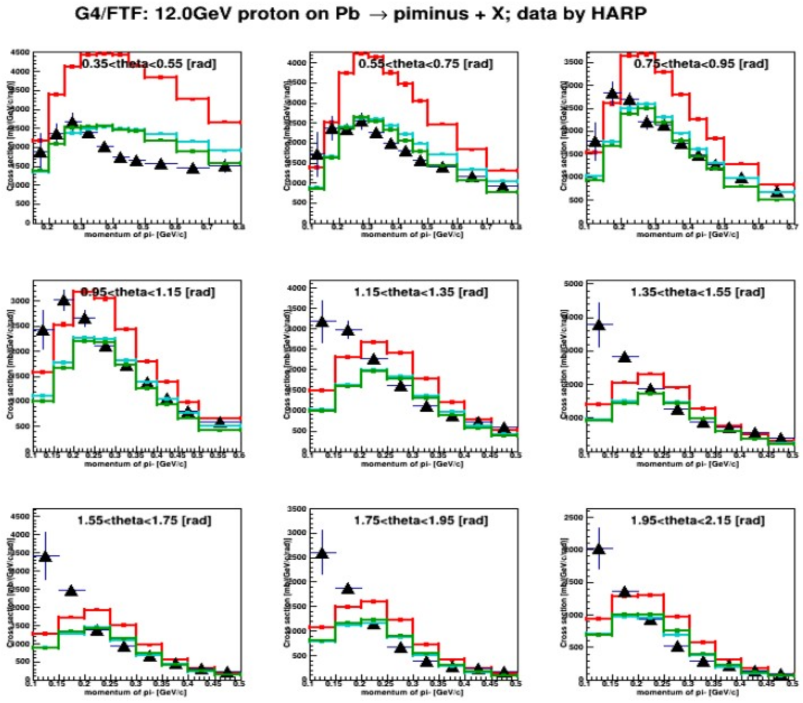
60GeV/c π^+ on C → π^+
Can we get the shape of the simulated spectrum right ?

Update on Tuning Geant4 FTF Parameters

Julia Yarba, Fermilab

Trying to change the thresholds in the **string mass sampling** to compensate for some discrepancies in the backward hemisphere, for the proton projectile tuning (tune1) → does not bring major benefits !

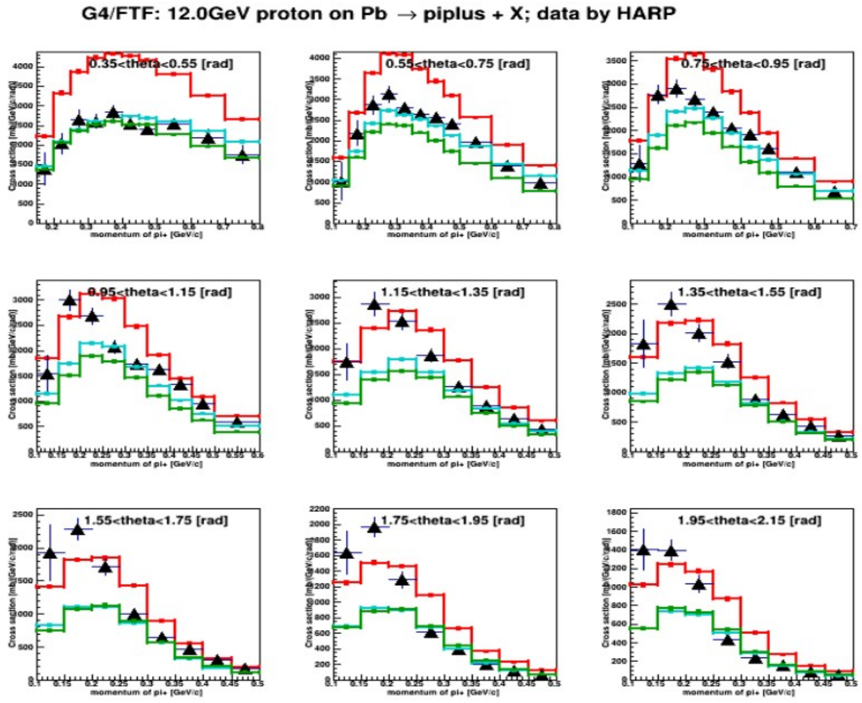
12 GeV/c proton on Pb (LA production of pions)



G4/FTF Default $\chi^2/NDF = 67.84$

G4/FTF tune1 $\chi^2/NDF = 10.48$

G4/FTF BestFit $\chi^2/NDF = 11.0$



G4/FTF Default $\chi^2/NDF = 22.59$

G4/FTF tune1 $\chi^2/NDF = 12.37$

G4/FTF BestFit $\chi^2/NDF = 7.71$

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)