Geant4 updates - Hadronic Physics

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Slides by Alberto Ribon
On behalf of the Geant4 Hadronic Working Group

Outline: latest changes, upcoming in 11.2

Models that can affect hadronic showers
Low-energy neutrons
Others
Tuning FTF Parameters
Emulating Nuclear Interaction Models
Interface to Fluka-Cern

Models that can affect hadronic showers

Quark-Gluon String (**QGS**) model

No recent physics developments

Fritiof (**FTF**) model

Developments made by Vladimir Uzhinsky included in G4 11.1

– Improved string fragmentation in FTF
- To better describe the production of strange mesons and hyperons in proton-proton interactions, as measured by the NA61/SHINE Collaboration
- Also improved leading particle spectra in meson-nucleon interactions

–Improved production of vector mesons and pseudo-scalar mesons
- Revised the mixing probability between vector mesons (ϱ° and ω), as well as the probabilities for the ratios between pseudo-scalar and vector mesons

–Extended and revised treatment of FTF annihilation (at all energies)
- To deal with the annihilation of light anti-hypernuclei
- General improvement of the algorithm used to sample kinematical variables

Hadronic Showers: Intra-nuclear Cascade Models

BERT (Bertini-like cascade)

Stable

– The most used, workhorse cascade model in HEP

BIC (Binary Cascade)

Stable

–Used in medical physics, and sometimes in HEP for evaluating systematic errors

INCLXX (Liege cascade)

Extension to anti-proton annihilations

– Annihilation at rest included in G4 11.2
– Great interest of the CERN AD experiments and some astro-particle experiments for low-energy anti-baryon annihilations
– Implementation by Ph.D. student Demid Zharenov (supervised by J.C. David), CEA Saclay

New, improved Fermi Break-Up model

Driven by the long standing issue #2263 (reported by Igor Pshenichnov)

– Wrong distributions of fragments for light ion interactions (medical and space applications): in general, physically, one expects that the higher the excitation energy the wider the list of open decay channels, and, hence, the larger fragment multiplicity. This was indeed correctly observed in G4 9.2, but not any longer in more recent versions of Geant4 (e.g. 10.4).

Higher number of fragments are now handled

Many more reaction channels are now considered

– 5421 (now) vs. 991 (before)

Included in G4 11.2

Technical improvements

For initialization

For print-out

For modern C++, more robust code, clean up and better comments

- Implementation by Vladimir Ivanchenko, in collaboration with J.M. Quesada

Available in G4 11.2:

Updated parameters of the (already existing) class **G4ChargeExchange**

–Note: this class is in models/coherent_elastic/ because it has some similarity with hadron elastic, but it is an inelastic-type of interaction, not elastic!
Implementation by Tim Lok Chau – CERN summer student supervised by Vladimir Ivanchenko

–Not (yet) used in any physics list

Introduced the new class **G4ChargeExchangeXS**

–Cross section for the charge-exchange process

–Not (yet) used by default in any physics list

Low-energy neutrons

Low energy neutrons: ParticleHP package

Ongoing Code Review:

- Avoid duplications
- Improve and modernize the old C++ code
- Consistency for initialization and multi-threading in other physics models
- Goal is code maintainability & CPU performance
- Except for few, deliberate cases, no effects are expected on the physics results
- Changes included progressively in nearly each monthly reference tag
- Huge work (and often unpleasant…) undertaken by Vladimir Ivanchenko

The main changes that can affect the physics results are related to the nuclear de-excitation part

- Introduce G4PhotonEvaporation in G4ParticleHPCapture
- Introduce G4Fragment (not yet used in HP)

In G4 11.2 changes that do not affect physics results are shared among all HP-based physics lists, while only in QGSP_BERT_HP we include the other changes

Accurate modeling of neutron elastic resonant scattering in heavy nuclei by the use of DBRC algorithm

- Major improvement made by Marek Zmeskal and Loic Thulliez (CEA Saclay)
- Relevant for the detailed simulation of nuclear reactors
  - Making Geant4 another step closer to MCNP and TRIPOLI

Available since G4 11.2

- By default, it is switched off
- It can be switched on, and its parameters can be set, via UI commands
  - */process/had/particle_hp/**use_DBRC***
  - */process/had/particle_hp/**SVT_E_max*** *value*
  - */process/had/particle_hp/**DBRC_A_min*** *value*
  - */process/had/particle_hp/**DBRC_E_min*** *value*
  - */process/had/particle_hp/**DBRC_E_max*** *value*

RadioactiveDecay is activated by default in all HP-based reference physics lists

Ongoing Code Review:

- Make it consistent with the implementation of both HP and nuclear de-excitation models
- Work done by Vladimir Ivanchenko, included in G4 11.2
- Not expected to affect the physics, but may improve the computing performance

- G4RadioactiveDecay : various technical improvements, in particular related to MT mode
- G4Radioactivation : C++ improvements
- G4BetaMinusDecay, G4BetaPlusDecay, G4BetaSpectrumSampler : implemented a thread-safe sampling method
- G4NuclearDecay, G4ITDecay : added new methods

Low energy neutrons: New "_HPT" Physics Lists

- For a precise modeling of thermal neutrons, i.e. with kinetic energy below 4 eV , a special treatment of neutron elastic scattering should be used
- Called **Thermal Scattering Law (TSL)**, based on the $S(\alpha, \beta)$ approach
- TSL not used in any of our HP-based reference physics lists
- However, we provide a physics constructor, G4ThermalNeutrons, that can be utilized on top of any HP-based physics list

```
physicsList → RegisterPhysics( new G4ThermalNeutrons );
```

- One **explicit** new reference physics list: QGSP_BIC_HPT: same as QGSP_BIC_HP, with TSL applied
- Other 7 reference physics lists **available via the physics list factory** *(env variable PHYSLIST for example):*

  - FTFP_BERT_HPT
  - QGSP_BERT_HPT
  - FTFP_INCLXX_HPT
  - QGSP_INCLXX_HPT
  - QGSP_BIC_AllHPT
  - Shielding_HPT (Shielding_HP alias of Shielding)
  - ShieldingM_HPT (ShieldingM_HP alias of ShieldingM)

Others

Others: ABLA

an alternative nuclear de-excitation model used in the Geant4 Pre-compound/De-excitation processes

- Up to G4 11.1: couple ABLA only to INCL
- Since G4 11.2, it is possible to couple ABLA to other hadronic models:
  - Intra-nuclear cascade models – BERT and BIC
  - String models – FTF and QGS
- New "experimental" reference physics list, QBBC_ABLA
  - Similar to QBBC, but with ABLA coupling for the four most common hadron projectiles: pion+, pion-, proton and neutron
  - "Experimental" here means that it is mainly for developers, for testing purposes, therefore not yet recommended for users

Coupling between ABLA and BERT

Via C++ interface: `G4CascadeInterface::useAblaDeexcitation();`

Via environmental variable: `export G4CASCADE_USE_ABLA=1`

Coupling between ABLA and BIC

Via C++ interface: `G4BinaryCascade( new G4AblaInterface );`

Coupling between ABLA and FTF & QGS

Via C++ interface:

```
G4TheoFSGenerator::SetTransport( new G4GeneratorPrecompoundInterface( new
G4AblaInterface ) );
```

Others: QMD

Quantum Molecular Dynamic

- Current status: physics constructor G4IonQMDPhysics for ion interactions used in **Shielding** physics list, with QMD utilized in the range 0.1 – 10 GeV
- The model has been stable since a number of years, with only a few bug fixes
- Ongoing active development has started, aimed to improve the model, mostly driven by medical physics applications

Contributors:

Akihiro Haga, Dousatsu Sakata, Yoshihide Sato (**Japan**)
David Bolst, Susanna Guatelli, Edward C. Simpson (**Australia**)

- Three lines of improvements:
  - Updating the Skyrme-type interaction
  - Forming a realistic initial state of nuclei involved in the collision:
    Alpha-cluster structure : 12C — 3 alpha clusters ; 16O — 4 alpha clusters
  - Finding the best model parameters

- Integration in Geant4 11.2

Others: Gamma/Lepton - nuclear interactions

On-going major effort by Vladimir Grichine to implement:

- Neutrino-nuclear interactions inside Geant4
  - Most Geant4 neutrino users currently rely on the interface between G4 and GENIE
  - Useful to have an alternative approach and inside Geant4
  - Neutrino oscillations in vacuum included in G4 11.2;
  - Next, neutrino oscillations in matter

- Gamma-nuclear interactions
  - The existing approach is based on the equivalent photon approximation
  - The alternative approach is based instead on generalized nucleon structure functions

- Electro / Muon / Tau - nuclear interactions
  - Currently, the electro-nuclear and muon-nuclear interactions are based on the equivalent photon approximation. Note that tau-nuclear is not present!
  - The alternative approach is based instead on generalized nucleon structure functions, and will cover also tau-nuclear interactions

Tuning FTF Parameters

Tunes in Geant4 Hadronic Models

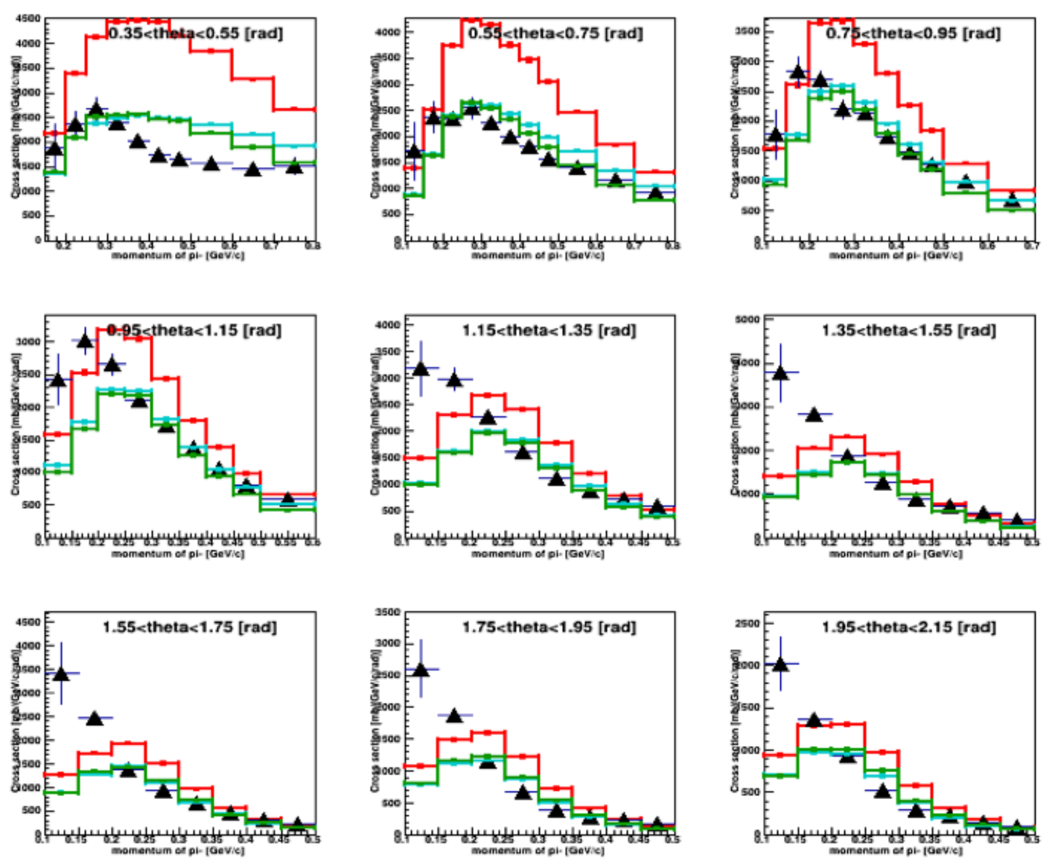
Julia Yarba, Fermilab

Critical questions: how sensitive are Geant4 hadronic models to the variations of model parameters ?

From release 10.4, Geant4 introduced configurable parameters which opens a possibility to:

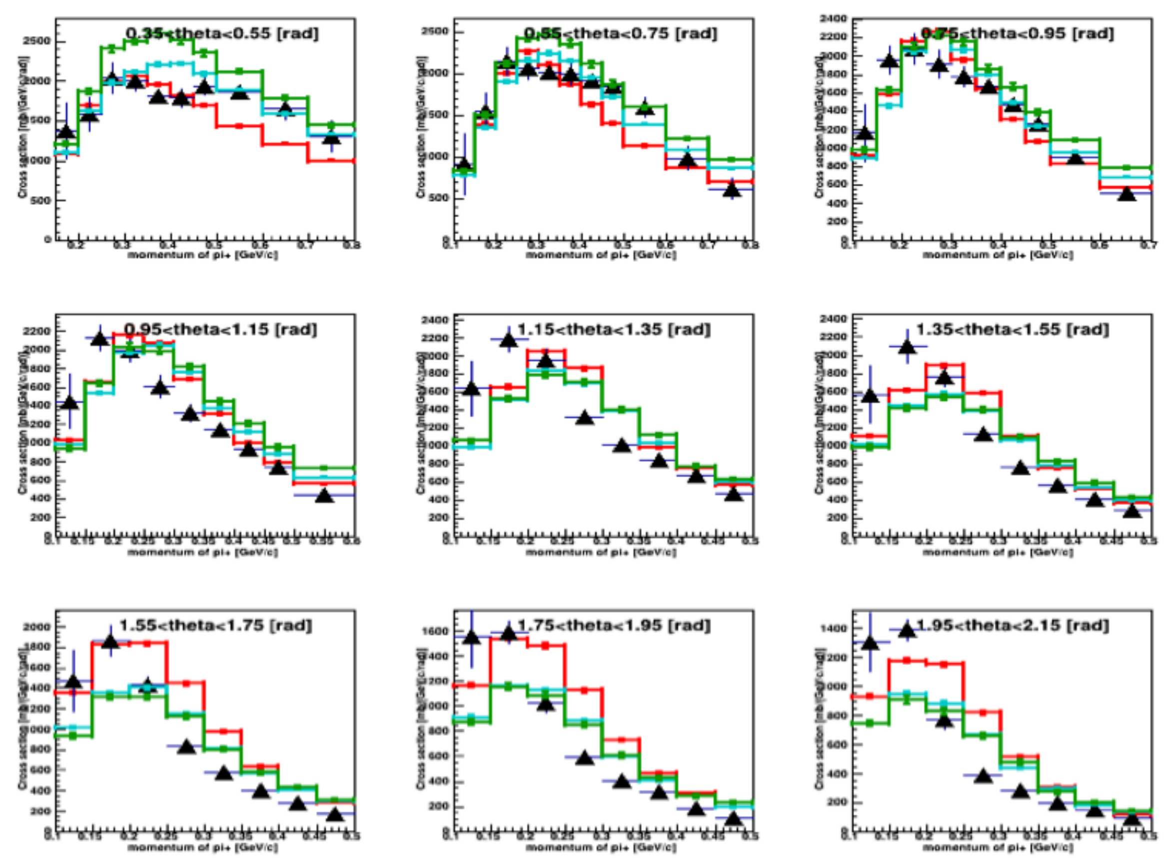
- Explore how much the simulated observables would change with variations of parameters
- Fit simulated distributions to experimental data and extract optimal values of the model parameters and the associated uncertainties

12 GeV/c proton on Pb (LA pion production)



G4/FTF Default $\chi^2/NDF = 67.84$
G4/FTF tune1 $\chi^2/NDF = 10.48$
G4/FTF BestFit $\chi^2/NDF = 11.0$

5 GeV/c π+ on Pb (LA pion production)



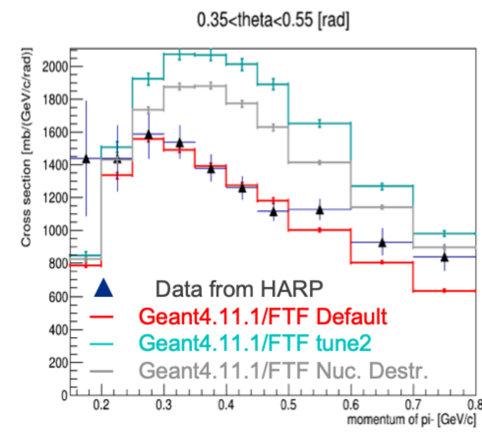
G4/FTF Default $\chi^2/NDF = 15.36$
G4/FTF tune2 $\chi^2/NDF = 12.2$
G4/FTF BestFit $\chi^2/NDF = 10.11$

Tunes in Geant4 Hadronic Models

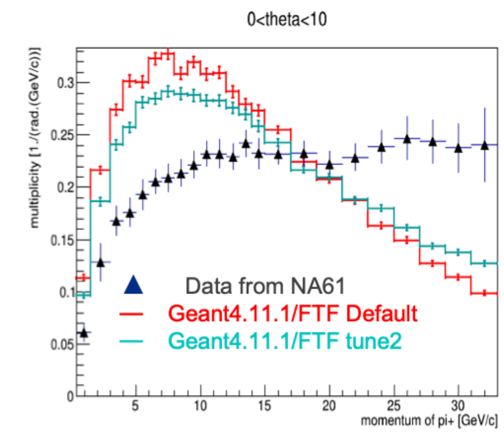
Julia Yarba, Fermilab

- Currently the focus is on FTF modeling of the quark-gluon string formation, specifically:
  - 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
- In general 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
- In some cases the MonteCarlo does not match the data “shape-wise”, no matter what

Some examples of concerns with tune1 and tune2



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 ?



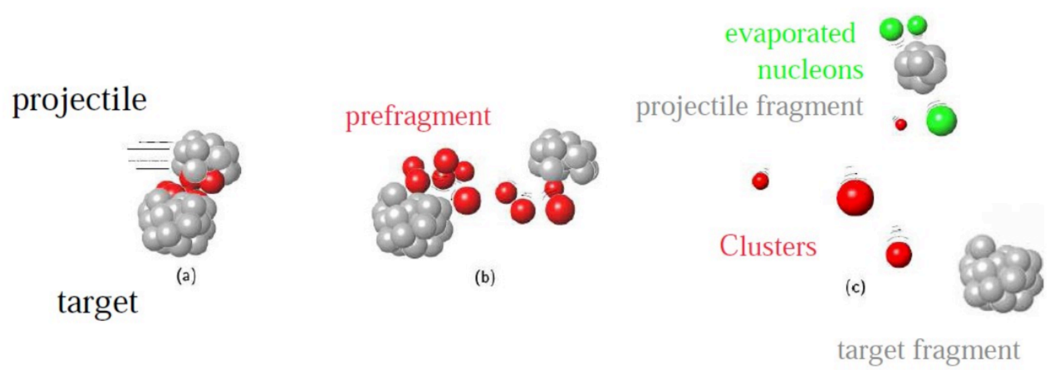
60GeV/c π^+ on C → π^+
Can we get the shape of the simulated spectrum right ?

Emulating Nuclear Interaction Models

Graph Neural Networks for fast emulation of nuclear interaction models

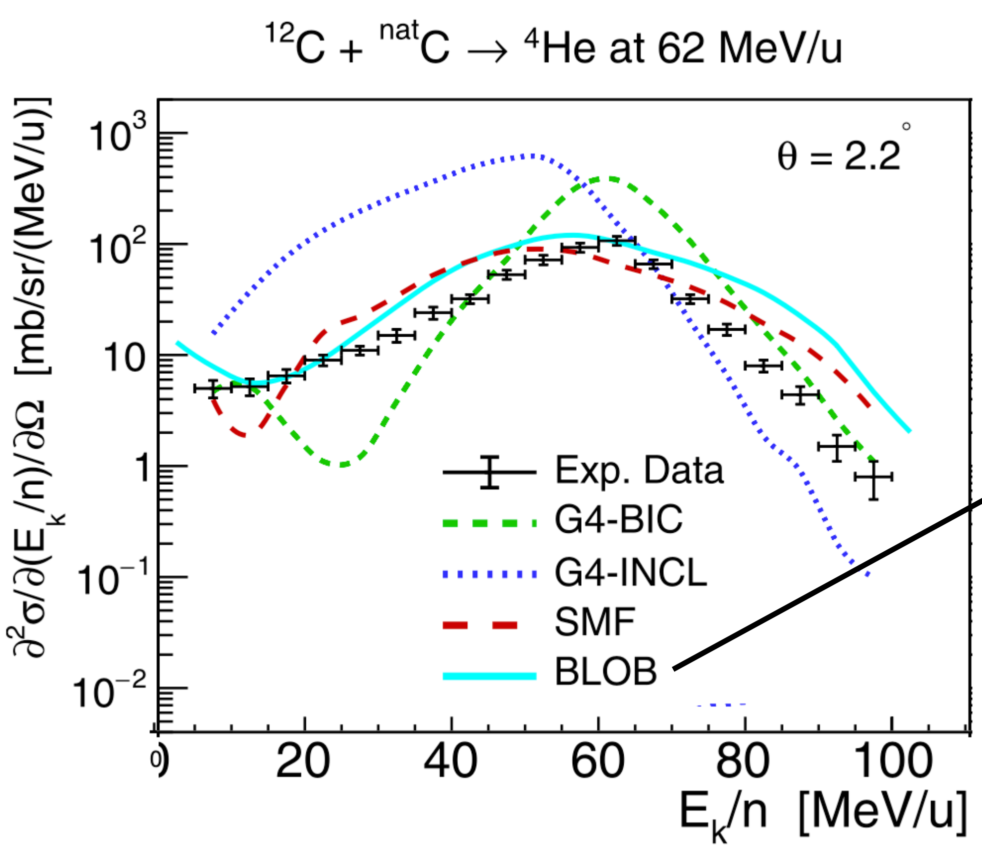
L. Arsini, B. Caccia, A. Ciardiello, M. Colonna, S. Giagu, C. Mancini Terracciano

- Nuclear interaction models are **slow**
- In particular the most sophisticated ones e.g. **QMD**



Trade off between computing **time** and **precision**

Use simpler models



Accurate | **Slow**

Order of minutes per interaction!

Graph Neural Networks for fast emulation of nuclear interaction models

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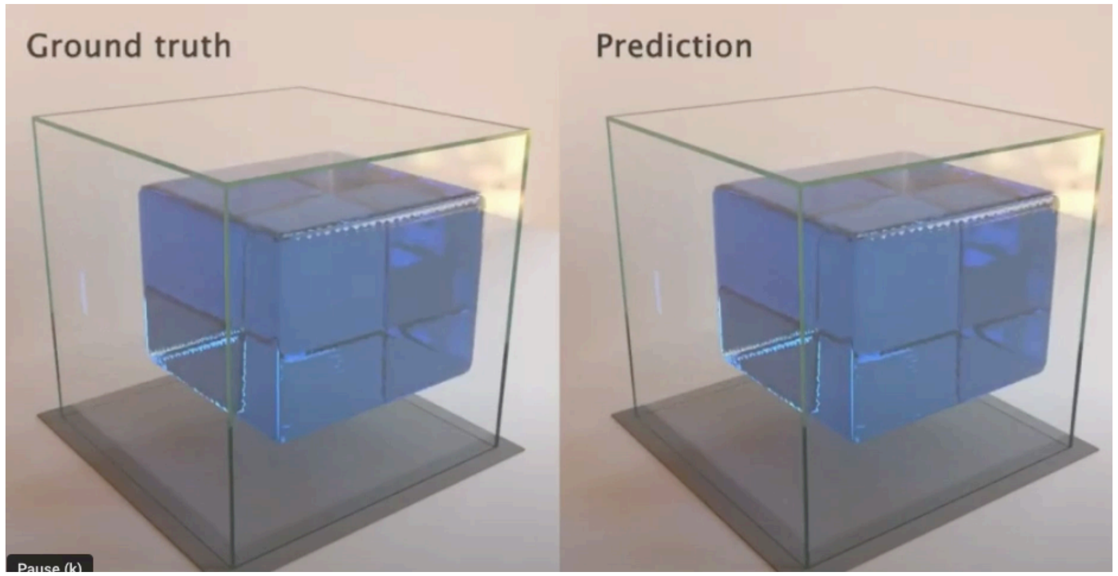
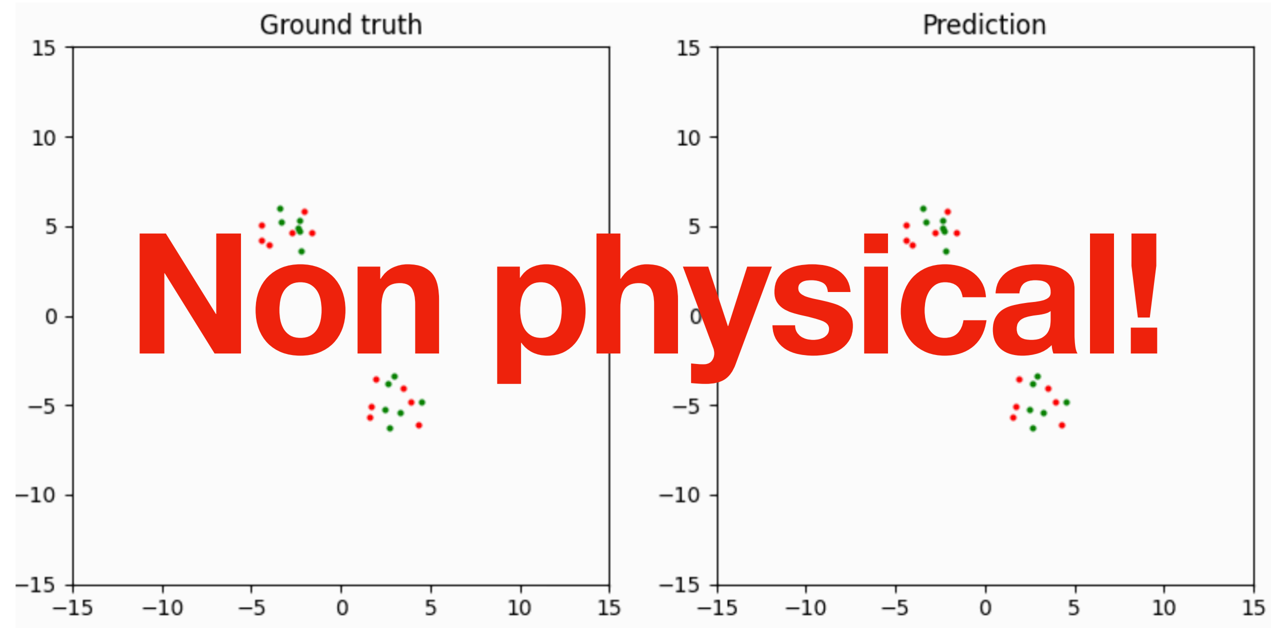
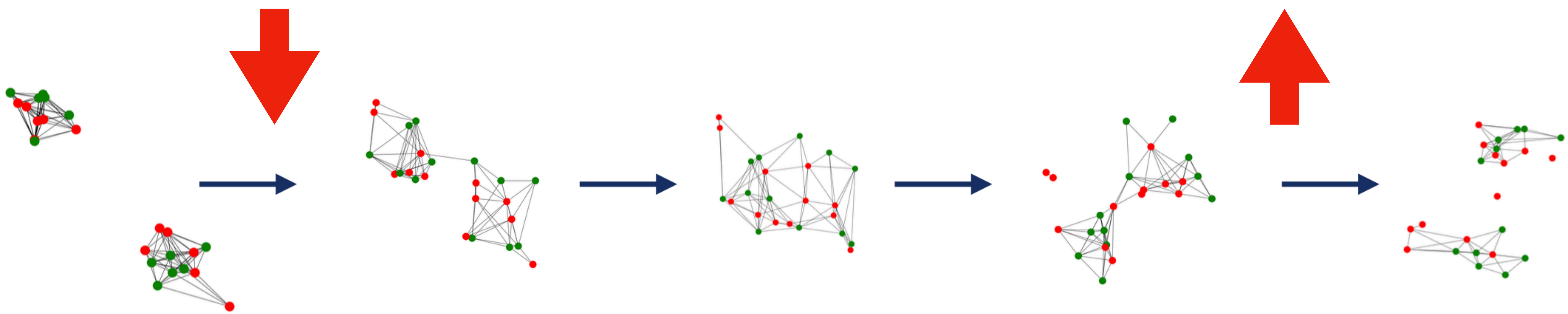
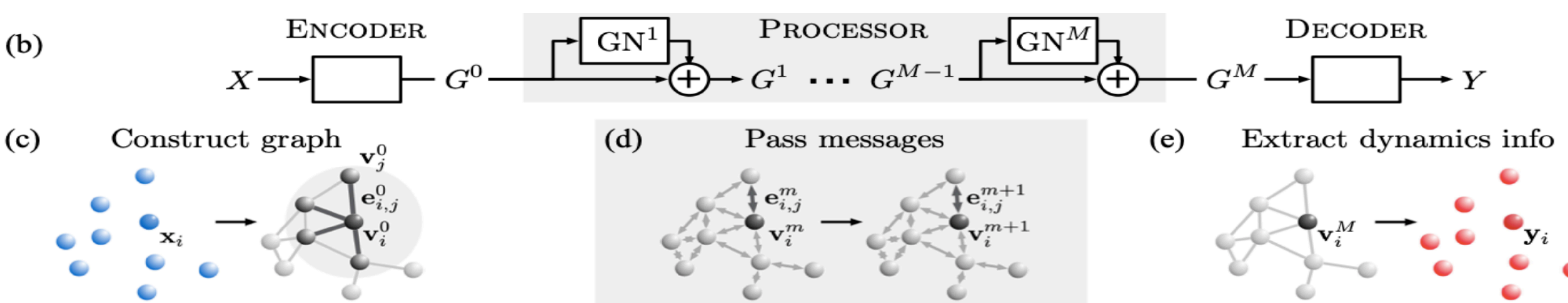






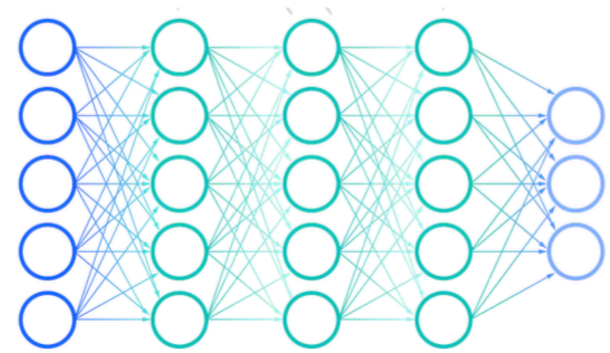


Each nucleon is a node of the graph

L. Arsini, B. Caccia, A. Ciardiello, M. Colonna, S. Giagu, C. Mancini Terracciano

Proposed Approach: emulate Potential

… and get more control of the Physics

$\{q, p\} \rightarrow$  $\rightarrow V_i$

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

↑

Bottleneck

Graph Neural Networks for fast emulation of nuclear interaction models

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Proposed Approach: emulate Potential

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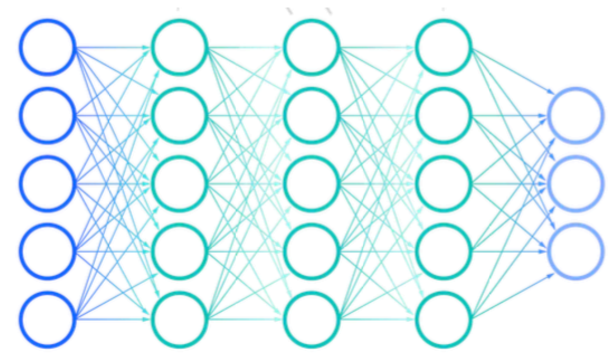
$\{q, p\} \longrightarrow$



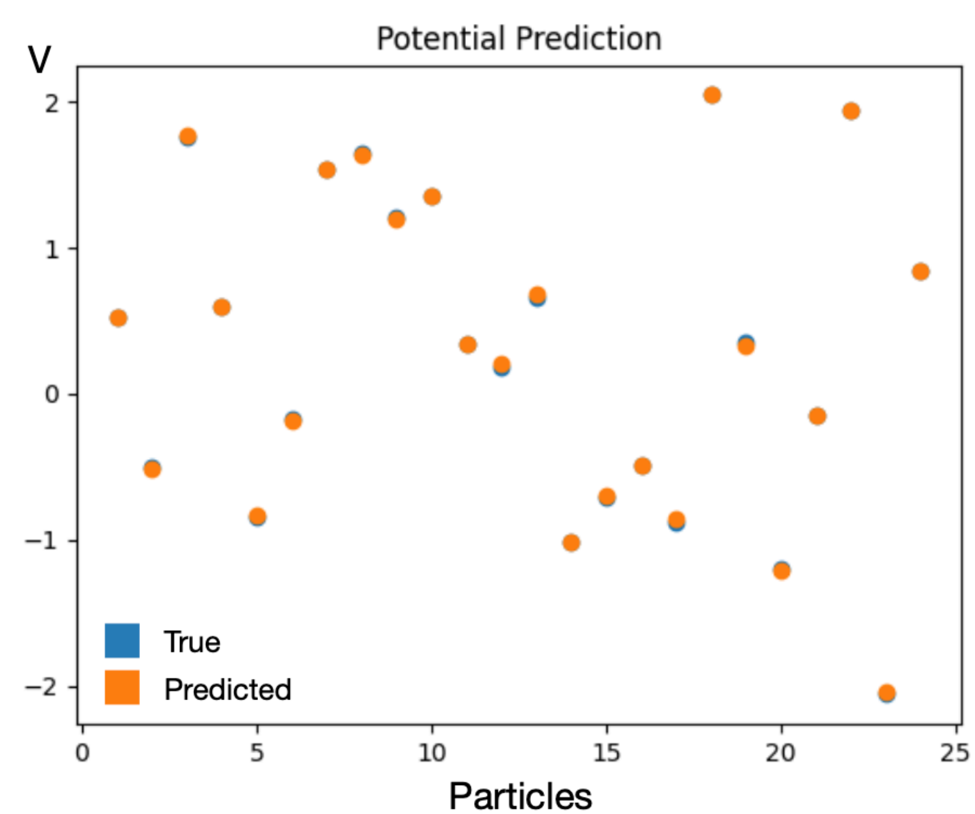
$\longrightarrow V_i$

Model: 5 layers MLP + ReLu + LayerNorm

Data: 23k stories
10 events
24 particles : ~5 M examples

Training: ~3 days training on Nvidia V100

Results: Mean Absolute Error: 0.0155



Preliminary Results

Interface to Fluka-Cern

FLUKA:

- General purpose Monte Carlo code for the interaction and transport of hadrons, leptons, and photons from keV (with the exception of neutrons, tracked down to thermal energies) to cosmic ray energies in any material.
- Accurate prediction of radiation doses
- Comparison with Geant4 not trivial, mostly due to having to re-write geometry / materials / fields

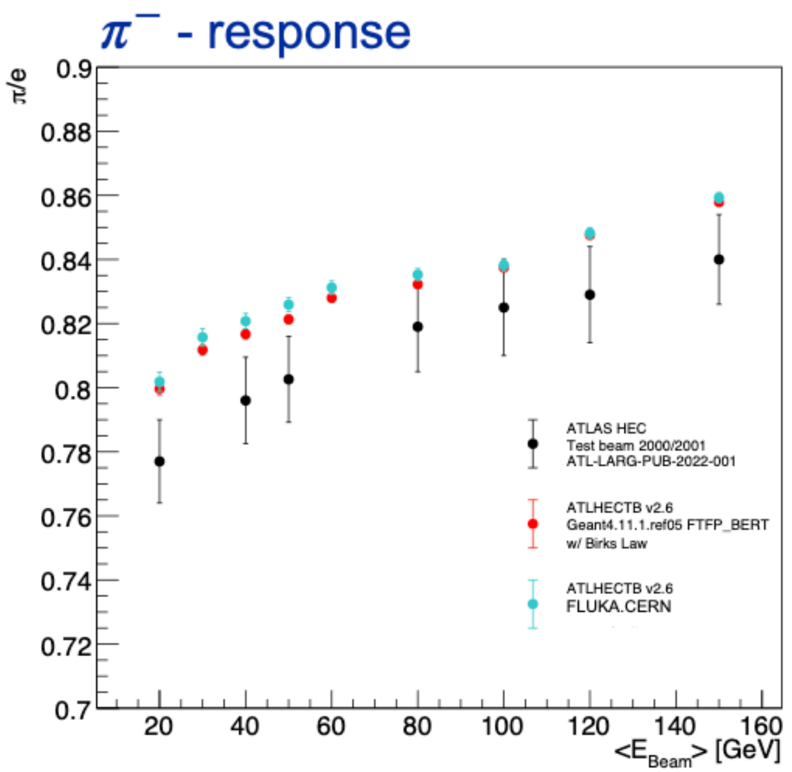
FLUKAHadronInelasticPhysics.cc

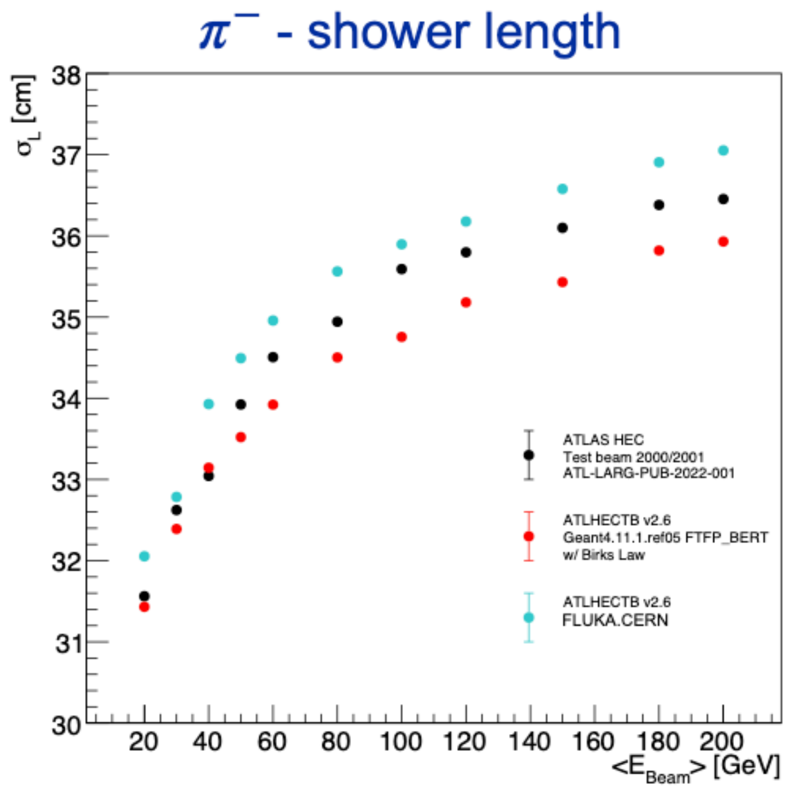
```
void FLUKAHadronInelasticPhysics::ConstructProcess() {
  //...

  const auto helper =
          G4PhysicsListHelper::GetPhysicsListHelper();

  // FLUKA hadron - nucleus inelastic XS
  const auto flukaInelasticScatteringXS =
                     new FLUKAInelasticScatteringXS();

  // FLUKA hadron - nucleus model
  const auto flukaModel =
                     new FLUKANuclearInelasticModel();

  // PROTON
  build_G4_process_helpers::buildInelasticProcess(
                                  G4Proton::Proton(),
                                  helper,
                          flukaInelasticScatteringXS,
                                  flukaModel);

  //...
}
```

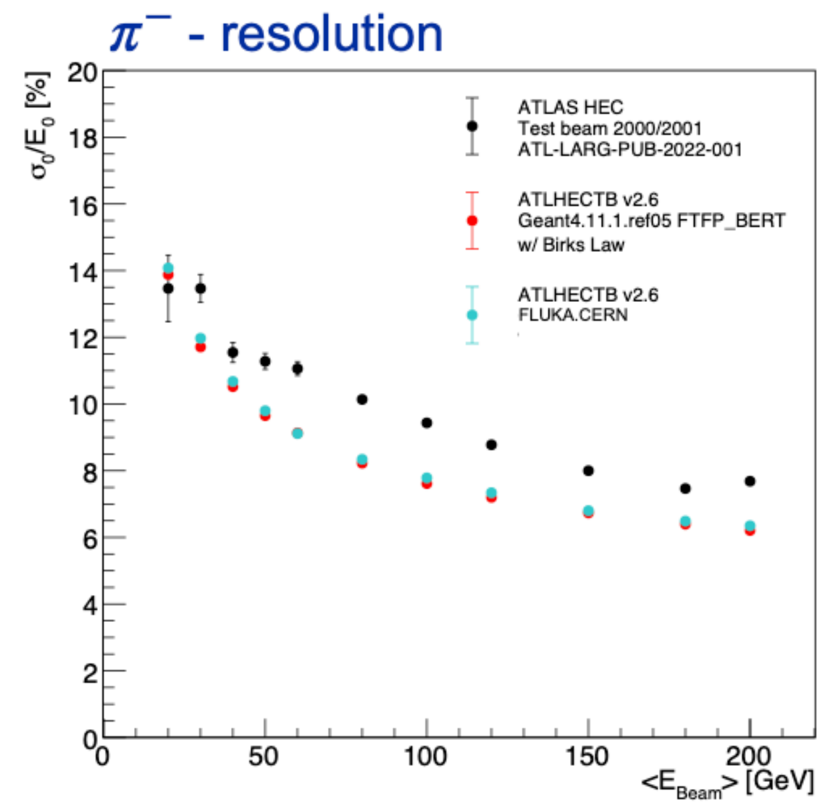
G4-to-FLUKA.CERN interface

- Used a custom FTFP_BERT Physics List that replaces the G4HadronPhysicsFTFP_BERT constructor with a new one that exploits the FLUKA.CERN interface
- User still needs to accept the FLUKA.CERN LICENSE
- Only works with Geant4.11.2
- Simulation must be run in single-threaded mode

G4-to-FLUKA.CERN interface







FLUKA.CERN and Geant4 are very close
They both scale well with Ebeam, which likely means that the π production is well modeled by both Monte Carlos

Energy profile as the energy fraction deposited in each layer

Geant4.10.4 (2017) was found to be in good agreement with ATLAS data but big drop in the hadronic signal fluctuations happened between Geant4 10.4 and 10.5 (2018)
Currently both Geant4 and FLUKA.CERN underestimate the HECresolutionby ≃15% –20%

New extended hadronic example, **FlukaCern**

- Showing how to use the new Geant4-FLUKA interface to get inelastic cross sections and final-states from Fortran Fluka-Cern
- Available in G4 11.2
- Work by Gabrielle Hugo (Fluka-Cern team)

Summary

Selected Ongoing Development

- Showers of QGSP_BERT vs. those of FTFP_BERT
  - A bit higher energy response, larger energy fluctuations, longer and narrower shower shapes
  - Good agreement up to G4 10.4 then: ~20% effect observed with FTF in ATLAS HEC and TileCal test-beams since G4 10.5
  - Comparisons with Fluka, using the new interface between Fluka-Cern and Geant4, show close agreement with Geant4
  - Found a new tune of the FTF model parameters which reproduces well the energy resolutions of ATLAS HEC and TileCal test-beams – i.e. similar to the old simulations up to G4 10.4

Summary of changes in hadronic showers since G4 10.1

- Hadronic showers kept stable from G4 **10.1** to **10.4**
  - Released the "production/stable" versions of the string models (FTF & QGS)
- Change of hadronic showers in G4 **10.5**
  - Finally release the development version of the string models (FTF & QGS)
  - Increased energy response to be "absorbed" by fitting Birks's parameter
- Change of hadronic showers in G4 **10.6**
  - Changed transition region between BERT and FTFP (from [3, 12] GeV to [3, 6] GeV)
- Stable hadronic showers in G4 **10.7**
  - Extension to charm & bottom hadron nuclear interactions
  - Only a small change (~% level) of hadronic showers for QGS-based physics lists
- Stable hadronic showers in G4 **11.0**
  - Validation and refinement of nucleus-nucleus interactions
  - Extension of the interface (for nucleus-nucleus, hypernuclei, etc.)
- Small changes in hadronic showers in G4 **11.1**
  - FTF- and QGS-showers getting a bit closer to each other
  - Complete, but simplified, treatment of light (anti-)hyper-nuclei