Status of Geant4 Hadronic Physics

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on behalf of the Geant4 Hadronic Physics Working Group

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Outline

The goal of this talk is to cover the main activities in the Geant4 Hadronic Working group since last year's Collaboration Meeting

- Models that can affect hadronic showers
  - String models, intra-nuclear cascade models, precompound/de-excitation, charge-exchange model
- Low-energy neutrons
  - Still a very active area this year!
- All others
  - Various topics, mostly unrelated to each other

Models that can affect Hadronic Showers

String Models

- Fritiof (**FTF**) model
  - No physics development after G4 11.1
  - Developments made by Vladimir Uzhinsky after Rennes and 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
      - For both FTF and QGS string fragmentation, to improve the description of NA61/SHINE data
        - 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
- Quark-Gluon String (**QGS**) model
  - No physics development after G4 11.1

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.beta; in-flight will be added for G4 11.2
    - Great interest of the CERN AD experiments and some astroparticle experiments for low-energy anti-baryon annihilations
    - Implementation by Ph.D. student Demid Zharenov (supervised by J.C. David), CEA Saclay

See talk by Demid Zharenov in this session !

Nuclear De-excitation

- 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)
  - Will be 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

Charge-Exchange Process (1/2)

- Motivations
  - As background for searching new physics in NA64 experiment at CERN
    - A more accurate description is needed with respect to what is currently available in Geant4
  - As a possible refinement of the simulation of hadronic showers in calorimeters
    - There are currently issues in the energy resolutions of ATLAS HEC and TileCal test-beams
- Charge mesons + nucleons → neutral mesons + nucleons
  - $\pi^- p \rightarrow \pi^\circ/\eta^\circ n$, $\pi^+ n \rightarrow \pi^\circ/\eta^\circ p$
  - $K^- p \rightarrow K^\circ n$, $K^+ n \rightarrow \underline{K}^\circ p$
  - Note: some of these processes are already partially included in the existing inelastic hadronic process – *e.g.* by the FTF string model and by the BERT intra-nuclear cascade model – so a separate process needs to be carefully evaluated to avoid "double counting"…
    - But the cross section of a separate charge-exchange process is tiny compared to the hadronic inelastic process...

Charge-Exchange Process (2/2)

- In G4 11.1.ref08 :
  - Introduced the new class ***G4ChargeExchangeXS***
    - Cross section for the charge-exchange process
    - Not (yet) used by default in any physics list
  - Updated parameters of the (already existing) class ***G4ChargeExchange***
    - Not (yet) used in any physics list
    - Note: this class is in *models/coherent_elastic/* because it has some similarity with hadron elastic, but it is an **in**elastic-type of interaction, not elastic!

- Implementation by Tim Lok Chau – CERN summer student supervised by Vladimir Ivanchenko

Interface to (Fortran) Fluka-Cern

- New extended hadronic example, ***FlukaCern***
  - Showing how to use the new G4-FLUKA interface to get inelastic cross sections and final-states from Fortran Fluka-Cern
  - Included since G4 11.1.ref05 by Gabrielle Hugo (Fluka-Cern team)
    - For more information, see G. Hugo's presentations last year in Rennes
    - For applications to hadronic showers *See talk by Lorenzo Pezzotti in this session !*

Hadronic Showers (1/2)

- Reminder:
  - Hadronic showers kept stable from G4 **10.1** to **10.4**
    - Released the “production/stable” versions of the string models (FTF & QGS) (snapshots of the development versions available in the beta releases)
  - 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-)hypernuclei

Hadronic Showers (2/2) *(see plots in backup slides)*

- Current hadronic showers up to now (*i.e.* G4 11.1.ref08):
  - Stable showers for both FTF- and QGS-based physics lists
    - Similar as those of G4 11.1.p02
  - Showers of QGSP_BERT *vs.* those of FTFP_BERT
    - A bit higher energy response, larger energy fluctuations, longer and narrower shower shapes
  - Main problem: too optimistic (narrow) energy resolutions
    - ~20% effect observed with FTF in ATLAS HEC and TileCal test-beams since G4 10.5
    - *See talk by Lorenzo Pezzotti in this session !*

Low Energy Neutrons

DBRC (Doppler Broadening Rejection Correction)

- 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)
    - See their presentation on January 18th https://indico.cern.ch/event/1237842/
  - Relevant for the detailed simulation of nuclear reactors
    - Making Geant4 another step closer to MCNP and TRIPOLI
- Available since G4 11.1.ref03
  - 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*

Code review of the ParticleHP package (1/2)

- Aimed to avoid duplications, improve and modernize the old C++ code, be consistent with what is done – *e.g.* for initialization and multi-threading – in other physics models. Goal is code maintainability & CPU performance
  - There are concerns about the code quality and computing performances
  - Huge work (and often unpleasant…) undertaken by Vladimir Ivanchenko – very much appreciated ! Except for few, deliberate cases, no effects are expected on the physics results
    - Only partial physics validation for 11.2.beta; more extensive one by experts is needed for 11.2
  - Changes included progressively in nearly each monthly reference tag
    - Removed many (~100) unused header files
    - Fixed several Coverity issues, in particular related to potential memory leaks
    - Simplified and improved physics data structures; replaced C++ arrays with *std::vectors*
    - Check only once and in one single class all the environmental variables
    - Consistent and simplified initialization
    - ...

Code review of the ParticleHP package (2/2)

- Other changes are planned
  - Some of them may be postponed after 11.2
  - *E.g.* remove a few obsolete classes (*e.g. G4StableIsotopes*);
    renaming of some classes;
    adopt a similar approach to cross sections as for *G4Neutron*XS* and *G4ParticleInelasticXS*;
    use consistently only isotope masses from Geant4, not from data;
    do not apply Doppler broadening (*i.e.* consider target nuclei at rest) when neutron projectile has kinetic energy above a certain threshold (~100 keV), to save expensive computations;
    ...
- 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)
  - …
- For G4 11.2, we are thinking to share among all HP-based physics lists the changes that do not affect physics results, while keeping in one single physics list (*e.g.* QGSP_BERT_HP) the other changes

… also reviewing RadioactiveDecay !

- RadioactiveDecay is activated by default in all HP-based reference physics lists, therefore it is natural to review its code to make it consistent with the implementation of both HP and nuclear de-excitation models
  - Work done by Vladimir Ivanchenko, included in G4 11.1.ref08
    - *G4RadioactiveDecay* : various technical improvements, in particular related to MT mode
      - Not expected to affect the physics, but may improve the computing performance
    - *G4Radioactivation* : C++ improvements
    - *G4BetaMinusDecay*, *G4BetaPlusDecay*, *G4BetaSpectrumSampler* : implemented a thread-safe sampling method
    - *G4NuclearDecay*, *G4ITDecay* : added new methods

New "_HPT" Physics Lists (1/2)

- Introduction
  - 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(α, β) approach**
  - This is not the case for 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);
  - Created 1 new physics list with neutron thermal scattering activated, as well as 7 new physics list names in the physics list factory, for easing the life of our users
    - Since G4 11.1.ref04

New "_HPT" Physics Lists (2/2)

- One explicit new reference physics list: *QGSP_BIC_HP**T***
  - Similar to *QGSP_BIC_HP* , with neutron thermal scattering included
    - Via the new class *G4HadronElasticPhysicsHP**T*** , which inherits from *G4HadronElasticPhysicsHP*
    - Available with or without the physics list factory
- Other 7 reference physics lists available only via the physics list factory
  - By specifying their name in the environmental variable *PHYSLIST*
  - The existing physics constructor *G4ThermalNeutrons* is registered on top of the corresponding HP-based reference physics lists
  - The names are: *FTFP_BERT_HP**T***
    *QGSP_BERT_HP**T***
    *FTFP_INCLXX_HP**T***
    *QGSP_INCLXX_HP**T***
    *QGSP_BIC_AllHP**T***
    *Shielding_HP**T*** (Shielding_HP alias of Shielding)
    *ShieldingM_HP**T*** (ShieldingM_HP alias of ShieldingM)

Others

Coupling ABLA with Cascade and String models (1/3)

- ABLA is an alternative nuclear de-excitation model available in Geant4
  - With respect to the Precompound/de-excitation used everywhere
  - Developed and maintained by the INCL group
- Used so far only with INCLXX
  - Not by default, but can be enabled via C++ interface:

G4INCLXXInterface::SetDeExcitation(new G4AblaInterface);

- Included since G4 11.1.ref03 some development of the hadronic framework to allow the coupling of ABLA with other hadronic models
  - Intra-nuclear cascade models – BERT and BIC
    - Triggered by the interested of Jose' Luis Rodriguez Sanchez
  - String models – FTF and QGS
    - *G4GeneratorPrecompoundInterface* inherits from *G4VIntraNuclearTransportModel* as *G4CascadeInterface* , *G4BinaryCascade* and *G4INCLXXInterface*

Coupling ABLA with Cascade and String models (2/3)

- 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));

Coupling ABLA with Cascade and String models (3/3)

- A new "experimental" reference physics list: QBBC_ABLA
  - With the development included since G4 11.1.ref03, it is possible and easy to couple ABLA with hadronic models at the process level, but it is cumbersome at the level of physics list
    - Because several files – in particular builders – need to be modified
  - Added since G4 11.1.ref04 a new, "experimental" (*i.e.* mainly for us, for testing purposes) reference physics list, *QBBC_ABLA*
    - Similar to QBBC, but with ABLA coupled to BERT, BIC, FTF and QGS – rather than to the usual Precompound/de-excitation – only for the four most common hadron projectiles: pion+, pion-, proton and neutron
    - The choice of this physics list (QBBC) and to restrict to these four hadron projectiles allows to minimize the number of changes and new files which are needed
      - Only two new classes (*QBBC_ABLA* , *G4HadronInelasticQBBC_ABLA*) and no changes to existing classes !

QMD (Quantum Molecular Dynamic) model

- Current status: physics constructor *G4IonQMDPhysics* for ion interactions used in *Shielding* physics list, with QMD utilised in the range 100 MeV – 10 GeV
  - Since Tatsumi Koi left SLAC, no new development, only a few bug fixes
- There is an on-going, very active development to improve the model, mostly driven by medical physics applications
  - *See talk by Yoshihide Sato in Parallel Session 3A – this afternoon*
    - 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 expected for Geant4 11.2

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 11.1.beta; 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

Emulating a slow hadronic model with **ML**

- On-going work by Lorenzo Arsini & Carlo Mancini to emulate a nuclear interaction model – such as QMD or BLOB – (*i.e.* precise but slow) using a Deep Learning approach
  - *See talk by Lorenzo Arsini in Parallel Session 3A – this afternoon*

Backup

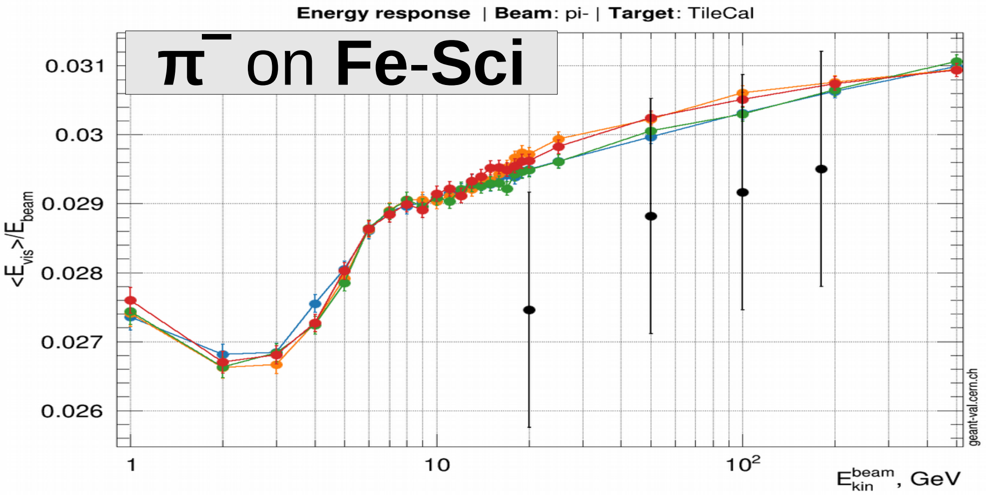
Pion– showers

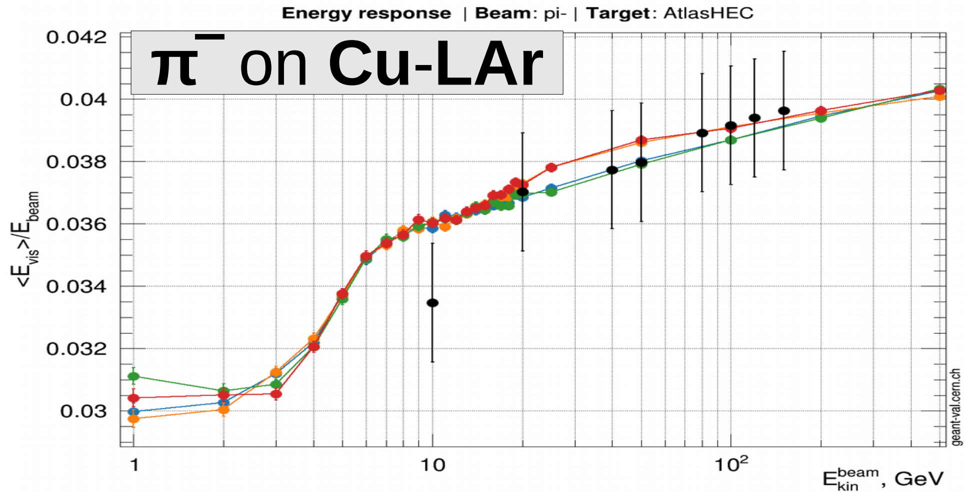
G4 11.1.p02 FTFP_BERT
G4 11.1.ref08 FTFP_BERT

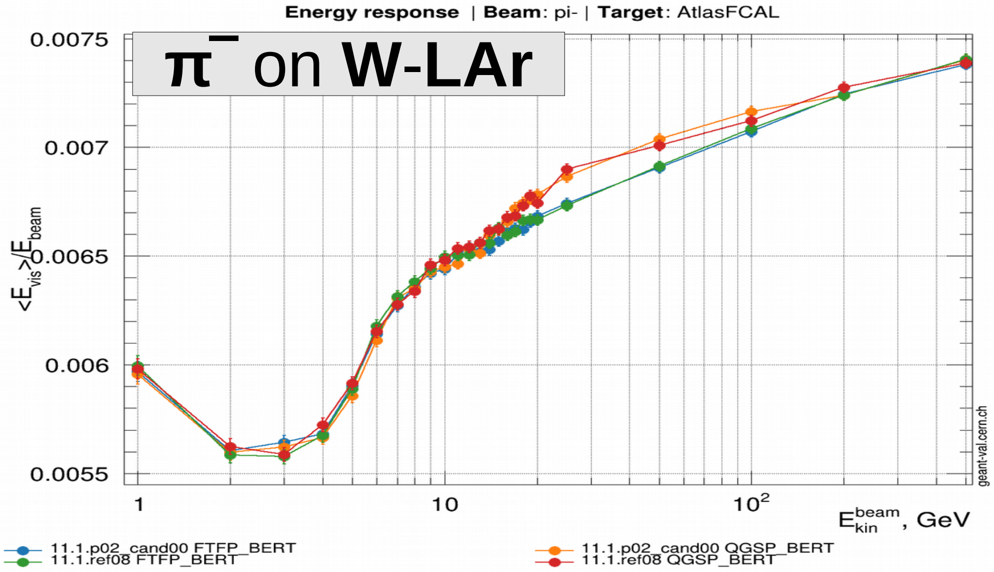
G4 11.1.p02 QGSP_BERT
G4 11.1.ref08 QGSP_BERT

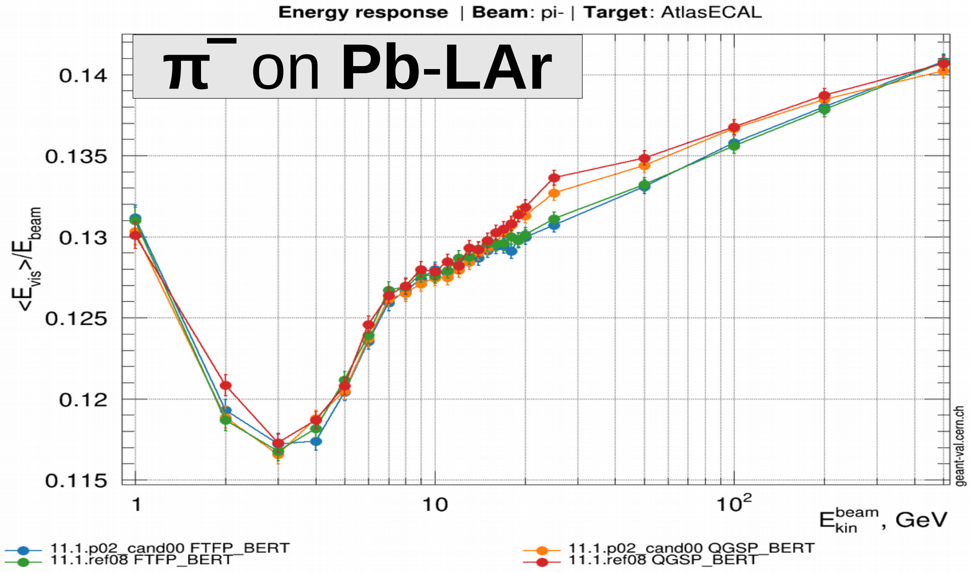
Note : conventional Birks treatment
(easier and no experimental h/e to fit !)

Energy Response

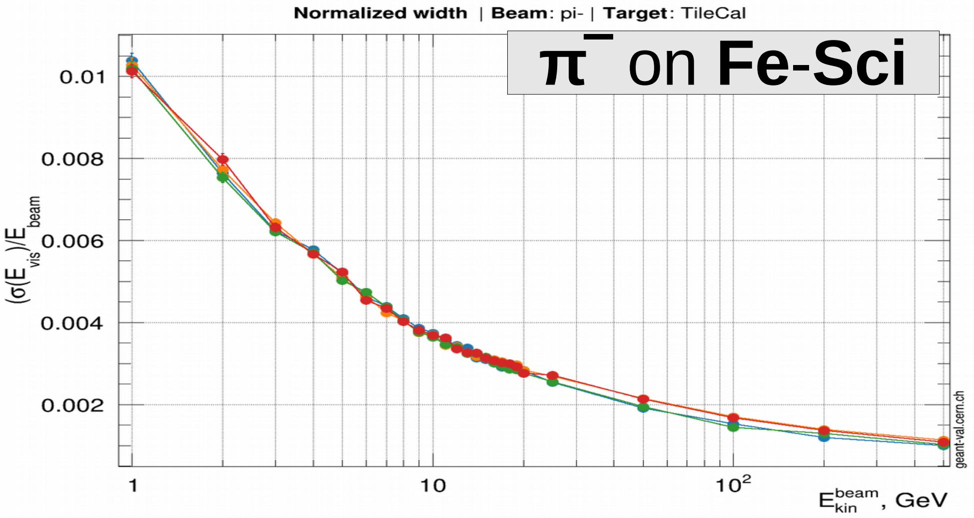


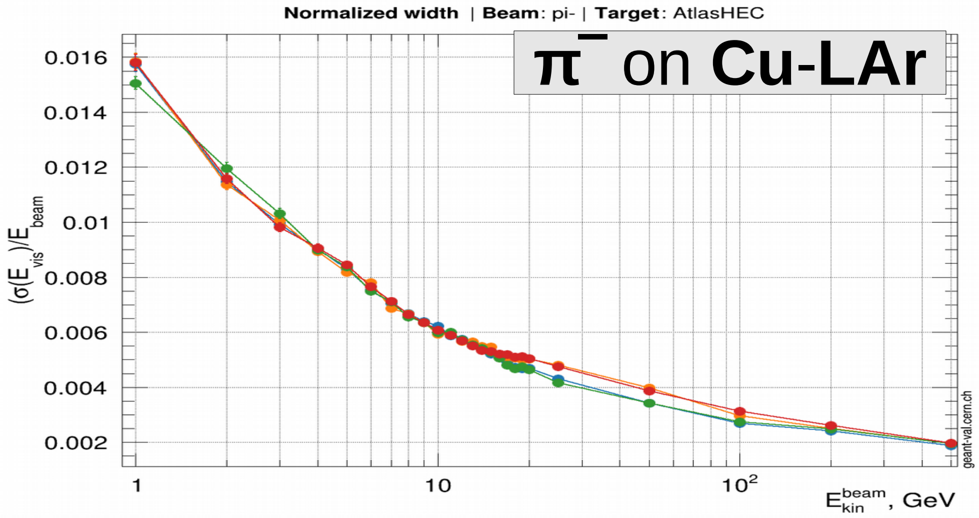


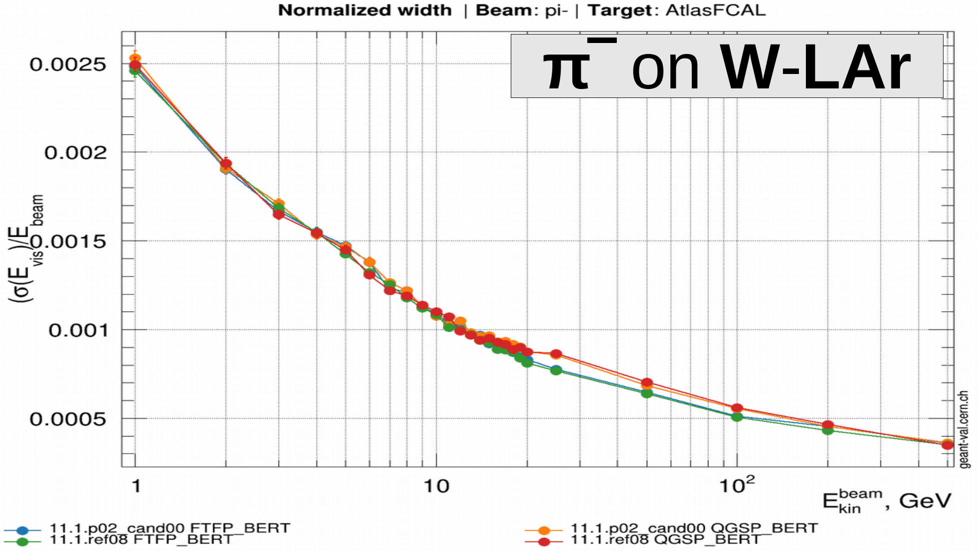


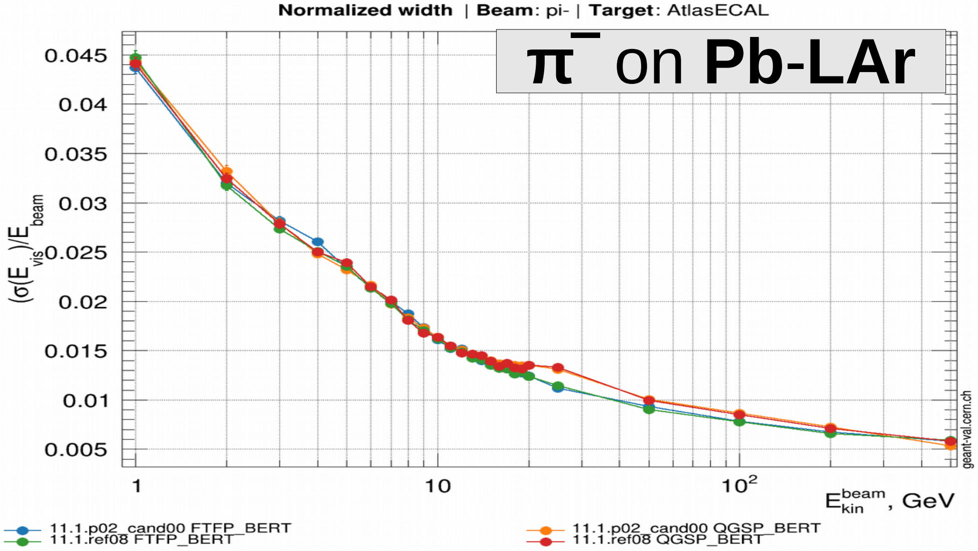


Energy Width

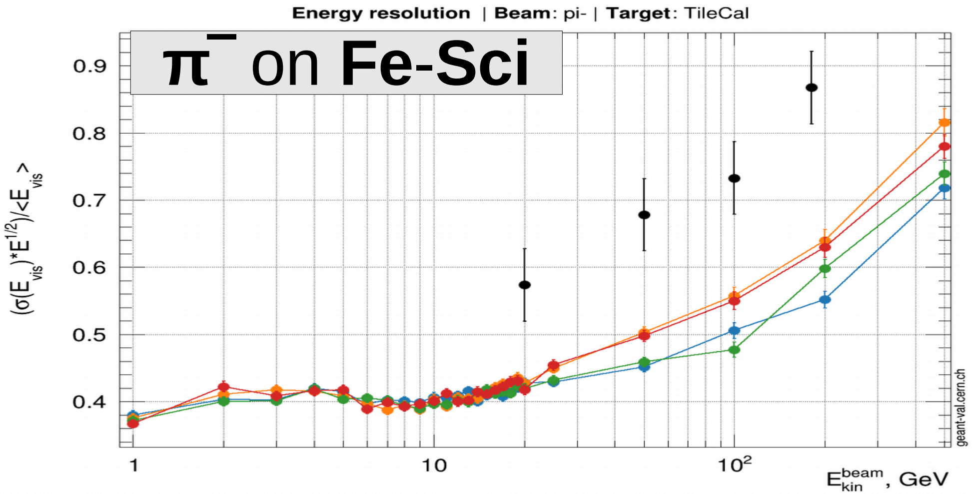


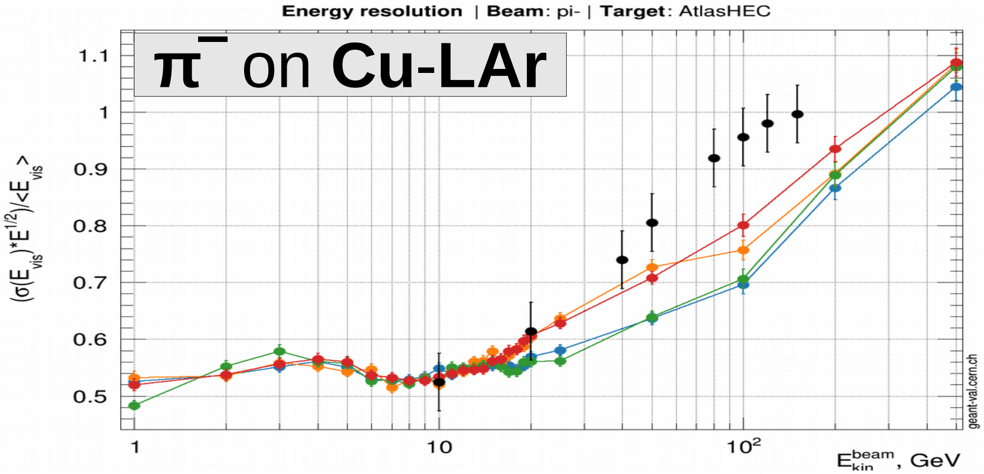


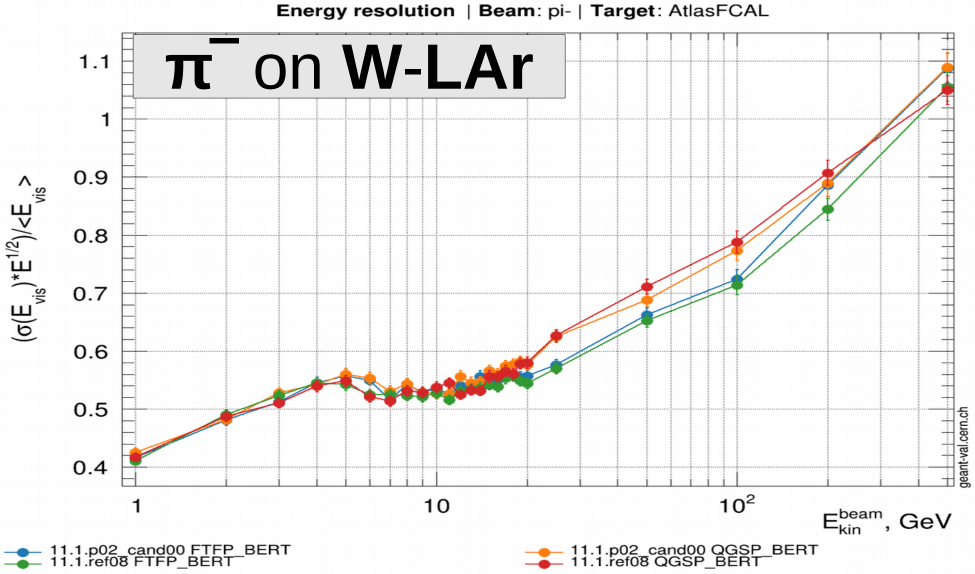


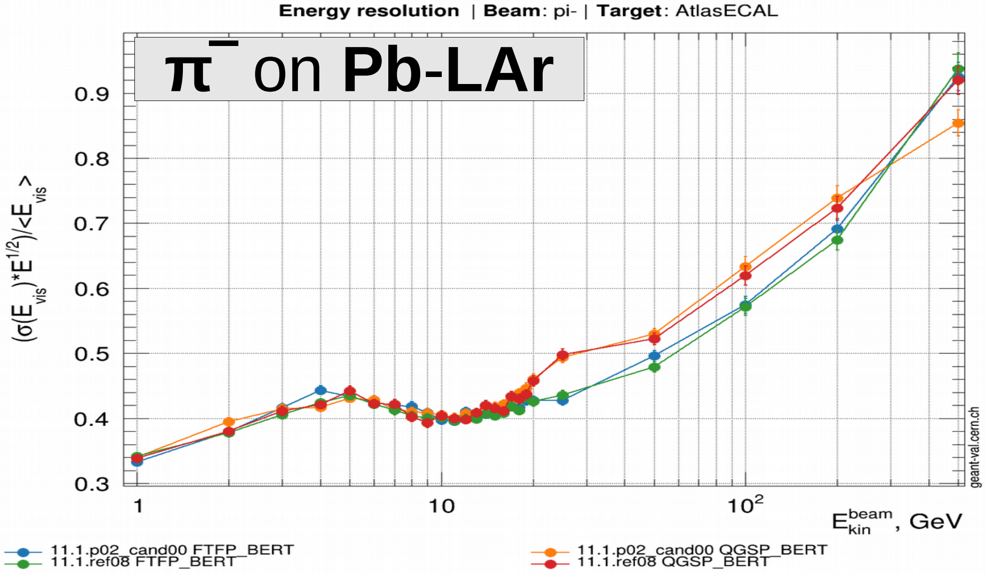


Energy Resolution

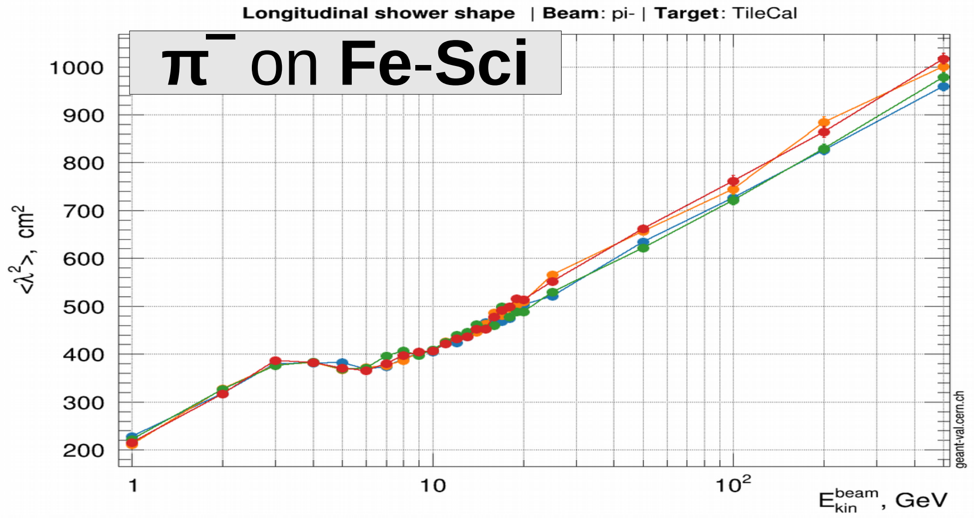


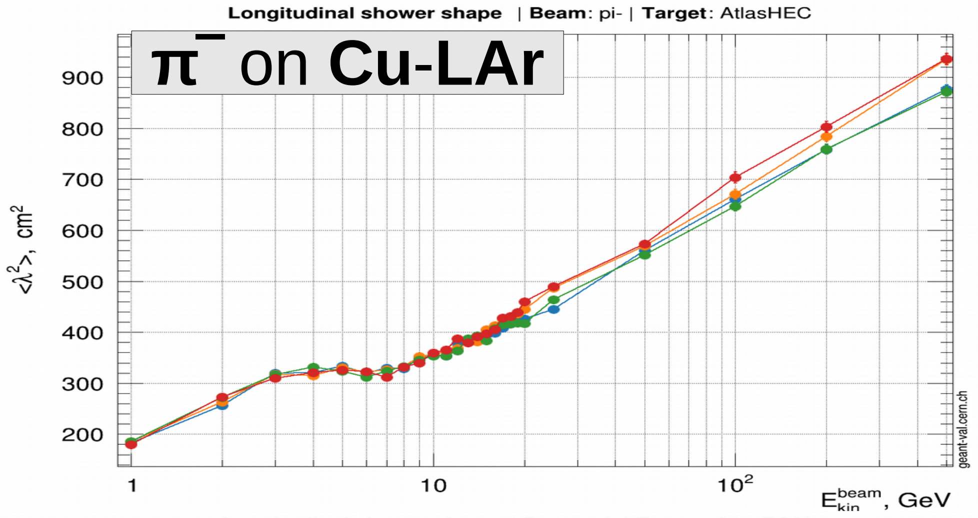


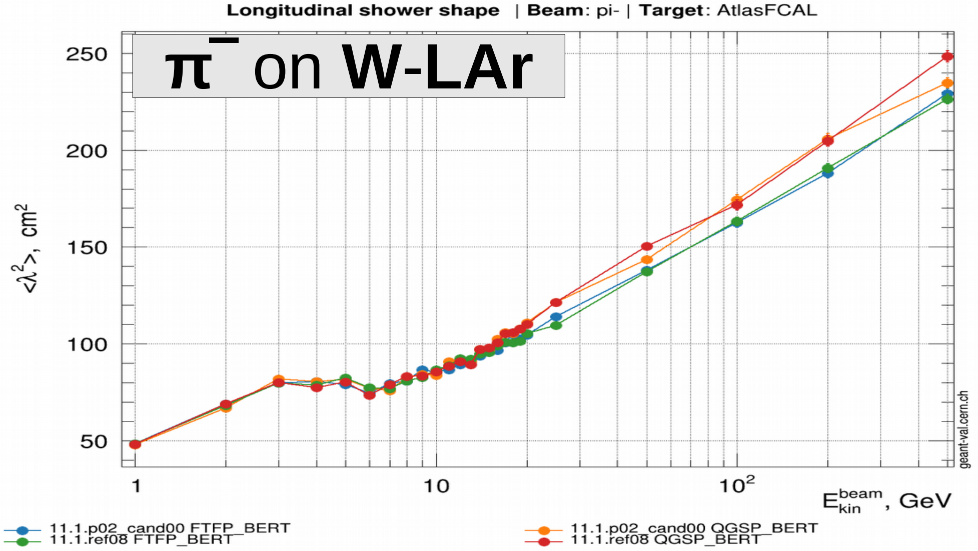


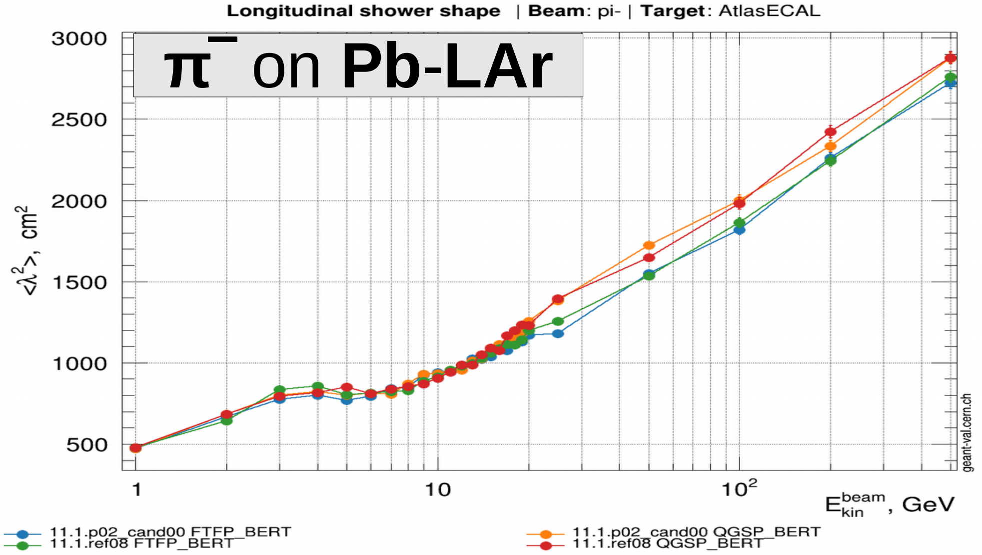


Longitudinal Shape









Lateral Shape