Status of Geant4 Hadronic Physics

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on behalf of the Geant4 Hadronic Physics Working Group

Geant4 Collaboration meeting, Rennes, 28 September 2022

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
- Low-energy neutrons
  - A lot of news!
- All others
  - Various topics, mostly unrelated to each other

Models that can affect Hadronic Showers

FTF (Fritiof) String Model

- Reminder
  - Up to ~ G4 10.1, revision of FTF by V. Uzhinsky improved both thin-target data and hadronic showers
  - Then, developments in the model driven by the goal of improving thin-target data led to worse hadronic showers (*i.e.* higher energy response)
    --> released “stable/production” version
  - Since G4 10.5, we continue the development and recommend a more consistent Birks quenching treatment for the energy response issue
  - In G4 10.6, started the extension for charm and bottom hadrons; refinement of nucleus-nucleus interactions; improved annihilation at rest of light anti-ions
  - In G4 10.7, completed the extension for charm and bottom hadronic interactions
- Main developments included in G4 11.0
  - Validation and refinement of nucleus-nucleus interactions
  - extended interface for (anti-)hypernuclei projectiles

Extensions of the FTF Interface

- Possibility to get the number of projectile/target spectator nucleons, the number of nucleon-nucleon collisions, and the impact parameter
  - Useful for nucleus-nucleus (validation) studies
  - The existing extended hadronic example Hadr09 has been updated to show how to access these new information provided by FTF
  - Introduced in G4 11.0, work by Vladimir Uzhinsky
- Possibility to control the diffraction dissociation for nucleon projectiles on target nuclei with baryon number larger than 10
  - By default, both projectile and target diffraction are switched off (but they are both active in the case of target nucleus with baryon number below or equal to 10);
    if instead the flag is set to "true",
    G4HadronicParameters::Instance()->SetEnableDiffDissociationForBGreater10(true)
    then both projectile and target diffraction are activated regardless of the target nucleus
  - Introduced in G4 11.1.beta by Laurie Nevay
- Possibility to specify an alternative set of parameters for the FTF model

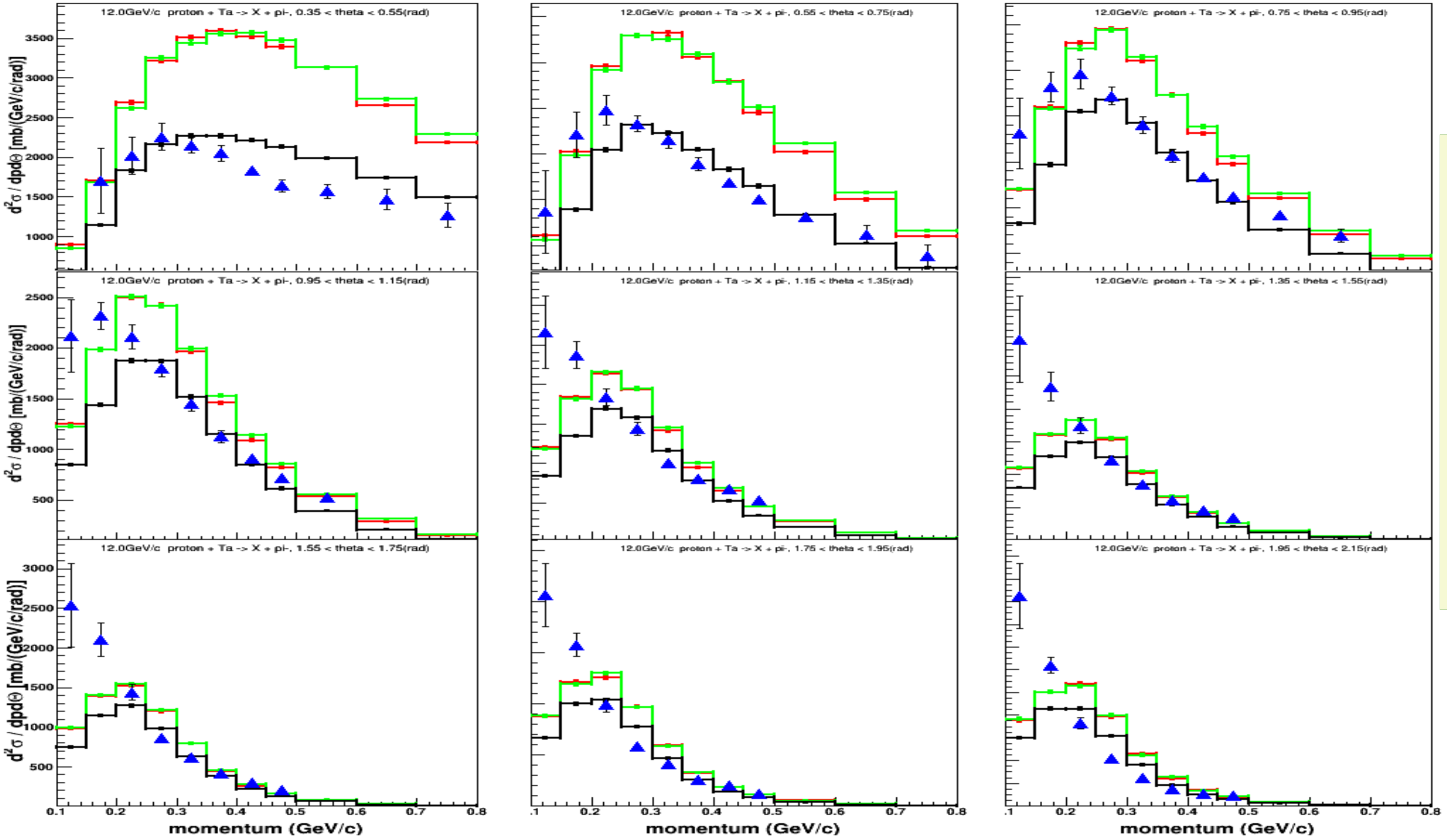
QGS (Quark Gluon String) Model

- Reminder
  - In 2014, V. Uzhinsky started to revised QGS according to the theoretical prescriptions of Kaidalov – as an alternative string model *w.r.t.* FTF
  - In G4 10.1 new version of the string hadronization
  - In G4 10.5 new version of the string formation
  - In G4 10.6 started extension for charm & bottom hadrons; various fixes
  - In G4 10.7 completed the extension for charm and bottom hadronic interac.
- Stable in G4 11.0
  - Minor fixes
- QGS becomes competitive with FTF above roughly 15 – 20 GeV
  - From thin-target data
  - For lab. projectile E_{kin} below these energies, FTF is better

On-going Developments in String Models

- Developments for the coming release, G4 11.1
  - Improved FTF fragmentation to better describe the production of strange mesons and baryons in proton-proton interactions, as measured by the NA61/SHINE Collaboration
    - Included in G4 11.1.beta, work by Aida Galoyan and Vladimir Uzhinsky
  - Tuned mixing between vector mesons (ρ°, ω), in the string fragmentation, to better describe NA61/SHINE experimental data
    - Included in G4 11.0.ref07, work by Aida Galoyan and Vladimir Uzhinsky
  - New singleton class *G4FTFTunings* to allow to specify alternative sets of FTF parameters, called "tunes"
    - Either via C++ interface: *G4FTFTunings::Instance()->SetTuneApplicabilityState(1,1)*
      or via (new) UI commands, either: */process/had/models/ftf/selectTuneByIndex 1*
      or: */process/had/models/ftf/selectTuneByName tune2022-v0*
    - Included in G4 11.0.ref07, work by Julia Yarba & A.R.

Tuning FTF Parameters (1/2)



ftfp vs HARP Data; χ^2/NDF calculated over LA theta bins
χ^2/NDF = 53.1522 for geant4-11-00
χ^2/NDF = 56.1516 for geant4-11-00-ref-06
χ^2/NDF = 9.4612 for 11.0.r06+tune2022-v0

- geant4-11-00
- geant4-11-00-ref-06
- 11.0.r06+tune2022-v0
- exp.data

FTF modeling of

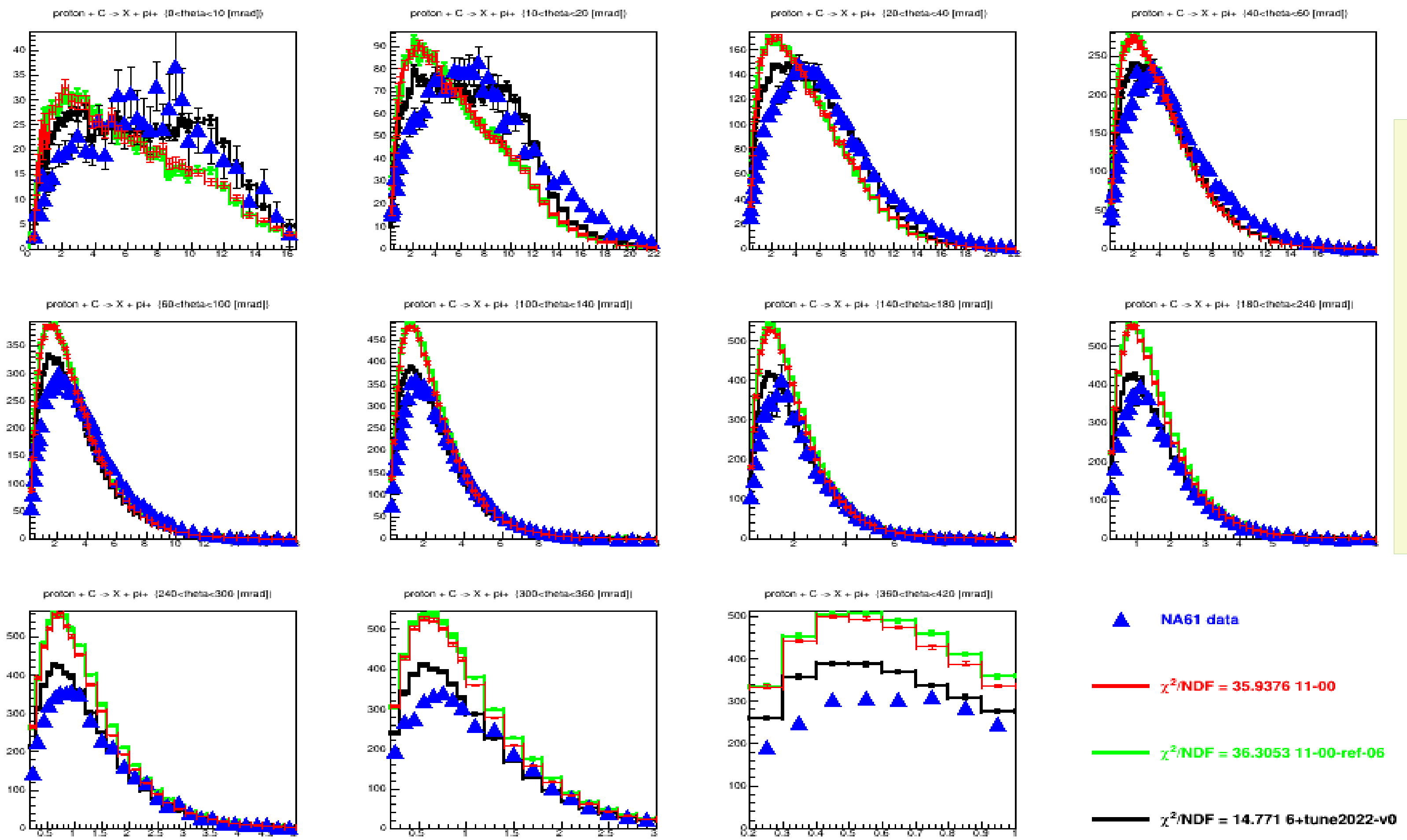
12 GeV/c proton + Ta --> pi- + X

data from HARP

J. Yarba's presentation at the hadronic group meeting on July 20th

Tuning FTF Parameters (2/2)

See also talks by V. Uzhinsky & J. Yarba in Hadronic Parallel Session 1B



FTF modeling of

31 GeV/c proton + C --> pi+ + X

data from NA61/SHINE

J. Yarba's presentation at the hadronic group meeting on July 20th

Intra-nuclear Cascade Models

- **BERT** (Bertini-like cascade) – Dennis Wright
  - Stable (the most used, workhorse cascade model in HEP)
- **BIC** (Binary Cascade) – Gunter Folger
  - Stable (in HEP used sometimes for evaluating systematic errors)
- **INCLXX** (Liege cascade) – CEA Saclay group (J.C. David *et al.*)
  - Recent and on-going developments:
    improved nuclear potential for Lambda particles (J.C. David *et al.*, included in G4 11.0);
    added implementation of hypercluster emission (J.C. David *at al.*, included in G4 11.0);
    extension to anti-proton annihilations (**Demid Zharenov**, planned for G4 11.1)
    - In HEP it is used by **ALICE** in the Tracker region (while using FTFP_BERT elsewhere)
    - Interest by ALICE and PANDA (at FAIR) on **hypernuclei** physics : both INCL and ABLA are capable to handle both projectile and target hypernuclei
    - Great interest of the CERN AD experiments and some astroparticle experiments for **low-energy anti-baryon annihilations**

See also talk by D. Zharenov in Hadronic Parallel Session 6B

Nuclear De-excitation

- Regular updates and improvements – V. Ivanchenko & J.M. Quesada
  - More robust code
    - For handling floating levels – coping with the data inconsistencies between G4LEVELGAMMADATA and G4RADIOACTIVEDATA
    - For handling unphysical fragments – both production and decay
  - Improved evaporation code
    - Better numerical integration, improved sampling, *etc.*
    - Included also improvements suggested by expert Geant4 users (A. Svetlichnyi, *et al.*)
  - Multi-Fragmentation
    - In general, it should be useful for heavy nuclei and high excitation energies
    - In practice, currently disabled through setting very high thresholds
    - Recent improvements, also thanks to suggestions by experts (I. Pshenichnov, *et al.*)
  - *See talk by V. Ivanchenko in Hadronic Parallel Session 3B*

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 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 showers in G4 **11.0**
    - Validation and refinement of nucleus-nucleus interactions
    - Extension of the interface (for nucleus-nucleus, hypernuclei, *etc.*)

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

- Current hadronic showers up to now (*i.e.* G4 11.0.ref07):
  - Stable showers for both FTF- and QGS-based physics lists
    - Similar as those of G4 11.0.p03
  - Showers of QGSP_BERT *vs.* those of FTFP_BERT
    - A bit higher energy response, larger energy fluctuations, longer and narrower shower shapes

Low Energy Neutrons

Important Fix in NeutronHP : too much Energy in Gammas

- Issue in NeutronHP for gammas too high in energy generated from G4NDL/Capture/FSMF6 data
  - Sven Menke (ATLAS) was trying to understand the big increase in Particle Flow seen in ATLAS with Shielding physics list between G4 10.1 and 10.6
  - The bug is present since a long time, but its effects were negligible before G4NDL4.6 ; Dennis Wright also contributed by further cleaning up the code of the two relevant classes: *G4ParticleHPContEnergyAngular* and *G4ParticleHPContAngularPar*
  - Protections in *G4ParticleHPContAngularPar* were added more recently to avoid rare crashes and non-reproducibility problems
  - All these fixes have been included also in G4 10.7.p04 and 11.0.p03

Gamma files in NeutronHP

- Inconsistencies found (by Geant4 user Artem Zontikov) in many files in: *$NEUTRONHPDATA/Inelastic/Gammas/*
  - Due to several mistakes, *e.g.* in the handling of floating levels
  - Note: these problems are not present in *$G4LEVELGAMMADATA* used by *G4PhotoEvaporation* !
- Proposal to use *G4PhotoEvaporation* for gamma de-excitations
  - Also in NeutronHP, neglecting *$NEUTRONHPDATA/Inelastic/Gammas/*
    - In principle, *$NEUTRONHPDATA/Inelastic/Gammas/* could be dropped, but...
- Fixing also the files in *$NEUTRONHPDATA/Inelastic/Gammas/*
  - For backward compatibility
  - Correct files already prepared by Artem Zontikov
    - By a new (improved and consistent) parsing of ENSDF data
  - Dennis Wright is working on these and could be included in *G4NDL**4.8***

Major Improvements for Thermal Neutrons

- Solved long-standing disagreements with MCNP & Tripoli codes
  - Over the years, closer matching for neutrons 4 eV < E_kin < 20 MeV between NeutronHP and MCNP & Tripoli codes, while for thermal energies E_kin < 4 eV significant differences remained
  - In G4 11.0, included major improvements in the treatment of thermal neutrons, made by Eric Dumonteil & Loic Thulliez (CEA Saclay)
    - Corrected the original treatment of the temperature interpolation when computing the neutron final state, with the temperature interpolation performed stochastically now
    - Rewritten the method *G4Nucleus::GetBiasedThermalNucleus()* according to the sampling of the Velocity of the Target nucleus (SVT) algorithm
    - Recent paper: NIM A, Volume 1027, 11 March 2022, 166187
    - *See also talks by them in the Hadronic Parallel Session 4B*
  - With these improvements and better thermal data libraries (see next slide) Geant4 starts to become on-par with reference codes such as MCNP and Tripoli4 for low-energy neutrons (< 20 MeV)

G4NDL**4.7**

- Similar to G4NDL4.6, but with an updated ***ThermalScattering*** data, obtained from thermal scattering data from JEFF-3.3 and adding the ENDF/B-VIII.0 materials not present in JEFF-3.3
  - Created by Eric Dumonteil & Loic Thulliez (CEA Saclay)
    - Included in G4 11.0.ref04 (and available to anyone in G4 11.1.beta)
  - Thermal neutrons are defined in G4 as neutrons with E_kin < 4 eV
  - Larger coverage of materials, and option to get more precise data
    - NJOY : LowPrecision: tol=0.02, N_mu=8 ; HighPrecision: tol=0.001, N_mu=32
  - 7 alternative thermal data libraries available for download
    - Pure: JEFF-3.3, ENDF/B-VII.1, ENDF/B-VIII.0; x LowPrecision and HighPrecision
    - Combined (JEFF-3.3 + ENDF/B-VIII.0, as the default but) HighPrecision
  - A new Python tool – on Gitlab, and well documented – has been created and is available to anyone to generate thermal data libraries

NCrystal

- Many developments; interface to Geant4 to be revised and improved
  - See presentation by Thomas Kittelmann (with contributions by Xiao Xiao Cai *et al.*) at the hadronic group meeting on September 14th
    - https://indico.cern.ch/event/1197295/
  - Open source backend providing thermal neutron scattering to MC codes
    - Not only Geant4, but also MCNP, PHITS, OpenMC, NJOY-Ncyrstal, *etc.*
    - Not only for crystals – despite the name – also for amorphous solids, liquids and gases
    - Extended data library : currently 132 materials
    - Sub-eV neutron scattering: rich connection to material structure
  - Interfacing NCrystal with Geant4
    - Aimed to be able to add NCrystal on top on any HP-based physics list
    - Need to mark NCrystal-enabled materials, to have a special treatment for these
    - Need to replace all "hadElastic" physics for low-energy neutrons in some materials
    - Goals: support for MT-mode, compatibility with parallel worlds, *etc.*

See also talks by them in Hadronic Parallel Session 4B

Others

Daughter Tracks of Short-lived Resonances

- NA61/SHINE requested to know whether two (or more) tracks are the daughters of the same short-lived parent resonance
  - Short-lived resonances (*e.g.* ω, Φ, ρ, Δ, *etc.*) don't have track objects
  - In G4 11.1.beta, added the following methods to G4Track :
    - *const G4ParticleDefinition* **GetParentResonanceDef()** const;*
      void SetParentResonanceDef(const G4ParticleDefinition parent);*
      *G4int **GetParentResonanceID()** const;*
      void SetParentResonanceID(const G4int parentID);
      G4bool HasParentResonance() const;
      G4int GetParentResonancePDGEncoding() const;
      G4String GetParentResonanceName() const;
      G4double GetParentResonanceMass() const;
  - Now when an hadronic model (FTF, QGS, BIC, INCL) creates an hadronic resonance, the Hadronic Framework is capable to propagate this information to the daughter tracks

Particle Fluence

- ATLAS observed recently a significant increase (up to ~50%) in **particle fluence** from Geant4 **10.1** to **10.6**
  - Radiation background studies made with the ***Shielding*** physics list
    - Which includes both NeutronHP and Radioactive Decay
  - Worrisome because “eats up the simulation safety factors of G4 10.1”
    - Most of the effect is seen for photons, electrons and neutrons
  - Particle fluence is the number of particle per unit of surface (cm^-2)
    - Can be estimated as the sum of track lengths on a volume divided by the cubic-volume
  - On-going investigations to understand what is causing the large increase
    - A large part of the increased particle fluence seems to be due to the change in neutron library, from G4NDL4.5 (mostly based on ENDF/B-VII.1) to G4NDL4.6 (mostly based on JEFF-3.3), and a few bugs in neutronHP causing an overestimated overall energy in gammas
- Created a new hadronic extended example ***ParticleFluence***
  - To monitor regularly particle fluence (not only hadronic showers!)

Neutron General Process

- New *G4NeutronGeneralProcess* combined process
  - Included in G4 11.0.ref07 by Vladimir Ivanchenko
  - Enabled, for the time being, only in QBBC physics list
  - Similar concept as for the "Gamma General Process"
    - Which has brought significant speed up in simulations!

  Reduced the number of calls to cross sections for separate processes of the same particle (gamma or neutron), using instead only the cross section of the combined process, when the step is limited by geometry (*i.e.* crossing a volume boundary)
    - Useful in particular in granular geometries
  - *See talk by V. Ivanchenko in Hadronic Parallel Session 3B*

Integral method for Hadronic Processes

- Provided full integral option for frequently used charged hadrons
  - Included in G4 11.0.ref05 by Vladimir Ivanchenko
  - Take into account the variation of the hadronic cross sections of charged hadrons along a step, due to the energy losses by ionization
    - Already included and important in EM physics
  - Negligible effects for hadronic showers in simplified calorimeters
  - *See talk by V. Ivanchenko in Hadronic Parallel Session 3B*

QMD (Quantum Molecular Dynamic) model

- 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 developments, only a few bug fixes
- The good news is that there is an on-going very active development to improve the model, mostly driven by medical physics applications
  - By Akihiro Haga and collaborators (D. Sakata, Y. Sato, D. Bolst, S. Guatelli, E.C. Simpson)
    - See recent presentation at the hadronic group meeting on August 17th : https://indico.cern.ch/event/1188742/
  - Three lines of improvements:
    - Updating the Skyrme-type interaction
    - Forming a realistic initial state of nuclei involved in the collision
    - Finding the best model parameters
  - Integration in Geant4 after 11.1

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
  - 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

Anti-Baryon Physics

- Three, unrelated bug-fixes by Vladimir Uzhinsky
  - Cross sections : correct treatment of the cross-sections of light anti-nuclei on hydrogen target
  - Elastic scattering : corrected computation of the highest momentum transfer for anti-baryon nuclear elastic scattering
  - Anti-baryon annihilation at rest in FTF : retrieved isotropic distributions of secondary particles

Light Hypernuclei and Anti-Hypernuclei

- ALICE requested to be able to transport light (anti-)hypernuclei
  - ALICE provided us with a list of 6 hypernuclei and their anti-particles
    - hypertriton (pnΛ) , hyperH4 (pnnΛ) , hyperalpha (ppnΛ) , hyperHe5 (ppnnΛ) , doublehyperdoubleneutron (nnΛΛ) , doublehyperH4 (pnΛΛ)
- EM interactions (ionization & multiple scattering) and decays of light (anti-)hypernuclei are included in G4 11.0.p03
  - Switched off by default; to turn it on:
    G4HadronicParameters::Instance()->SetEnableHyperNuclei(true);
  - For the time being, extremely simplified treatment of the decays
    - Lambda decays to either proton+pion- (63.9%) or neutron+pion0 (35.8%), with 50% probability to find the nucleon as final state outside the nucleus
- Hadronic interactions planned for G4 11.1

Hadronic Interactions of Light (anti-)Hypernuclei

- FTF and INCL models are already capable to handle light hypernuclei projectiles, and for FTF, also light anti-hypernuclei
  - Of course, a lot of testing is needed!
- We cannot use BERT, but we can use FTF down to ~100 MeV, and below use a dummy model that returns the projectile unchanged
  - As we did for charm and bottom hadrons
- For excited hyper-fragments, we can force the prompt transition to the ground state via gamma emission
  - Plus a dummy mechanism to avoid unknown residual hypernuclei
- Need to extend our Glauber-Gribov cross sections
  - *G4ComponentGGNuclNuclXsc* , *G4ComponentAntiNuclNuclearXS*

Testing & Validation

- A major effort, involving a large fraction of the Hadronic WG
  - Regular campaigns carried out at CERN (G. Folger, D. Konstantinov, V. Ivanchenko, L. Pezzotti, A.R. *et al.*) and in US (S. Banerjee, J. Yarba, *et al.*)
  - New calorimeter test-beam set-ups are progressively included (L. Pezzotti – see next talk in this Session)
- Key role of our validation & testing suite, ***geant-val****.cern.ch*
  - On-going work to include new tests and migrate old ones
  - Striving to enlarge the group of contributors and maintainers of this vital tool, in particular looking at young people
  - See talk by Dmitri Konstantinov in Plenary Session 2

Last slide: About the 2 following Talks of this Session

- **Lorenzo Pezzotti** is going to tell us about the Geant4 physics validation activity through calorimeter test-beams, and their integration in our validation & testing suite, ***geant-val.cern.ch***

- **Gabrielle Hugo** is going to tell us about the **Fluka-Cern** project, its status and plans, as well as very interesting synergies with us

Backup

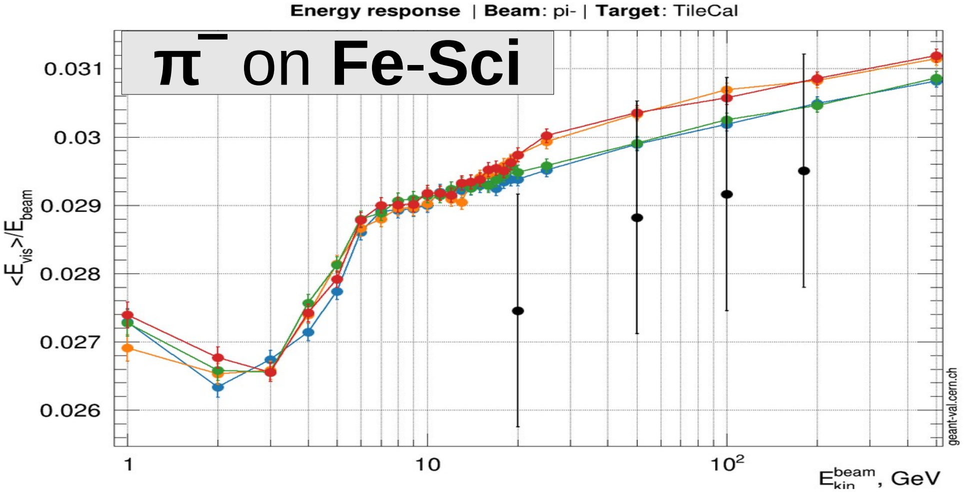
Pion– showers

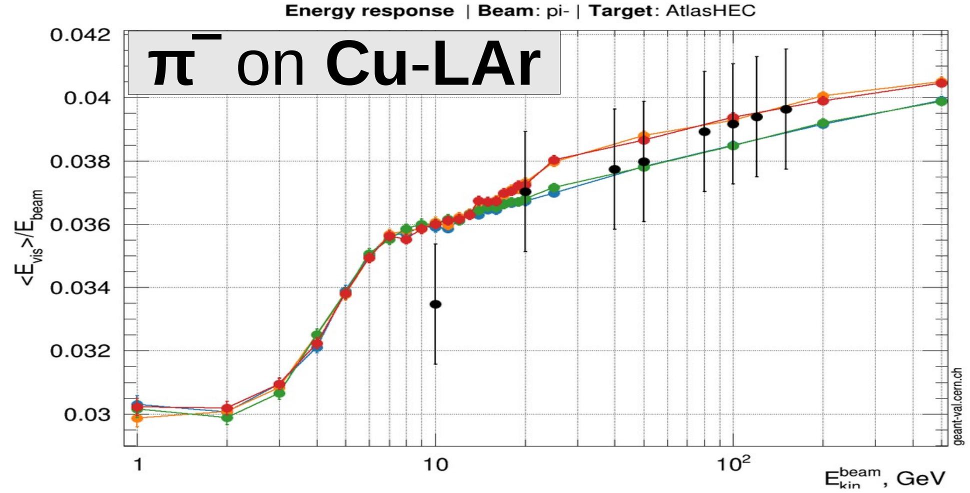
G4 11.0.ref07 FTFP_BERT
G4 11.0.p03 FTFP_BERT

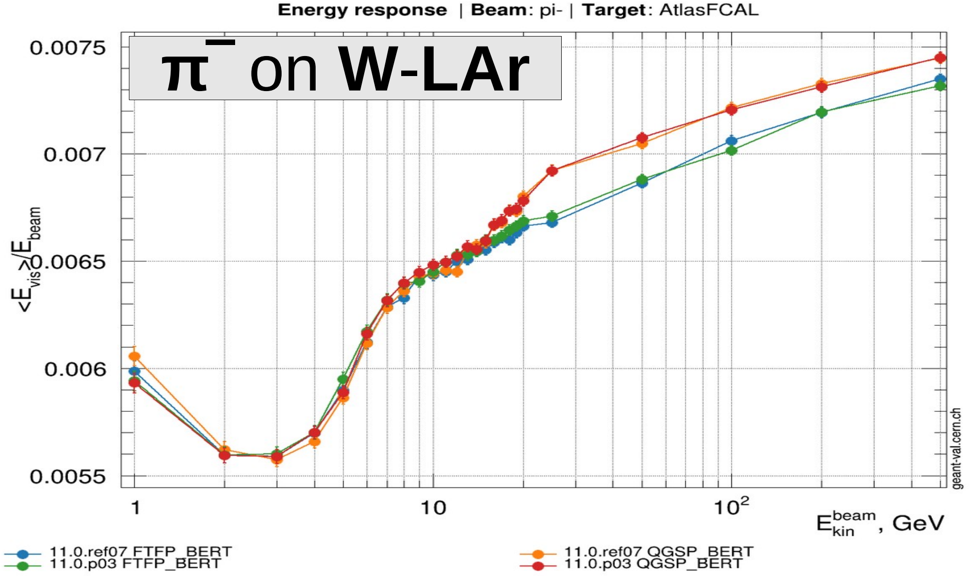
G4 11.0.ref07 QGSP_BERT
G4 11.0.p03 QGSP_BERT

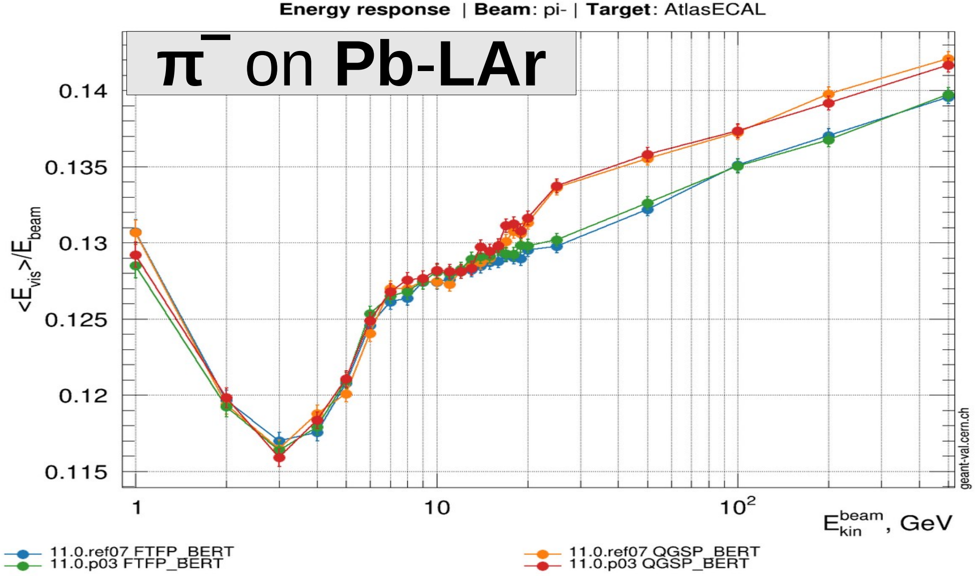
Note : conventional Birks treatment
(easier and no experimental h/e to fit !)

Energy Response

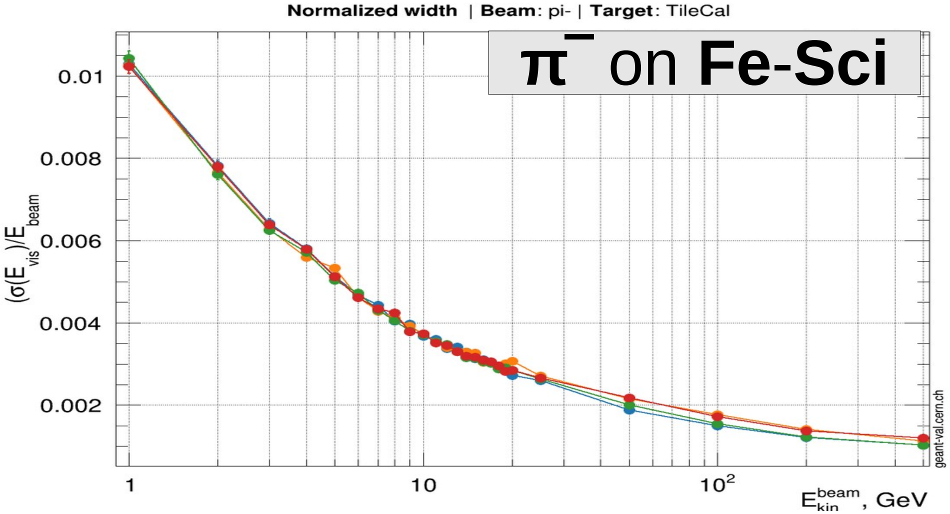


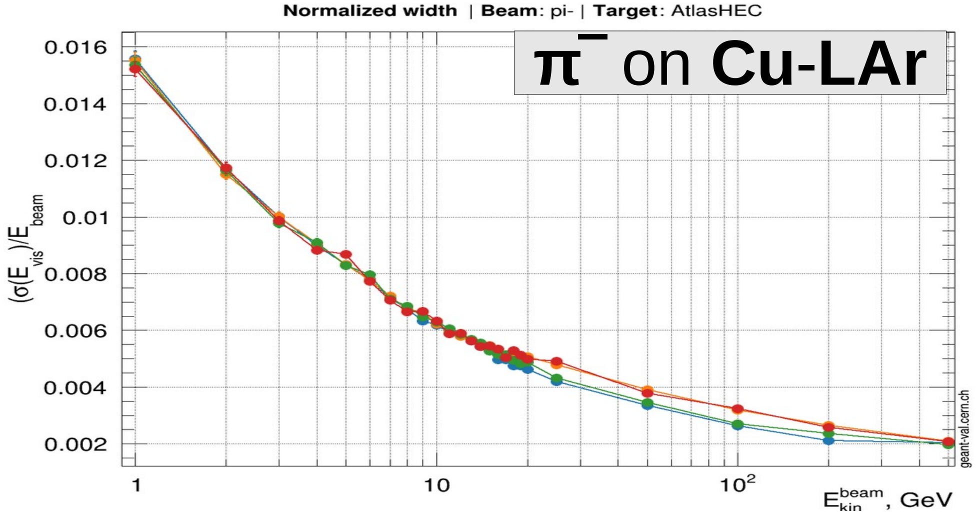


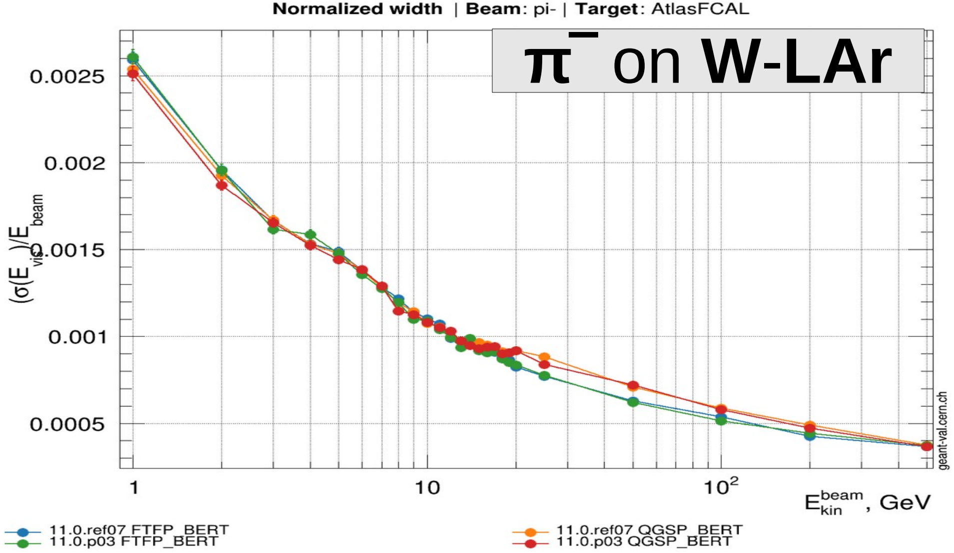


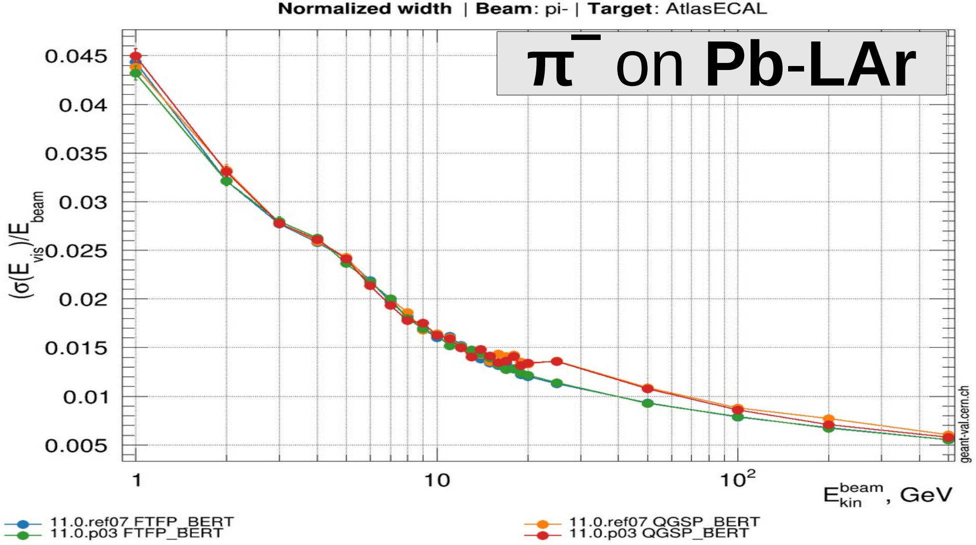


Energy Width

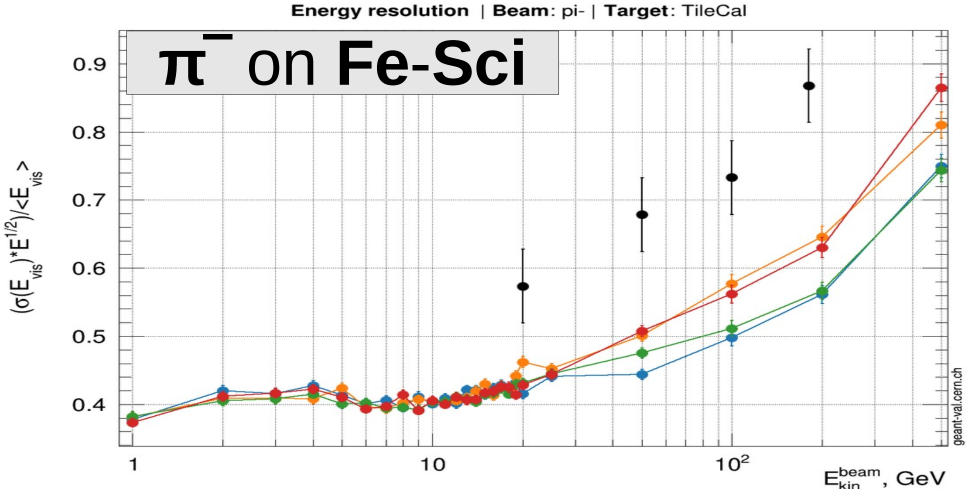


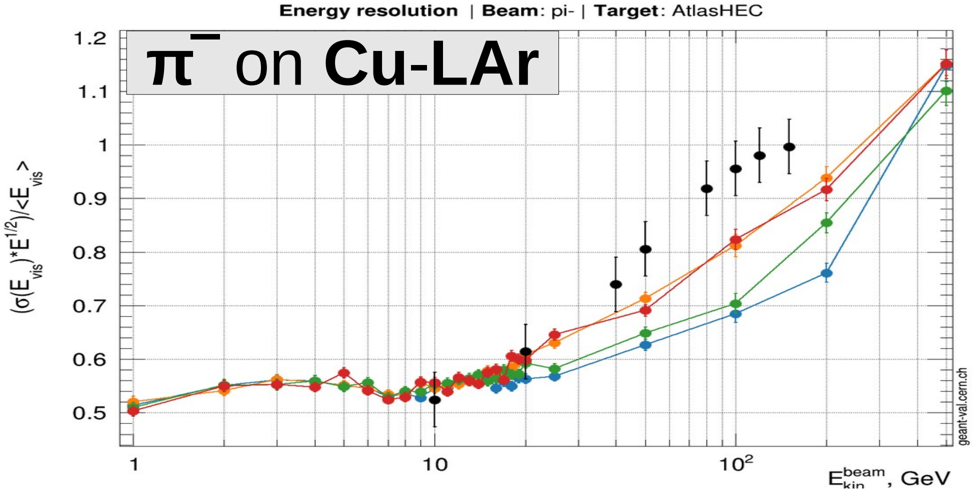


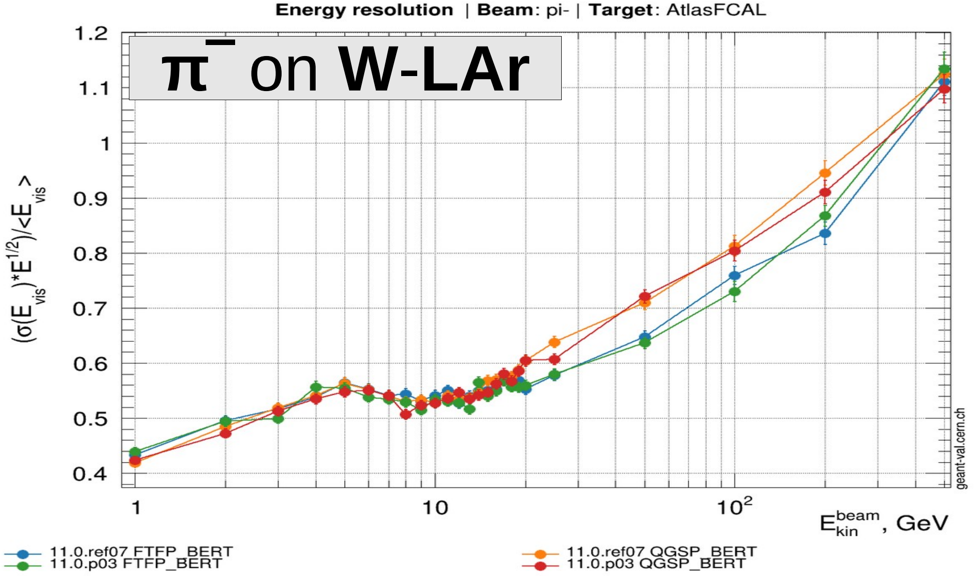


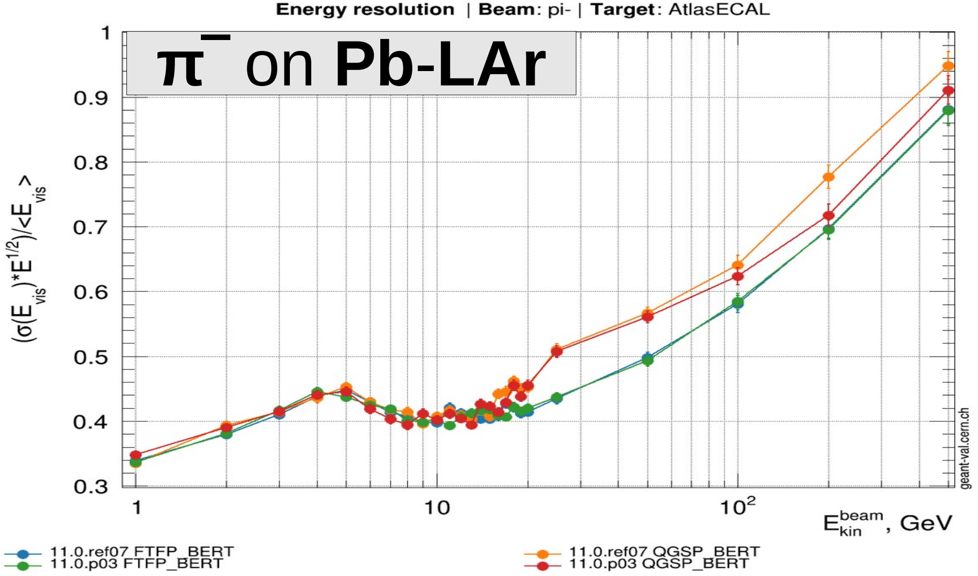


Energy Resolution

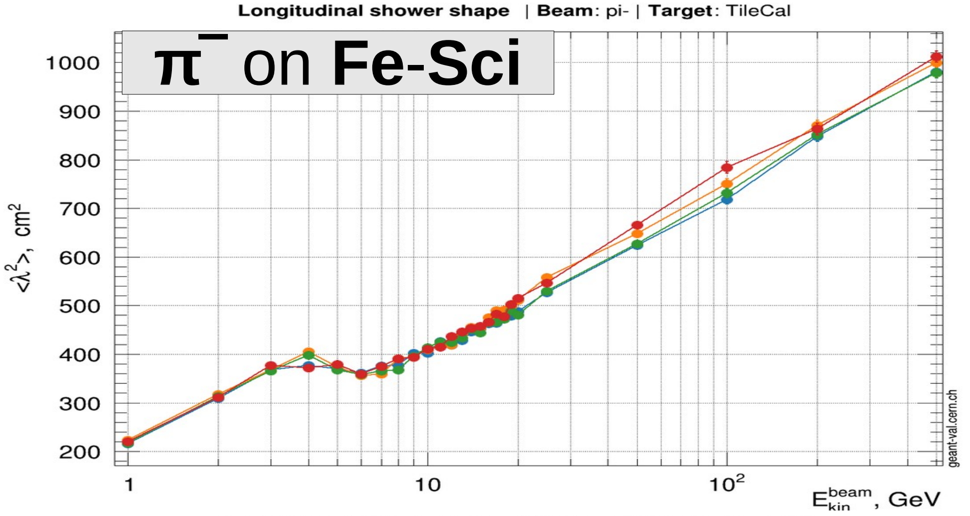


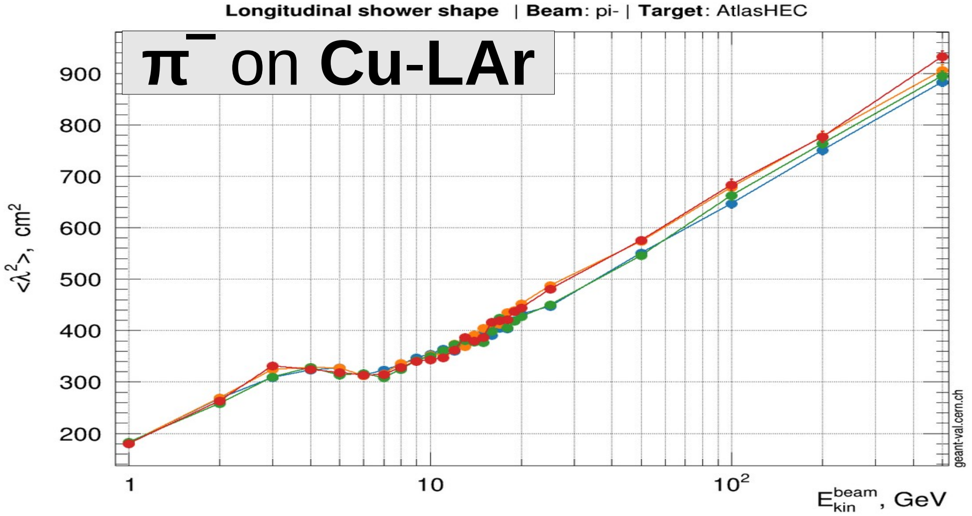


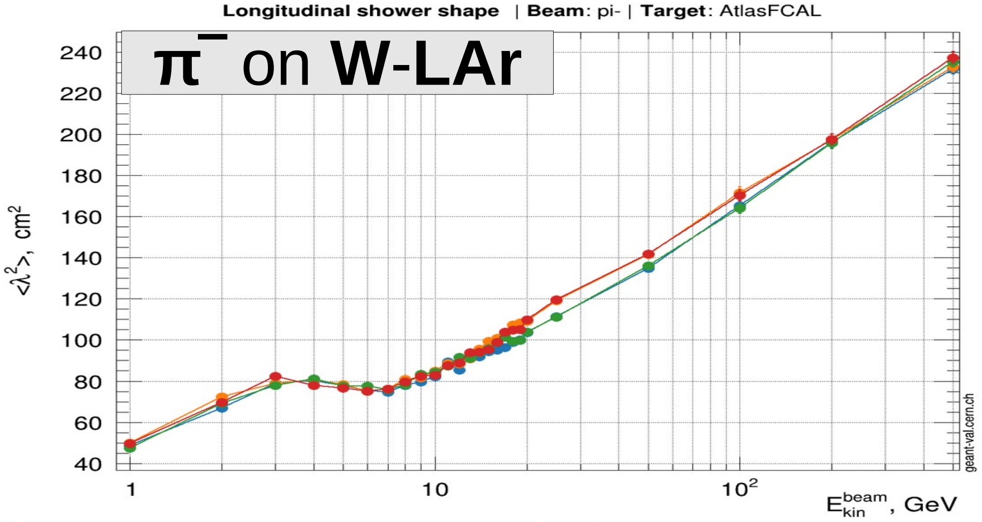


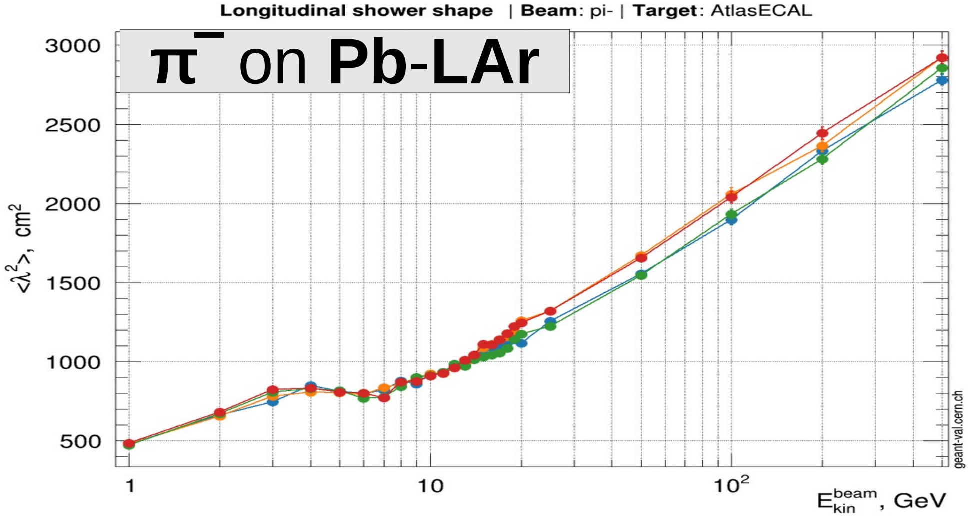


Longitudinal Shape









11.0.ref07 FTFP_BERT
11.0.p03 FTFP_BERT
11.0.ref07 QGSP_BERT
11.0.p03 QGSP_BERT

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11.0.p03 QGSP_BERT

Lateral Shape