Geant4 physics: issues, progress, development

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Goal

The first comparisons between simulations and LHC collision data show good agreement: this is the best reward for all people working in simulation!

Nevertheless, from test-beam data we know some limitations of Geant4 physics: in this talk you will see what we are doing to address them.

Our goal is to provide detector simulations which help the LHC physics analyses and are not the dominating source of systematic errors → constraints on both accuracy and CPU performance of simulations

Outline

Not a complete overview, focus on remaining physics issues

- Introduction
- G4 Electromagnetic Physics
  - Electromagnetic lateral shower
  - Bremsstrahlung
  - Multiple scattering
- G4 Hadronic Physics
  - Fritiof (FTF)
  - Bertini (BERT)
  - Precompound/evaporation (PRECO)
  - High Precision low-energy neutrons (HP)
  - Kaons, hyperons, anti-baryons, light anti-ions
  - Forward physics
  - Other models, transition between models, physics lists
- Conclusions & Outlook

Models, Processes, Physics Lists

- Physics models = *final state generators*
  - Validated and tuned by Geant4 developers with thin-target data

- Physics process = *cross section* + *final state model*
  - Different physics models can share the same cross sections

- Physics list = *a complete list of physics processes associated to each particle present in the simulation*
  - Chosen by users: tradeoff accuracy vs. speed
  - Geant4 offers some reference physics lists ready to be used
  - Validated by the users with (test-beam and/or collision) data

Main achievements

Main achievements of Geant4 physics for LHC applications, in chronological order

- Inclusion of Bertini intranuclear cascade model
- Improvement of quasi-elastic
- Full coverage with only theory-based models (no dependence from parameterized models)
- More accurate simulations of nuclear interactions of: kaons, hyperons, anti-baryons, and light anti-ion

Remaining issues

Remaining issues of Geant4 physics as identified by the LHC experiments, from test-beam data and collision data

- **EM** : - electromagnetic shower lateral leakage (R_{95} ~1 - 2 %)
  - multiple scattering in thin layers (impact parameter resolution in VELO)
- **HAD** : calorimeter observables of hadronic showers
  - energy response (+ 1 - 5 %)
  - energy resolution (- 10 %)
  - longitudinal shower profile (± 10 - 20 %)
  - lateral shower profile (- 10 - 20 %)

Hadronic interactions of “other particles” :

- kaons, hyperons, anti-baryons, light anti-ion

G4 Electromagnetic Physics

Foreword on electromagnetic physics

- Electromagnetic physics must be validated accurately before the validation of hadronic physics
  - electromagnetic component in a hadronic shower: π^0 -> γ γ
  - visible energy of hadrons is from ionization (and brem.)

- For the main observables, Geant4 electromagnetic physics describes the experimental data with accuracy **< 1%**

- We concentrate here only on the weakest points of G4 electromagnetic physics, where the disagreement with data is above 1%, and work is on-going to progress
  - These issues are due to a fast and approximate description, or because of medium and atomic physics effects

Electron shower lateral leakage

ATLAS, CALICE, and CMS report that Geant4 electron shower lateral profiles agree on the core but are slightly (1 - 2%) narrower in the tails

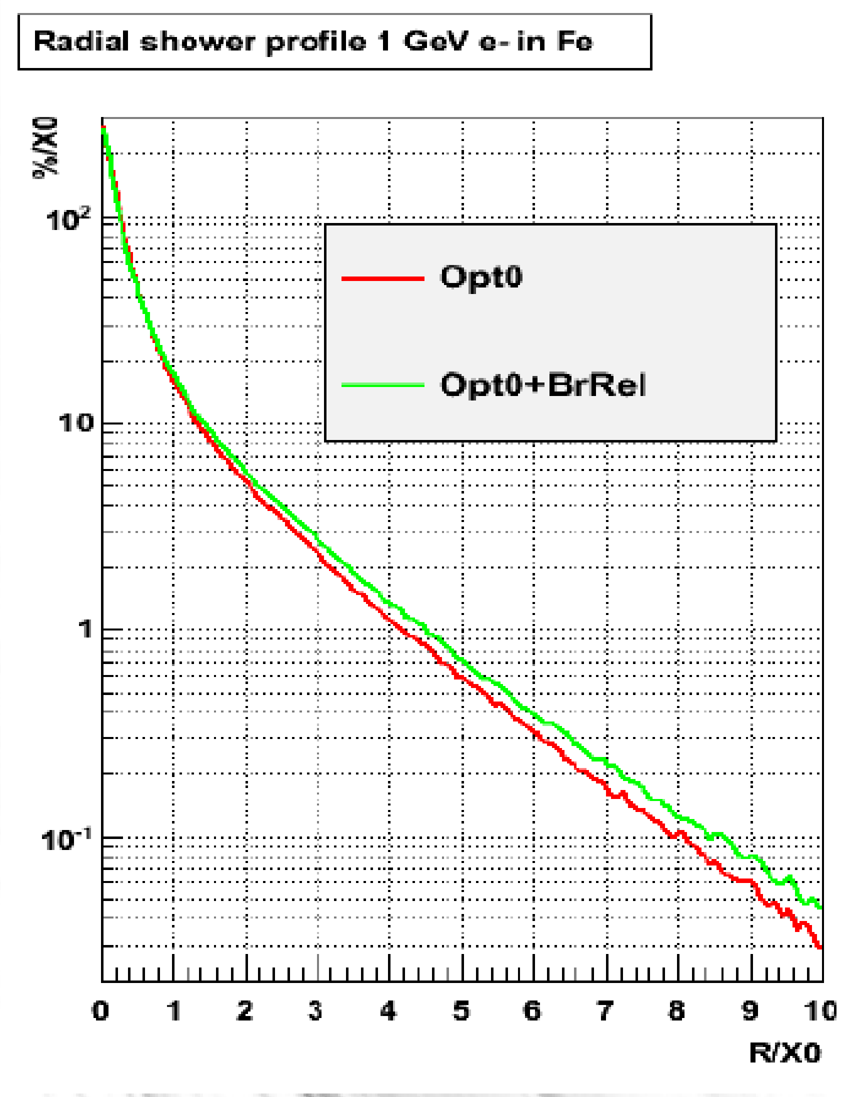
Studies of the effect of various EM options on the lateral shower profile of electrons in calorimeters:

- Model combinations
- Step limitation
- Cuts
- Multiple scattering (msc95, WVI, GS)
- Polarization models
- Bremsstrahlung models (Penelope, Livermore), and angular generators (Tsai, 2BS, Grichine)
- Low-energy extrapolation of relativistic Bremsstrahlung model

--> only the last one shows some effect

Effect of low-energy extrapolation of relativistic bremsstrahlung on radial electron shower profile

By lowering the applicability energy limit of the relativistic brem. model, the radial electron shower profile gets wider



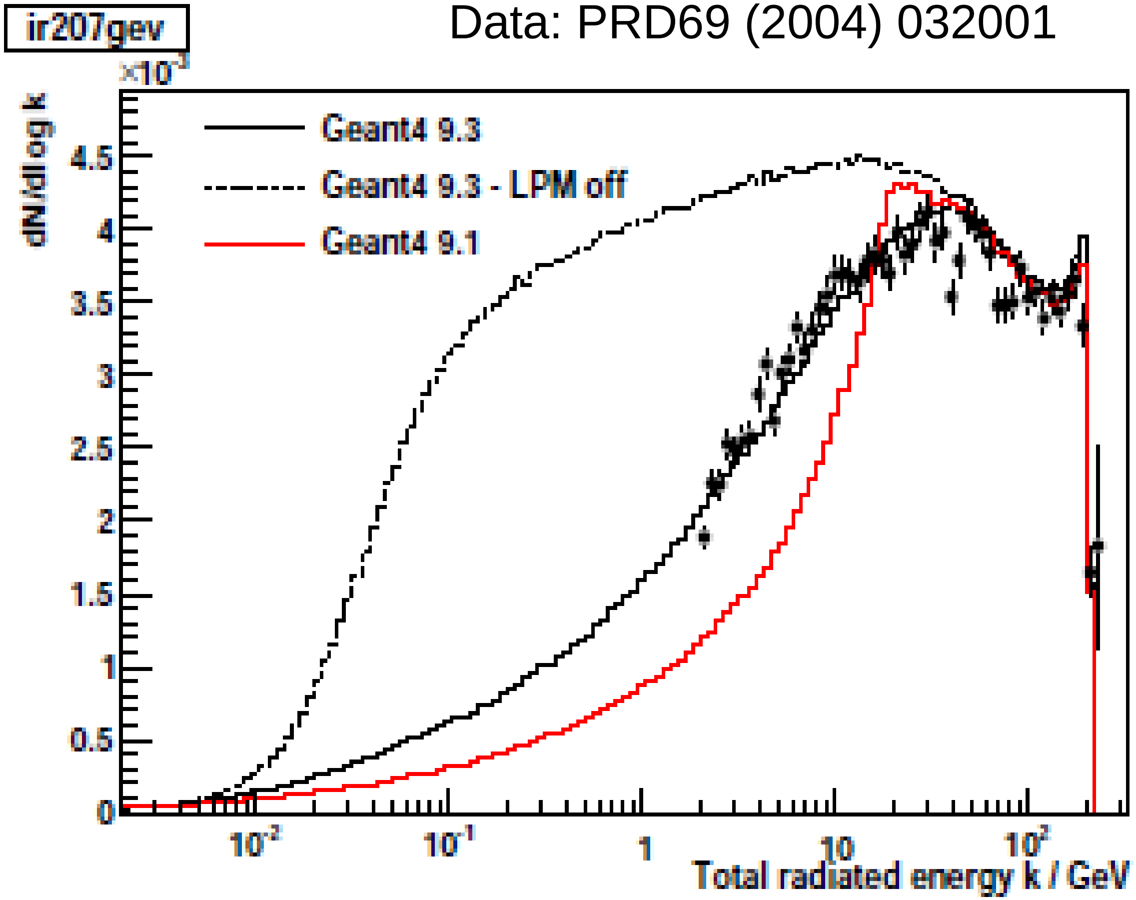
Bremsstrahlung

GLAST test-beam data (CERN 2004) showed that Geant4 bremsstrahlung model needed to be improved

Since G4 9.3, a new relativistic bremsstrahlung model is present, with LPM and density effects, and complete screening, valid for E > 1 GeV

Work in progress to create a new low-energy, non-relativistic bremsstrahlung model

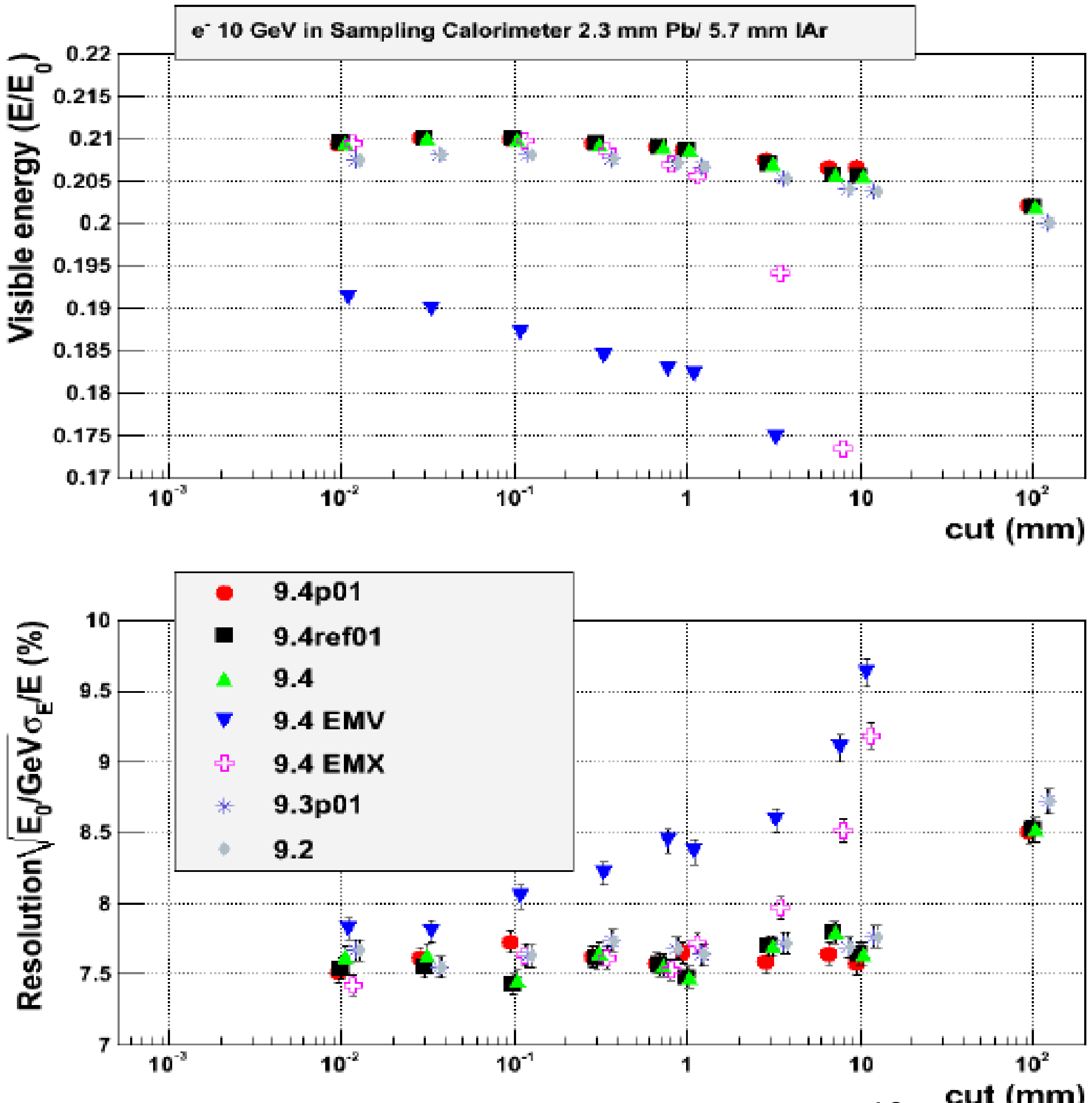
Data: PRD69 (2004) 032001



Effect of Multiple Scattering on visible energy

Simplified calorimeter Pb-LAr ("ATLAS barrel")

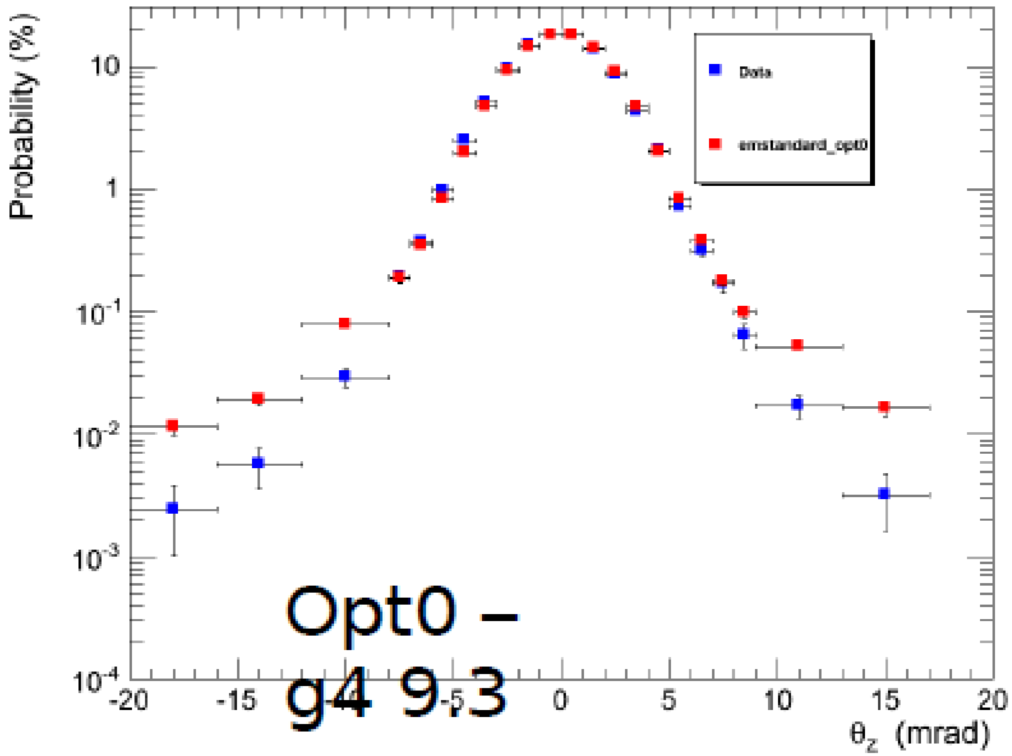
Visible energy and resolution are stable within **1%** since G4 8.3

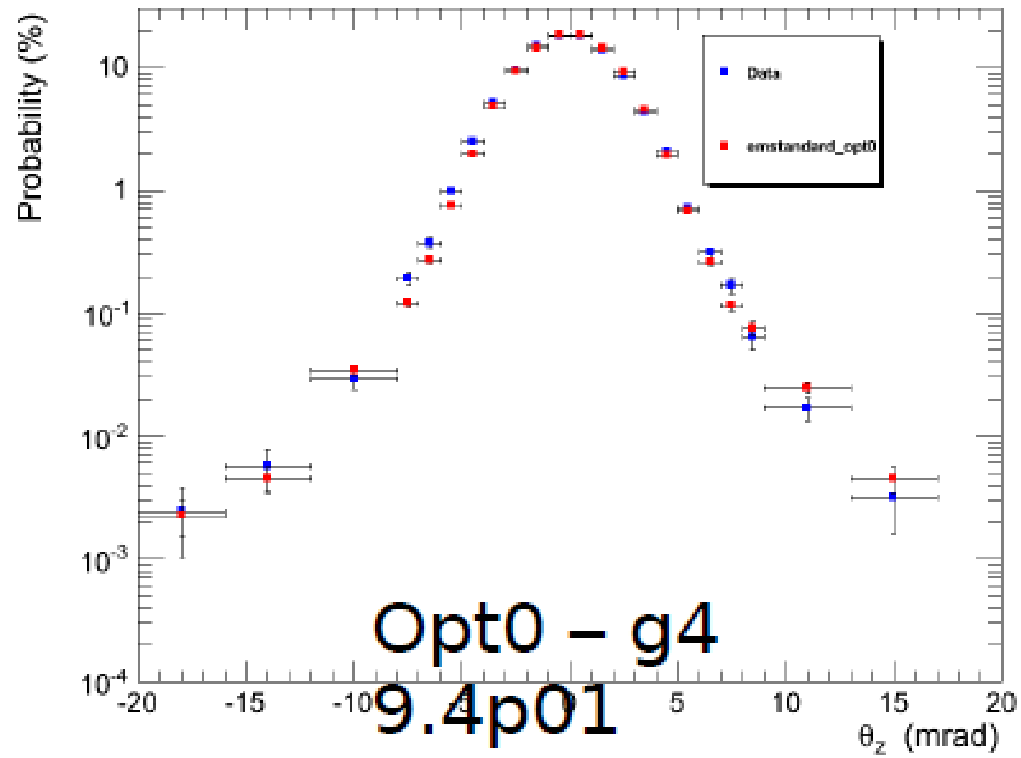


Multiple Scattering

- Modeling of multiple scattering (MSC) of electrons is critical for both CPU performance and calorimeter response
- Earlier versions of MSC showed unphysical dependence of the calorimeter visible energy on the range cut
- Significant improvements over the years
- In G4 9.2 separation of MSC for electrons, muons, and hadrons, to allow for specific tuning of each type
- Recent issue of impact parameter resolution vs. Pt in VELO (LHCb vertex detector)

Multiple scattering of 7 GeV/c μ on Cu





Data: NIM A 234 (1986) 518

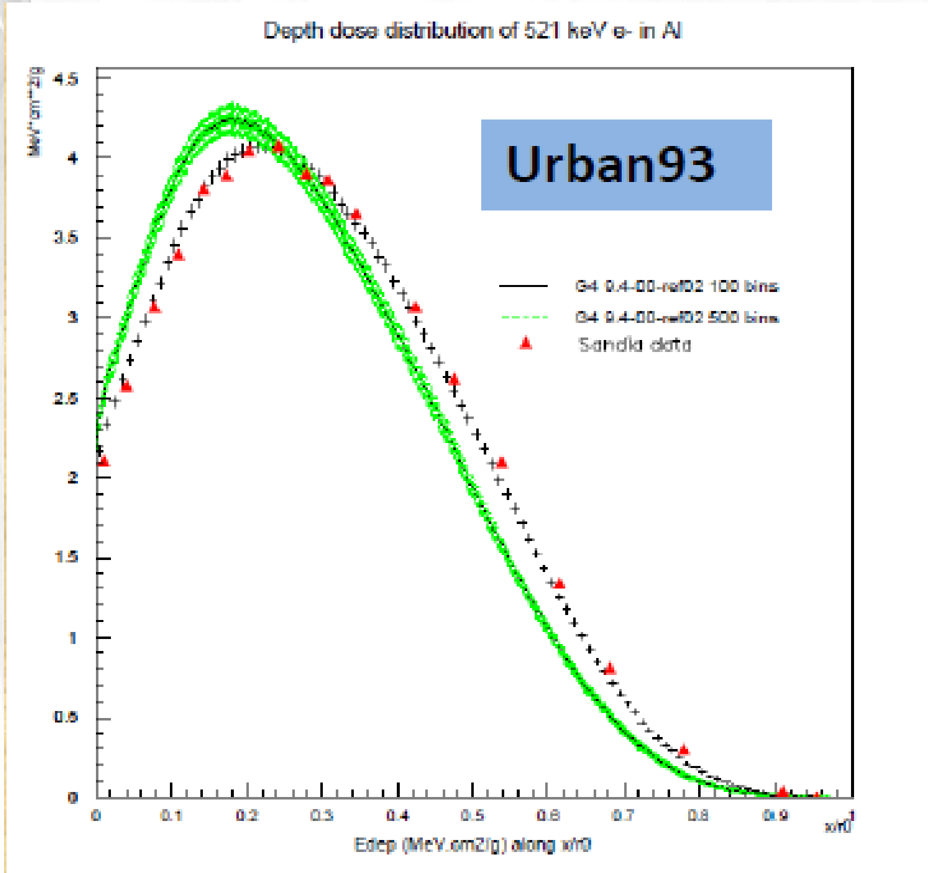
Good description of the core; improving in the tails in G4 9.4

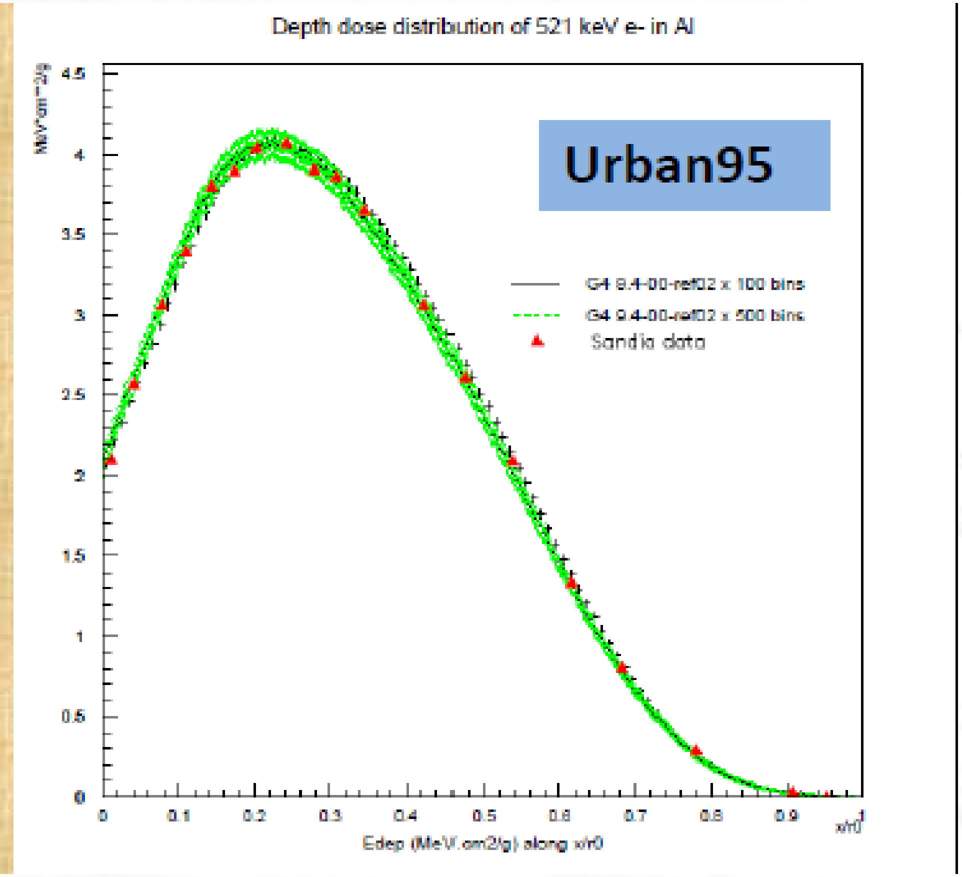
MSC : recent developments

- New G4UrbanMscModel95 will be the default in G4 9.5 (available in development tag 9.4.ref08)
  - improved lateral displacement
  - allow fluctuations in straggling
  - improved large-angle tails
- Validation tests show similar or improved results with respect to the previous default model, G4UrbanMscModel93
  - G4UrbanMscModel93 will be kept for backward compatibility

0.5 MeV electron transport in Al with step limitation

▲ : Sandia data **+++** : 100 steps **---** : 500 steps





Urban95 is more stable than Urban93 for step size change

EM Options

- Baseline (default)
  - Used in production by ATLAS
  - Available in QGSP_BERT , QGSP_FTFP_BERT , FTFP_BERT

- Fast (option1)
  - Used in production by CMS and LHCb
  - Available in _**EMV** variants of the physics lists
  - Fast due to simple step limitation, cut used by photon processes, WentzelVI model of multiple scattering for muons and hadrons
  - Good for crystals, not for sampling calorimeters

- Accurate (option3)
  - The most precise EM simulation offered by Geant4, regardless of speed
  - Available in _**EMY** variants of the physics lists

G4 Hadronic Physics

Foreword to hadronic physics

- hadron – nucleus interactions of interest for detector simulation (e.g. hadrons in a jets crossing a calorimeter) cannot be computed by pQCD, so we need to rely on hadronic models

- There are several hadronic models
  - Limited in **projectile type** , **energy** , **target nucleus**
  - Need to combine more models to cover the whole range of hadronic interactions
  - Choice of the models depend on the application: tradeoff between accuracy and speed

- Accuracy of hadronic physics depends strongly on the observable. We concentrate here on:
  - Calorimeter observables relevant for LHC physics

Issues <---> Models

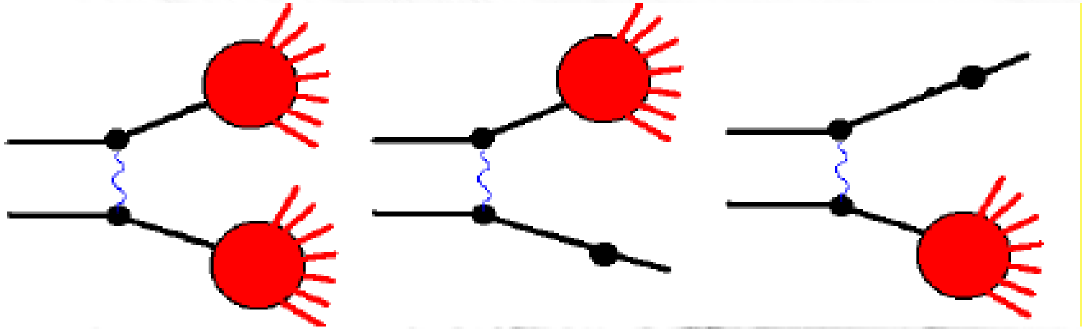
- **Energy response**
- **Energy resolution**
- **Longitudinal shower profile**
- **Lateral shower profile**

- **Fritiof** (**FTF**)
- **Bertini** (**BERT**)
- **Precompound** (**Preco**)
- High Precision (**HP**)
  low-energy neutrons
- Forward physics
  elastic, q.elastic, diffraction

Fritiof (FTF) model

- **High-energy string model**
- Valid for any hadron with E_{kin} **3 GeV - 1 TeV**
- Important for:
  - energy response
  - energy resolution
  - shower shapes

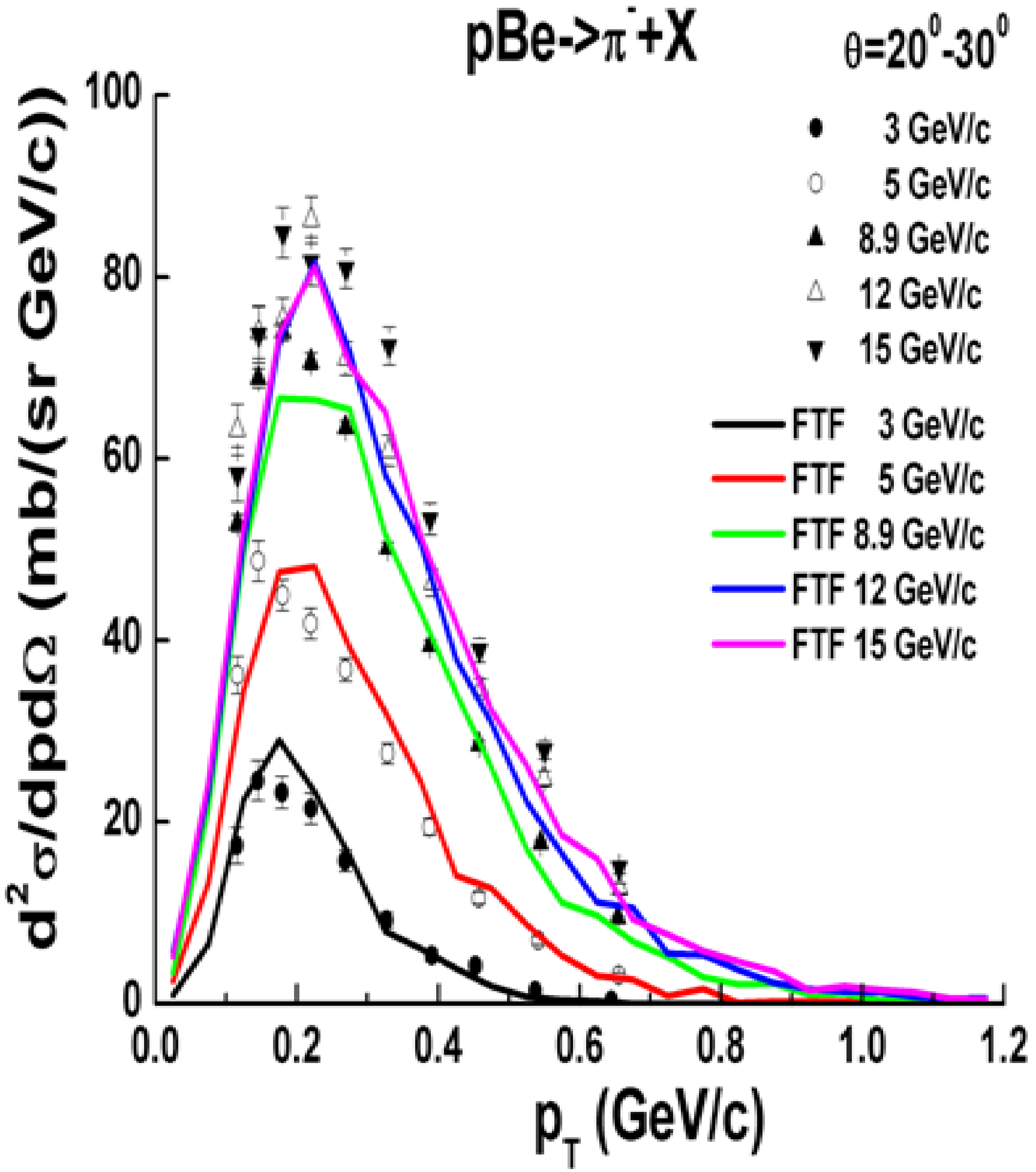
Note: renew interest on this model after discontinuities in the energy response vs. beam energy in QGSP_BERT



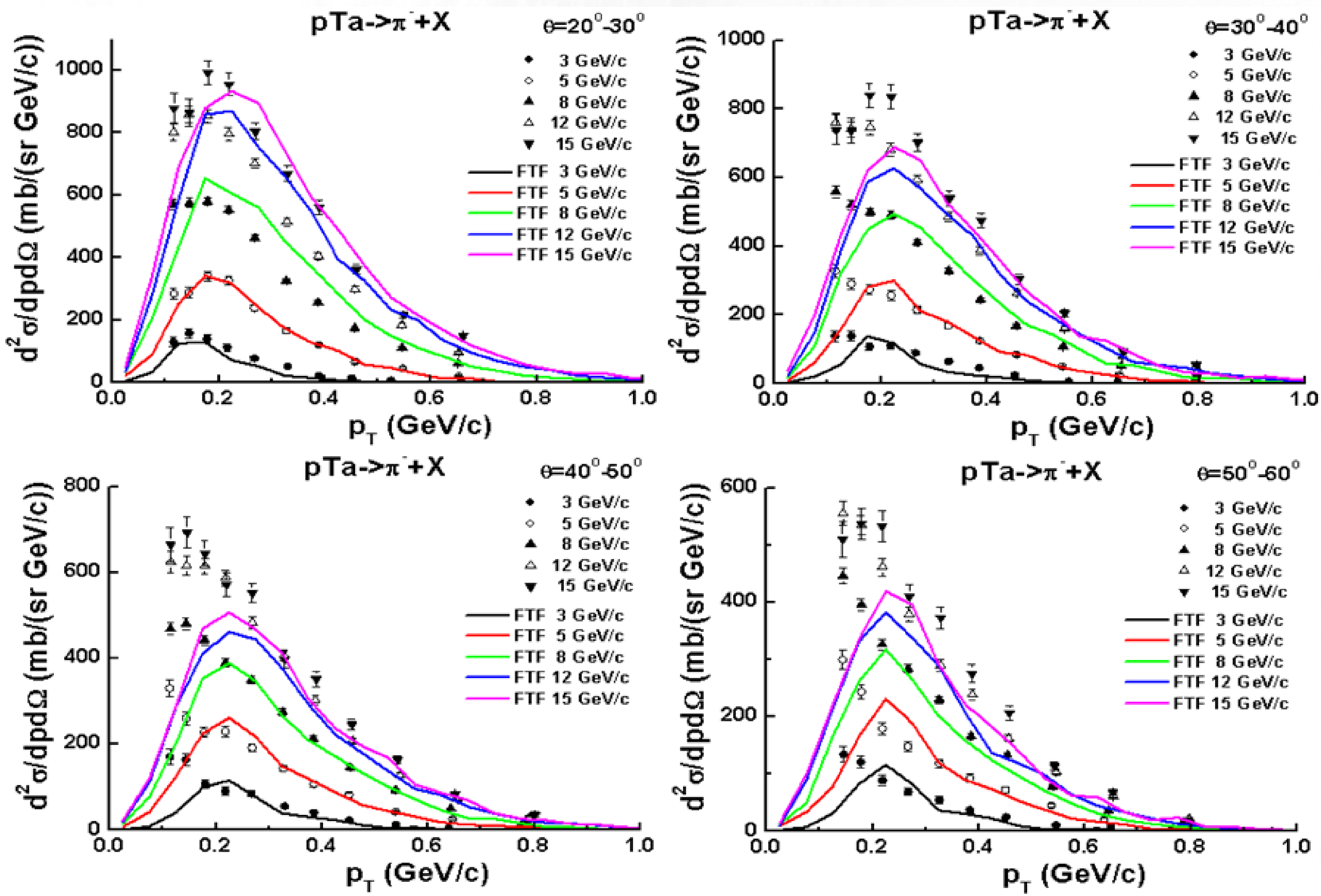
Main FTF developments

- Addition and tuning of Reggeon Cascade
    - describes high energy cascading as a repeated exchange of quarks between nucleons (in a nucleus)
    - allows better nuclear destruction/de-excitation after the initial high energy interaction
- Added quark exchange for **low-mass string** formation
- Improved **low-mass string** fragmentation
- These improvements allowed to extend FTF to much lower energies (**~ 3 GeV**) for nucleons, pions, and hyperons
    - **HARP-CDP data** used for tuning cascade and low mass strings
- Now, FTF merges more smoothly with Bertini

FTF tuning/validation with HARP-CDP data



FTF tuning/validation with HARP-CDP data

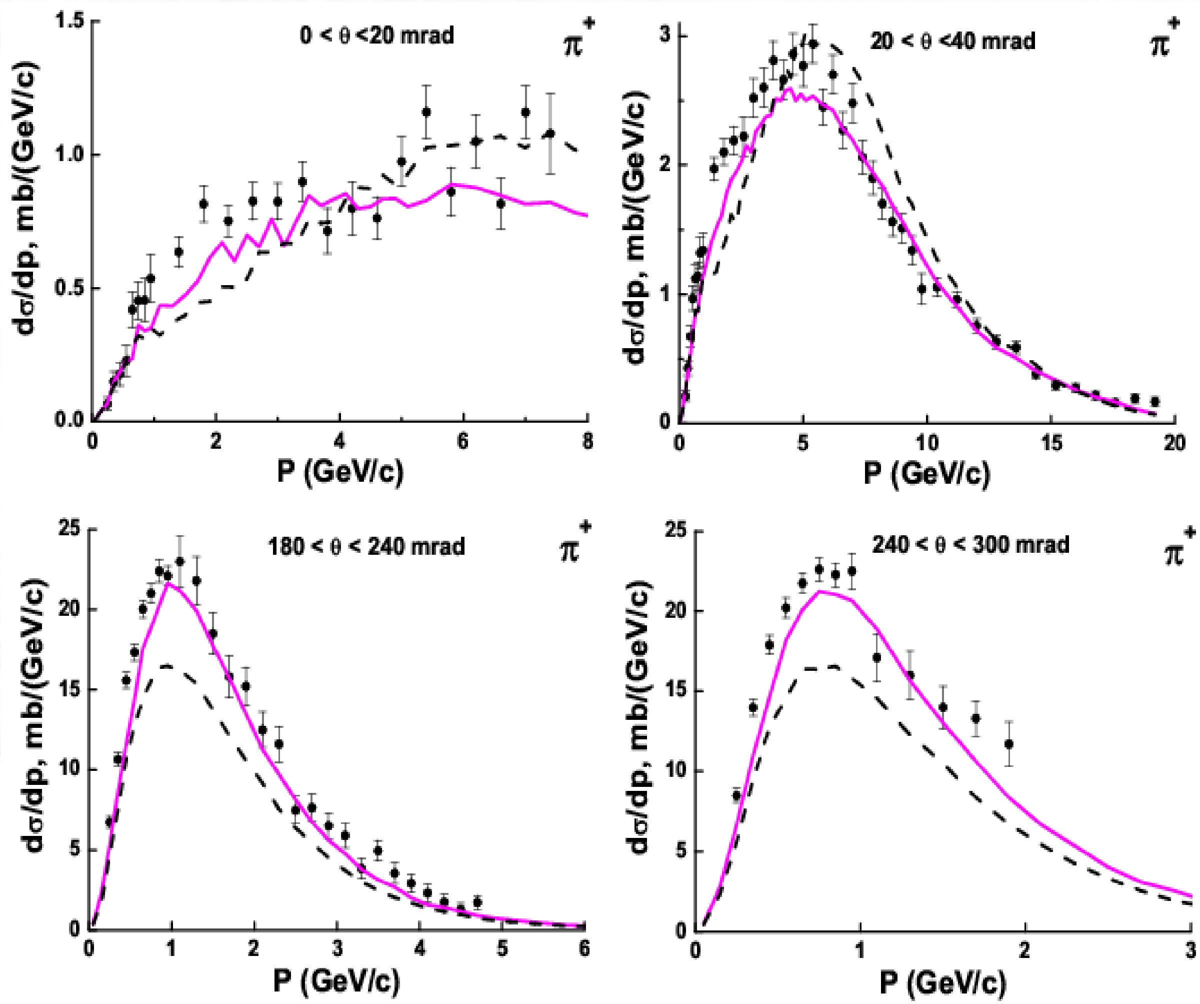


FTF thin-target validation

31 GeV/c p + C → π± + X , **NA61/SHINE**

- **FTF G4 9.4**
- FTF G4 9.2

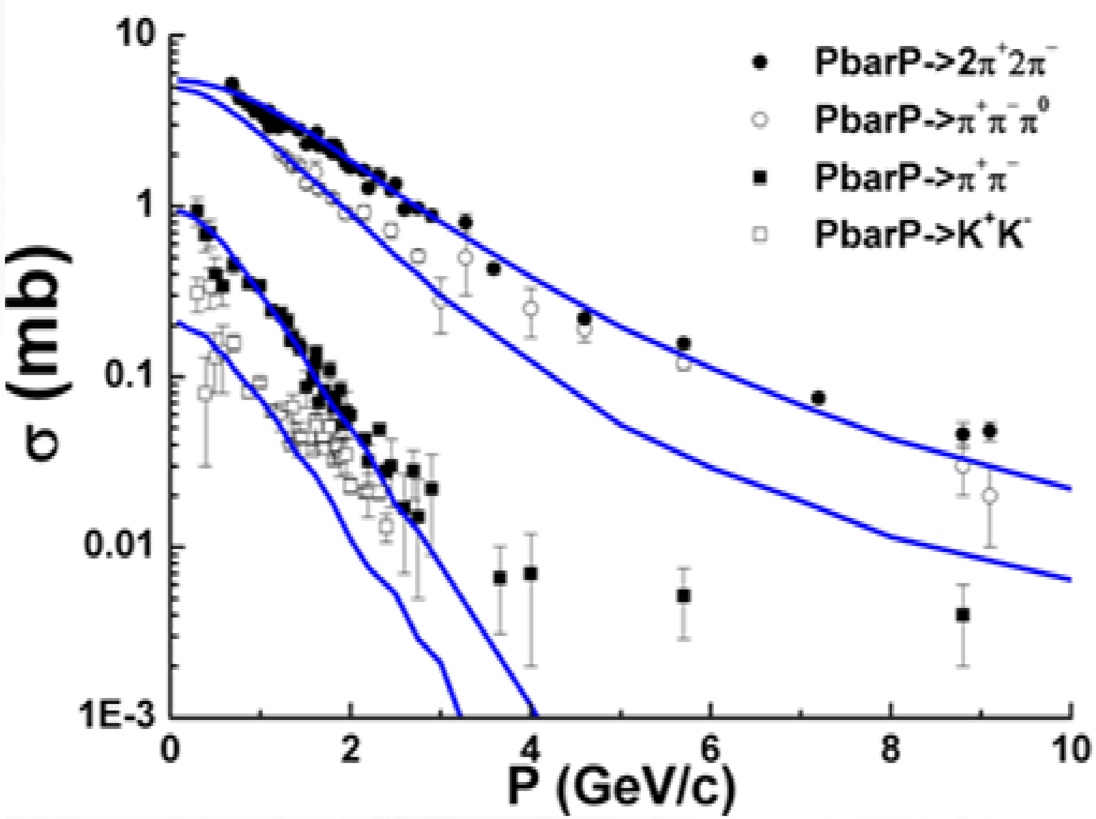
FTF improved significantly

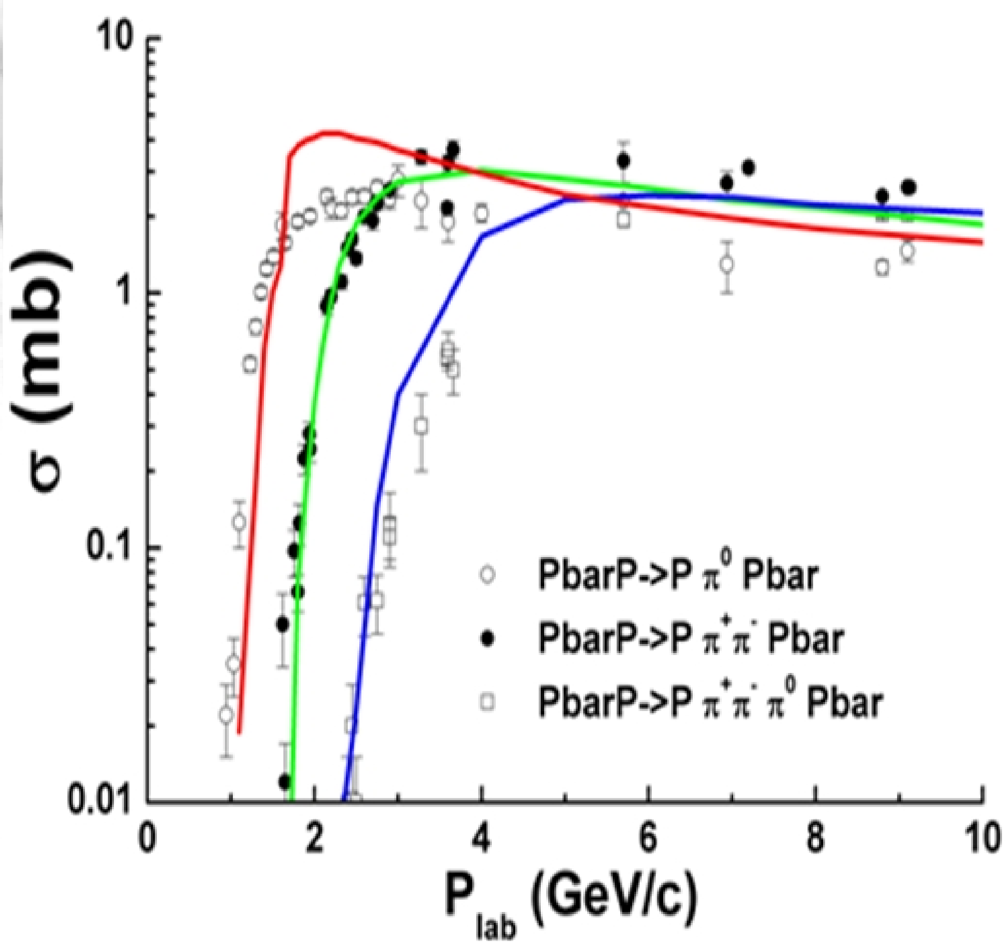


FTF extension to anti-matter

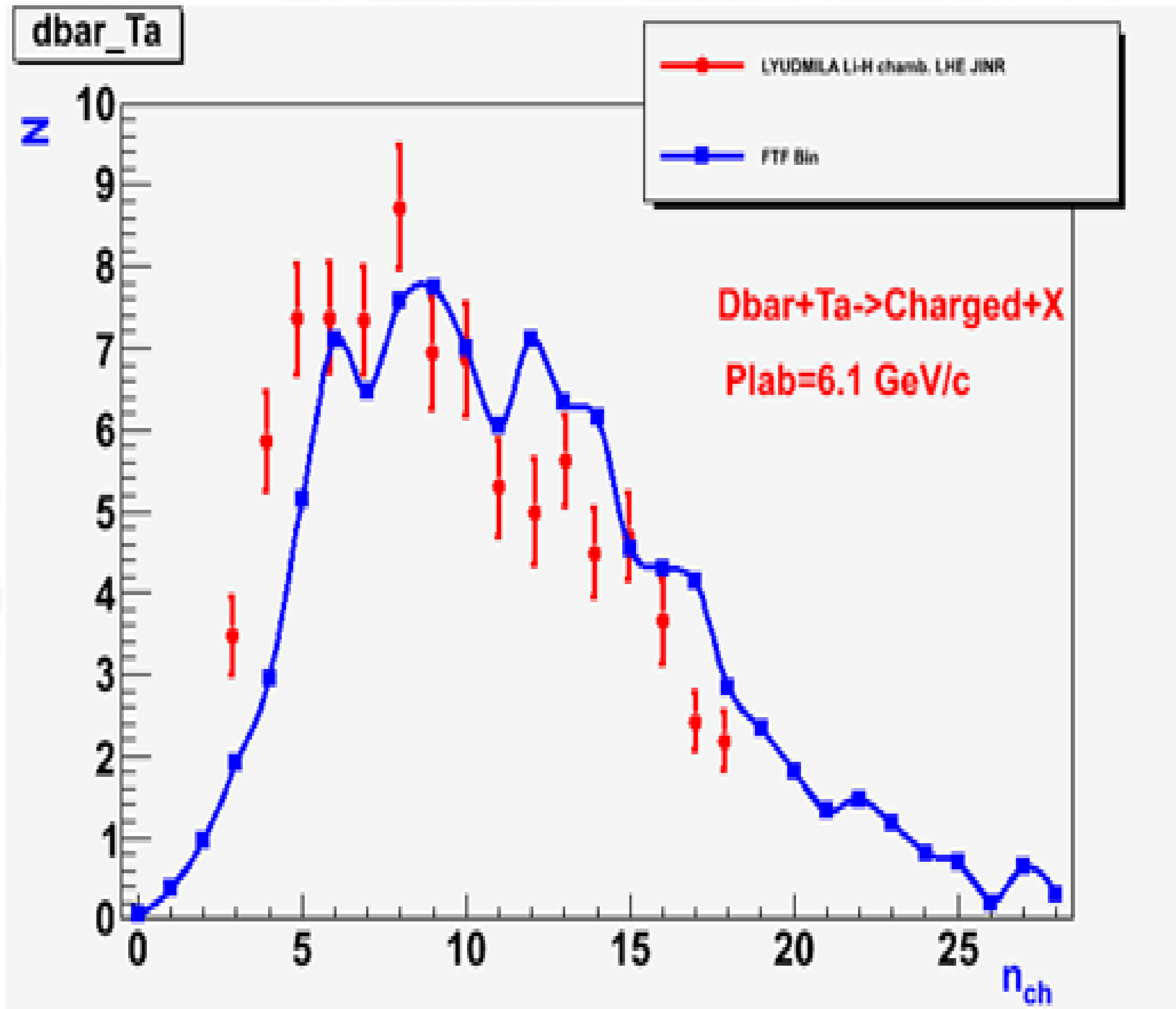
- Anti-baryon (p,n,Λ,Σ,Ξ,Ω) and light anti-ion (d,t,3He,α) nuclear interactions, available in G4 9.5.beta
  (and development tags since April)
  - Requested by ALICE and now under validation
  - New cross sections
  - Final state generation down to zero incident energy
  - Valid from **0** to **1 TeV/c/nucleon**
- Nucleus-nucleus interactions also available
  - Requested by NA61/SHINE
- Further validation & tuning needed

FTF p̲ - p validation



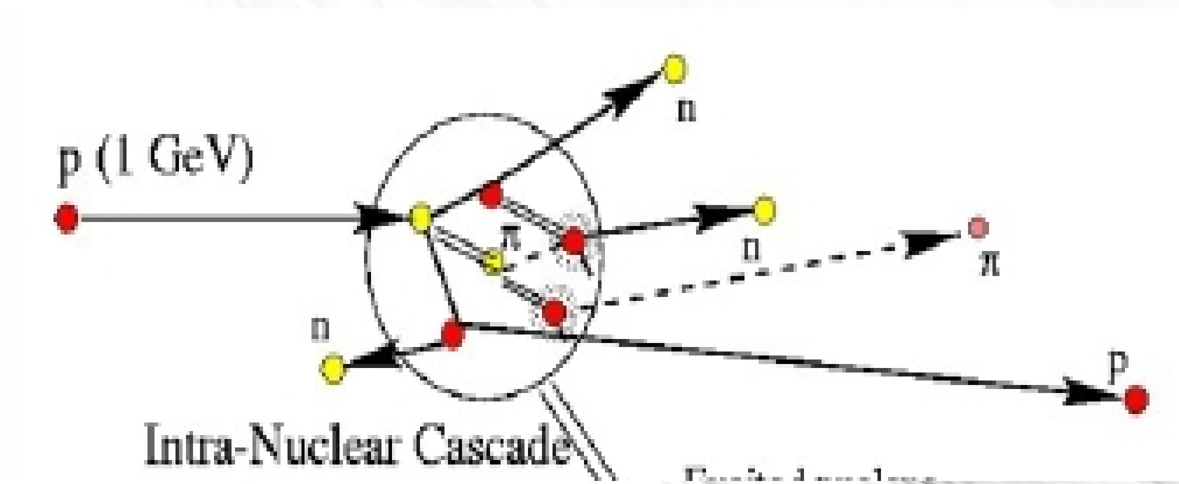


FTF d - Ta validation

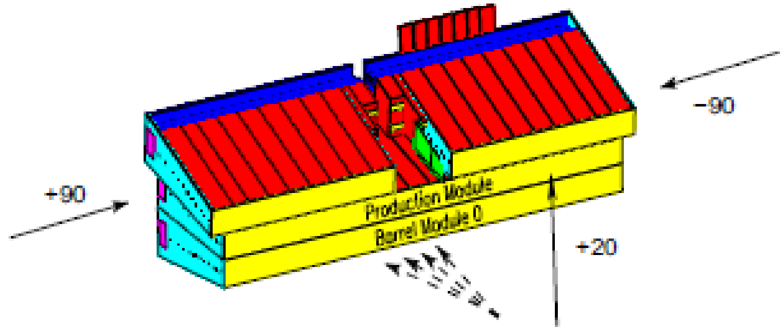


Bertini (BERT) model

- **Intranuclear cascade model**
- Geant4 implementation of early codes (1960s)
- Valid for p, n , π, K, hyperons with E_{kin} **< 10 GeV**
  - *has its own internal version of precompound and evaporation*
- Important for:
  - radial shower profile
  - energy response
  - energy resolution

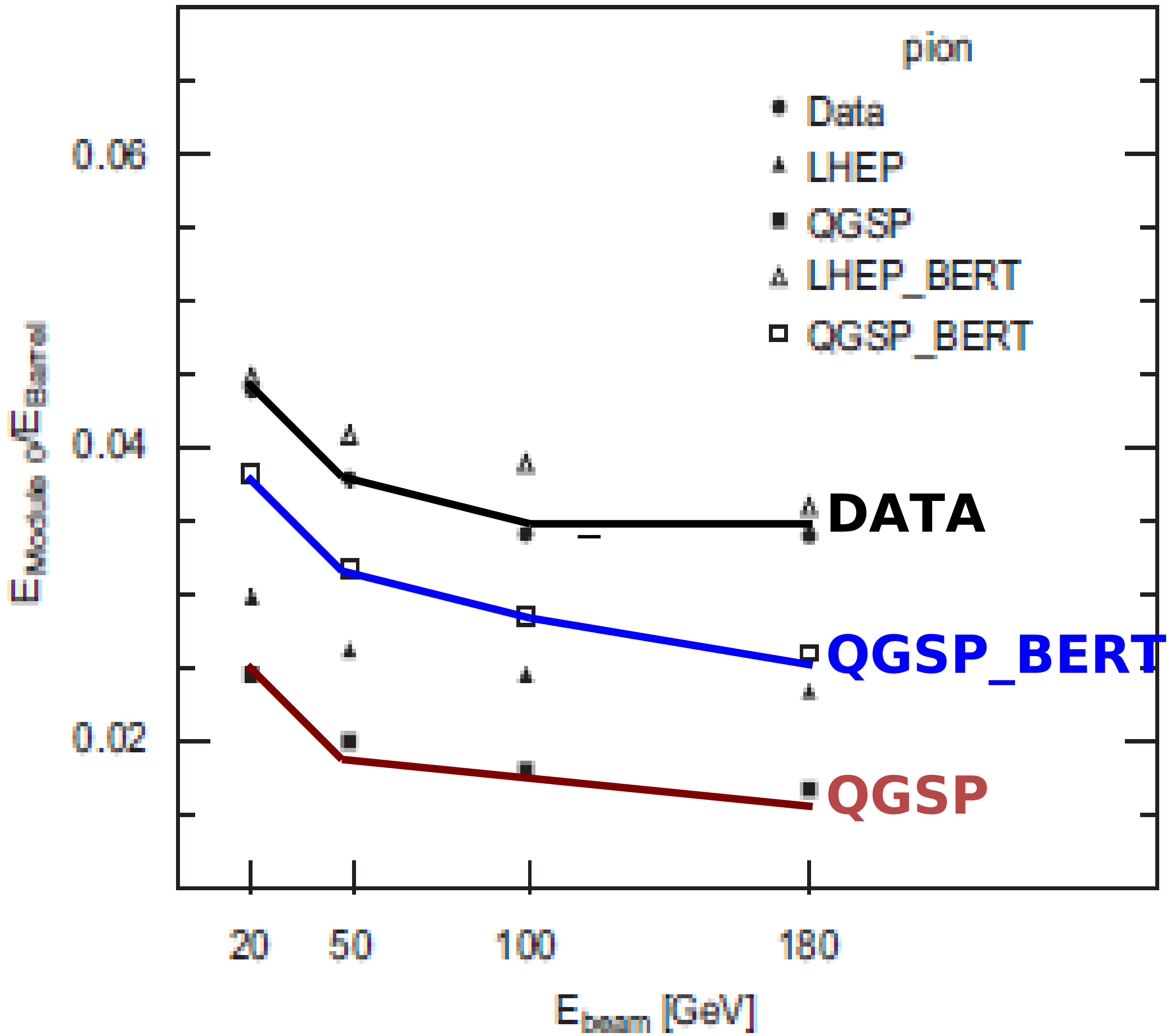


BERT: effect on lateral shower profiles

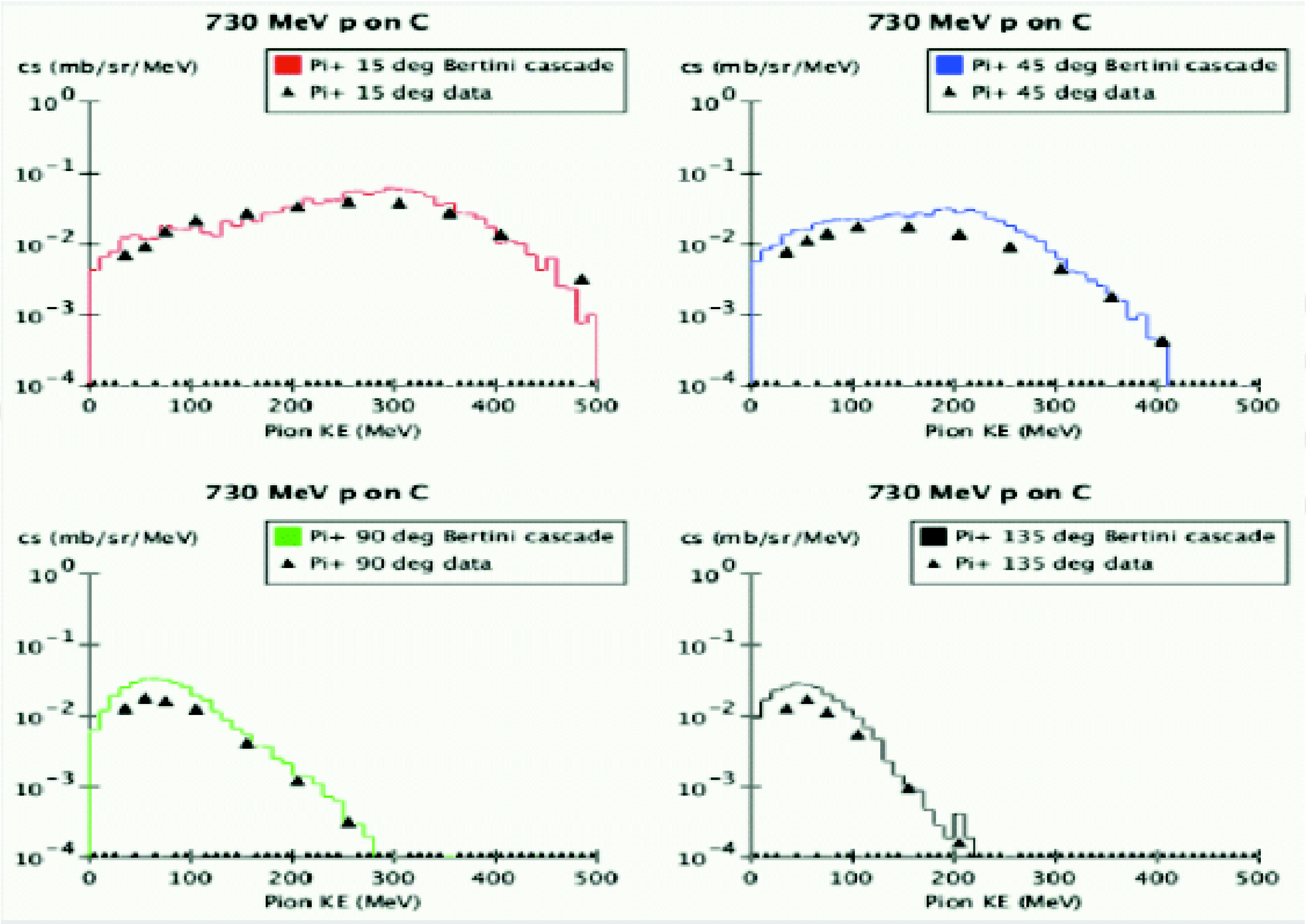


ATLAS TileCal
test-beam @90⁰
NIMA 615
(2010) 158

QGSP_BERT
is wider
than QGSP



BERT validation with thin-target data

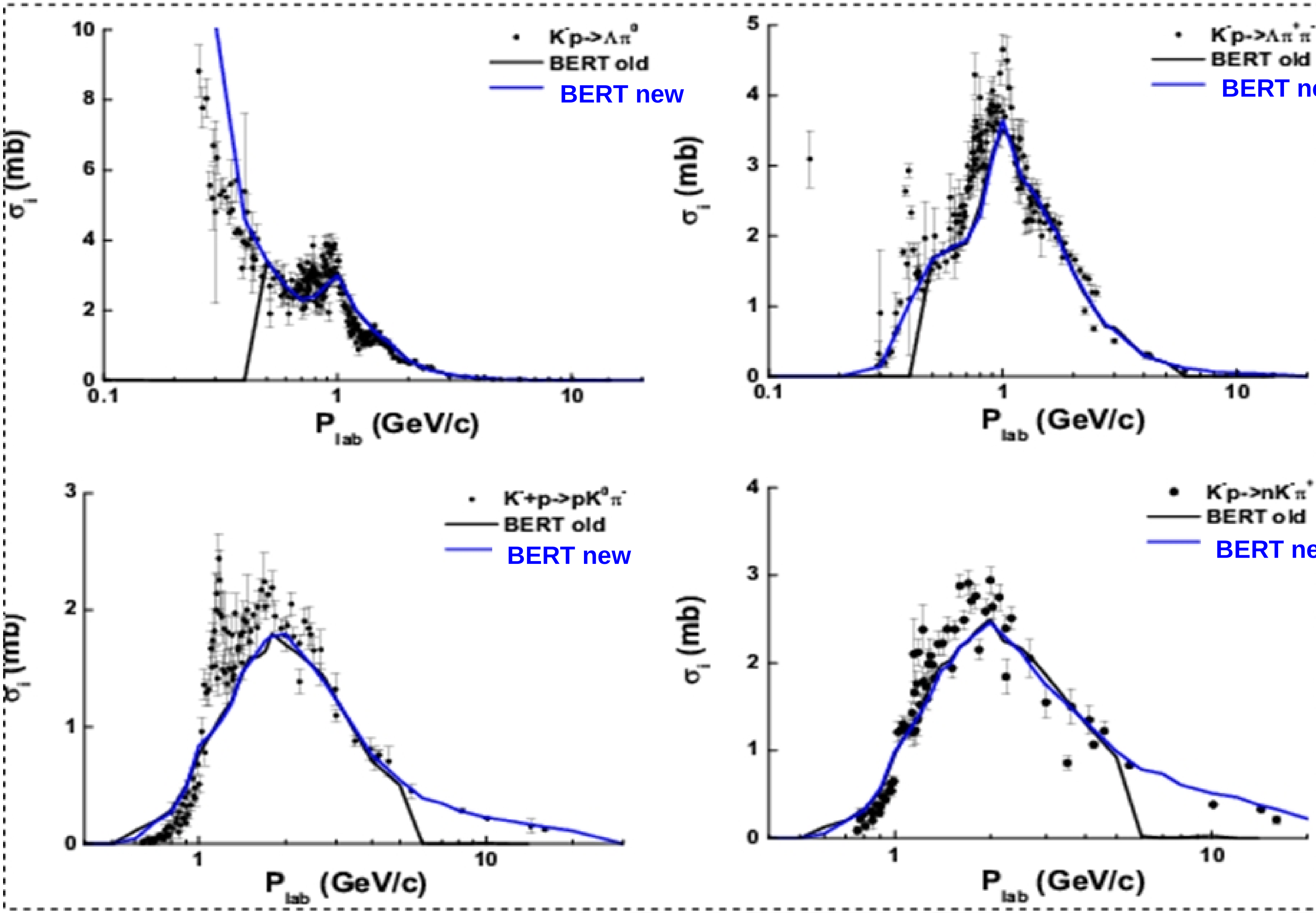


BERT physics developments

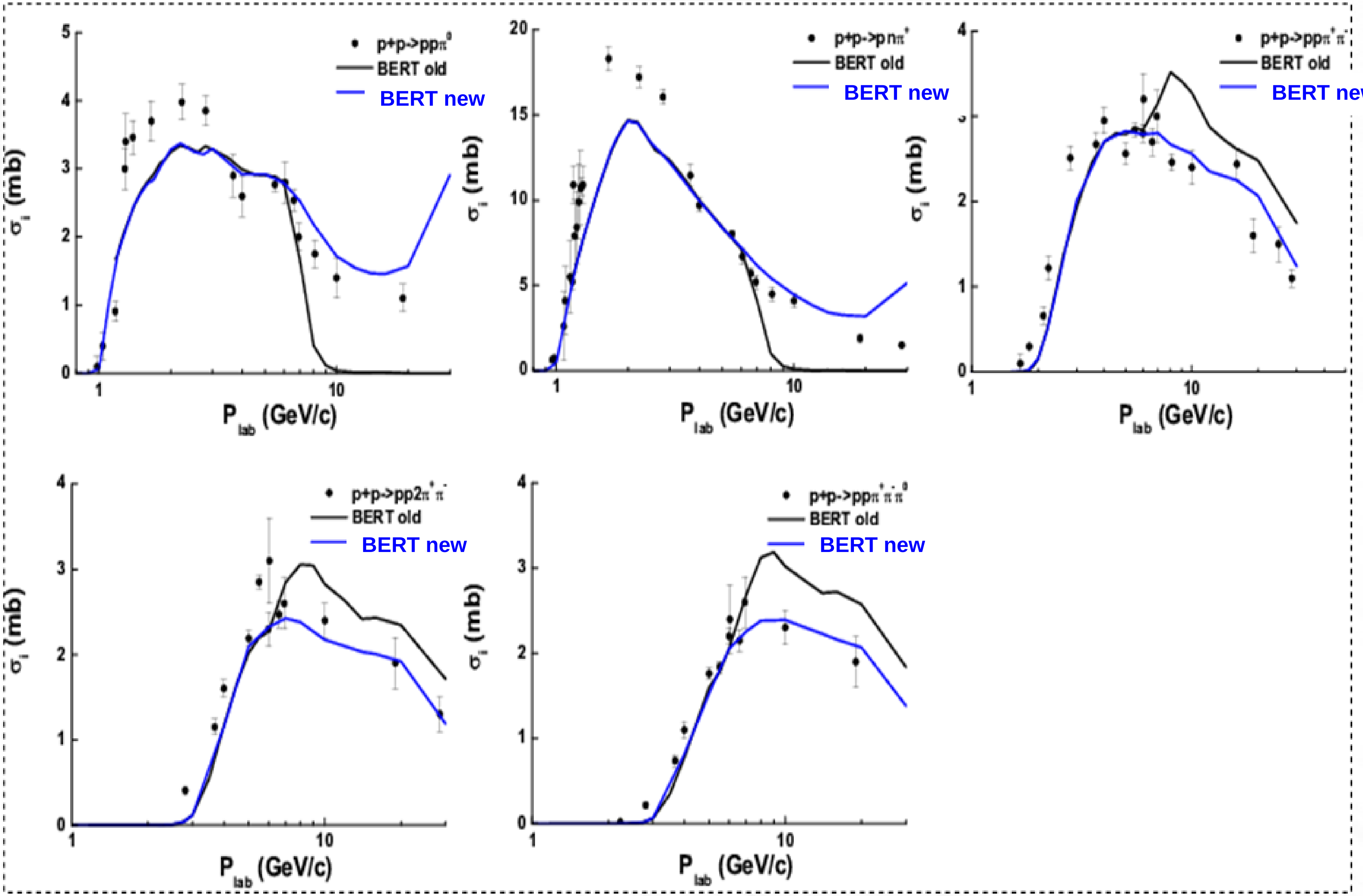
- Revision of internal cross sections
- Trailing effect added
  - Well-known effect of local density reduction in nuclear medium following an individual scatter within nucleus -> predicts fewer final state nucleons
  - Still optimizing parameters for this effect
- Supports re-scattering of secondaries from string models
  - High energy scatter on nucleon produces fragments either inside or outside the target nucleus
  - Needed for smooth, physical transition from string models (FTF, QGS) to Bertini cascade

Note: the above physics developments have been possible thanks to significant improvements in the code structure

BERT improvements

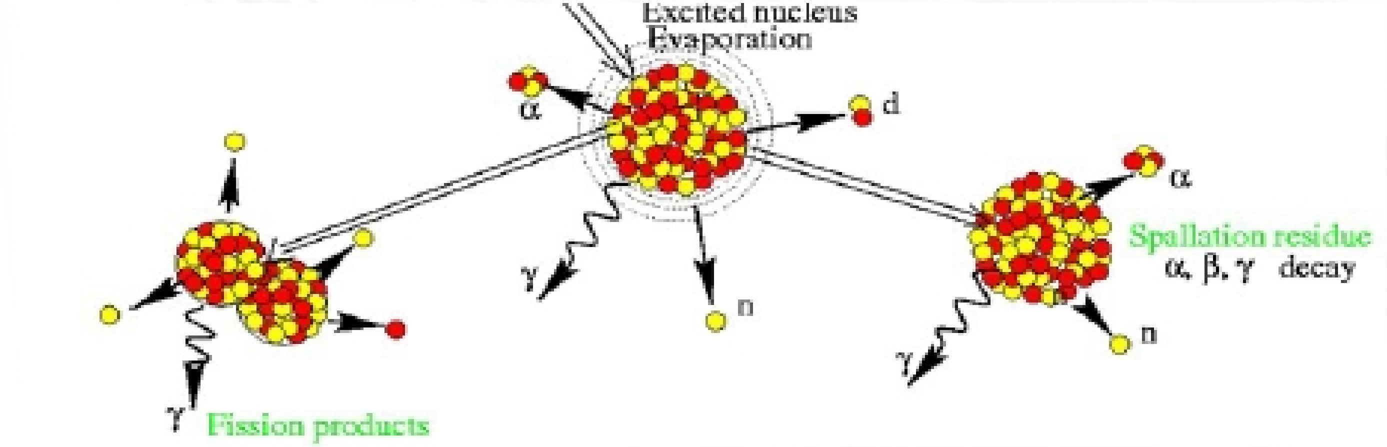


BERT improvements



Precompound / evaporation (Preco)

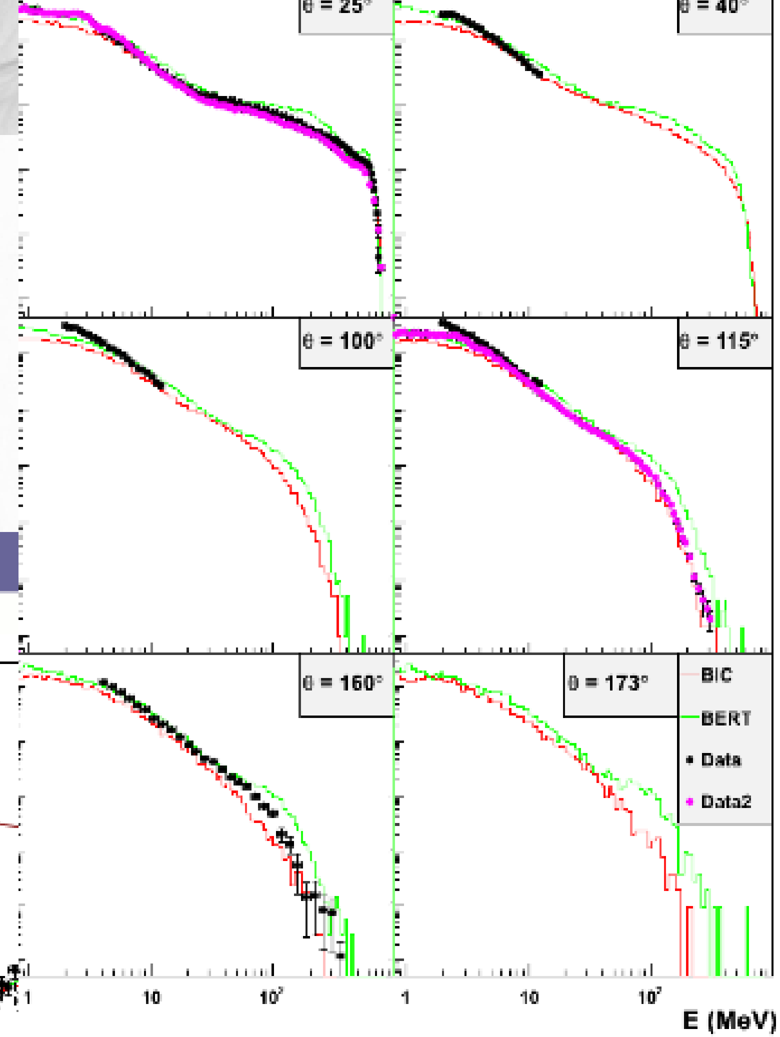
- **De-excitation nuclear model**
- Valid for any excited nucleus
- Important for:
  - energy response
  - energy resolution



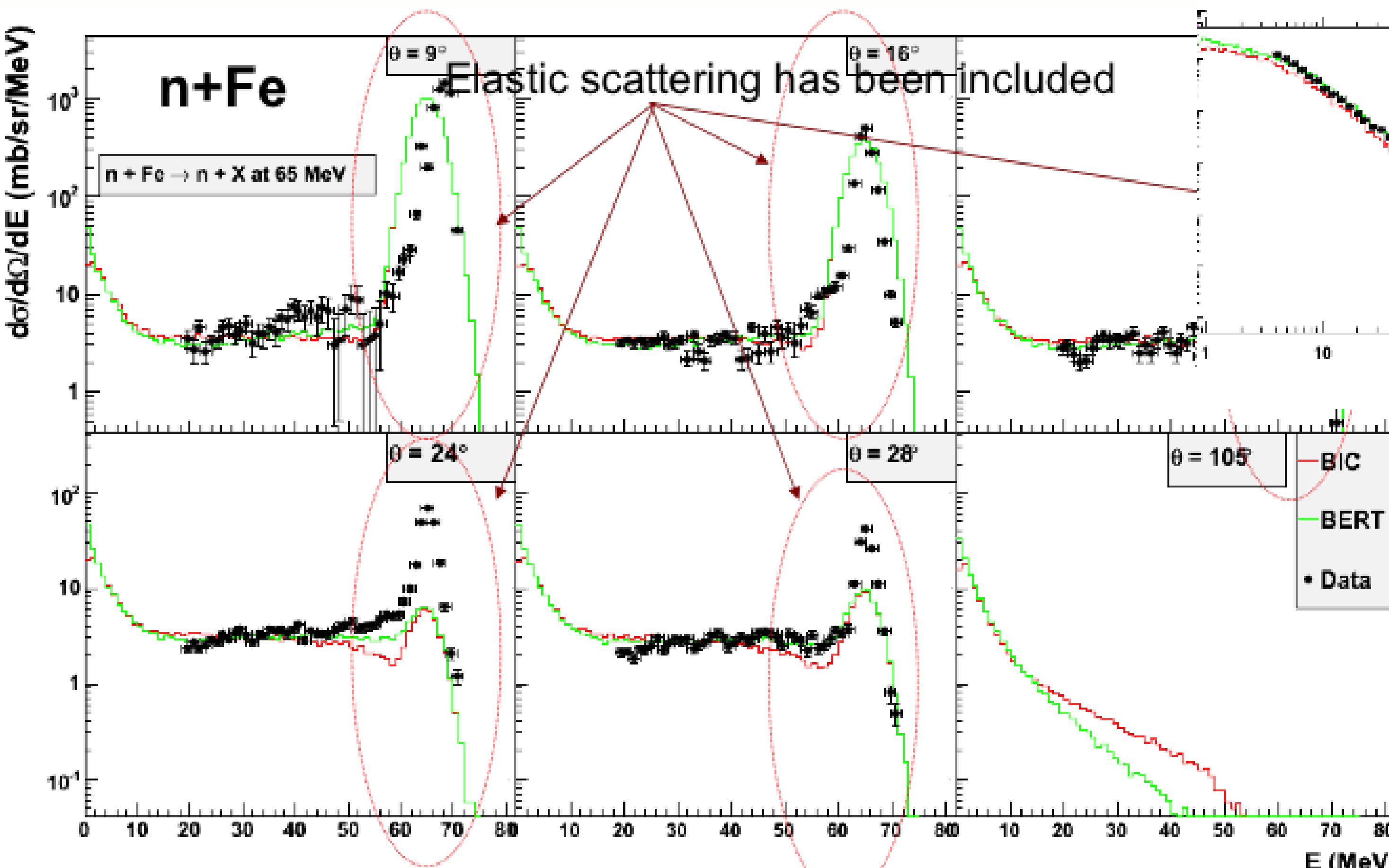
Precompound

- Precompound stage = pre-equilibrium
- Competition between
  - particle emission
  - internal transition between exciton states
- Generate “higher” energy secondaries
- Revised transition probabilities & exit condition

Validation: neutron production p + Fe -> n + X @800 MeV

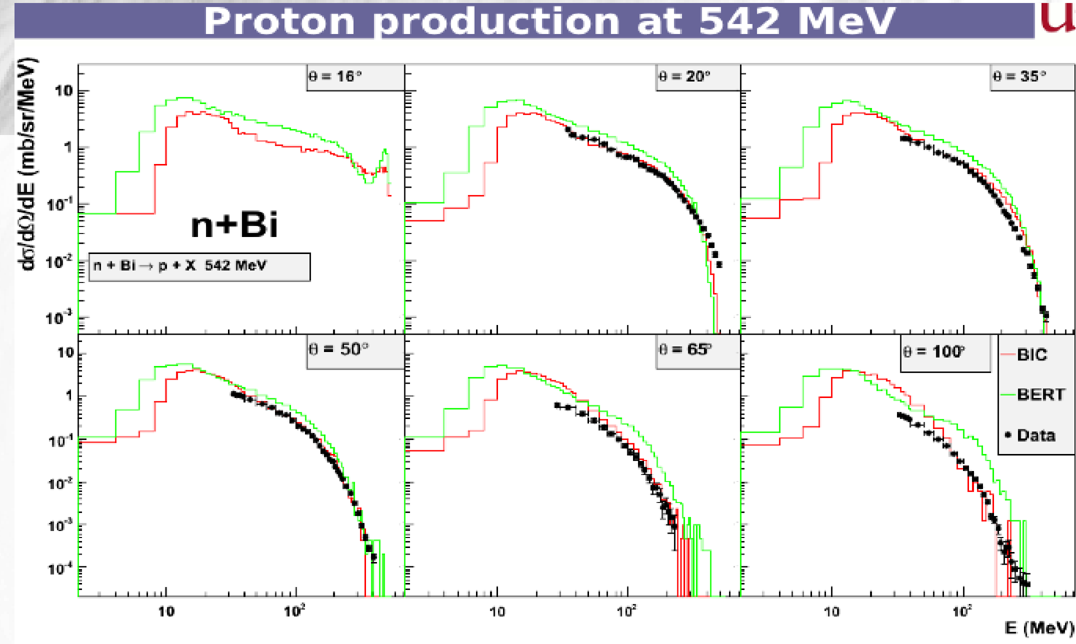


Neutron production at 63 MeV



BIC -> PRECO

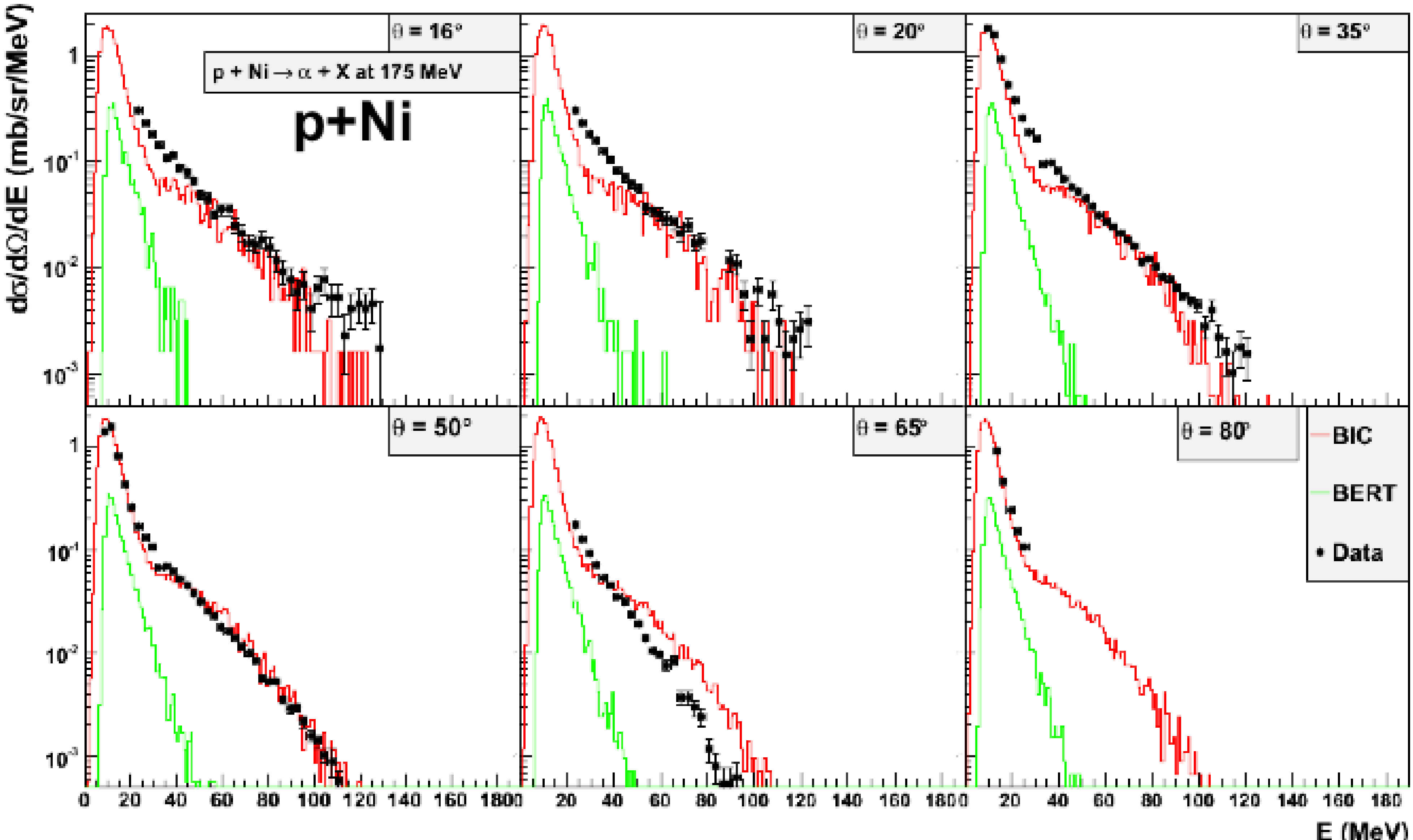
BERT has its own internal preco



De-excitation

- Most processes revised:
  - Fission
  - Fermi-breakup (light nuclei)
  - Evaporation WE (Weisskopf-Ewing): n, p, d, t, He^3, α
  - Photon-evaporation
- New “hybrid” evaporation
  - Uses revised GEM (Generalized Evaporation Model) to emit heavy fragments (Z < 13 and A < 29)
- Large number of comparisons to IAEA spallation benchmark

Alpha production at 175 MeV



BIC -> PRECO

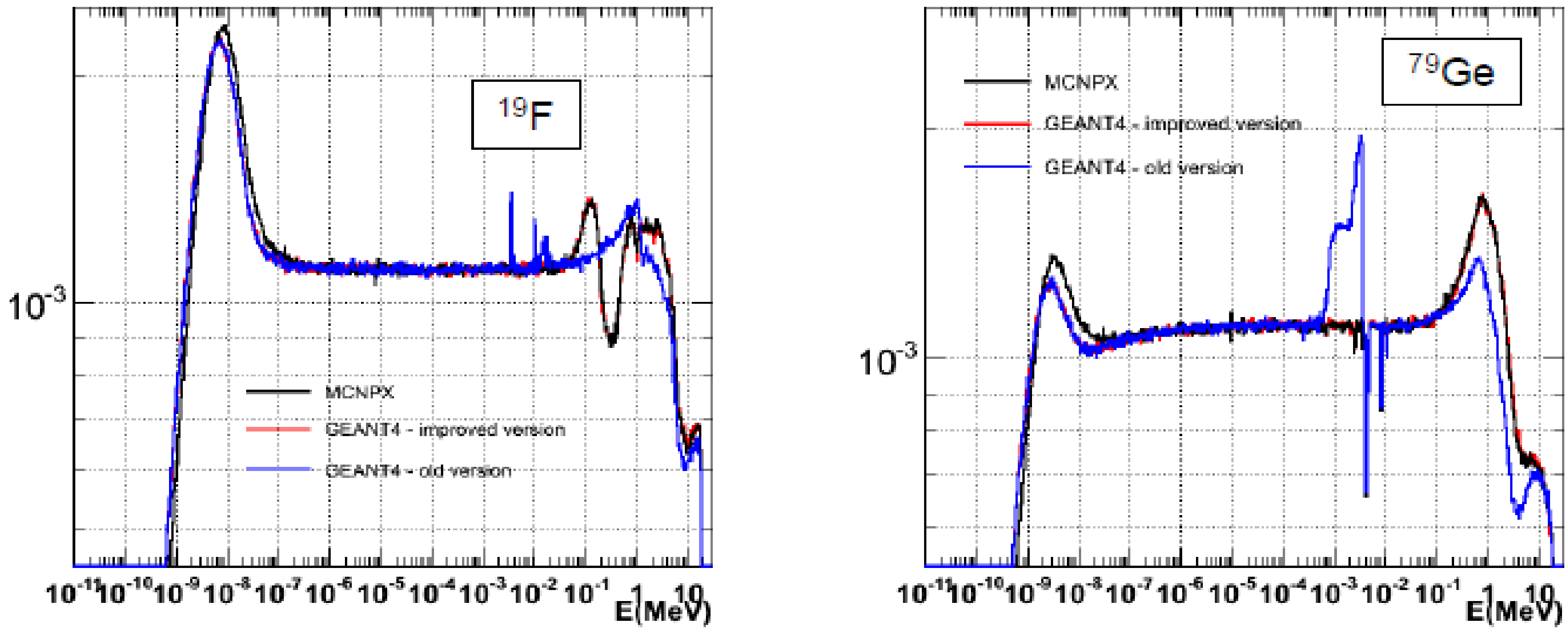
BERT has its own internal preco

High Precision low energy neutrons (HP)

- The standard simulation of neutrons in Geant4 does not provide an accurate simulation below $\lesssim$ **10 MeV**
- The High Precision (**HP**) option of Geant4 allows a detailed data-driven transportation of neutrons with **E_{kin} < 20 MeV**
- Relevant for:
  - Better (wider) lateral hadronic showers
  - Time-dependent hadronic shower development
  - Background radiation studies
- Recent improvements
  - Updated neutron libraries : **ENDF-VII.0**
  - More isotopes included: **395** , from $^{1}H_{1}$ to $^{255}Fm_{100}$
    - * previous version has 181 isotopes
  - Code (several bug fixes, and new capabilities added)
  - Studies to reduce its CPU impact

Comparing G4 HP old & new with MCNPX

First time that G4 HP gets very close to MCNPX !



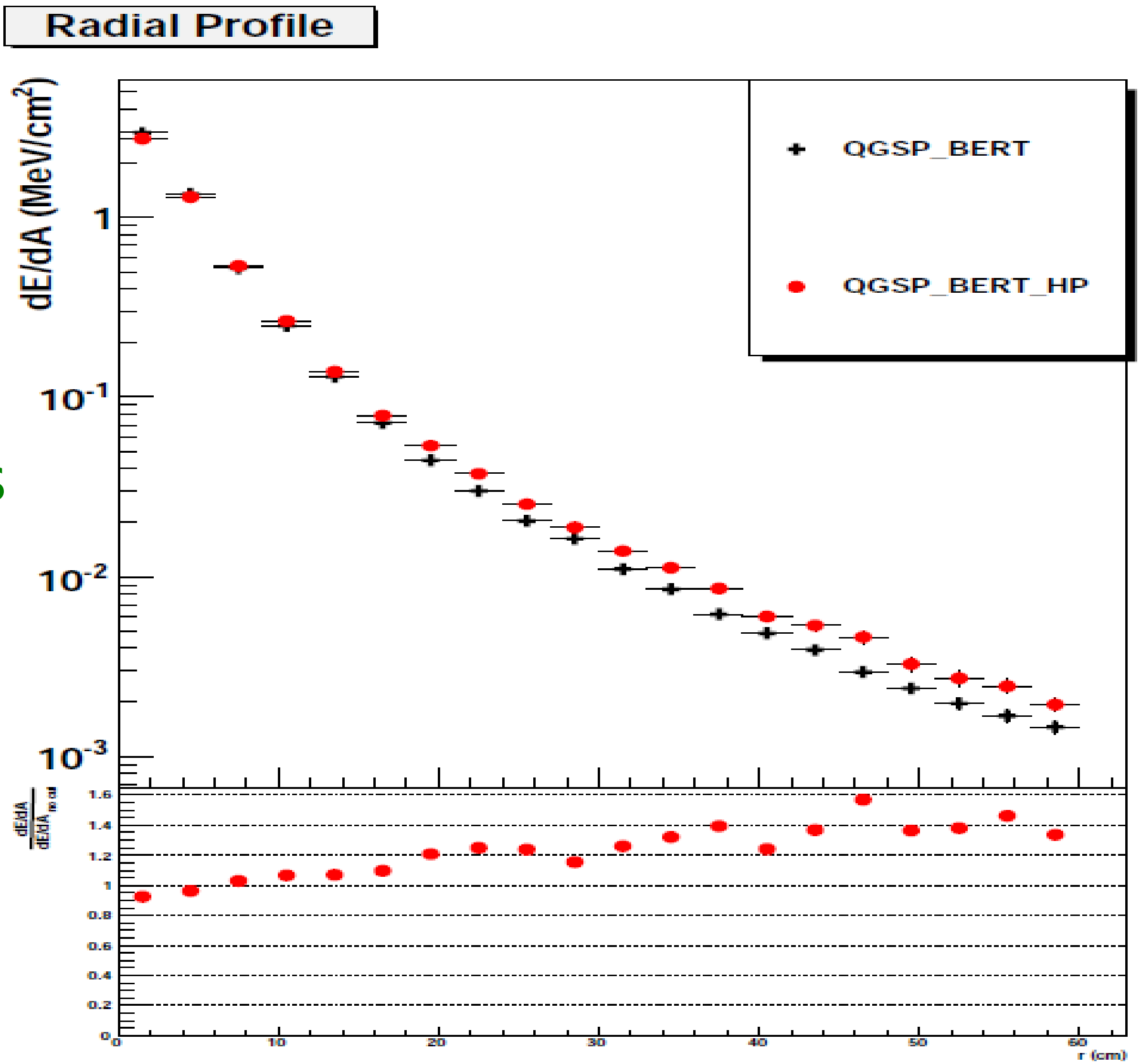
Outgoing neutron spectrum after incident neutron (Ekin < 20 MeV) interactions with a target (19F, left, 79Ge right).
The new G4 HP version is closer to MCNPX than the older G4 HP version

Effect of HP on lateral shower profile

8 GeV π- on a simplified calorimeter Pb-LAr

HP produces wider showers

Notes:
- No timecut
- Energy deposit in the halo is very small (compatible with noise/pileup/UE)



Kaons, hyperons, anti-baryons, light anti-ions

- Kaons and antiprotons are non-negligible jet components
- Interest on hadronic interactions in thin layers (tracker), both cross sections and final states, for several hadrons:
  - $\pi^\pm$, **$k^\pm$** , **k^0** , p , n , **Λ** , Σ , Ξ , Ω

  and also for anti-baryons and light anti-ions
  - **p** , n , Λ , Σ , Ξ , Ω and d , t , 3He , α
- New focus in Geant4 to develop better models for these particles than the available old parameterized model (LEP) But limited data is available for validation
- For these particles **CHIPS** and **Fritiof** provide better options than LEP, available in **QGSP_BERT_CHIPS** and Fritiof-based physics lists **FTFP_BERT** , **QGSP_FTFP_BERT**

Forward physics

- Hadronic elastic scattering, and hadronic quasi-elastic scattering have been revised. These improved the longitudinal shower profiles, especially for pions
  - Further refinement of quasi-elastic in QGS is on-going, thanks to a recent feedback from NA61 on h-A interactions

- For **protons**, the agreement with data is less good

- Further progress on longitudinal shower profiles is expected from improvement of diffractive processes

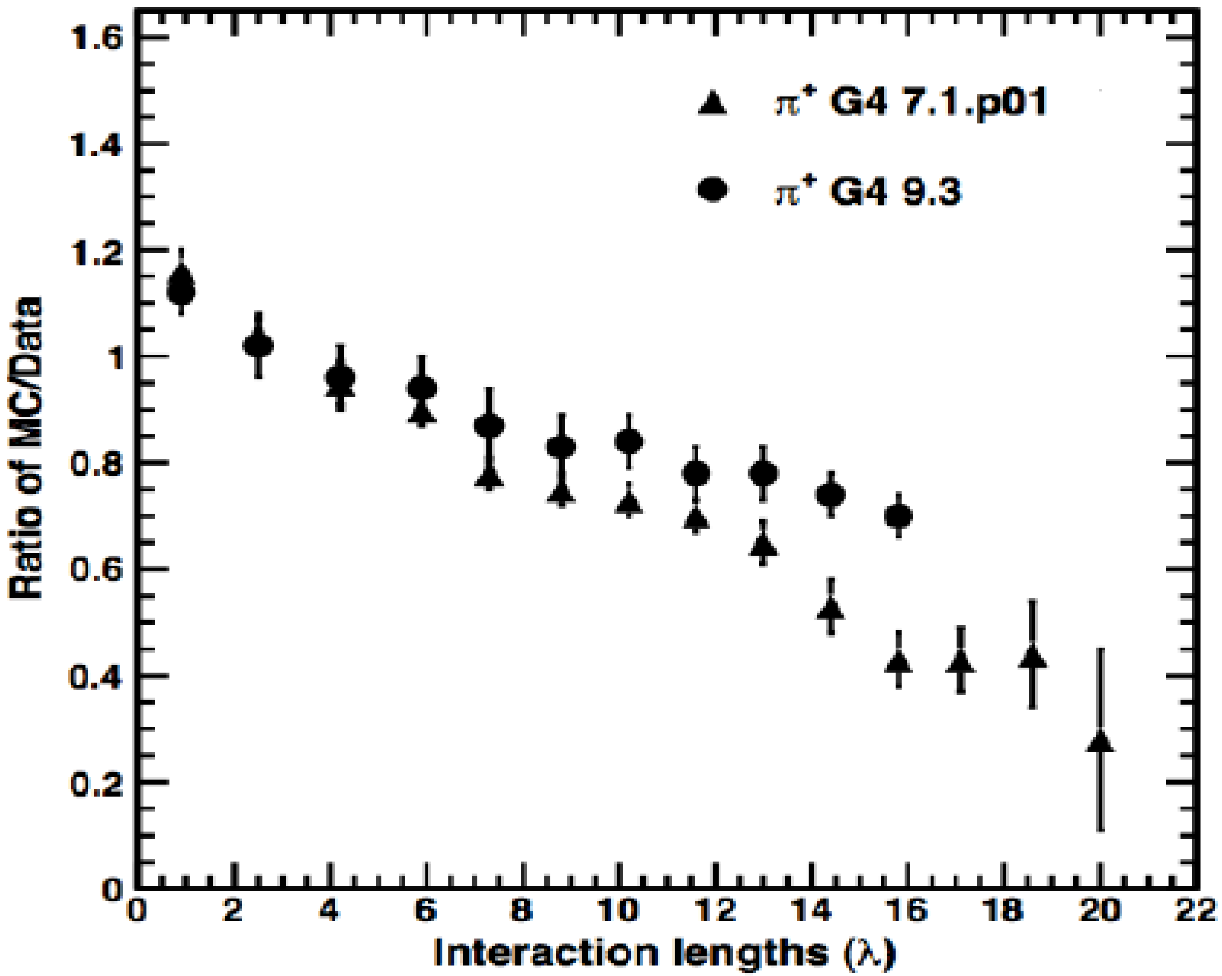
Effect of quasi-elastic on longitudinal shower profile

ATLAS TileCal
test-beam @90°

G4 7.1.p01 : OFF
quasi-elastic

G4 9.3 : ON
quasi-elastic

quasi-elastic
produces
longer showers

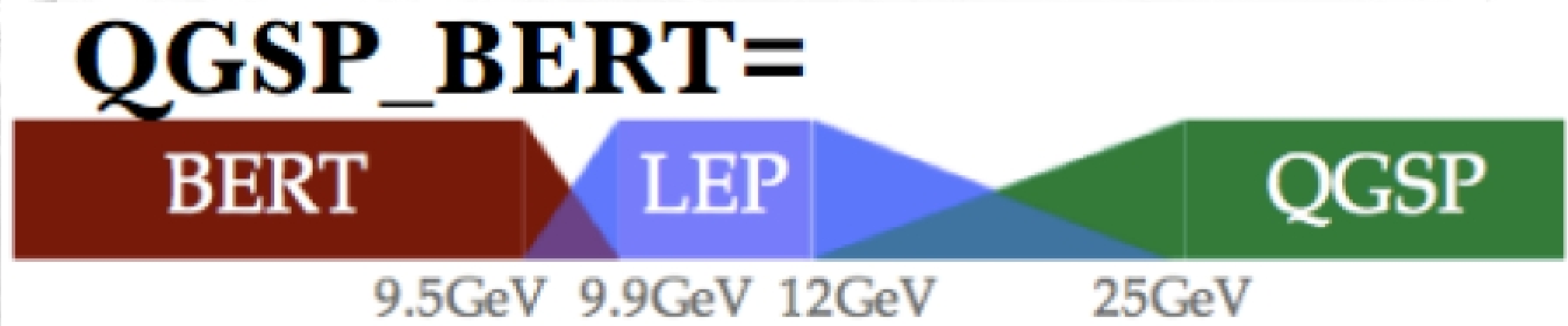


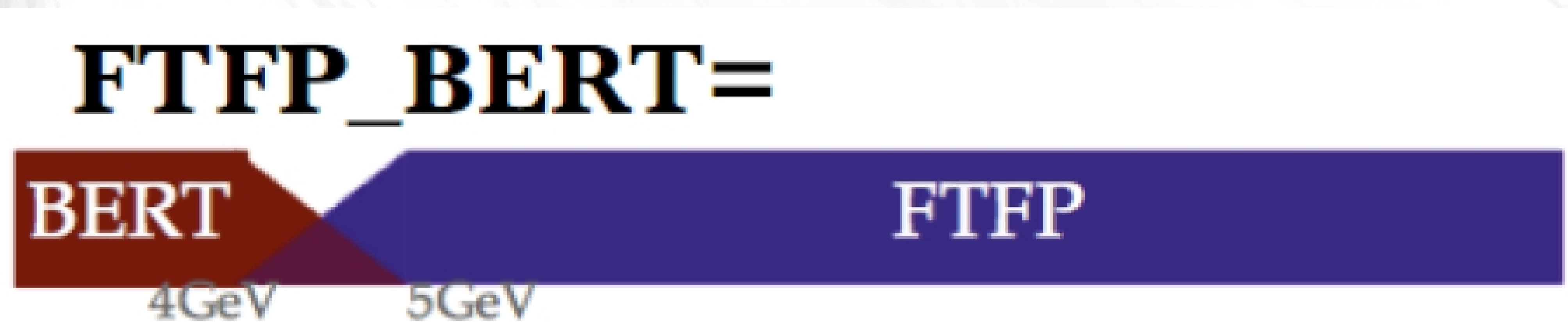
Other models

- CHiral Invariant Phase Space (**CHIPS**) model : used for gamma-nuclear, nuclear capture of negative charged hadrons at rest, quasi-elastic in QGS, p-A and n-A elastic, kaon and hyperon nuclear cross sections
- Quark Gluon String (**QGS**) model : current default high-energy generator used in production physics list QGSP_BERT; it is an alternative string model to FTF
- BInary Cascade (**BIC**) model : intranuclear cascade model, more theoretical motivated than the phenomenological Bertini cascade model
  - provides accurate simulation of protons and neutrons ≤ 1 GeV
  - used in FTF_BIC for re-scattering of secondaries produced by FTF
- Low / High Energy Parameterized (**LEP**, **HEP**) models: Geisha-equivalent in Geant4, fast but very rough

Assembling Models in Physics Lists

Transition between models





Coupling and Mixing between models

How models are assembled is critical: this is as important as the models themselves!

- **Coupling** between models: the output of one model is fed in input to another one, e.g.
  - QGSP : Precompound de-excite the residual nucleus after the high-energy projectile collision on the target nucleus described by the Quark-Gluon-String model
  - FTF_BIC : Binary cascade re-scatters the secondaries produced by Fritiof

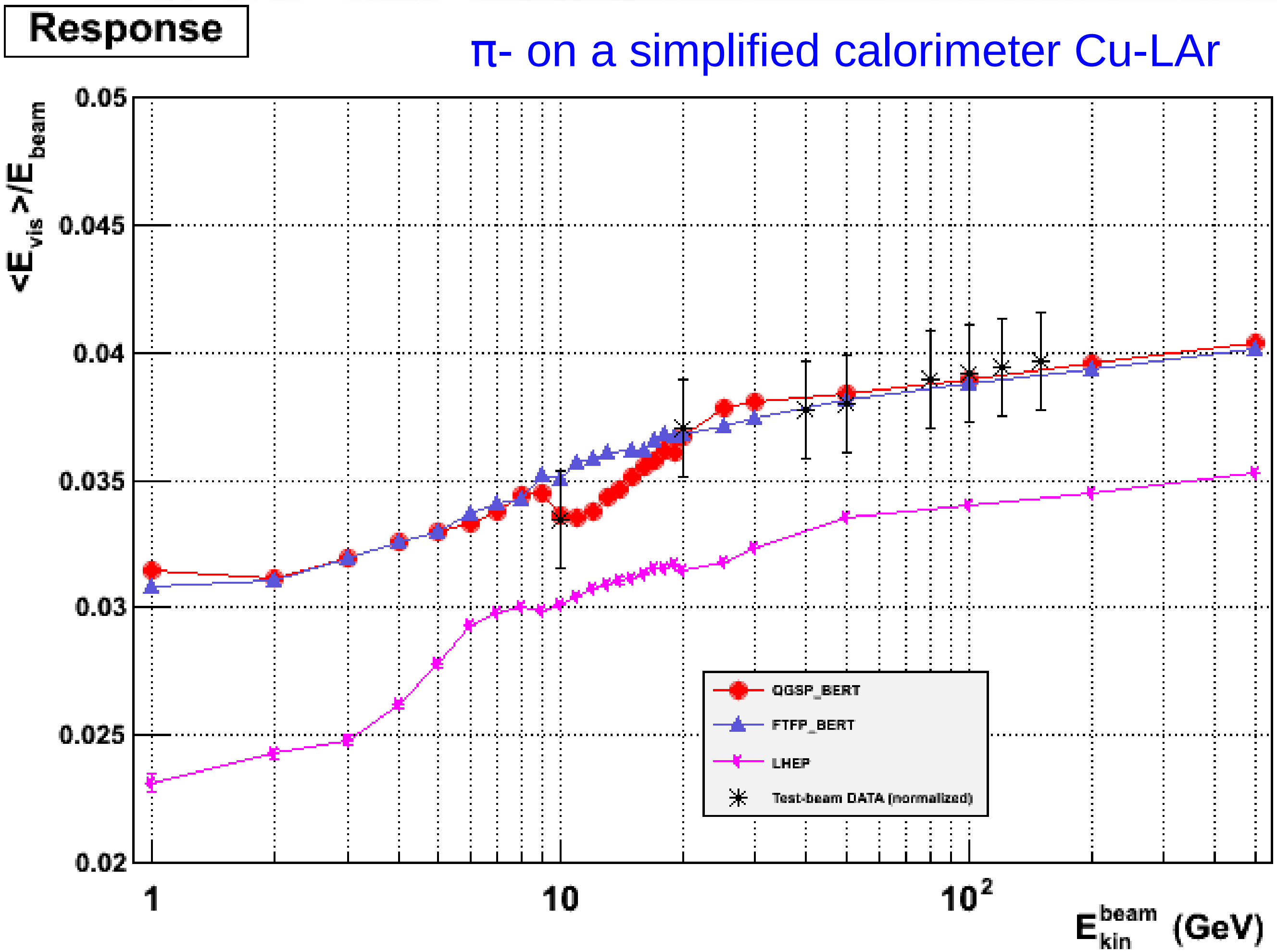
  Note: no coupling between FTFP and BERT in FTFP_BERT !

- **Mixing** between models: for each interaction in a given energy region, one of two models is chosen randomly, in order to have a smoother transition, e.g.
  - QGSP_BERT : QGSP and LEP mix in the interval 12 - 25 GeV
    LEP and BERT mix in the interval 9.5 - 9.9 GeV
  - FTFP_BERT : FTFP and BERT mix in the interval 4 - 5 GeV

Transition: String ↔ Cascade

- It is a challenge to have a smooth transition between high-energy (string) models and low-energy ones
  - transition between particle physics and nuclear physics
- The **old solution** was to use the parameterized model **LEP** in this intermediate region
  - very rough model, produces unphysical discontinuities, e.g.
  - calorimeter energy response as a function of the beam energy
- The new solution is the direct transition from Fritiof to Bertini, without LEP
  - allowed by the recent improvements in FTF, BERT and Preco
  - outcome: smooth observables as a function of the beam energy

Energy response vs. beam energy



FTFP_BERT has a smoother energy response than QGSP_BERT

Physics Lists for Production

- Evolution of Geant4 physics lists used in production by LHC experiments:
  LHEP -> **QGSP** -> **QGSP_BERT** -> **FTFP_BERT**

- For LHC, Geant4 provides 3 production physics lists (starting with version 9.4):
  1) **FTFP_BERT** : *recommended*
  2) **QGSP_FTFP_BERT** : *transition / conservative*
  3) **QGSP_BERT** : *legacy / stable*

- The spine of Geant4 hadronic physics is made of the following models: **FTF** , **BERT** , **Preco**

- Our approach is to remove dependencies on weaker models and weaker implementations (i.e. with software issues)

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Conclusions

Conclusions & Outlook

- Significant progress in Geant4 physics has been driven and validated in the last ~10 years by the LHC test-beams, which will remain extremely valuable for G4 validations
- Further progress will also come from feedback provided by LHC collision data and especially by CALICE test-beams
- Geant4 provides 3 production physics lists, stable but not frozen, with incremental physics improvements aimed to address the issues reported by the experiments
- Development effort is concentrated in a few key models which are the spine of Geant4 physics: **FTF**, **BERT**, **Preco**
- Geant4 offers also some alternative options (e.g. QGS , BIC , etc.) useful for systematic studies and for physics understanding and development

BACKUP Slides

Geant4 MSC models

Model	Particle type	Energy limit	Specifics and applicability
Urban (Urban 2006)	Any	-	Default model, (Lewis 1950) approach, tuned to data, used for LHC production.
Screened Nuclear Recoil (Mendenhall and Weller 2005)	p, ions	< 100 MeV/A	Theory based process, providing simulation of nuclear recoil for sampling of radiation damage, focused on precise simulation of effects for space app.
Goudsmit-Saunderson (Kadri 2009)	e+, e-	< 1 GeV	Theory based cross sections (Goudsmit and Saunderson 1950). EPSEPA code developed by Penelope group, final state using EGSnrc method (Kawrakov et al. 1998), precise electron transport
Coulomb scattering (2008)	any	-	Theory based (Wentzel 1927) single scattering model, uses nuclear form-factors (Butkevich et al. 2002), focused on muons and hadrons
WentzelVI (2009)	any	-	MSC for small angles, Coulomb Scattering (Wentzel 1927) for large angles, focused on simulation for muons and hadrons.
Ion Coulomb scattering (2010)	ions	-	Model based on Wentzel formula + relativistic effects + screening effects for projectile & target. From the work of P. G. Rancoita, C. Consolandi and V. Ivantchenko.

Monopoles in Geant4

Geant4 provides an example

examples/extended/exoticphysics/monopole

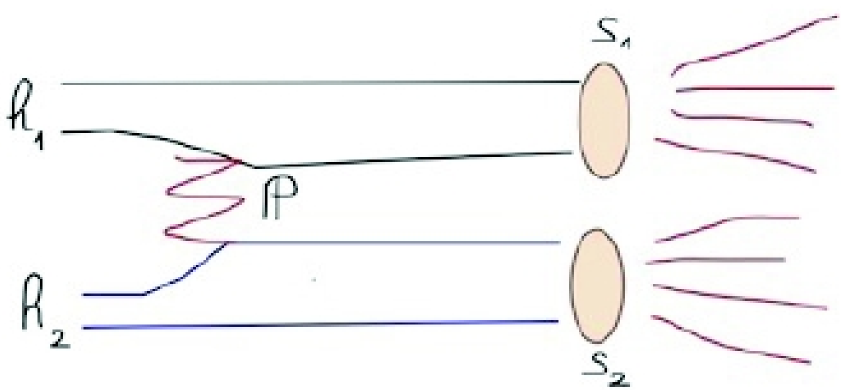
that demonstrates:

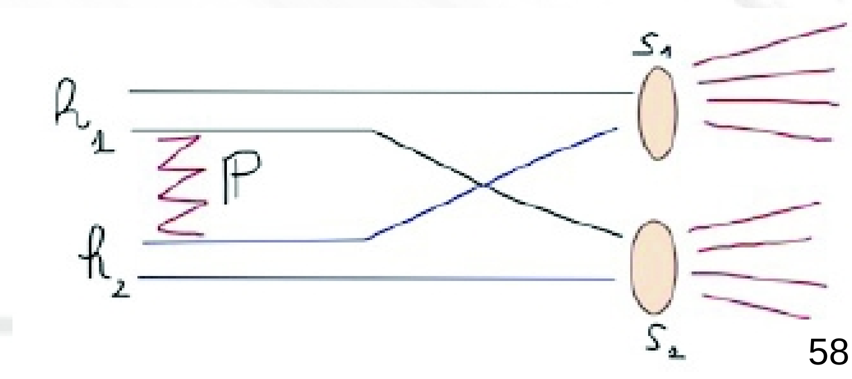
- How to define a monopole as G4 particle
  - may have different mass, electric and magnetic charge
- Special transportation process for a monopole
- Special process and model for monopole ionization
- How to create a Physics List builder for a monopole

Work done in close collaboration with ATLAS and CMS

FTF (1)

- Valid for any hadron projectile with E_{kin} 3 GeV - 1 TeV
- Selection of collision partners: projectile, nucleon
- Splitting of nucleons into quarks and diquarks
- Formation and excitation of strings
- String hadronization/fragmentation
  - Extends between constituents
  - Insert q-$\underline{q}$ pair , u : d : s : qq = 1 : 1 : 0.27 : 0.1
  - At break: new string plus hadron
    - * gets $P_{||}$ from sampling fragmentation functions
    - * Gaussian P_T , $<P_T^2>$ = 0.5 GeV^2





FTF (2)

- Build up 3D model of nucleus
  - Large boost collapses nucleus to 2D
- Calculate impact parameter with all nucleons
  - Calculate hadron-nucleon collision probabilities
  - Multiple collisions are allowed
  - Use gaussian density distributions for hadrons and nucleons
- Sample number of strings exchanged in each collision
- String formation and then fragmentation into hadrons
- Remnant nucleus
  - After the HE interaction is performed an exited nucleus remains
  - De-excitation via precompound model
- Under developing/testing: re-scattering
  - Use Binary Cascade or Bertini to propagate string fragments in nuclear media

BERT (1)

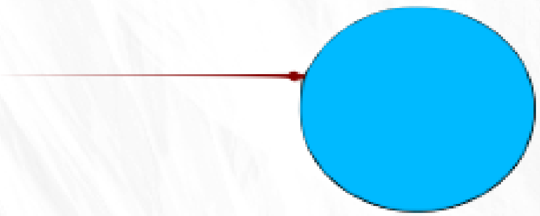
- Solution to the Boltzmann equation (on average)
- No scattering matrix calculated
- Geant4 implementation of early codes (1960s)
- Valid for p, n , π, K, hyperons with $E_{kin} < 10$ GeV
- Core:
  - Use free-space cross sections to generate secondaries
  - Cascade in nuclear medium
  - Pre-equilibrium and evaporation of residual nucleus is embedded
  - Detailed 3D model of nucleus

BERT (2)

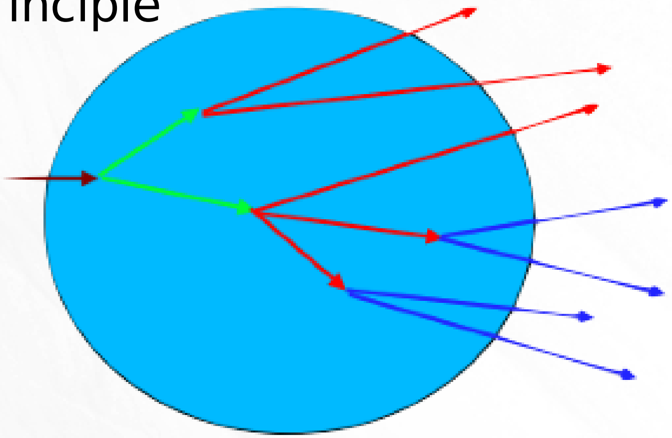
- Incident particle penetrates nucleus, propagates in a density-dependent nuclear potential
- All hadron-nucleon interactions based on free-space σ, angular distributions, etc., but consider Pauli exclusion principle
- Each secondary is propagated in nuclear potential until re-interacts or leaves nucleus
- Particle-hole excitons are created during cascade

BERT + Preco

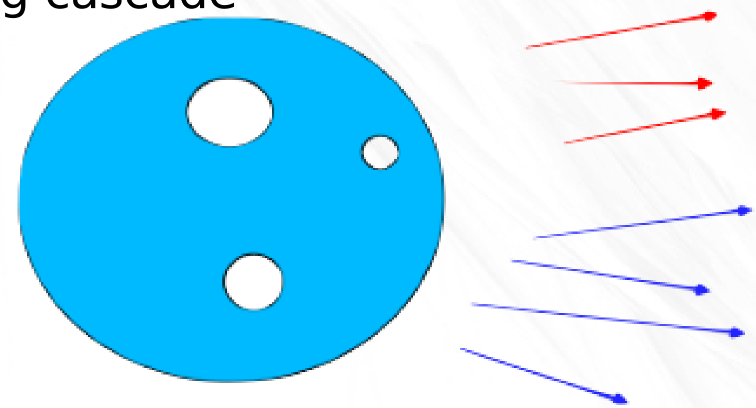
Hadron penetrates nucleus
Nucleus: density-dependent potential



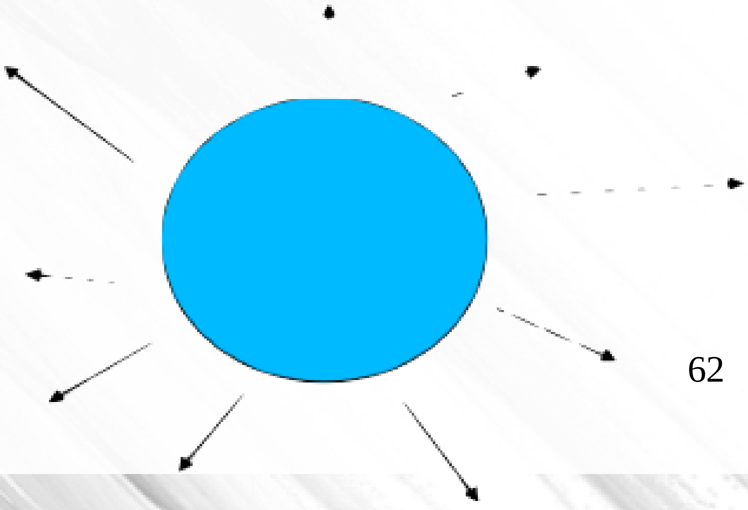
Free-space σ and angular distributions
Pauli principle



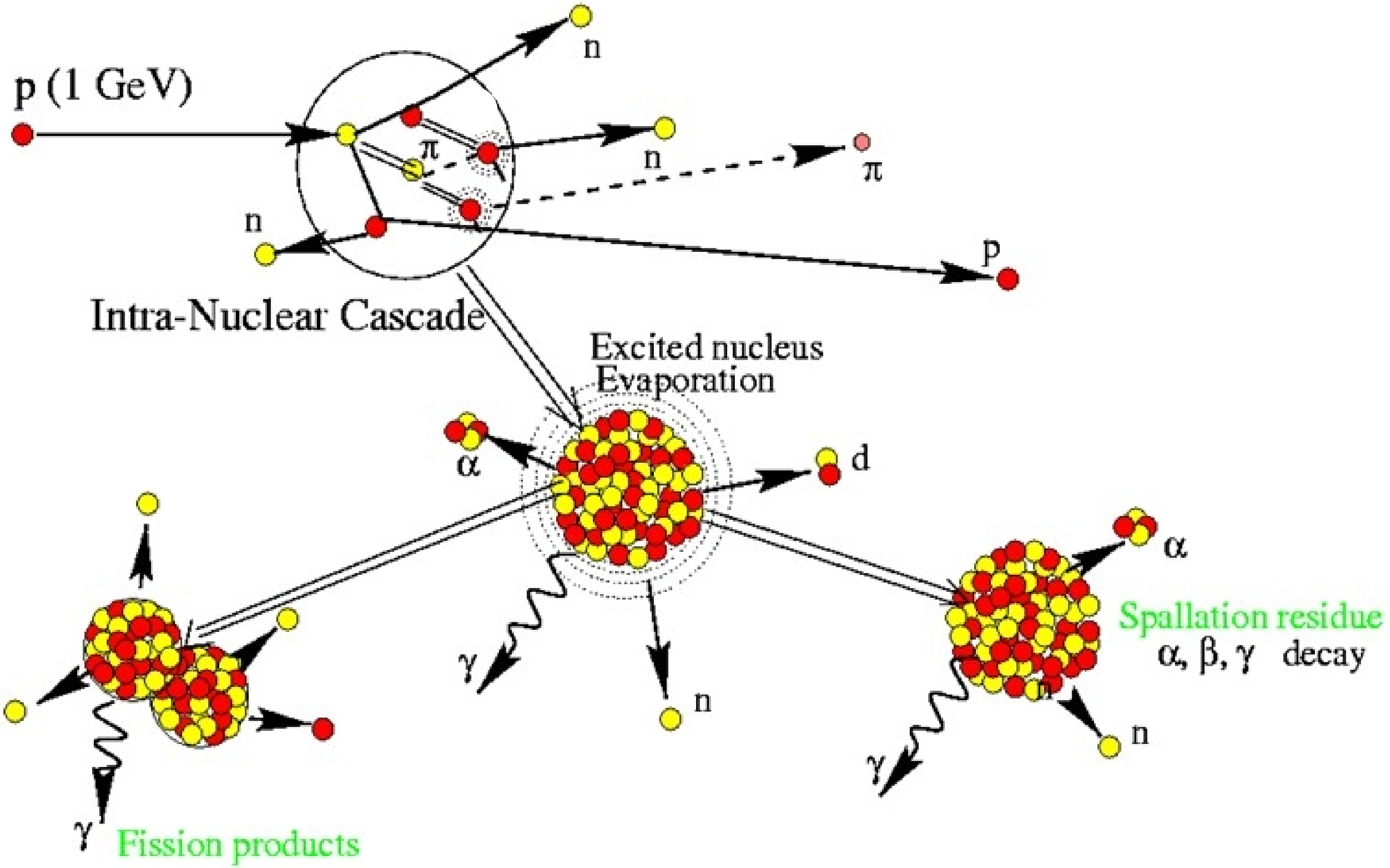
Particle-hole excitations are created during cascade



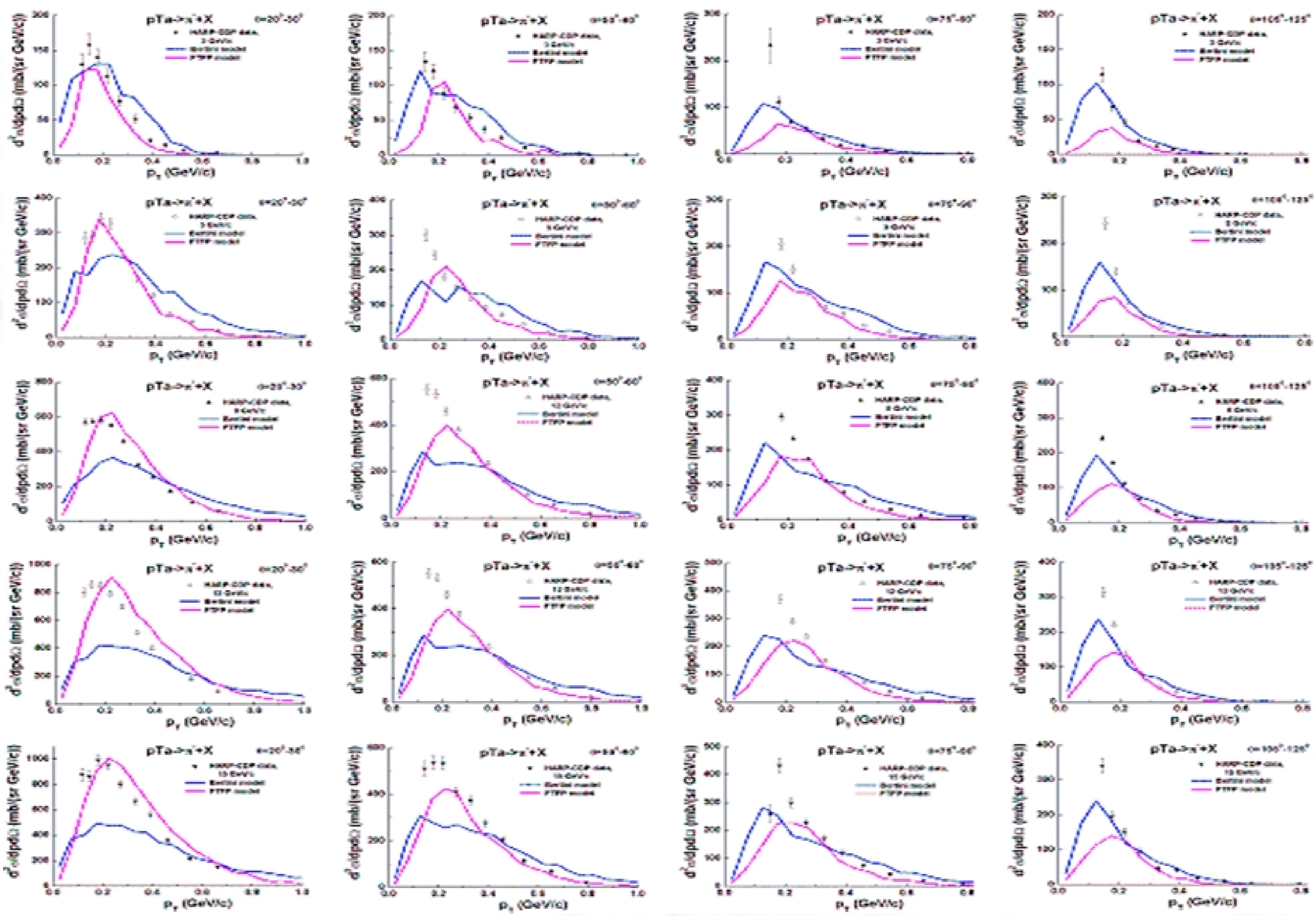
Nucleus is de-excited



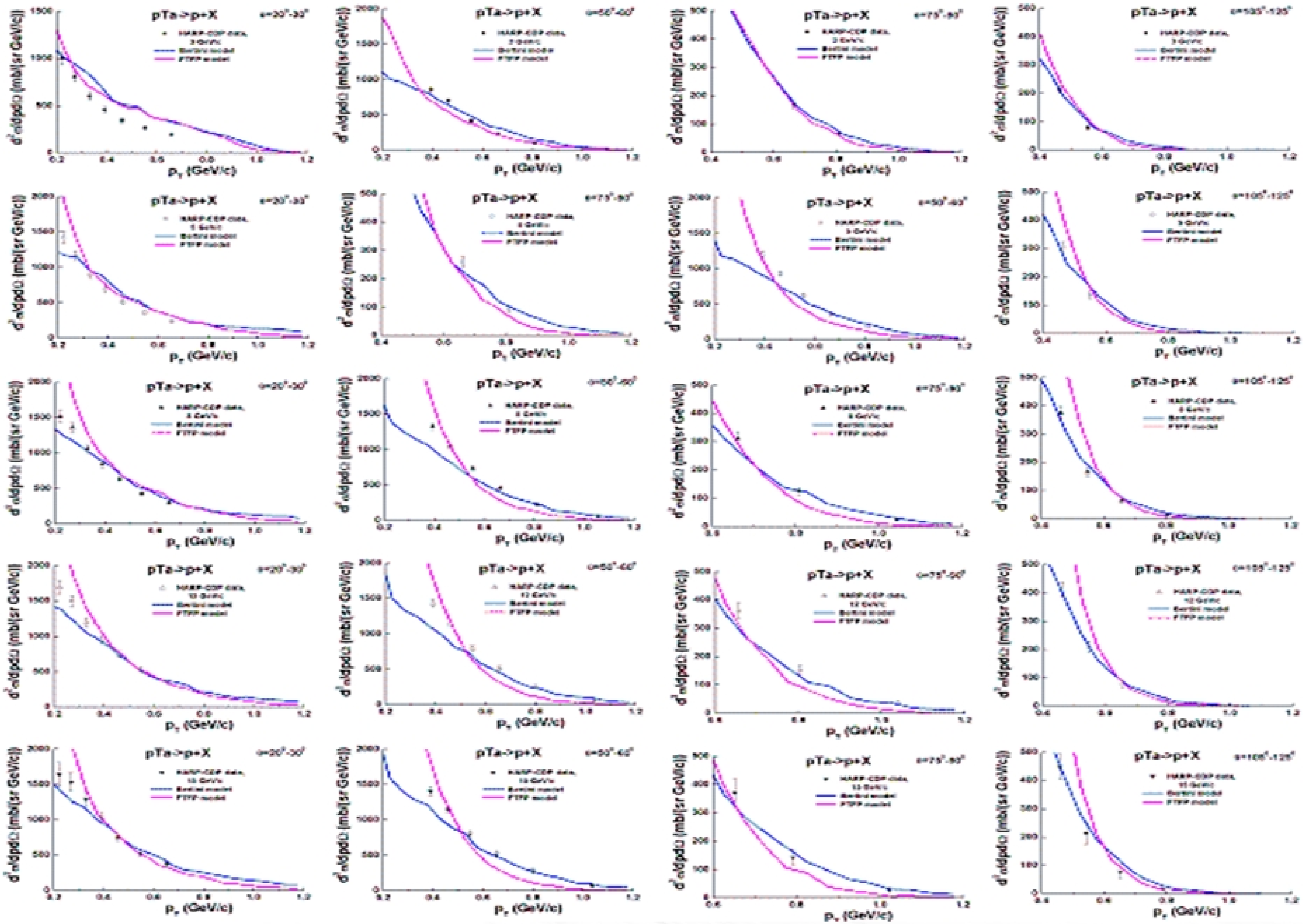
BERT + Preco


p (1 GeV)
n
n
π
π
n
p
Intra-Nuclear Cascade
Excited nucleus
Evaporation
α
d
α
Spallation residue
α, β, γ decay
γ
n
γ
n
γ
Fission products

FTF , BERT vs HARP-CDP data



FTF , BERT vs HARP-CDP data



Preco: pre-equilibrium

Native pre-equilibrium de-excitation model in Geant4 is a version of standard exciton model. Key ingredients:

- Internal transition rates:
  - CEM (Cascade Exciton Model): default
  - Blann-Machner's parameterization
- Emission rates:
  - Nucleon emission in standard exciton formulation
  - Complex particle emission (d, t, 3He, 4He) from CEM

The pre-equilibrium phase continues until:

number of excitons ≤ *number of excitons in equilibrium*

then transition to equilibrium

Preco: equilibrium

Five processes are considered:

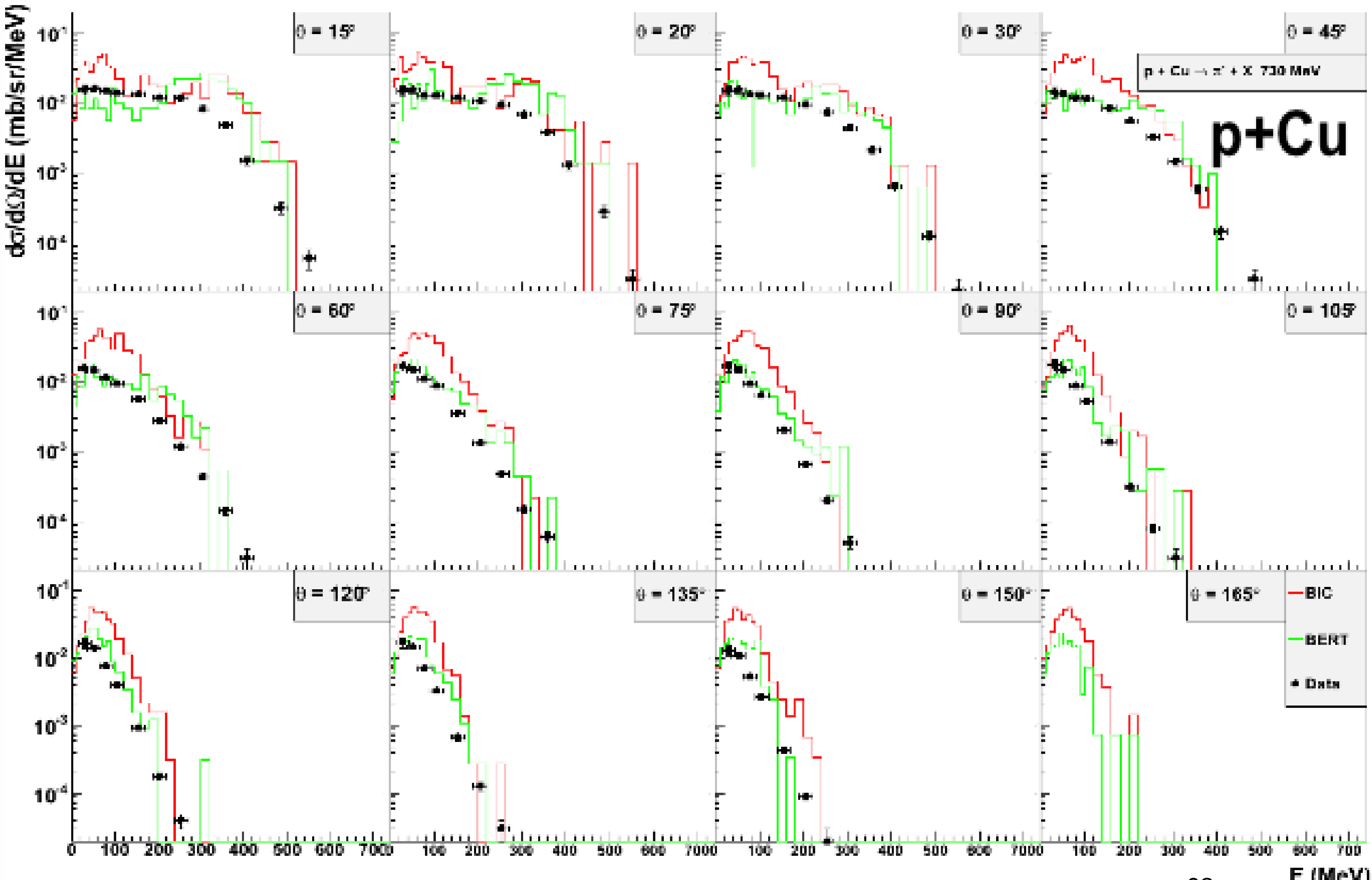
Alternates:

- Fermi Breakup , for $Z < 9$ and $A < 17$ (Botvina et al)
- Statistical Multifragmentation, for $E^*/A > 3$ MeV (Botvina et al)

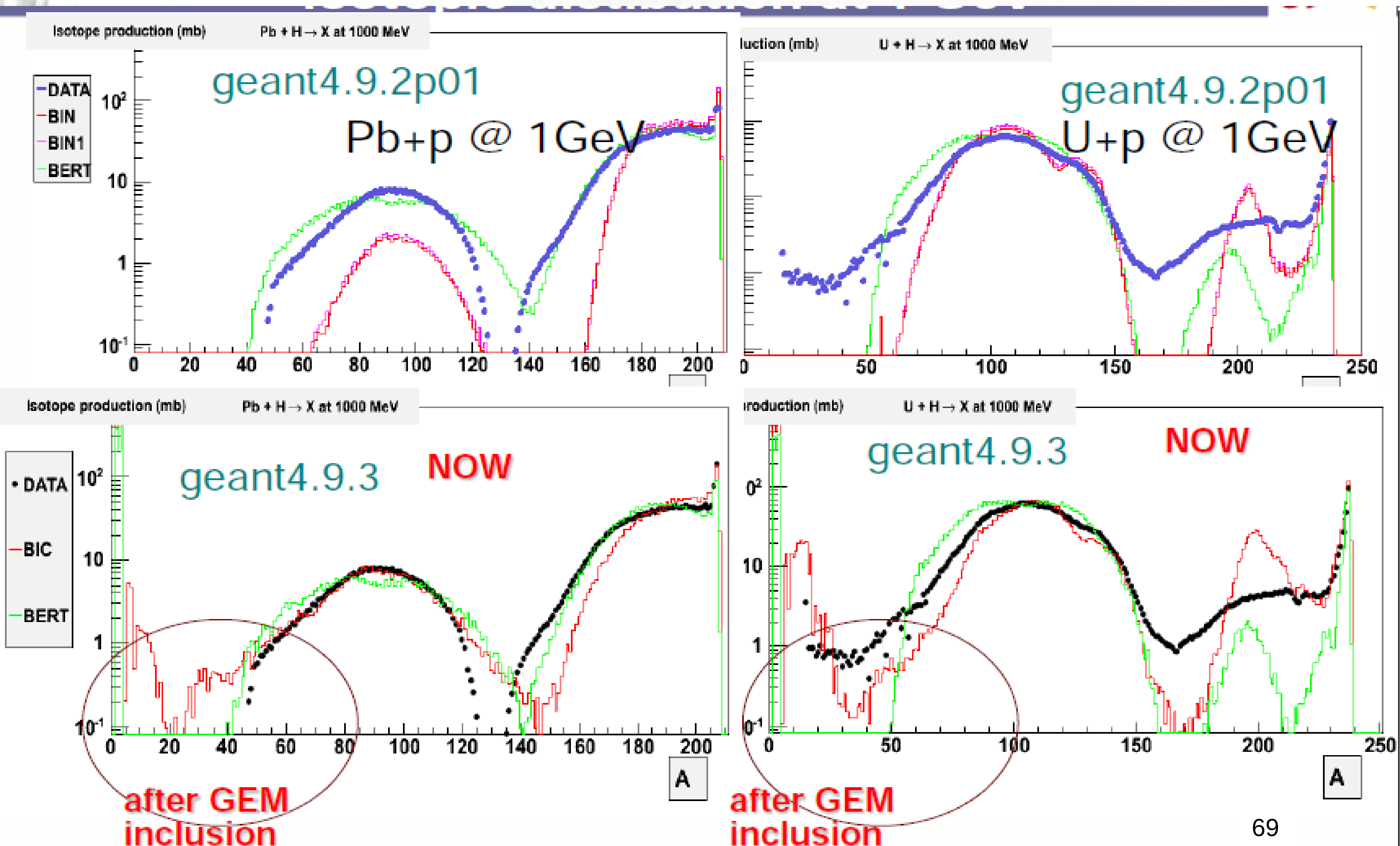
Competitors:

- Fission (Bohr-Wheeler model + Amelin prescript.)
- Particle Evaporation:
  - Evaporation Model WE (Weisskopf-Ewing) (evaporation of: n , p , d, t, 3He , α)
  - Generalized Evaporation Model GEM (Furihata) (heavier ejected fragments: $Z < 13$ and $A < 29$)
- Photon Evaporation:
  - Discrete (tabulated E1,M1, E2)
  - Continuum (GDR strength)

Pion production at 730 MeV



Isotopic distribution at 1 GeV



Proton production at 542 MeV