Status of Geant4 simulation for calorimeters

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CHEF-2019: Calorimetry for High Energy Frontier
25-29 November 2019, Centennial Hall, Kyushu University, Japan

Outline

- Introduction
- Electromagnetic (EM) physics in Geant4 10.6
- Hadronic physics in Geant4 10.6
- How to configure and optimize Geant4 physics?
  - Physics accuracy
  - Birks quenching
  - CPU efficiency
- Summary

Introduction

- CERN LHC Run-2 2015-2018 collected data at 13 TeV
  - Geant4 9.6 and Geant4 10.X have been used
    - CMS experiment used 10.0p02, 10.2p02, 10.4p03 and ~100 B events produced
  - Geant4 team was trying to keep stable results between Geant4 10.1-10.4
    - Some developments were not in the official release, others were included but either not activated or not used in main Physics Lists
- Now there is the Large Shutdown of LHC until 2021
  - Geant4 10.6 will include all modifications accumulated over last few years
    - Will be release 6th of December 2019
    - We would appreciate if issues in Geant4 10.6 will be early reported
  - We may expect some differences in simulation results both in EM and hadronic compared with Geant4 10.4
    - in calorimeters, in backscattering, and in other observables

EM physics in Geant4 10.6

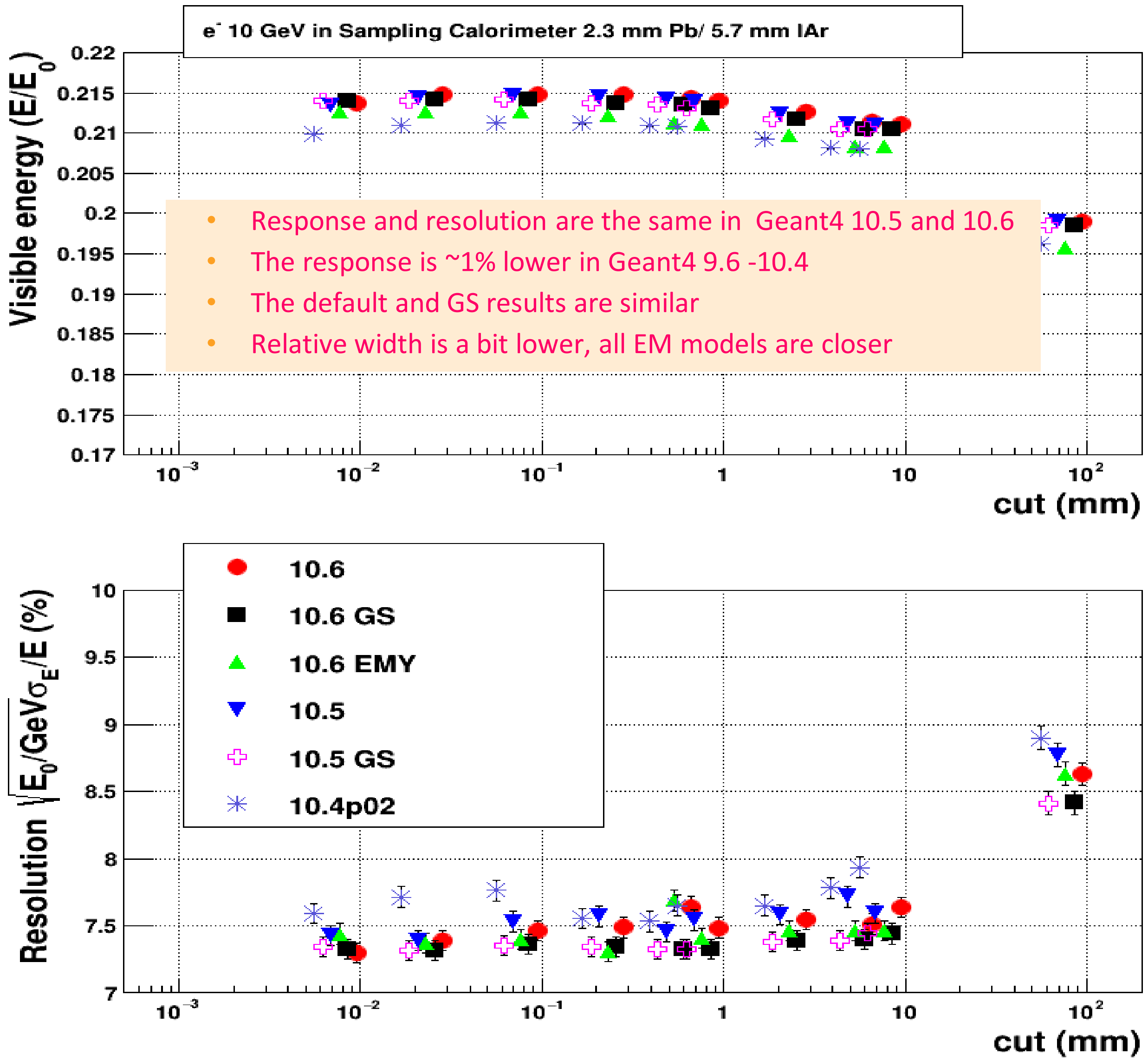
Main recent developments:

- code optimization and speed-up
- addition of rare processes
- addition of next to leading order corrections
- development of low-energy processes

EM model developments

- Models of single and multiple scattering for e+-
  - Improved sampling of displacement for the G4UrbanMscModel
  - Added Mott corrections to G4WentzelVIModel used for simulation of multiple scattering of e+- above 100 MeV
  - G4ScreenedMottCrossSection – use G4MottData shared between threads and implemented more optimal computations
- Gamma models and bremsstrahlung
  - G4ModifiedTsai – use as the default angular generator for bremsstrahlung and pair production
    - Since Geant4 9.6 G4DipBustGenerator was the default
  - G4BetheHeitlerModel, G4PairProductionRelModel – improved
    - screening function and LPM suppression approximations
- New models:
  - G4BetheHeitler5DModel - accurate sampling of 5D final state considering nuclear recoil and polarisation
  - G4LindhardSorensenModel – ion ionisation above 10 MeV/u
  - 3-gamma annihilation model

Cut dependence of ATLAS-type simplified calorimeter response



Optimization and speed-up for 10.6

- EM physics software was reviewed, and several optimizations were introduced into the toolkit
  - At any step of each track EM energy loss, ranges, cross sections are recomputed using internal tables
  - Energy scales of tables are logarithmic over particle kinetic energy
    - Main optimization is in computing logarithm only once if the energy is the same
    - This also allows to simplify the interpolation algorithm, reducing by 1 factor 10 the number of lines of code executed at each step
- Benchmark results for CMS geometry without hit creation:
  - ~8% faster for Mac Book Pro (Mac OS 10.13.2) 2.8 GHz i7
  - ~5 % faster for AMD (SLC6 gcc8.2.0) 3.5 GHz

NIEL Calculator For Radiative Background Studies

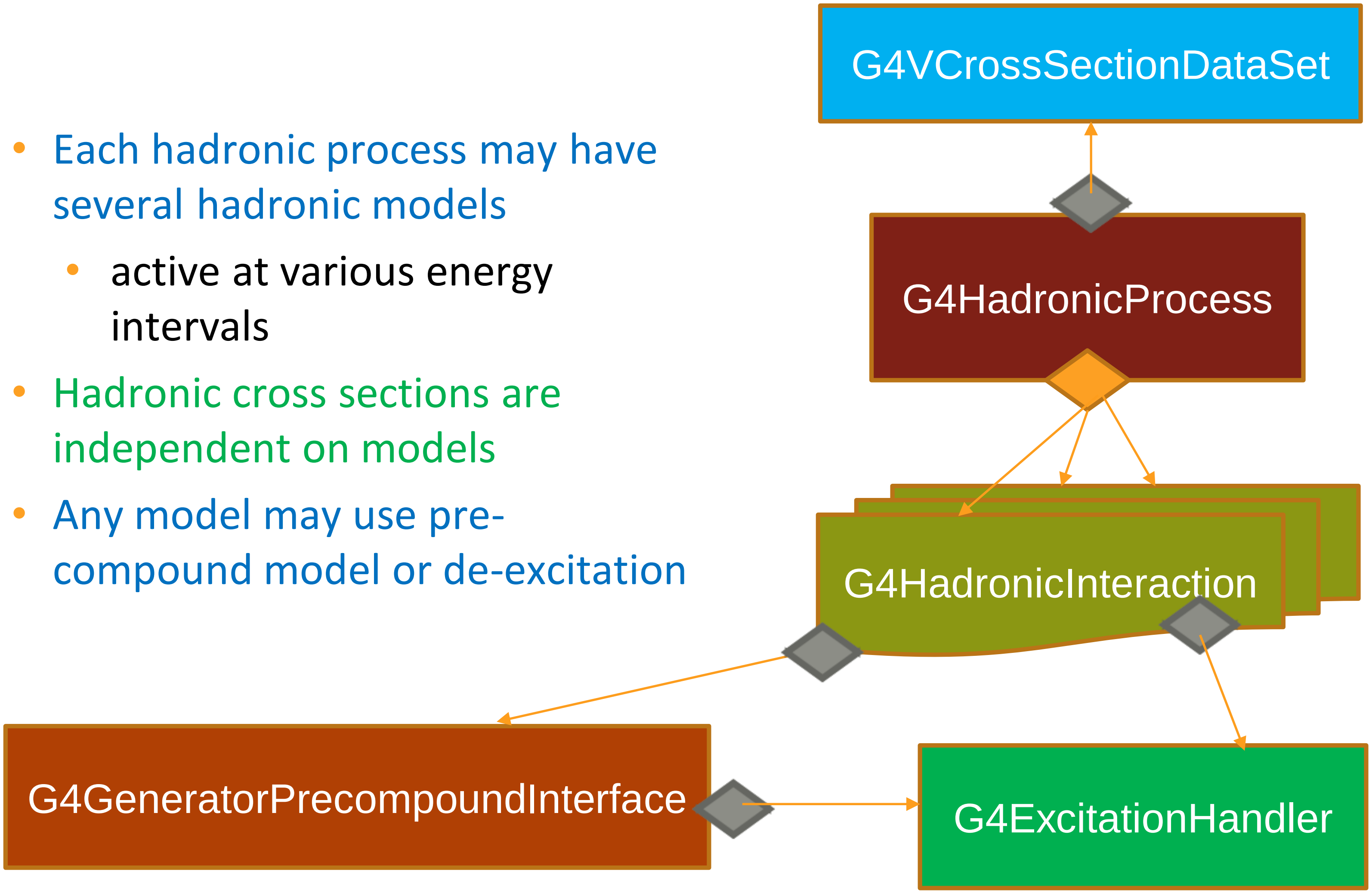
- Before Geant4 10.6 user had to correctly combine tracking cuts and production thresholds in EM physics definition
  - Non-ionizing energy loss (NIEL) is available in Geant4 user actions from the G4Step object
    - This value depends on "*cut in range for proton*"
  - Production of recoil ions should be also counted in user actions
  - This method seems to be complicated and not obvious to a user
- As an alternative, G4NIELCalculator helper class is introduced in 10.6
  - This class calculates NIEL at a step independently on cuts
    - Example how to use is in TestEm1
  - This class uses G4VEmModel which provides NIEL computation
    - The default model is G4ICRU49NuclearStoppingModel

Hadronic physics in Geant4 10.6

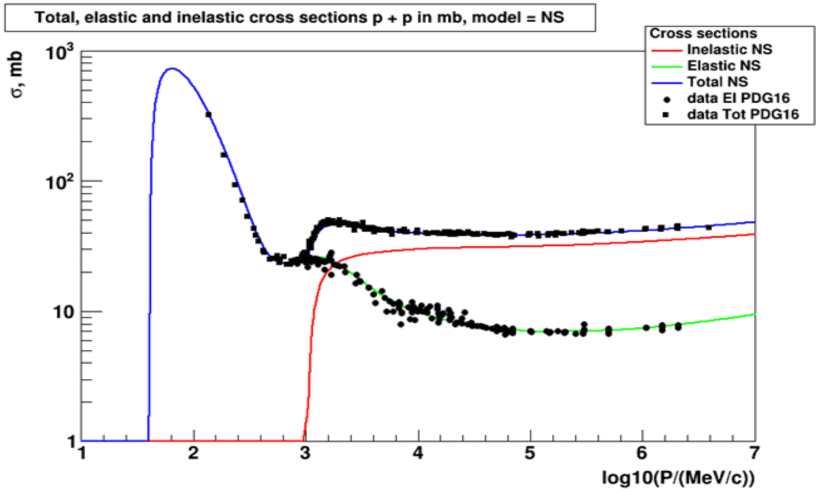
Main recent developments:
- FTF and QGS string models
- de-excitation module and radioactive decay
- Hadron and ion cross sections
- high precision (HP) data driven models

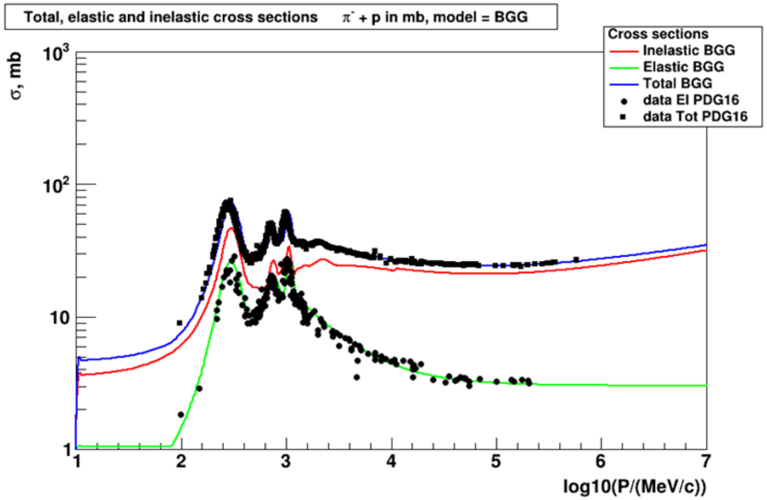
Geant4 hadronic physics design

- Each hadronic process may have several hadronic models
  - active at various energy intervals
- Hadronic cross sections are independent on models
- Any model may use pre-compound model or de-excitation

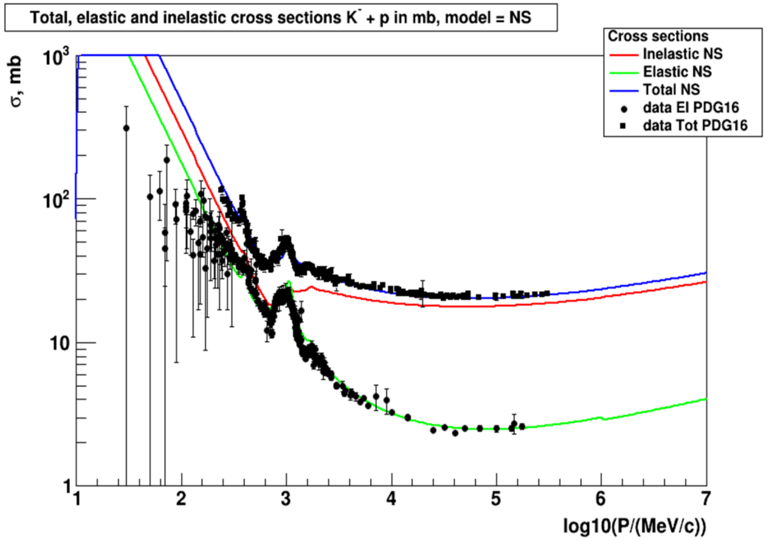


Hadron-nucleon cross sections





- Parameterization of PDG2016 data for hadron-nucleon cross section are done for p, n, pions and kaons
- Scaling of cross sections for hyperons, charmed and bottom mesons and baryons



Geant4 hadronic cross sections

NIM A 835 (2016) 186-225

- In Geant4 10.6 the Glauber-Gribov cross sections will be used for all hadrons at any energy:

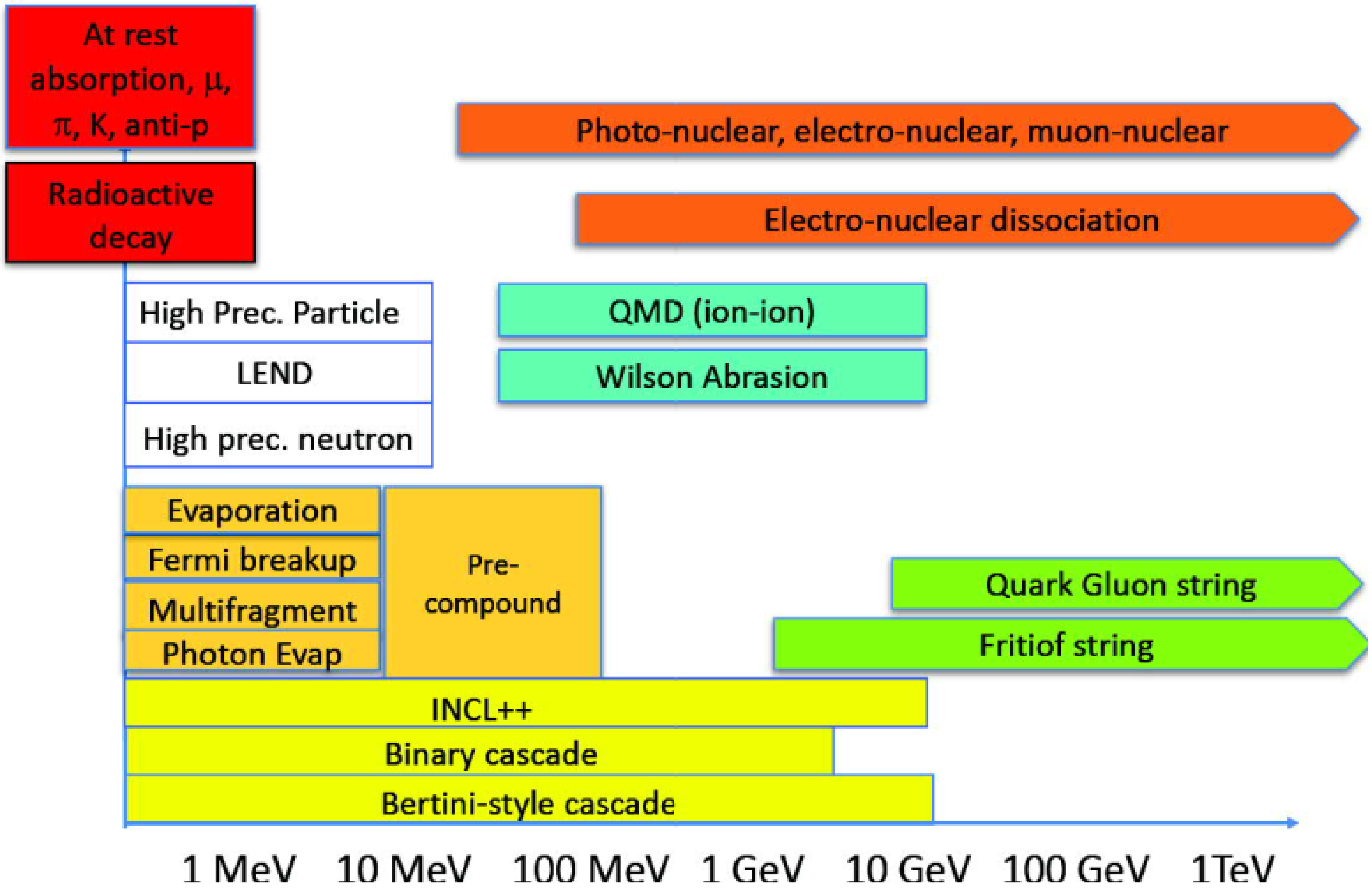
$$\sigma_{tot}^{hA} = 2\pi R^2 \ln\left[1 + \frac{A\sigma_{tot}^{hN}}{2\pi R^2}\right], \quad \sigma_{in}^{hA} = \pi R^2 \ln\left[1 + \frac{A\sigma_{tot}^{hN}}{\pi R^2}\right],$$

$$\sigma_{prod}^{hA} = \pi R^2 \ln\left[1 + \frac{A\sigma_{in}^{hN}}{\pi R^2}\right], \quad \sigma_{el}^{hA} = \sigma_{tot}^{hA} - \sigma_{in}^{hA}, \quad \sigma_{qe}^{hA} = \sigma_{in}^{hA} - \sigma_{prod}^{hA},$$

$$\sigma_{sd}^{hA}(hA \to XA) = \pi R^2 \left\{\alpha - \ln\left[1 + \alpha\right]\right\}, \quad \alpha = \frac{A\sigma_{tot}^{hN}}{2\pi R^2 + A\sigma_{tot}^{hN}}.$$

- Based on elementary hadron-nucleon cross sections and nuclear radius parameterisations
  - Barashenkov parameterisation for moderate energies 20 MeV – 20 GeV for p, n, π+, π-
    - Below 20 MeV n, p, d, t, He3, He4 cross sections per isotope are taken from the HP data and provided in G4PARTICLEXS2.1 dataset
  - Coulomb barrier for positively changed
  - Similar formulas for ion-ion cross sections
- The accuracy for hadron-nuclear and ion-ion cross sections may be estimated on level 5-10%
  - Limited by lack of data and data accuracy
  - Neutron cross sections depending on target isotopes may be are more accurate

Geant4 hadronic models



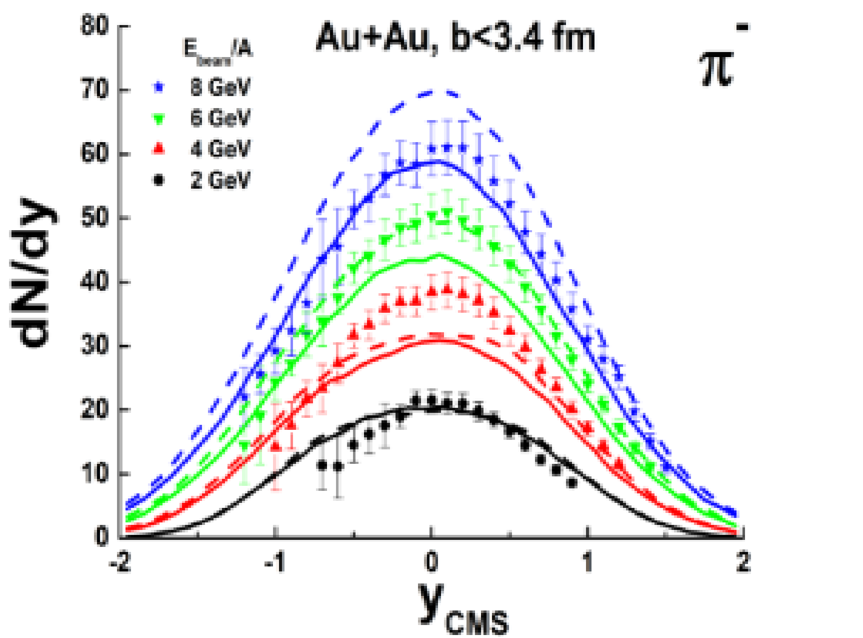
String Models Developments

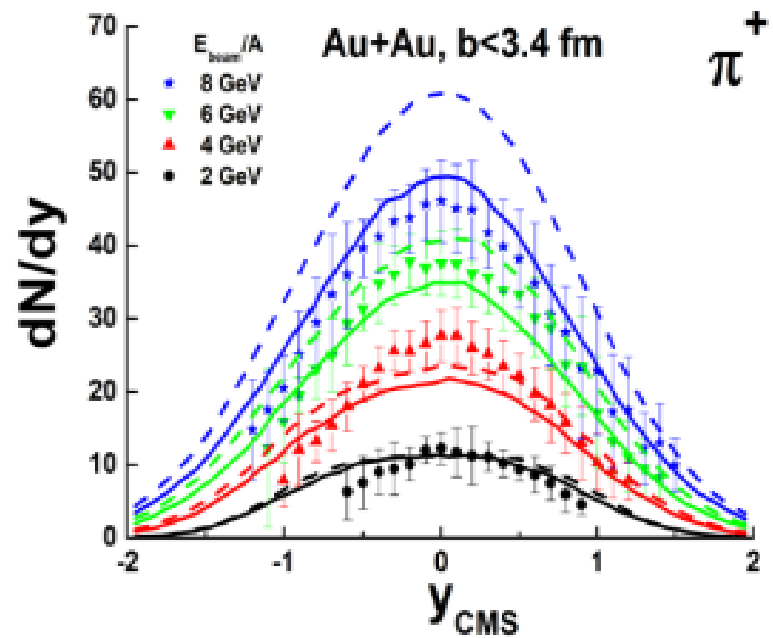
- Since 10.5 development versions of FTF and QGS are moved to the production release
  - Between 10.1 and 10.4 we tried to keep stability for simulation of Run-2
- FTF improved for
  - thin target benchmarks
  - Introduced rotating strings and smearing of resonance masses
  - Interactions of light anti-ions
  - Introduced a coalescence model for ion-ion interactions
  - Introduced production of charmed and bottom mesons and baryons
- QGS
  - Improved thin target benchmarks
  - Provide narrower shower and increased visible energy
  - Introduced production of charmed and bottom mesons and baryons
- In 10.6 unified transitions between models for all particles are established
  - between FTF and QGS is 12-25 GeV
  - between cascade and FTF is 3-6 GeV

FTF string model improvement for pion production in ion-ion collisions

Results of the improvements for E895 exp.

J. L. Klay et al., Phys. Rev C 68, 054905 (2003)
Charged pion production in 2A to 8A GeV central Au+Au Collisions,





Solid line – Geant4 10.6, dashed line – Geant4 10.4
Results become better for high energies T > 6 GeV

Pre-compound model and de-excitation module

- Established set of model parameters for PRECO and DEEX and user interface to these parameters
  - Has been extended in 10.6
- Renewed internal data structure for nuclear levels for 10.6
  - G4ENDSFSTATEDATA, G4LEVELGAMMADATA, G4RADIOACTIVEDATA are coherent
  - New data format was introduced in Geant4 10.3
  - All components of PRECO and DEEX use this data and not hard-coded numbers
- Provided long-lived isomer production
  - Added floating level states
  - Long lived isomers may be tracked by Geant4
- Provided correlated gamma emission for radioactive decay
  - Is disabled by default but may be enabled by a flag
- The reorganisation was completed in general for Geant4 10.4
  - However, many fixes are introduced in 10.6

How to configure and optimize Geant4 physics in 10.6?

Geant4 simulation may be more accurate and faster in production if fine tuning of configuration parameters is done for each calorimeter of an experiment

Physics Lists for Calorimeters

- Geant4 recommended Physics List is FTFP_BERT
  - For detailed studies of new calorimeter response FTFP_BERT_EMZ may be used
    - More accurate EM physics
    - Substantial slow down of simulation
  - For high energy projectile QGSP_FTFP_BERT may be tried
    - Above 25 GeV QGS string model
  - FTF_BIC and QBBC may be recommended for more accurate fragmentation below 1 GeV
  - FTFP_INCLXX provides more accurate production and interaction of light ions
    - Is slower than the default physics
- Radioactive decay may be added on top of any Physics List
  - Long lived isomers will be produced and tracked

Comments on Birks quenching

- In recent years, we observed that developments in the FTF model improving thin target data have a larger disagreement with the testbeam/large-scale experiment data for calorimeters
  - More visible energy and less fluctuations
  - We have made several investigations:
    - Check on production of π°
    - Tuning of model parameters driven by light targets
    - Use Binary Cascade (BIC) instead of Bertini (BERT) for nucleons below a few GeV
    - Refined hadron elastic
    - More accurate models provide worse results
- For scintillator-based calorimeters, the coefficient used for Birks quenching was obtained from old measurements, by fitting under the assumption of no delta-ray emissions
  - This implies that the Birks coefficient is underestimated
- We suggest to retune Birks parameters
  - Ideally fit this parameter from the e/h (test-beam) data of the actual calorimeter
  - ΔE in test-beam analysis and in MC production should be computed in a similar way
    - Cut in range should be the same

$$\Delta E\_visible = \frac{\Delta E}{1 + K * \frac{\Delta E}{\Delta x}}$$

How to speed-up simulation of an actual detector?

- In Geant4 10.6 following customization options for EM physics are recommended:
  - Production thresholds (cuts in range) per G4Region
    - Increased cuts provide faster simulation
  - Tracking cuts per particle type
  - General process for gamma may be enabled
- Different multiple scattering parameters may be tuned per G4Region (per sub-detector)
  - RangeFactor, GeomFactor, Stepping algorithm, Lateral displacement
  - New in 10.6: SafetyFactor , LambdaLimit
- User may design EM physics constructor with multiple scattering models for e+- separately configured per G4Region
  - There is also helper class G4EmConfigurator which may be called from user application
  - CMS and ALICE already use this possibility in production

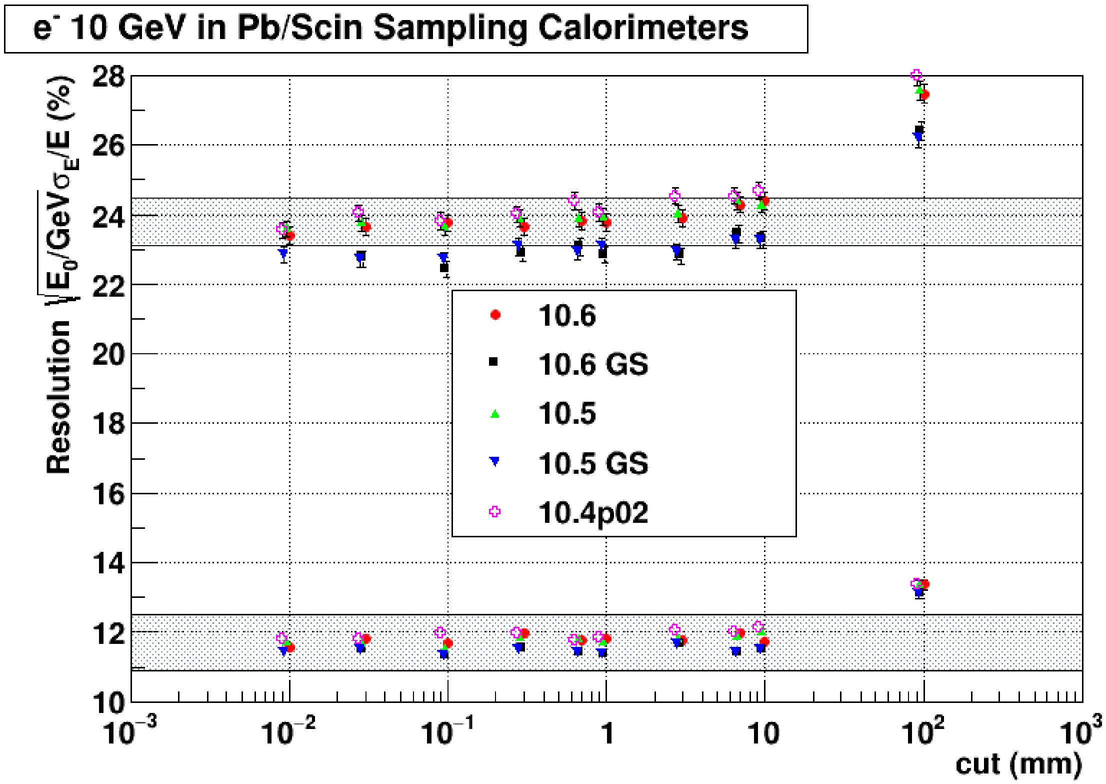
Summary

- A new version Geant4 10.6 will be available in December 2019
  - It is likely the last release of the 10 series
  - It will include all available updates of EM and hadronic physics
  - Assumed to be used for LHC Run-3 simulations
  - We propose to use 10.6 for calorimeter R&D studies
- Several EM physics models were enhanced
  - Multiple scattering
  - New 5D model for gamma conversion
  - 3-gamma annihilation
- Substantial progress in hadronic models
  - FTF and QGS string models
  - Consistent use of nuclear data in the de-excitation module and in the radioactive decay
  - Nuclear data updated
  - Glauber-Gribov cross sections are used in all Physics Lists except HP cross sections below 20 MeV
- We also bring to your attention to the Birks quenching parameters

Backup:
selected validation results

Resolution of Pb/Sc calorimeters

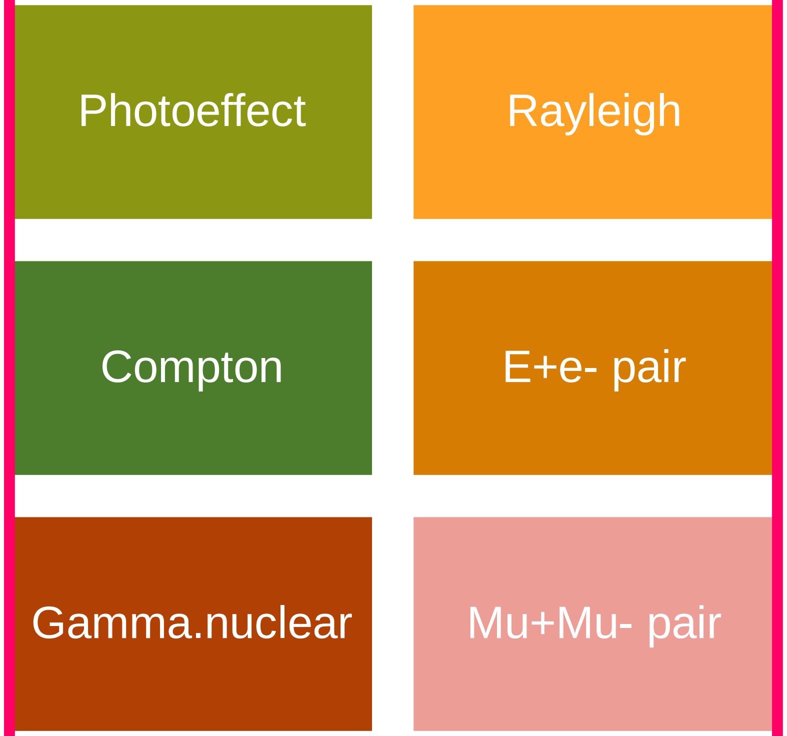
Bernardi E. et al. 1987 Nucl. Instrum. Meth. A 262, 229



- Resolution for 10.6 is narrower but within data errors
  - Effect is larger for lower sampling fraction (thicker scintillator)
  - Due to G4UrbanMscModel modification of lateral displacement sampling algorithm to provide more accurate backscattering

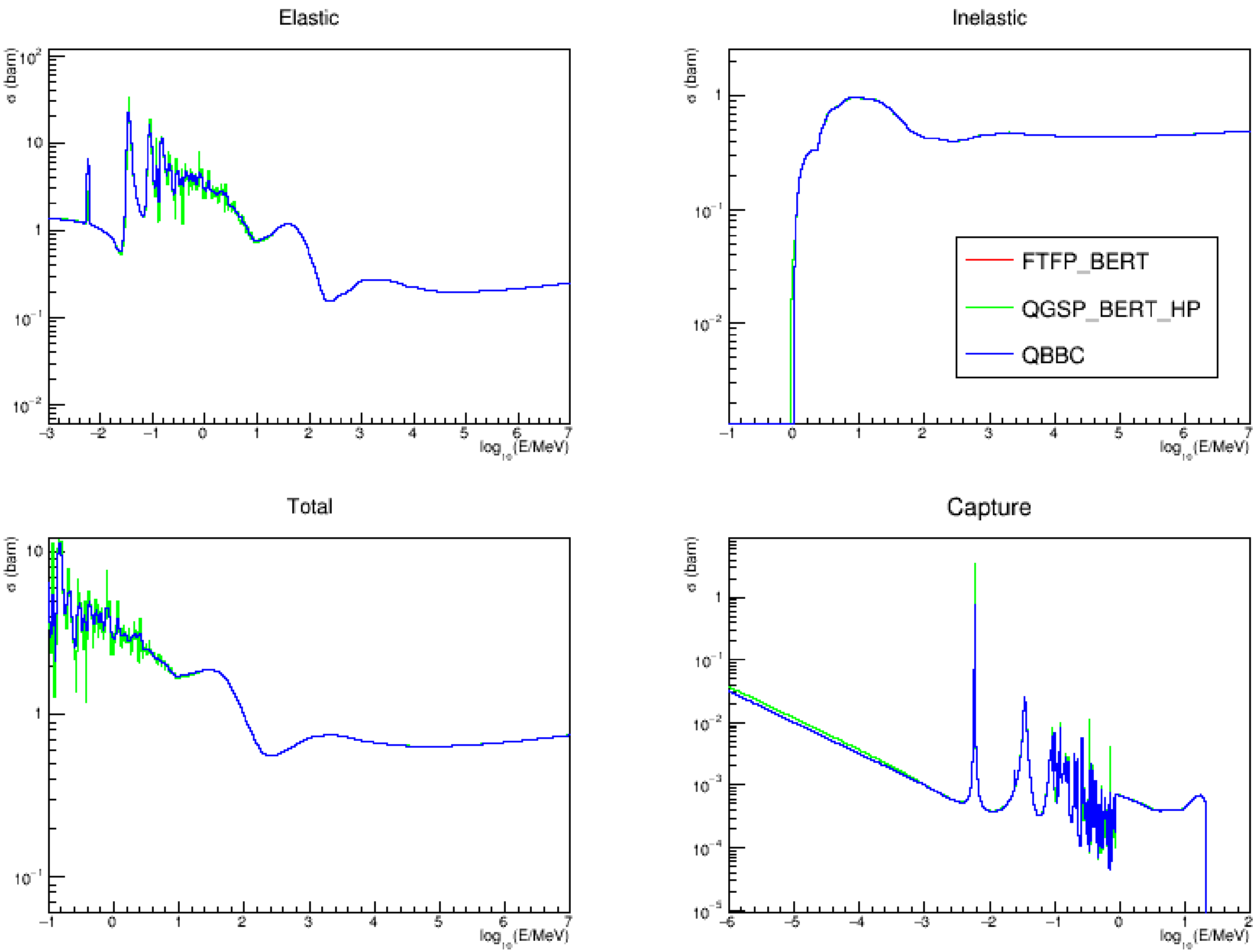
G4GammaGeneralProcess

- G4GammaGeneralProcess



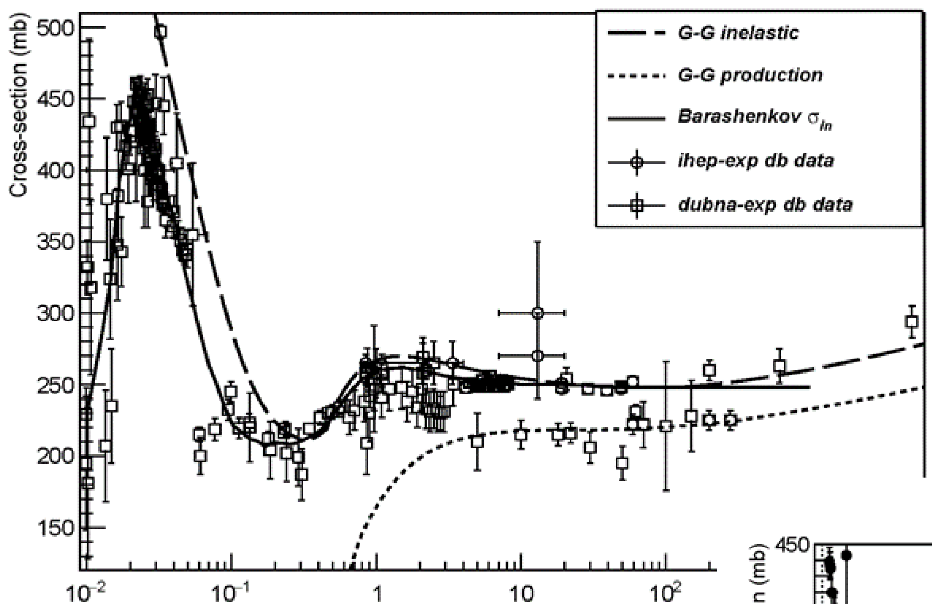
- SteppingManager see only 1 physics process
  - Only 1 mean free path
  - Plus transportation
- Enabled via UI command
  - In 10.6 will be optional in general, UI command may be used to enable
  - Will be defaults for Opt1 EM physics
- Reduced number of instructions
  - Advantage in CPU ~5%
  - Extra PhysicsTables shared between threads – a bit more memory
- Final numbers for CPU/memory should be checked by users

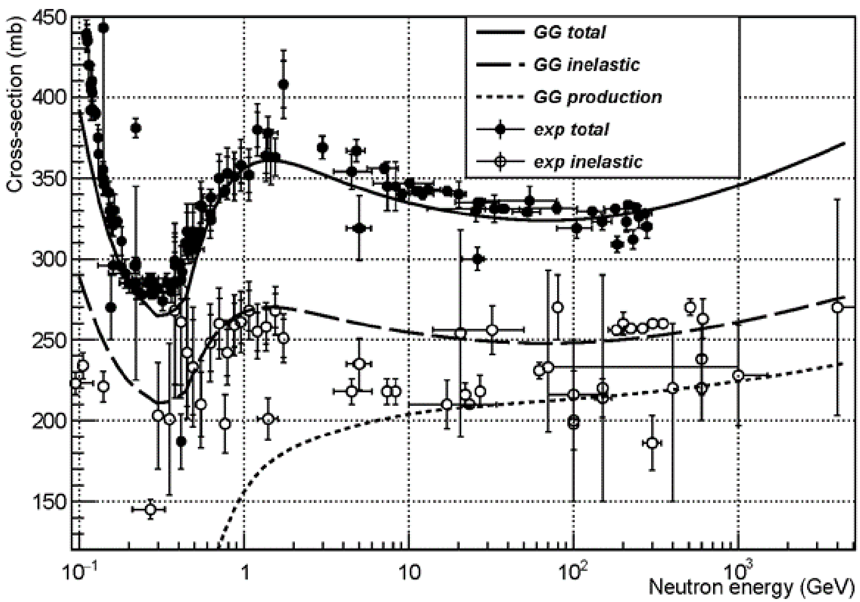
Neutron x-sections in Aluminum



HP and non-HP cross sections are similar

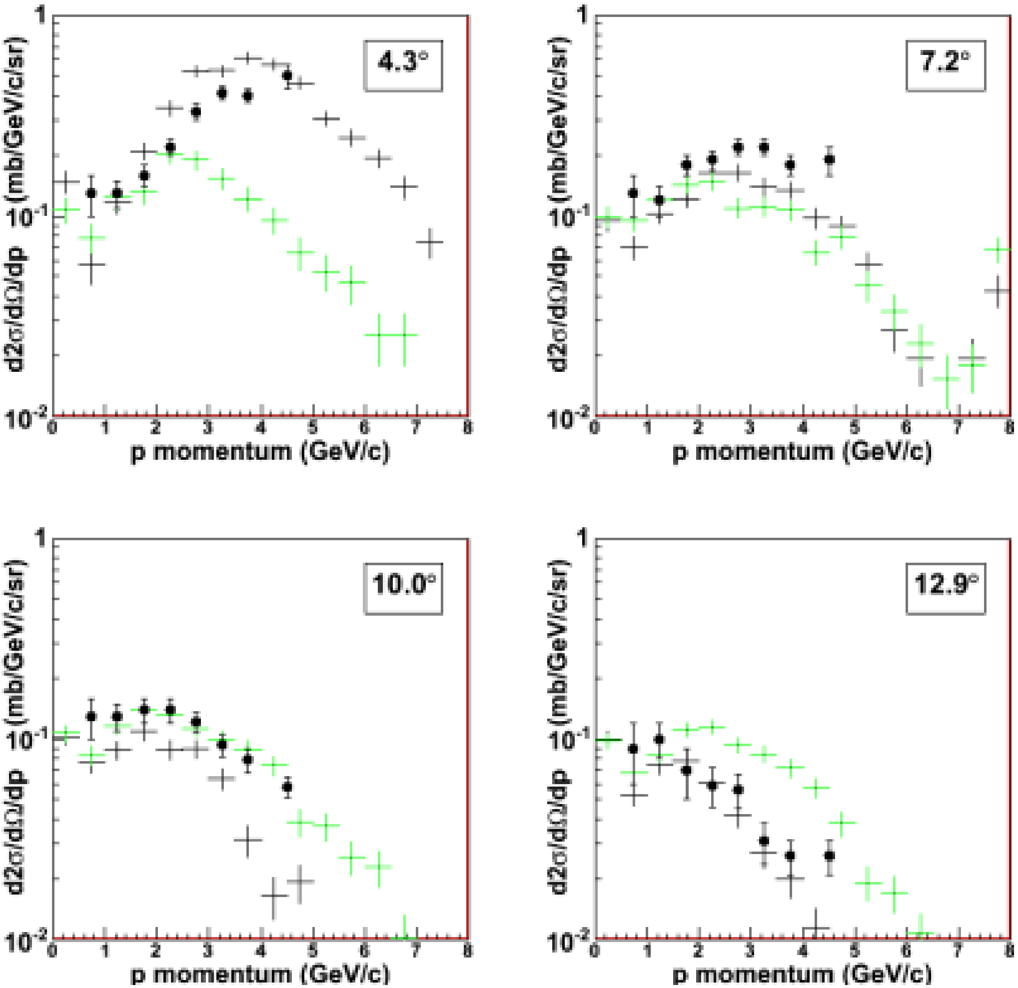
Proton and neutron cross sections off Carbon





The Bertini Cascade updates

Biased Phase Space p + C -> p + X @ 8 GeV/c



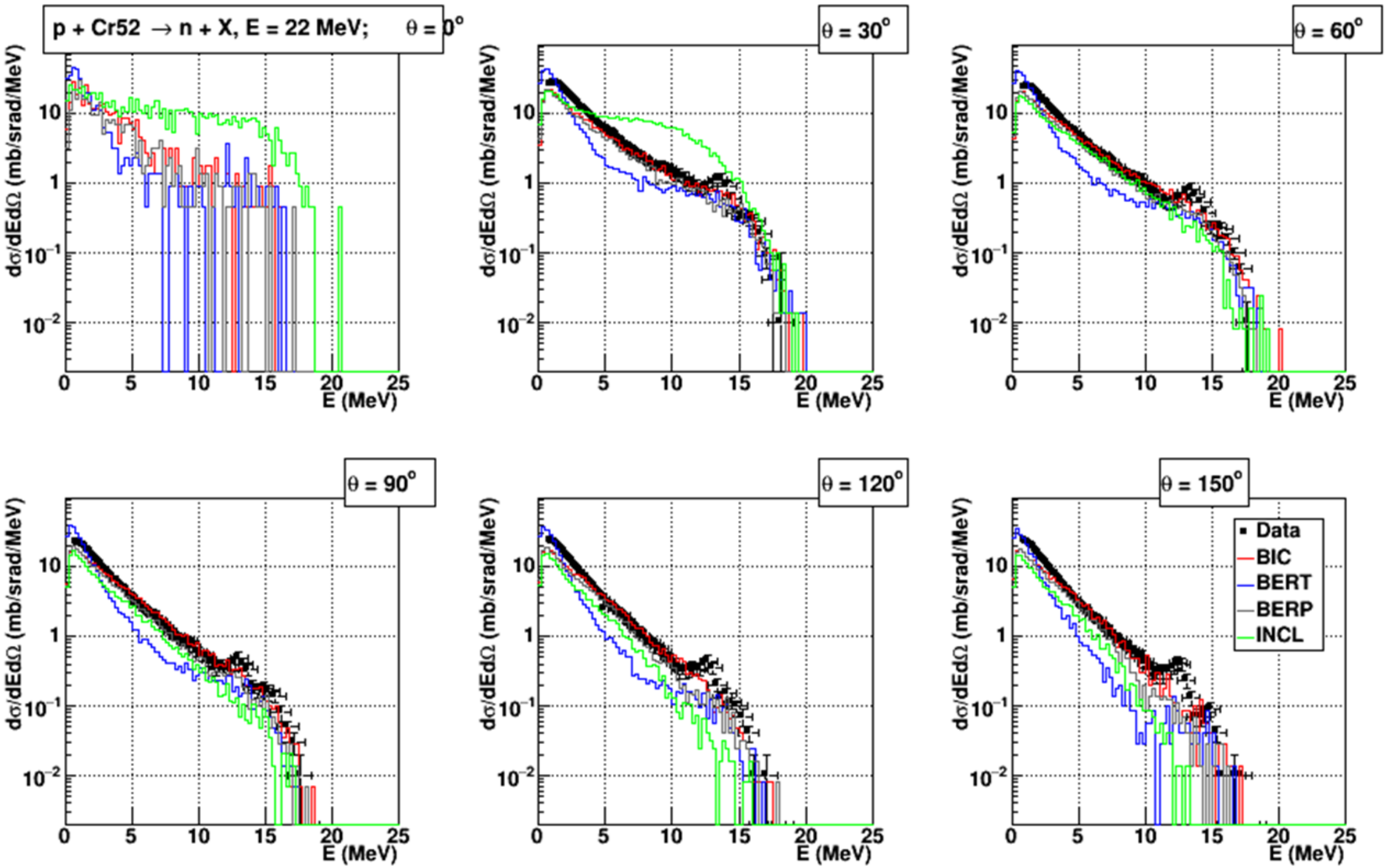
HARP data:
black dots

Original Bertini generator :
green crosses

Biased phase space:
black crosses

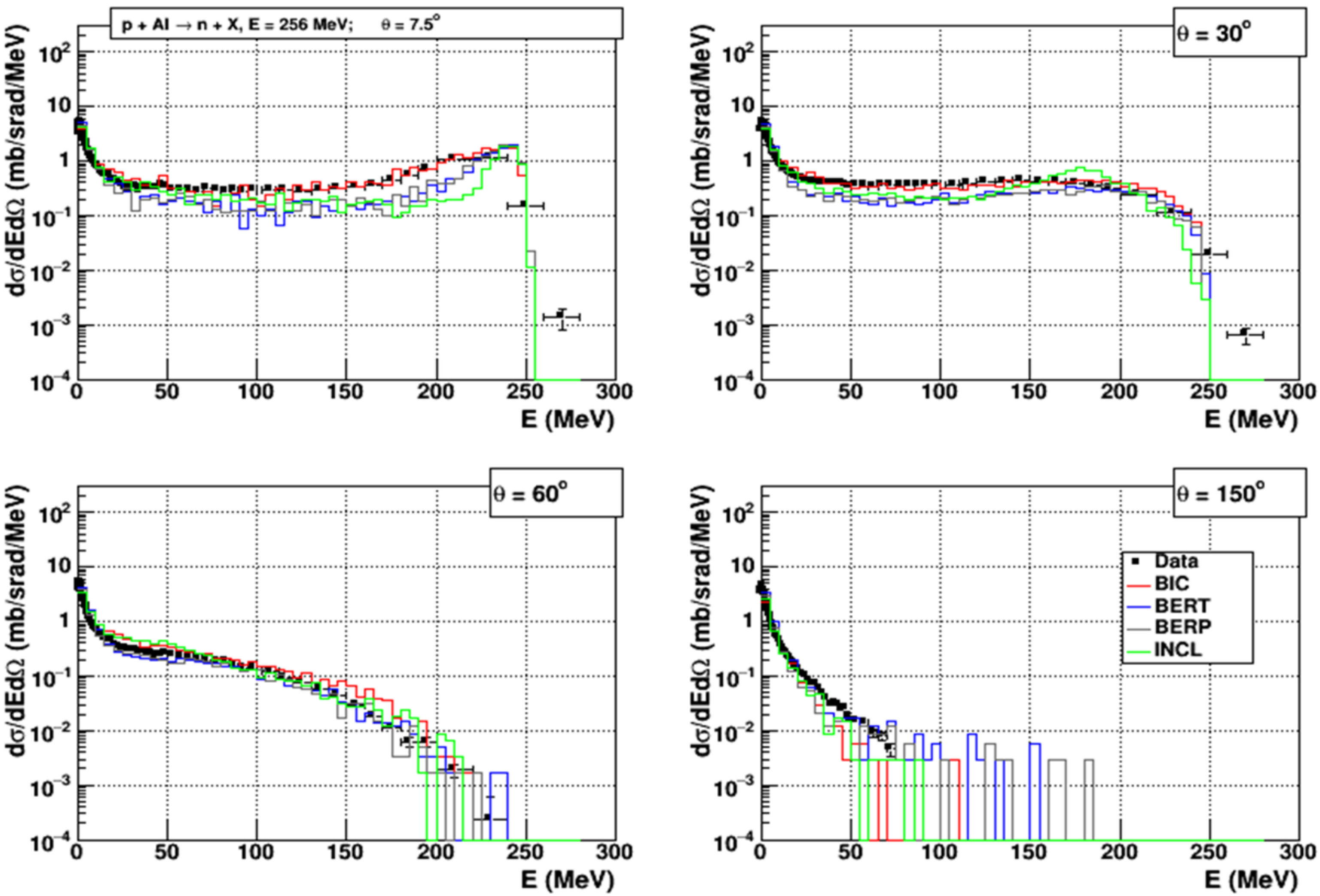
Double differential neutron production cross section for 22 MeV protons in ^{52}Cr target

N.S.Biryukov et al., Sov. J. Nucl. Phys. 31 (1980) 3



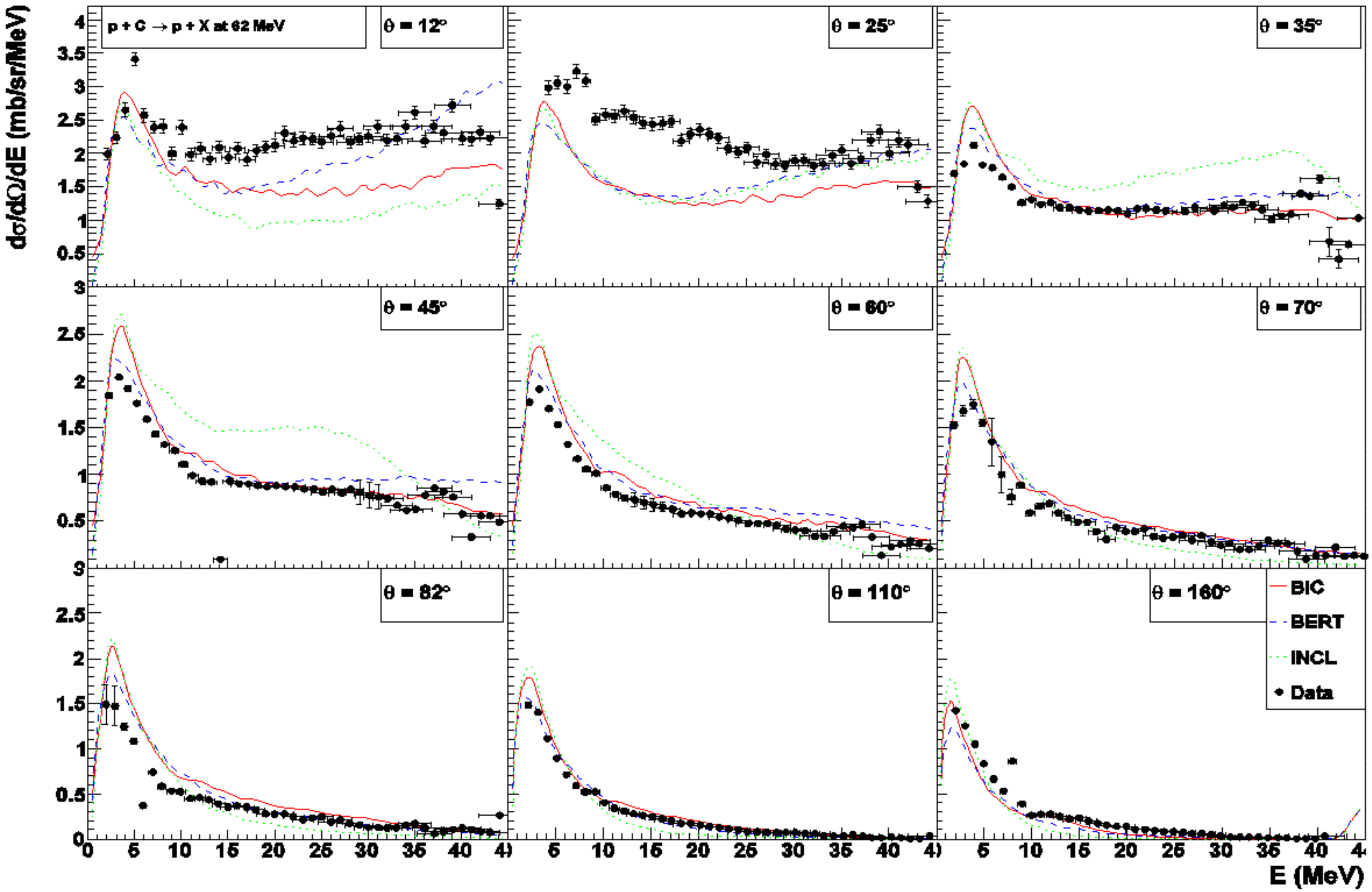
Double differential neutron production cross section for 256 MeV protons in Al target

M.M.Meier et al., Nucl. Sci. Engeneering 110 (1992) 289



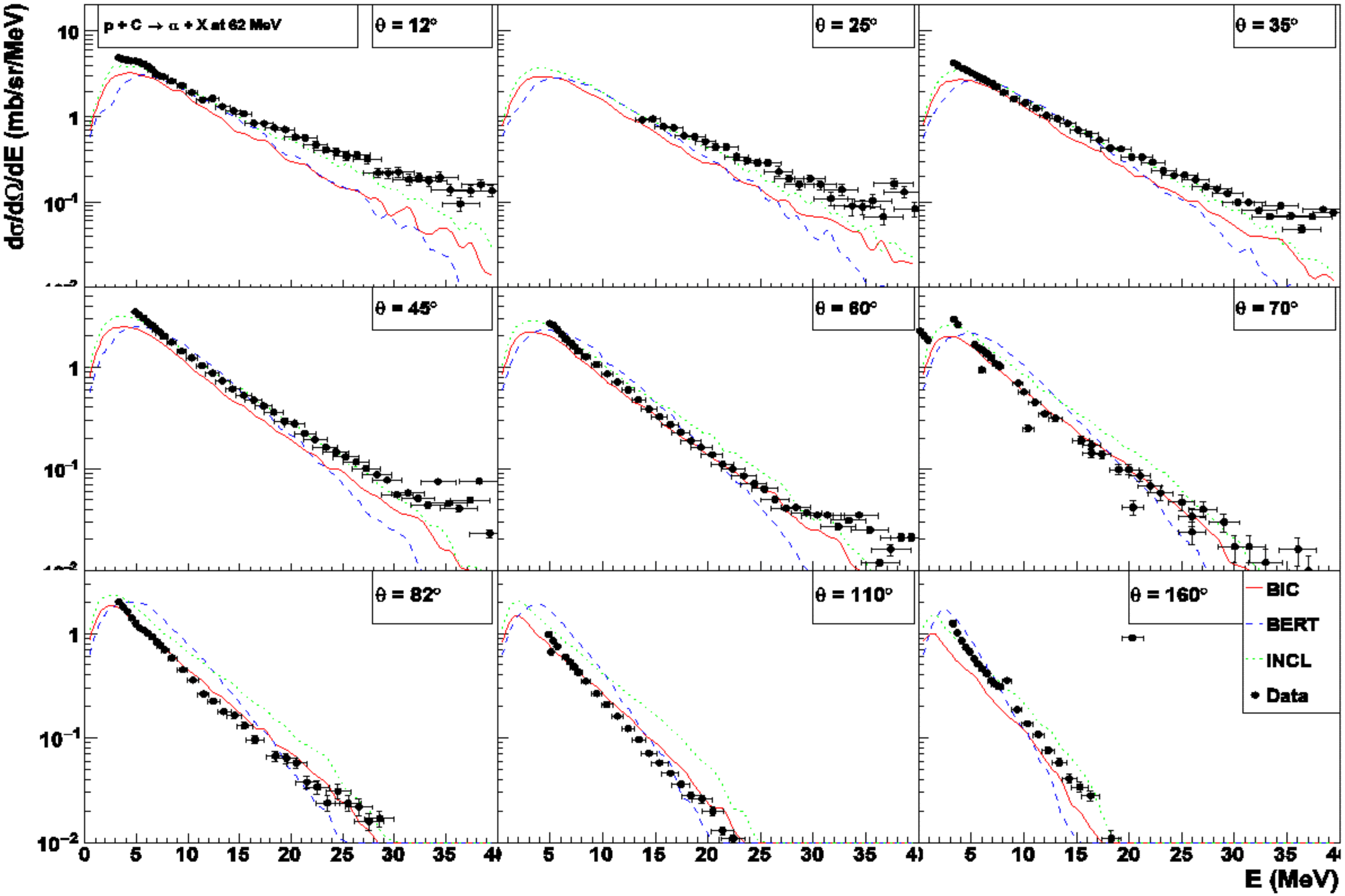
Double differential proton production cross section for 62 MeV protons in carbon target

F.E.Bertrand & R.W.Peelle, Phys. Rev. C 8 (1973) 1045



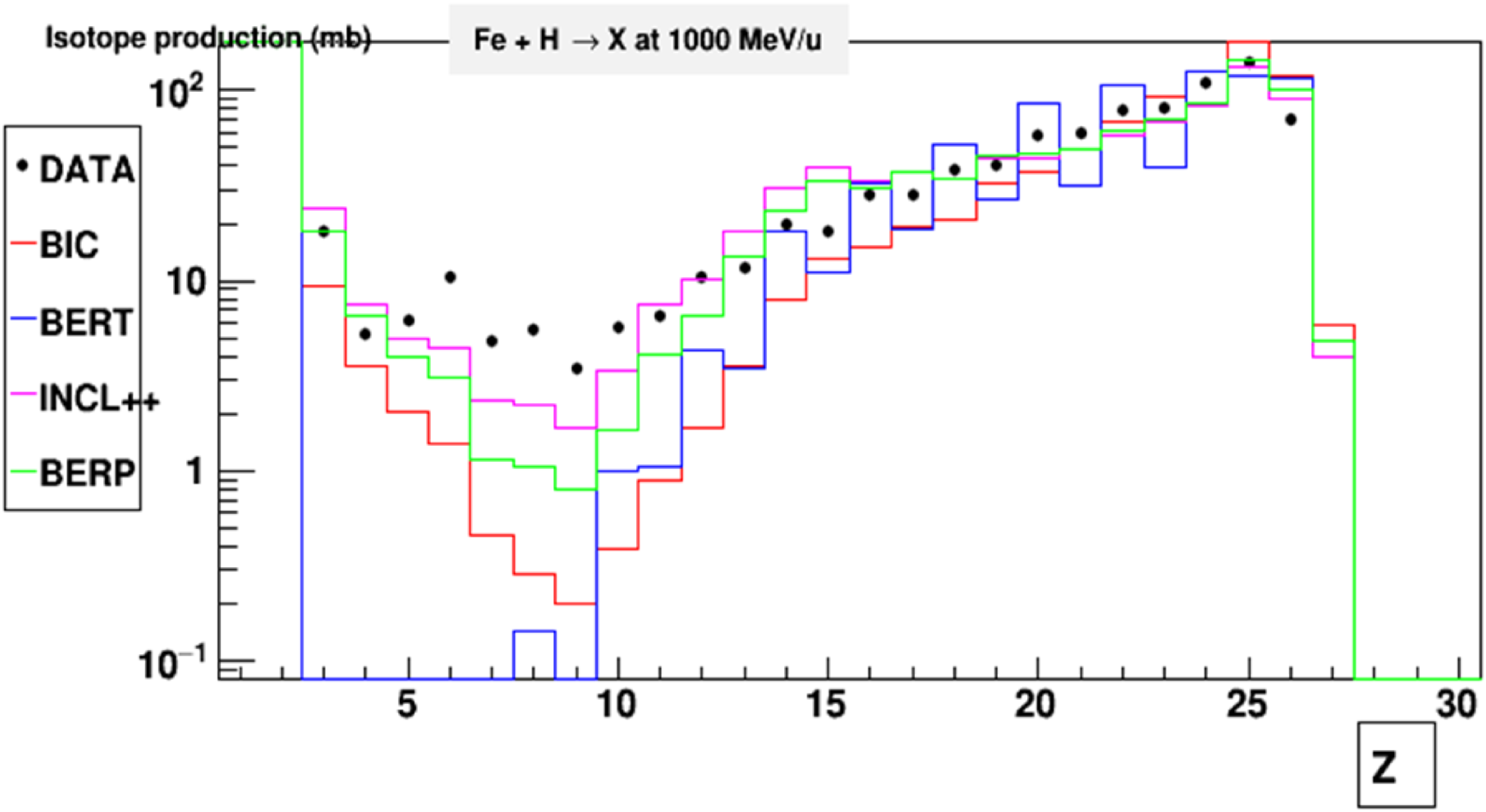
Double differential alpha production cross section for 62 MeV protons in carbon target

F.E.Bertrand & R.W.Peelle, Phys. Rev. C 8 (1973) 1045



Isotope production by 1 GeV protons in Fe target

C.Villagrasa et al., AIP Conference Proceeding 769 (2005) 842



- At this and previous plots INCL++ demonstrates more accurate simulation for ion components
- The binary cascade predictions improve when multi-fragmentation sub-model is enabled