Geant4 10.6 status for medical applications

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Outline

- Introduction
- Electromagnetic (EM) physics in Geant4 10.6
- Hadronic physics in Geant4 10.6
- How to configure and optimize Geant4 physics?
- Summary

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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 includes all modifications accumulated over last few years
    - It was released 6th of December 2019
  - 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 evolution

- Consolidation of Geant4 EM sub-packages was done for Geant4 9.6
  - Common interfaces for Standard, Livermore, Penelope models
    - Full set of models
    - Similar results
- In Geant4 10.1 full migration of EM physics to multi-threading
- G4EmParameters was introduced instead of G4EmProcessOptions in Geant4 10.2
  - Required by MT mode
  - Fully implemented in 10.4
- In Geant4 10.5
  - we updated lateral displacement algorithm for G4UrbanMscModel
  - G4GoudsmitSoundersonMscModel is used in Opt4 EM physics
  - Added ICRU90 data
  - Added 3-gamma annihilation
  - Added 5D gamma conversion model

Hadronic physics evolution

- FTF string model becomes the default since 10.0
  - FTFP_BERT is the default PhysicsList
- Substantial revision of handling of ions and isotopes was started after Geant4 10.2
  - For MT mode all components of low-energy hadronic physics should be coherent
    - The same list of isomers for all sub-models
    - The same nuclear transition energies in FermiBreakUp, GEM, Radioactive decay
  - Migration was completed in general in 10.4
    - Some bug fixes were done in newer releases
- In Geant4 10.5 all developments for FTF and QGS string models were included

EM physics in Geant4 10.6

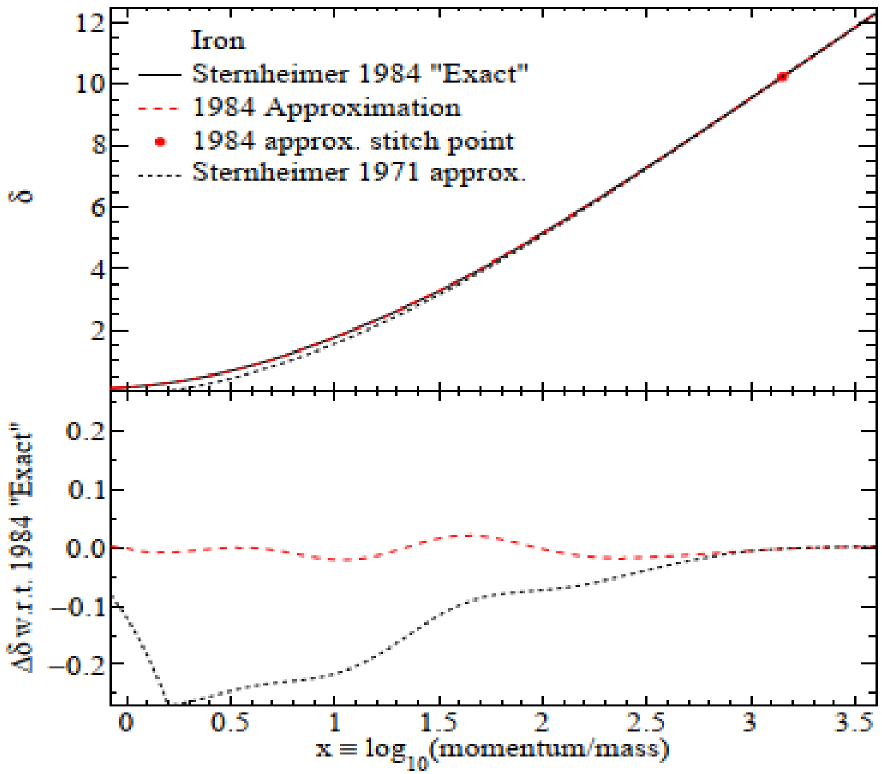
Main recent developments:

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

Updates of Geant4 Materials

- New static methods added
  - *G4Material::GetMaterial(const G4String&, G4double density)*
  - *G4Material::GetMaterial(G4double Z, G4double A, G4double density)*
  - *G4Material::GetMaterial(size_t nComponents, G4double density)*
  - These methods may help to reduce duplicate material definitions in HEP detector descriptions
- New class G4DensityEffectCalculator (Matthew Strait, University of Minnesota, USA)
  - Based on R.M. Sternheimer publications as our default but do not use parameterisation, instead resolving non-linear equation
  - By user request compute density effect correction on fly without any parameterisation
    - New UI command "/material/g4/enableDensityEffOnFly material_name"
- For the default computation of the density correction for compounds the logic was changed
  - If a compound is not inside NIST materials DB but some element dominates in the mass fraction (>90 %), then density correction is based on parameterisation for this pure element available in Geant4

Accuracy of the new approach for Fe (M. Strait)



- Pure iron: 1984 approximation is quite close to the exact solution
- Impure iron (say, steel): 1971 approximation, up to 1.3% off

- Patch already used by NOvA to obtain improved $\mathrm{d}E/\mathrm{d}x$ in steel by up to 1.3%
  - Important because this difference cannot be calibrated out in a neutrino experiment
  - Same will be true for DUNE at the level of 0.6%

EM model developments

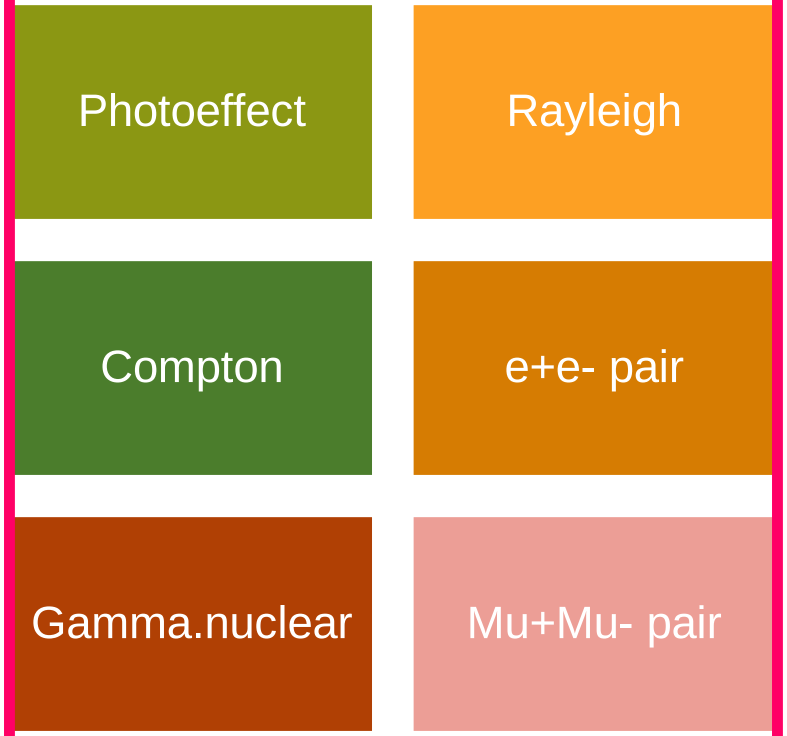
- Models of single and multiple scattering for e+-
  - Improved sampling of displacement for the G4UrbanMscModel
  - Added Mott corrections to G4WentzelVIModel used for simulation of multiple scattering of e+- above 100 MeV
  - G4ScreenedMottCrossSection – use G4MottData shared between threads and implemented 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

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

General Gamma Process

- G4GammaGeneralProcess



- SteppingManager sees only 1 physics process
  - Only 1 mean free path
  - Plus transportation
- Enabled via UI command
  - In 10.6 it is optional in general, UI command may be used to enable it
  - /process/em/UseGeneralProcess true
  - Is the default 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

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

Geant4-DNA developments for 10.6

- Physics
  - Atomic deexcitation & radioactive decay benchmarks
  - New models for electrons in gold
  - Checking and validation of sub-excitation electron thermalization models
  - New models for electrons in DNA material
  - Evaluation of proximity functions (extended example « microprox »)
- Chemistry
  - Influence of physics models and chemistry parameters on the simulation of radiochemical yields
  - Porting of TOPASnBio IRT & alternative versions to Geant4
- Geometries & damage
  - Evaluation of DNA damage in a fractal nucleus geometry
  - Dnadamage1 example

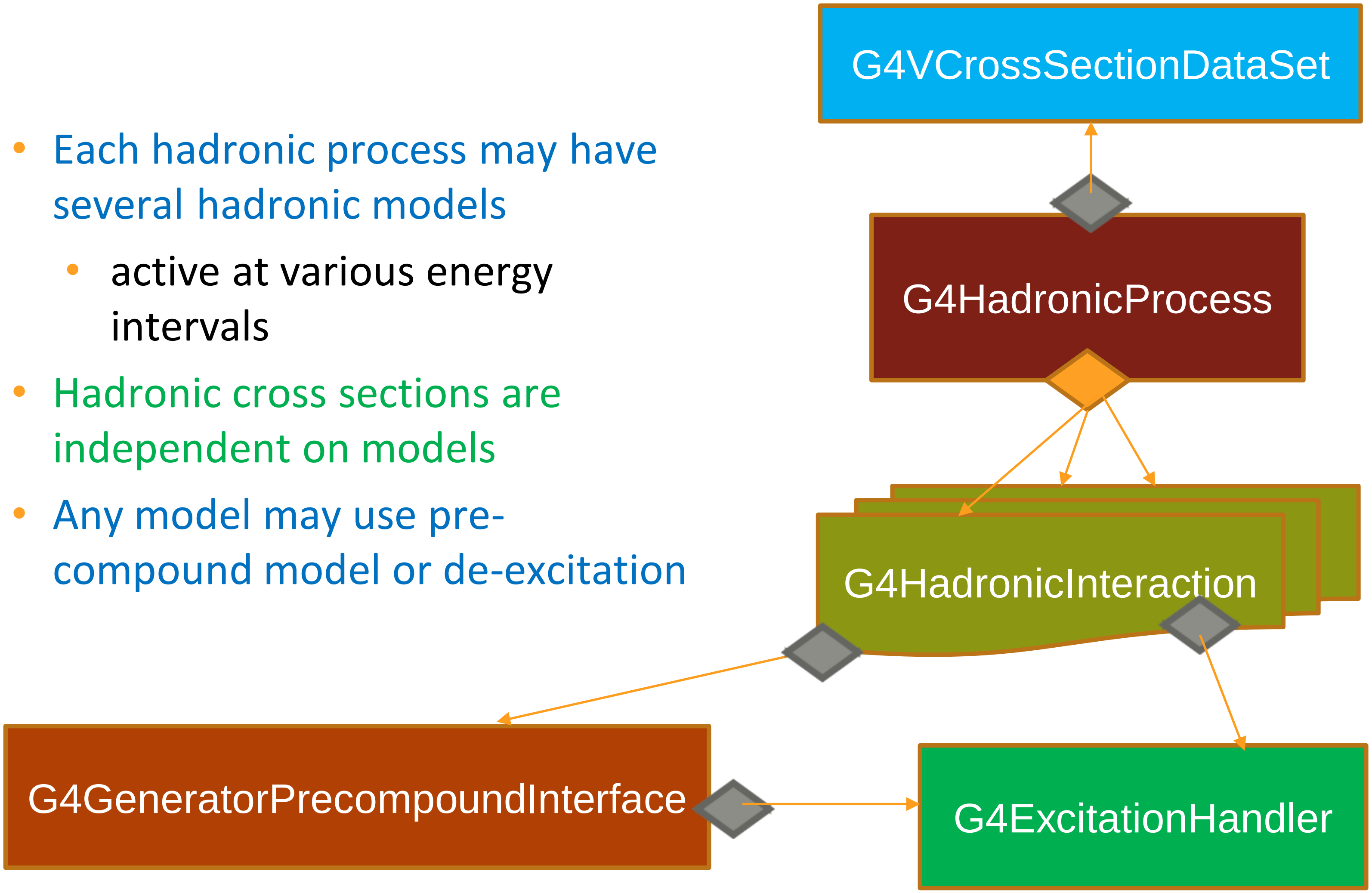
Hadronic physics in Geant4 10.6

Main recent developments:

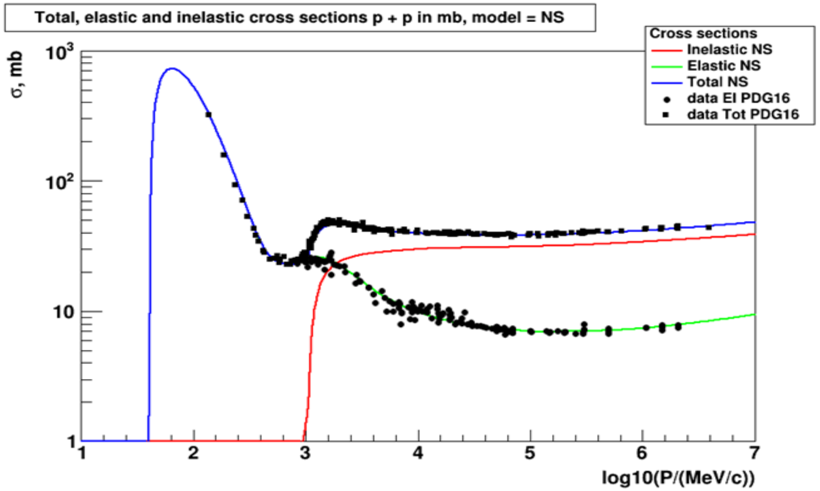
- FTF and QGS string models
- de-excitation module and radioactive decay
- Hadron and ion cross sections
- high precision (HP) data driven models

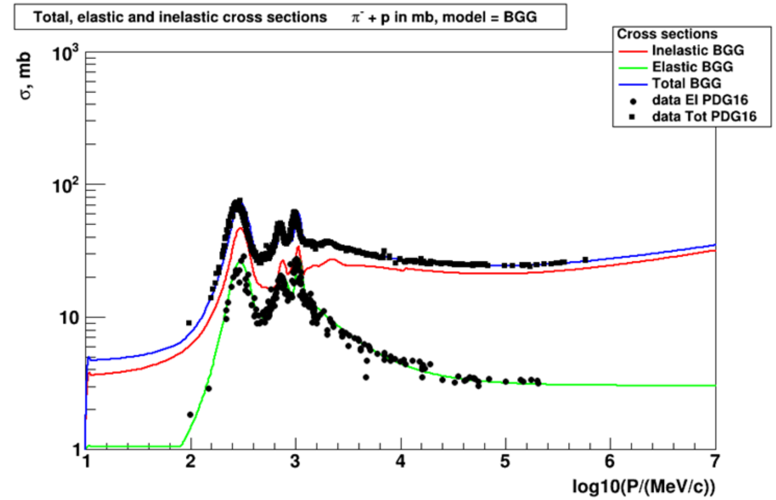
Geant4 hadronic physics design

- 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

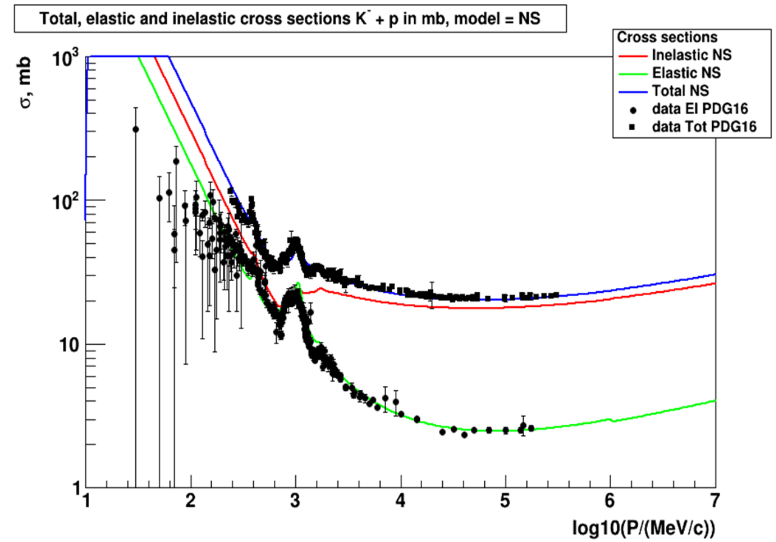


Hadron-nucleon cross sections





- 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:

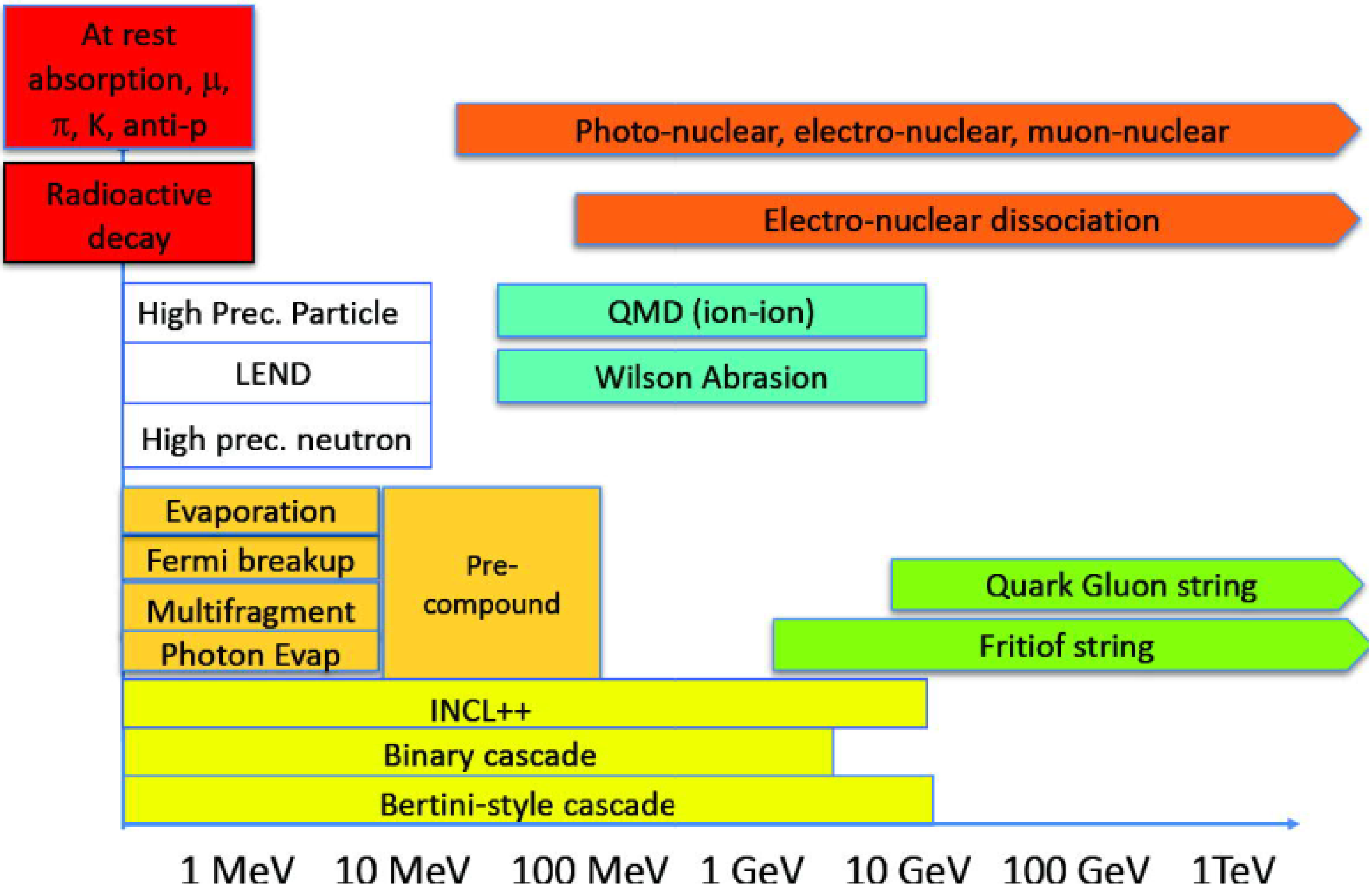
$$\sigma_{tot}^{hA} = 2\pi R^2 \ln\left[1 + \frac{A\sigma_{tot}^{hN}}{2\pi R^2}\right], \quad \sigma_{in}^{hA} = \pi R^2 \ln\left[1 + \frac{A\sigma_{tot}^{hN}}{\pi R^2}\right],$$

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

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

- 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



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

Configuration of EM physics

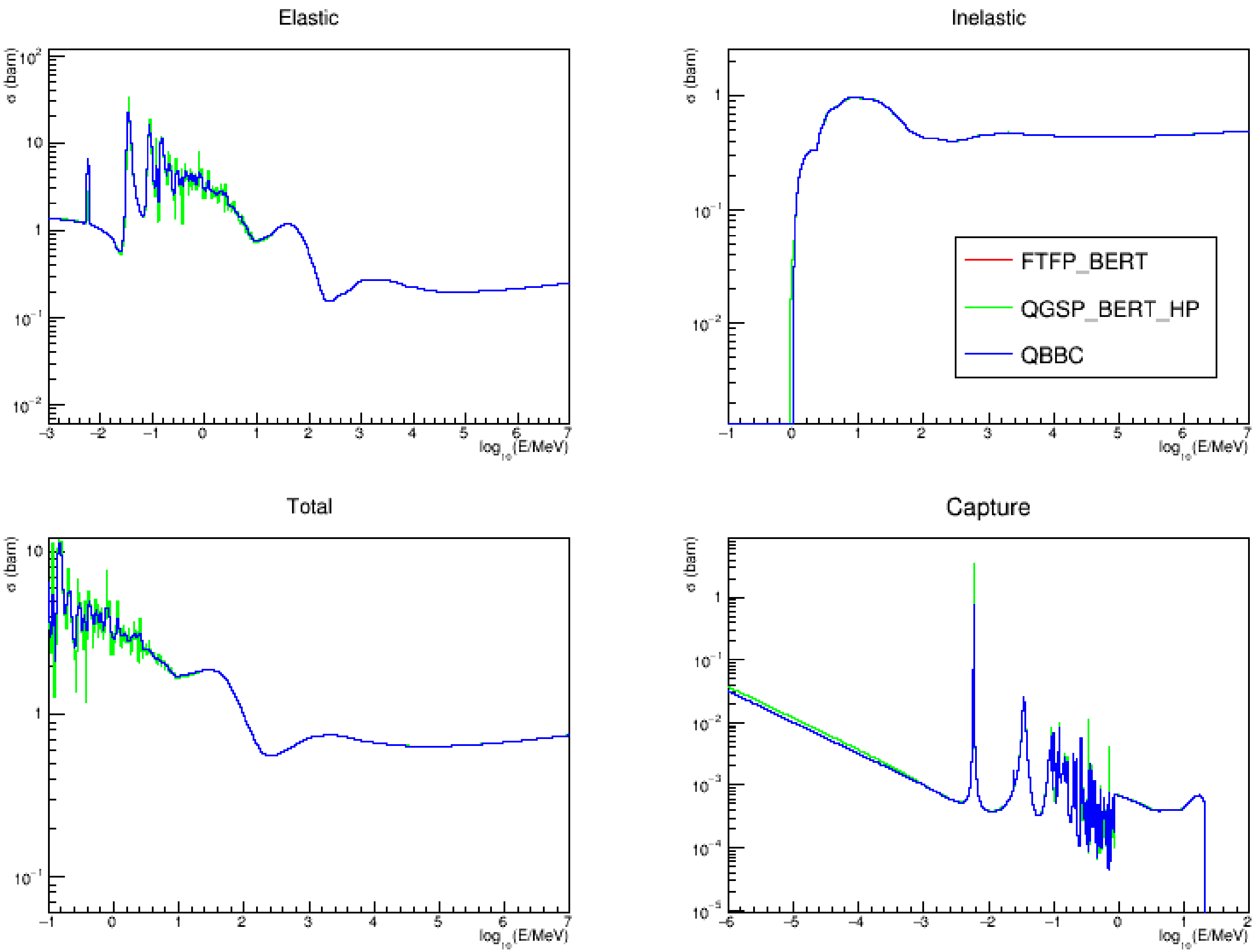
- A set of EM physics constructors are provided together with each recent Geant4 version
  - The default (Opt0) EM physics is optimized for use in HEP
  - There are variants Opt1 (EMV) and Opt2 (EMX) with simplified multiple scattering and other options
  - The alternative Opt4 (EMZ) physics is a combination of the most accurate EM models
    - Is recommended for R&D and detector performance studies
    - For 10.6 will use 5D gamma conversion model
    - It is substantially shower than the default EM physics
- On top of any EM physics configuration it is possible to customize EM parameters via UI commands and C++ interface
  - G4EmParameters class may be called
  - EM physics configuration and PAI ionization model may be defined for one or more G4Region(s)
    - This feature is used already by ALICE and CMS

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

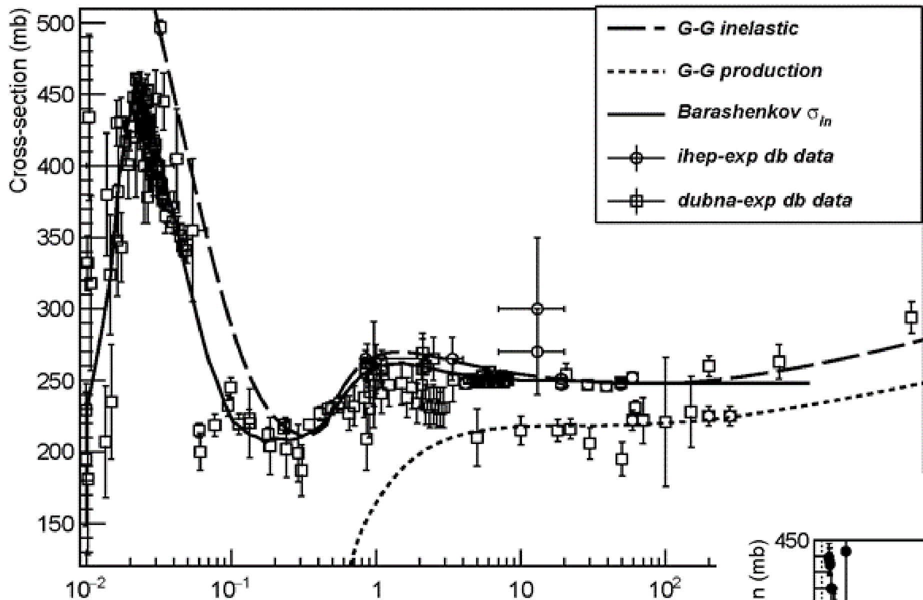
Backup:
selected validation results

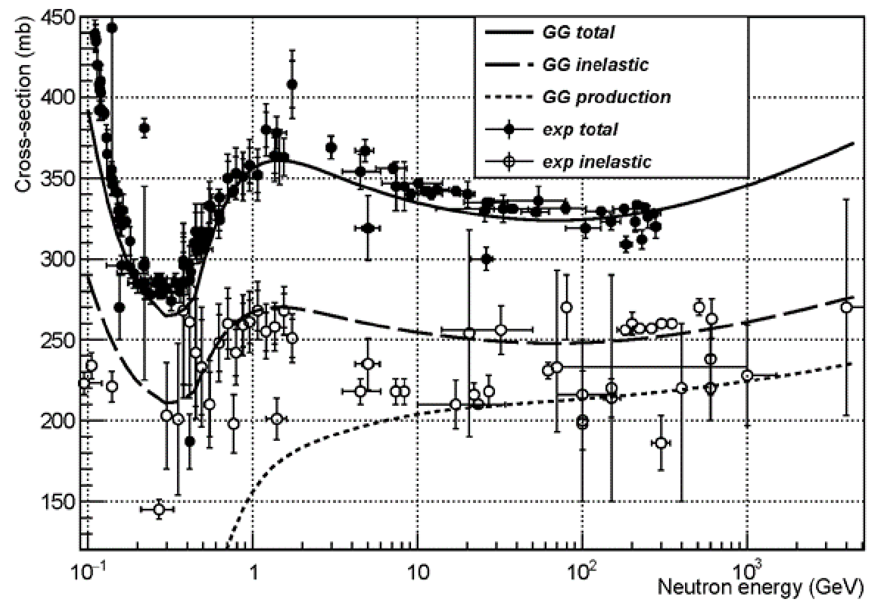
Neutron x-sections in Aluminum



HP and non-HP cross sections are similar

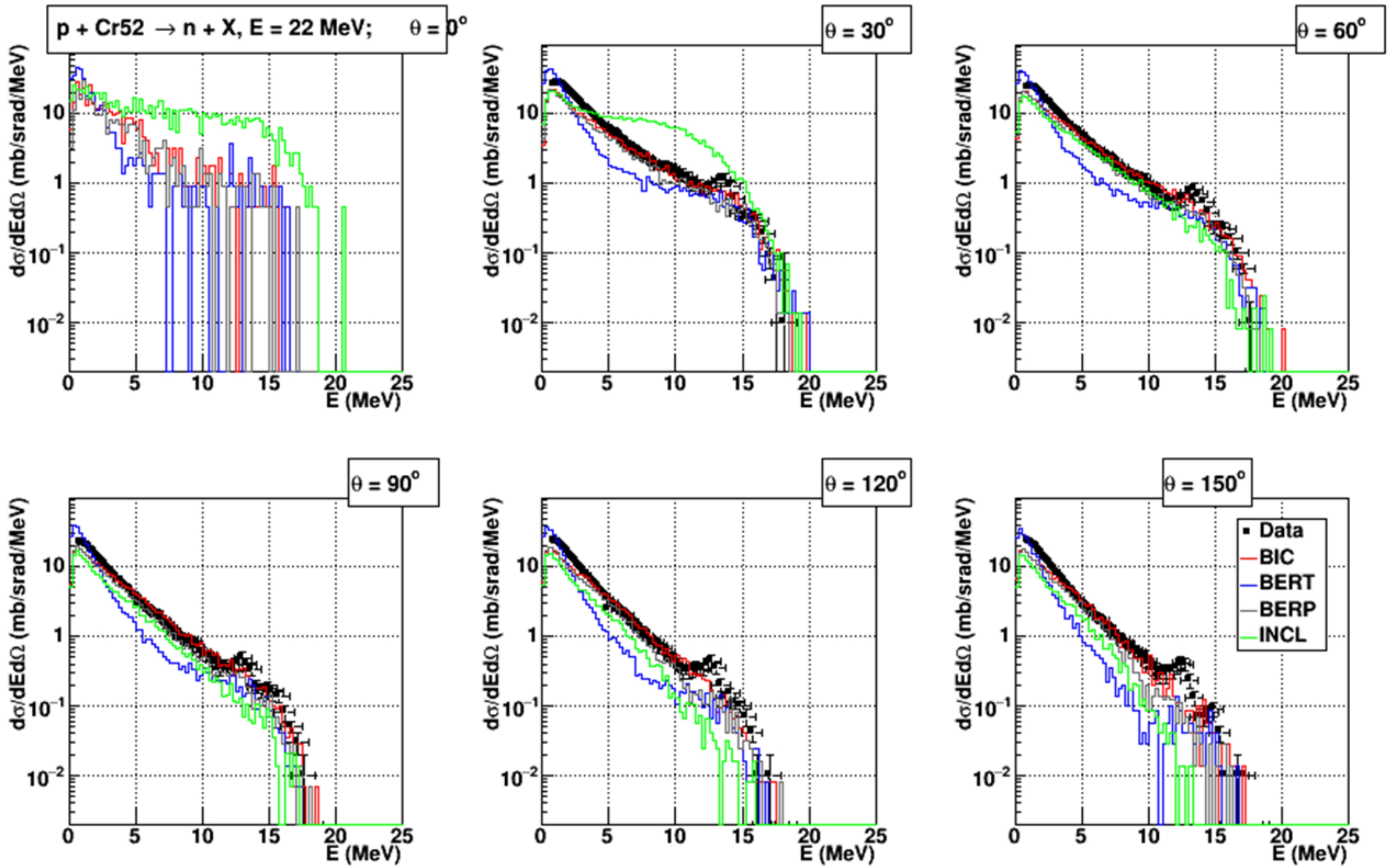
Proton and neutron cross sections off Carbon





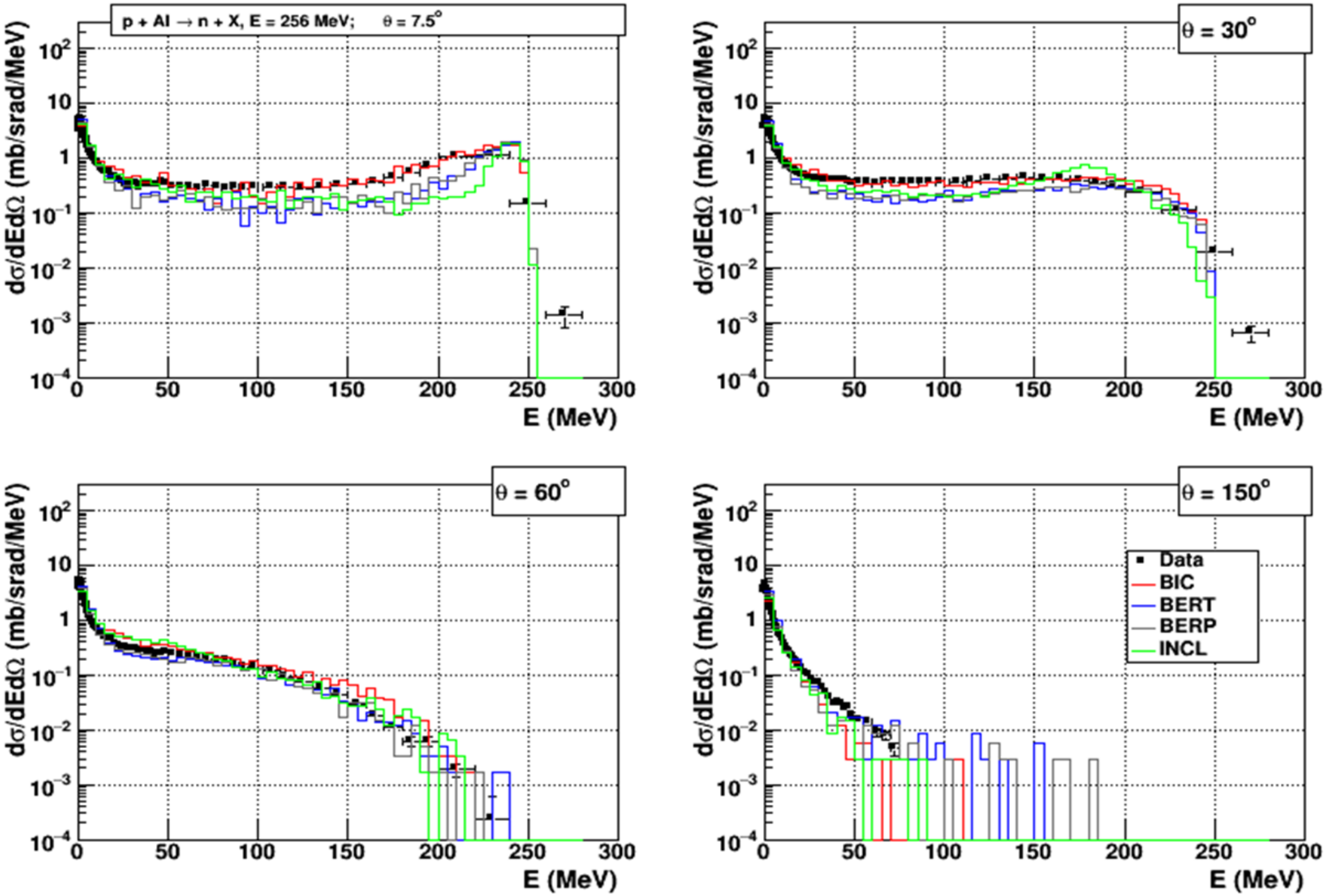
Double differential neutron production cross section for 22 MeV protons in ^{52}Cr target

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



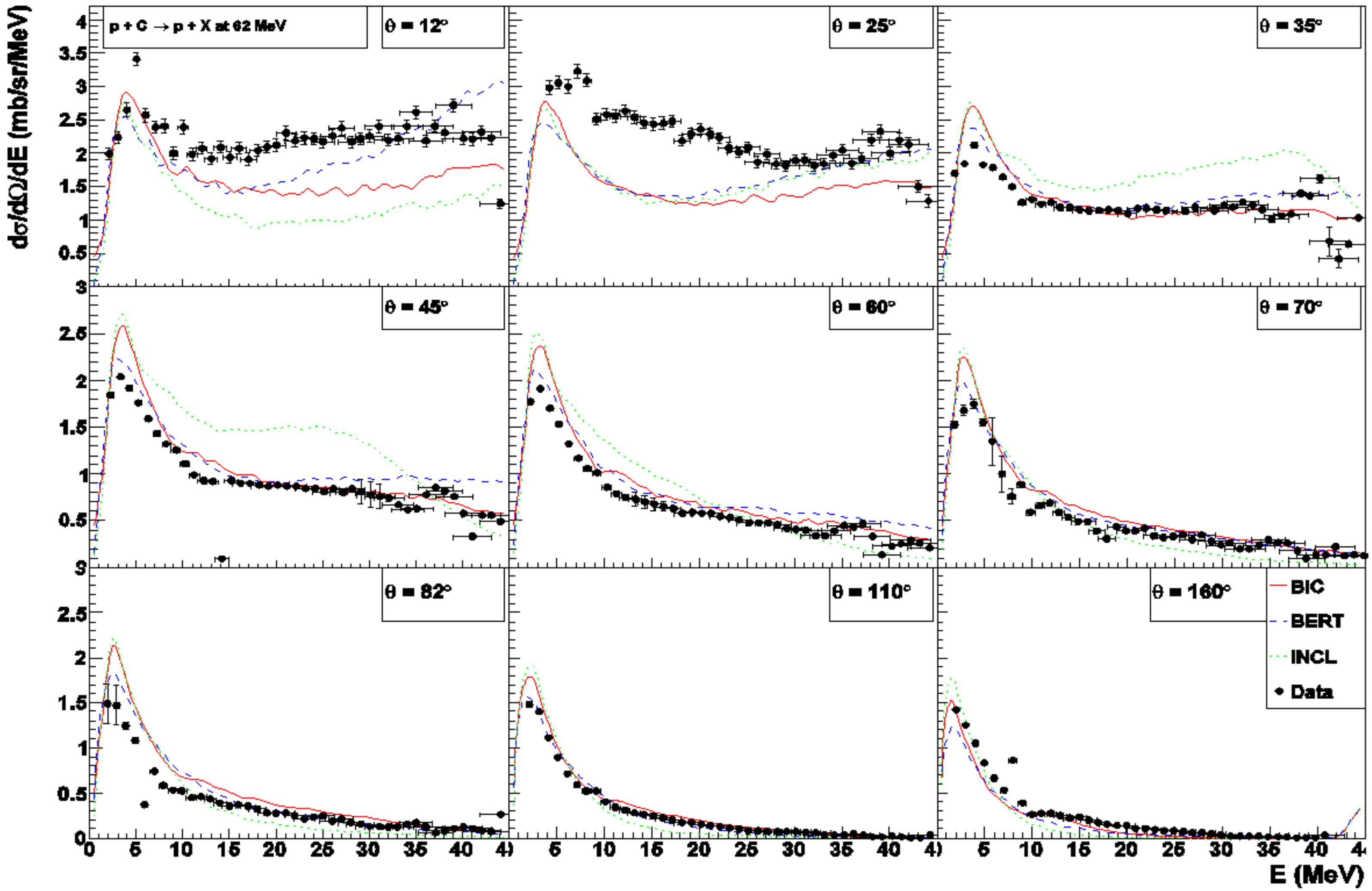
Double differential neutron production cross section for 256 MeV protons in Al target

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



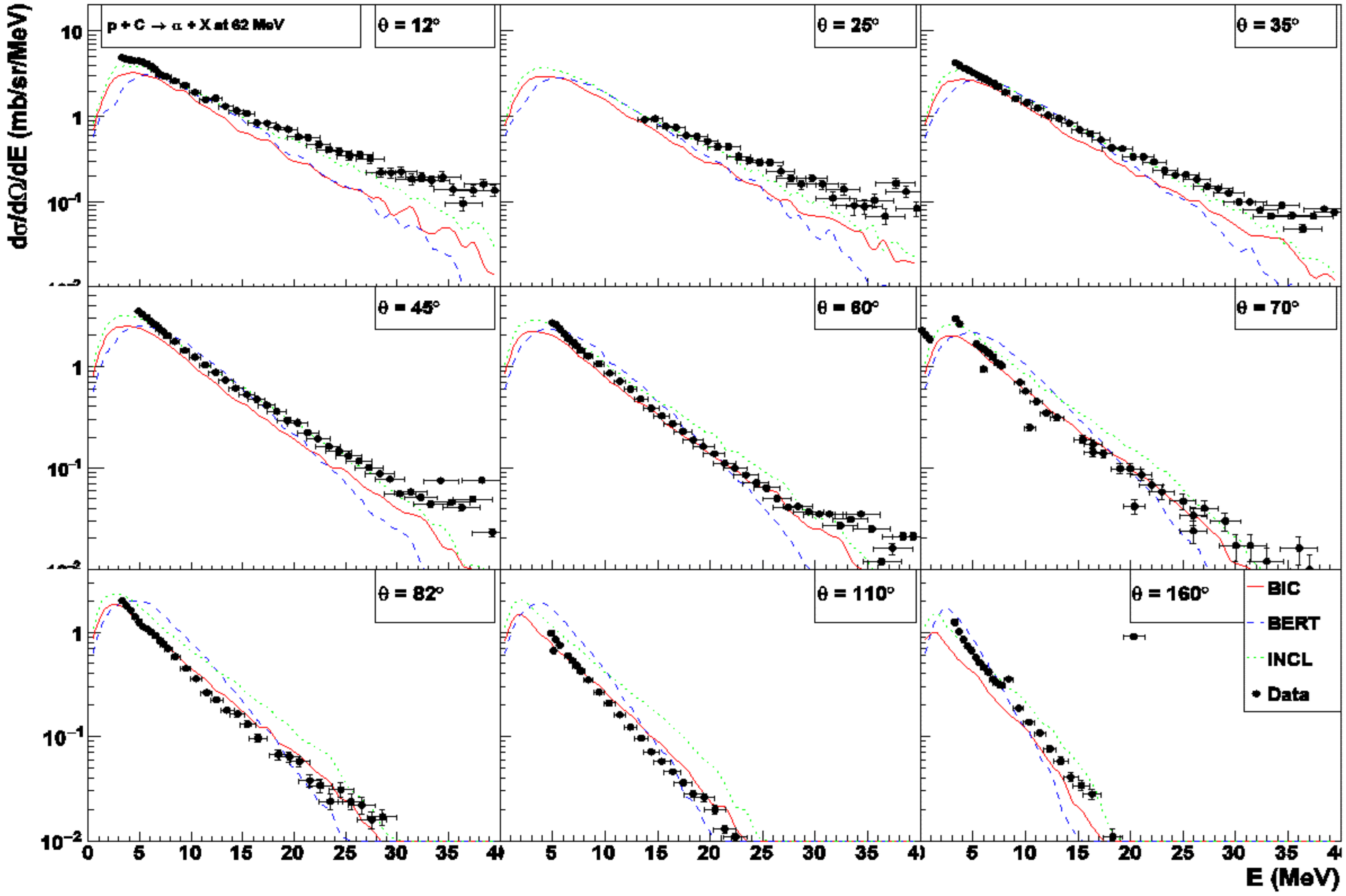
Double differential proton production cross section for 62 MeV protons in carbon target

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



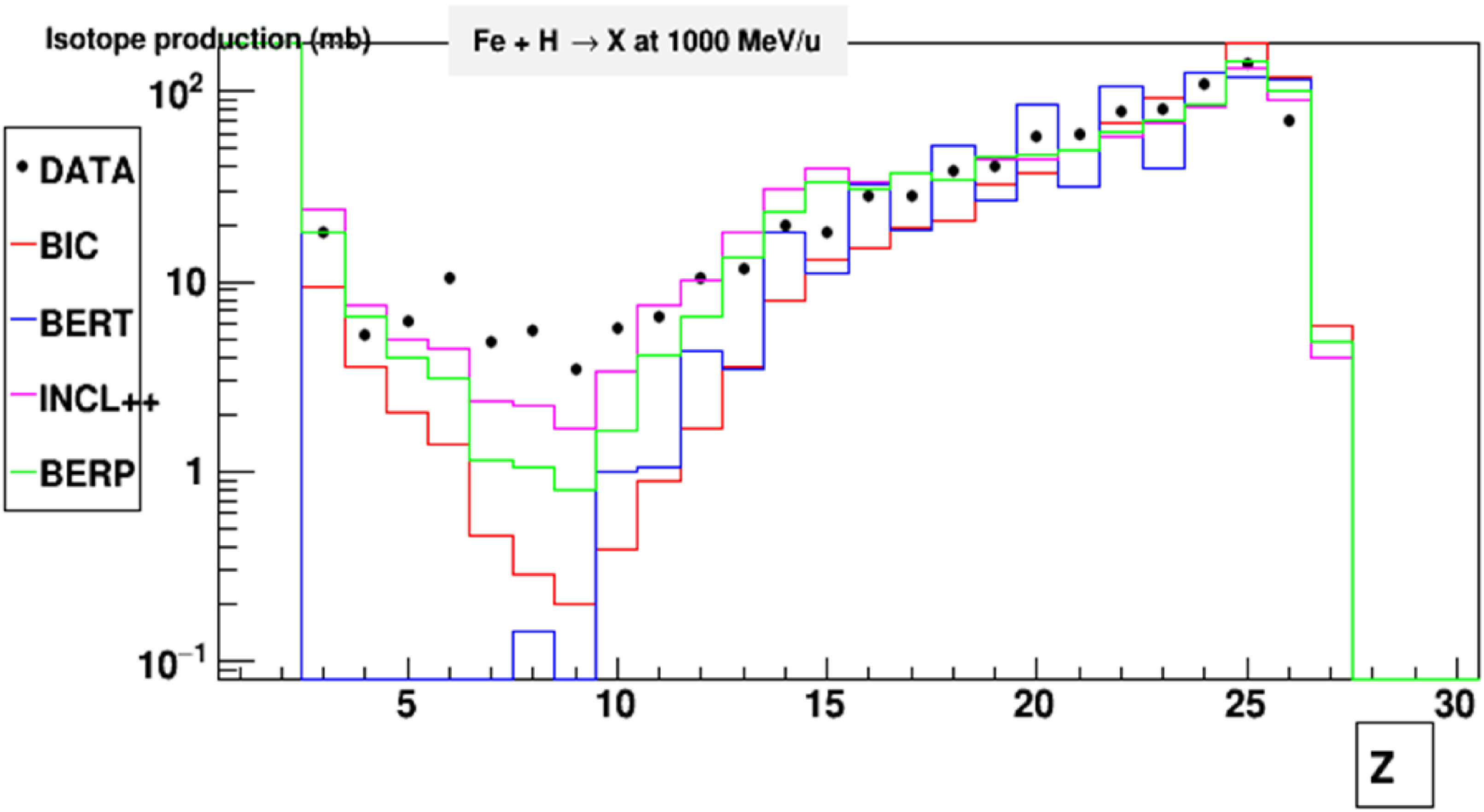
Double differential alpha production cross section for 62 MeV protons in carbon target

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