GEANT4: Models and links to cosmic rays, gamma rays, and accelerator physics

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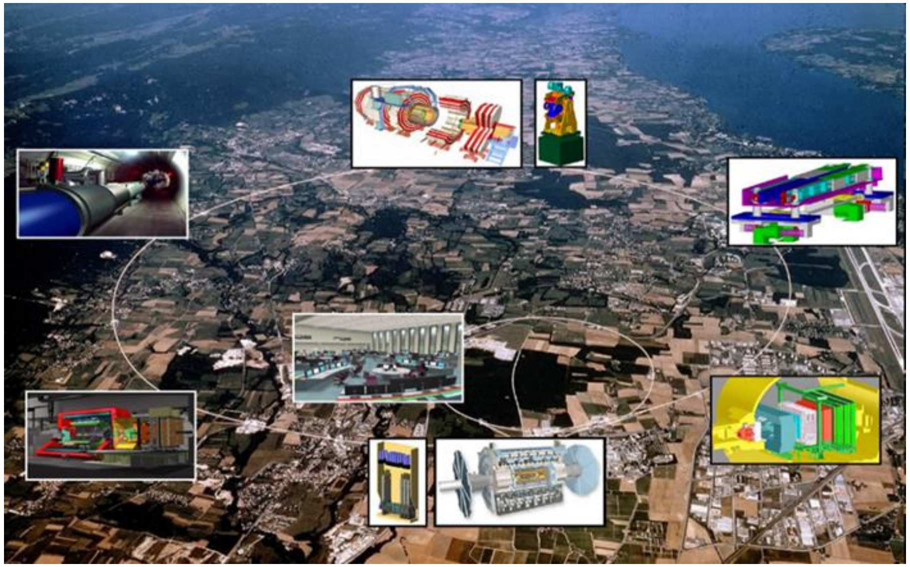
XSCRC2019: Cross sections for Cosmic Rays @ CERN
13-15 November 2019, CERN

Outline

- General Introduction
  - Geant4 history
  - Geant4 version 10.X
- Geant4 physics design
  - Configuration of physics
- Electromagnetic physics
  - EM sub-libraries
  - Specific models
- Hadronic physics
  - Hadronic final states
- Hadronic cross sections
- Summary

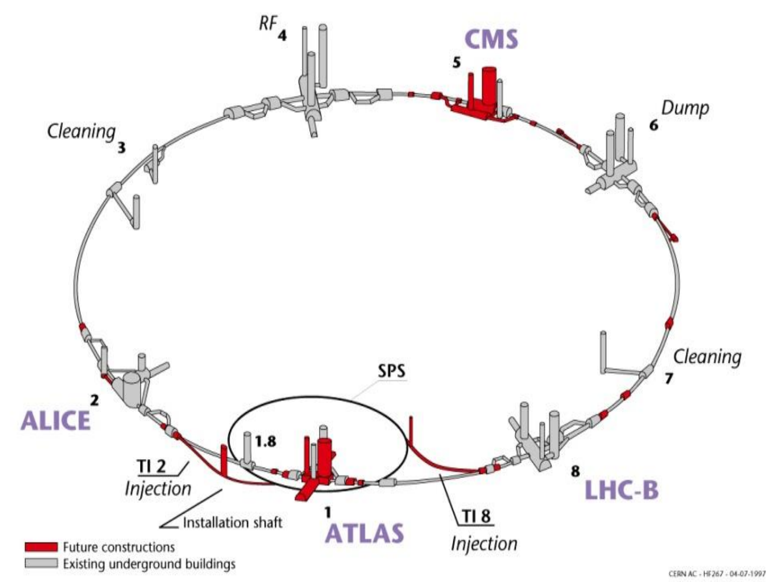


In this talk we will focus only on some physics aspects of Geant4 relevant to the workshop goals

Geant4 History

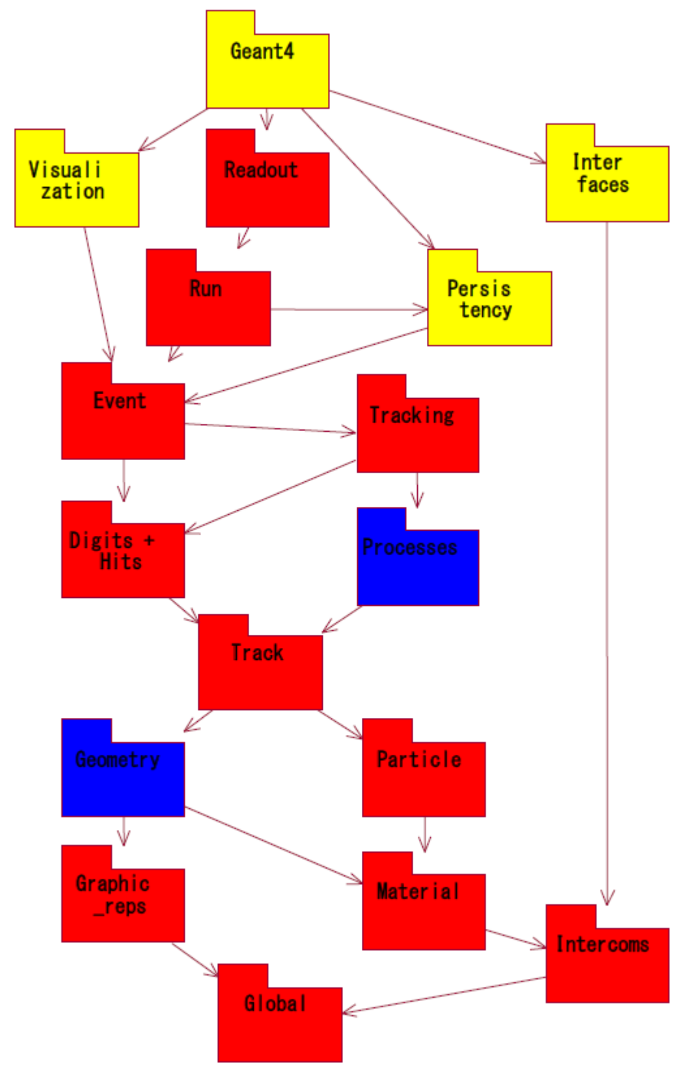
- Dec 1994 - Project start
- ...
- Dec 1998 - First Geant4 public release - version 0.0
- …
- Dec 2010 - Geant4 version 9.4 – RUN 1 LHC
- ...
- Dec 2012 - Geant4 version 9.6 – consolidation of 9.X
- Dec 2013 - Geant4 version 10.0 - multi-threading
- ....
- Dec 2018 – Geant4 10.5
  - April 2019 10.5p01
- Geant4 developments were strongly supported by HEP community
  - LHC experiments have always been the goal
  - Space and medical user communities also contribute significantly to Geant4 developments
  - Main publication: «Geant4 - a simulation toolkit» NIM A 506 (2003) 250 (> 10000 citations) http://www.sciencedirect.com/science/article/pii/S0168900203013688

Layout of the LEP tunnel including future LHC infrastructures.



What is Geant4 toolkit?

- Monte Carlo toolkit for simulation of particle transport in matter
  - Consists of 17 categories with well defined and stable interface
- Flexible geometry
  - Many different shapes
  - GDML exchange formal
- Tracking in electric and magnetic field
  - Including spin precession
- Wide variety of visualization and I/O options
- Built in scoring and analysis
- Many physics models
  - Electromagnetic physics
    - including Geant4-DNA extension
  - Hadronic physics
    - Including low-energy neutron transport and radioactive decay
  - Optical physics
  - Phonon physics

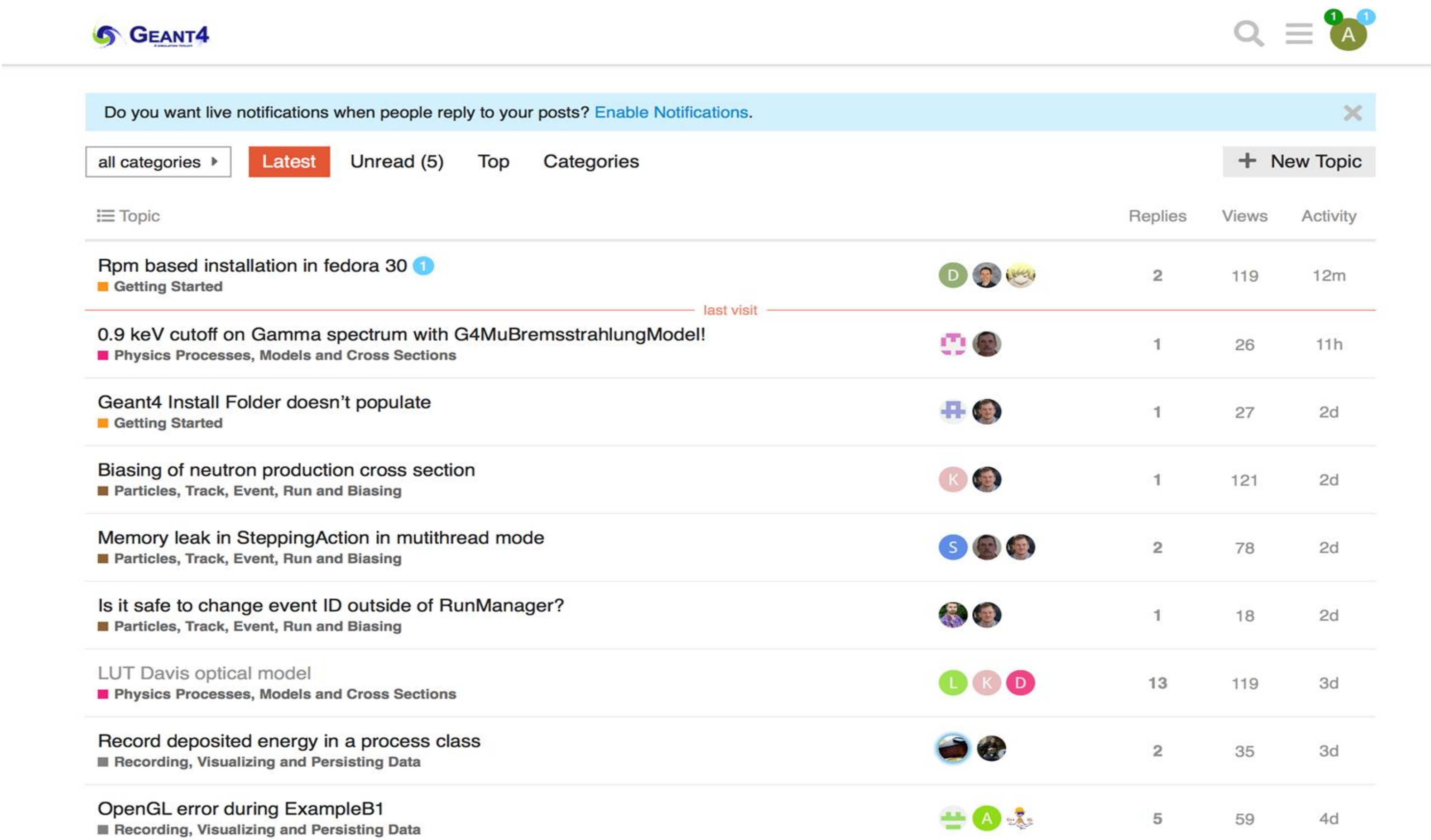


Geant4 Version 10 Series

- Geant4 version 10.0 was released on December 2013
  - Introduction of the multithreaded (MT) mode
    - Event level parallelism
  - Many users have successfully migrated to version 10 series and started to use it in the MT mode.
    - CMS is ahead of other LHC experiments using 10.X:
      - ~100 billions events produced using Geant4 for Run-2
      - current CMS production 10.4.p03-MT
    - ATLAS production version 10.1p03
    - LHCb and ALICE are using 10.X as well
- Geant4 10.6 (December,6 2019) will be available soon
- Details of version 10 are described in
  - J. Allison *et al.*, "Recent Developments in Geant4", NIM A 835 (2016) 186-225 http://www.sciencedirect.com/science/article/pii/S0168900216306957

Geant4 web interfaces are updated

- New Geant4 web design and user documentation: http://geant4.web.cern.ch/
- Discourse – new user forum system: https://geant4-forum.web.cern.ch



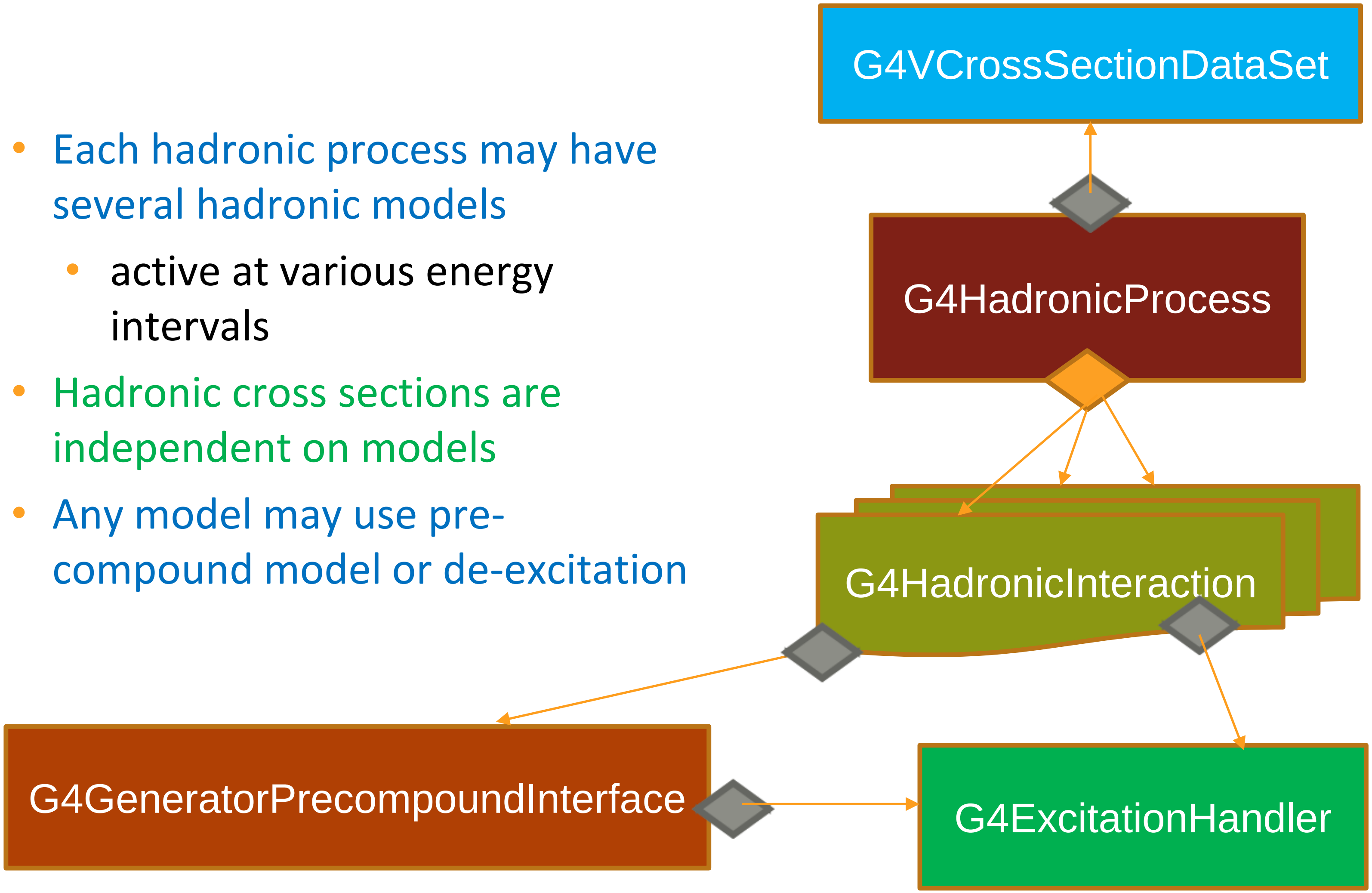
Geant4 physics design

Main approach:

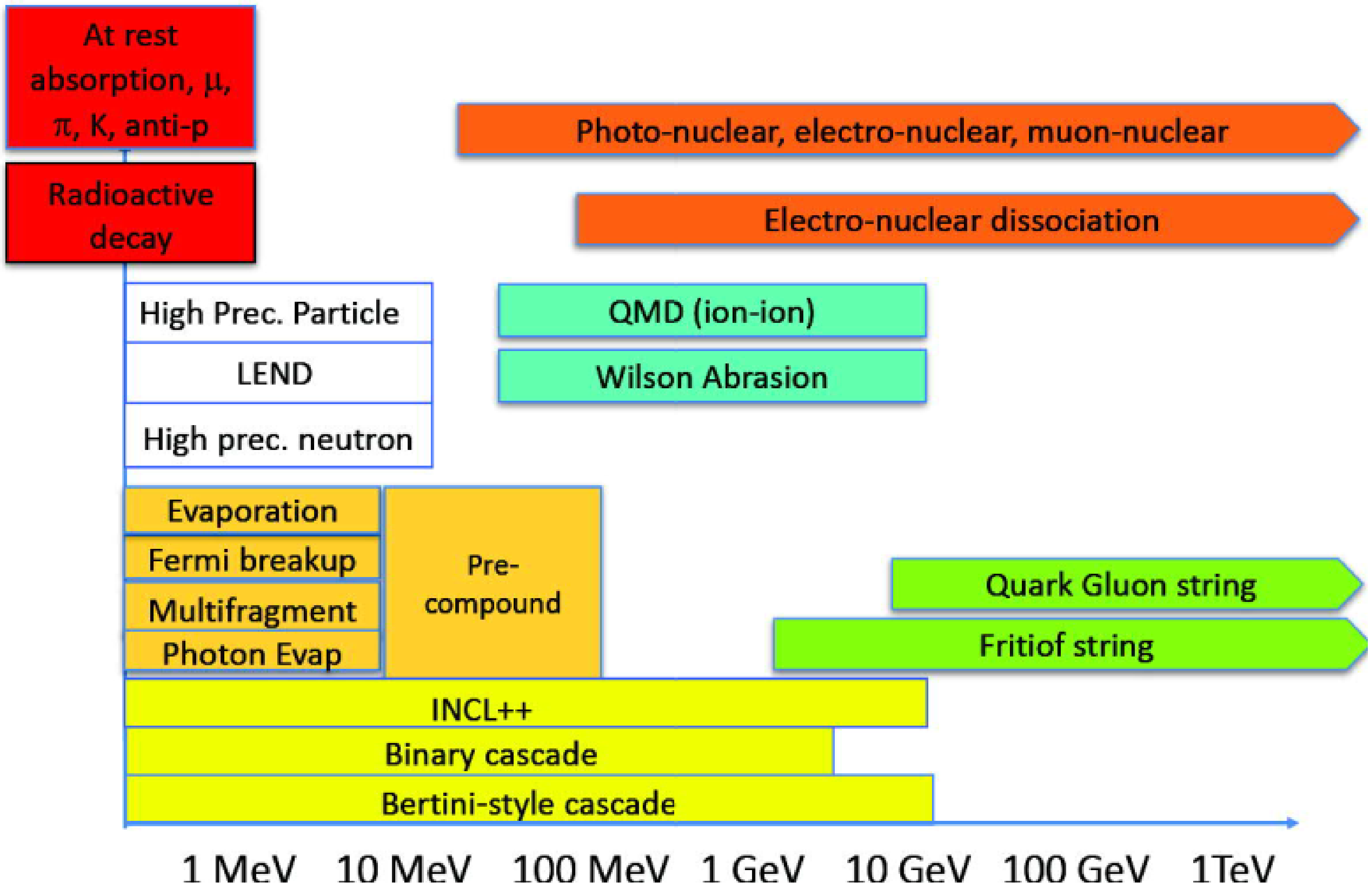
- abstract interface to physics
- stable for the long period of time

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

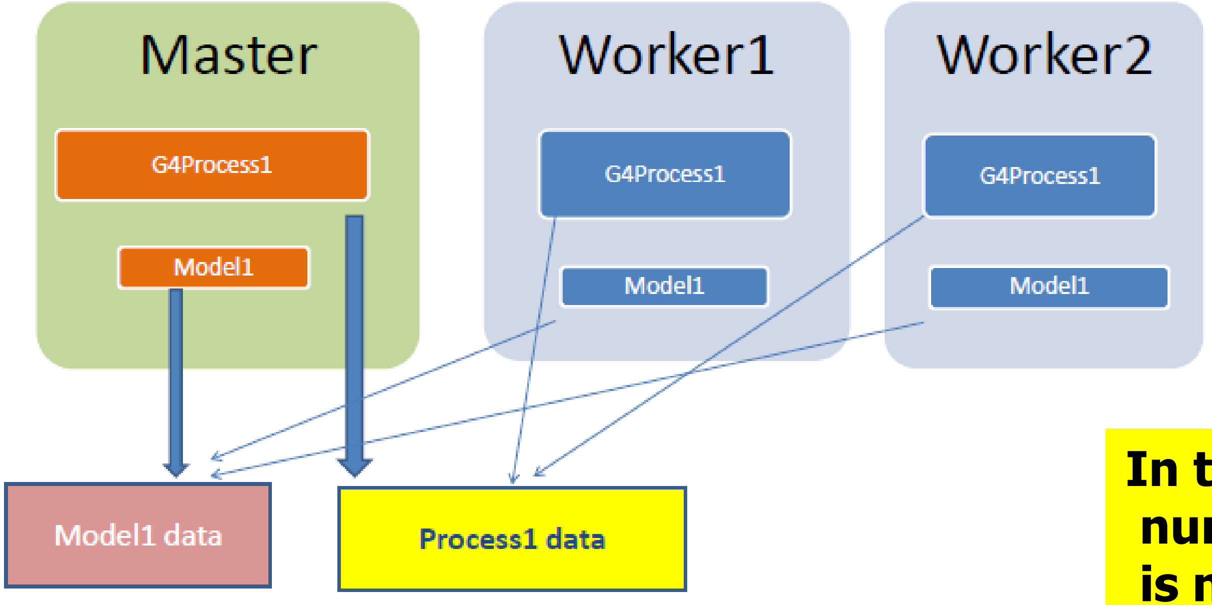


Geant4 hadronic models



EM Data Sharing for Geant4 MT

- The scalability of Geant4 10.X application in the MT mode depends on how effectively data management is performed
- Shared EM physics data:
  - tables for cross sections, stopping powers and ranges are kept by processes
  - Differential cross section data are kept by models
  - Material propertes are in material data classes
  - EM parameters established for Physics Lists in the G4EmParameters class



Tables are filled by Master and have read-only access in run time

In this scheme number of threads is not limited

Geant4 physics configuration

- Organized via abstract interfaces
- Physics List class is responsible for configuration of physics
- Geant4 provides several reference Physics Lists
  - Since version 9.6 Geant4 default is FTFP_BERT
  - Components of a reference Physics List:
    - Electromagnetic physics (EM)
    - Photo- electro-, muon- nuclear interactions
    - Hadron elastic
    - Hadron inelastic
    - Stopping processes
    - Ion processes
    - Neutron limiter
- User may customize a reference Physics List
  - For example, add optical physics
  - May choose one of alternative EM configurations
  - May use UI macro command or C++ interface to tune EM parameters
    - For example, cuts per detector region
- User may combine custom configuration from components
  - It is possible to add custom component
- User may use fully custom physics list

Validation of Geant4 physics

- For each new version of Geant4 a set of tests are executed
  - Integration tests
  - Regression tests
  - Tests versus data
- General approach of Geant4:
  - Physics models are tuned only for thin target tests or to theoretical predictions
    - This allows to keep prediction power of the toolkit
  - We prefer leave some inaccuracy of simulation than add not well justified tuning
- Test results are available:
  - http://cern.ch/geant4/publications_validations/testing_and_validation
- Publications:
  - http://cern.ch/geant4/publications

Electromagnetic physics

Main recent developments:

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

Geant4 EM libraries

- Low-energy
  - Livermore library γ, e- from 10 eV up to 1 GeV
  - Livermore library based polarized processes
  - PENELOPE code rewrite , γ, e- , e+ from 100 eV up to 1 GeV (2008 version)
  - hadrons and ions up to 1 GeV
  - atomic de-excitation (fluorescence + Auger)
- Geant4-DNA
  - microdosimetry models for radiobiology (Geant4-DNA project) from 0.025 eV to 10 MeV
- Adjoint
  - Reverse Monte Carlo processes and models to track from the volume of interest back to source of radiation
- Utils
  - general EM interfaces
- Standard
  - γ, e± up to 100 TeV
  - hadrons up to 100 TeV
  - ions up to 100 TeV
- Muons
  - up to 1 PeV
  - energy loss propagator
- X-rays
  - X-ray and optical photon production processes
- High-energy
  - processes at high energy (E>10GeV)
  - physics for exotic particles
- Polarisation
  - simulation of circular polarized beam transport
- Optical
  - optical photon interactions

New standard EM models in 10.5

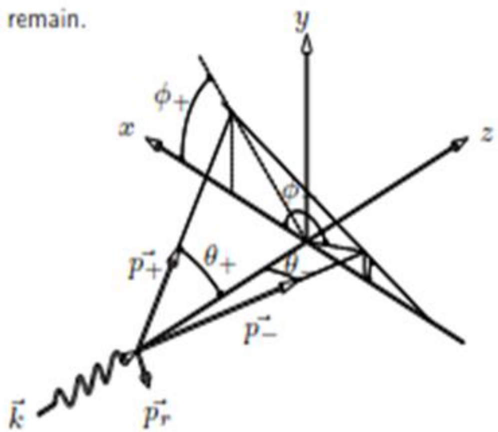
- G4BetheHeitler5DModel
  - Accurate sampling of final state
  - Nuclear recoil and polarisation are taken into account
- Ion ionisation based on Lindhard-Sorensen theory
  - G4LindhardSorensenModel – parameterisation above 10 MeV
  - G4AtimaEnergyLossModel – implementation of ATIMA code in C++
  - G4AtimaFluctuations – relativistic ion energy loss fluctuations
- 3-gamma annihilation model
  - G4eplusTo2GammaOKVIModel and G4eplusTo3GammaOKVIModel classes implement 2-gamma and 3-gamma positron annihilation in fly and at rest
  - Probability of 3-gamma final state depends on cut for 3d gamma energy

Gamma conversion to lepton pair model

by D. Bernard and I. Semeniouk (LLR, CNRS/IN2P3, Ecole Polytechnique)

A 5D phase space

- 3 particle final state, $4 - 1 = 3$ free parameters for each one.
- energy-momentum conservation fixes 4 of them.
- $3 \times 3 - 4 = 5$ variables remain.



- $+, -, r$ = positron, electron, recoil. ϕ azimuthal, θ polar angles.
- $\Omega \equiv (\phi_+, \phi_-, \theta_+, \theta_-, x_+ \equiv E_+/E_\gamma)$

The model was developed for e+e- pair production but is applicable to muon pair production

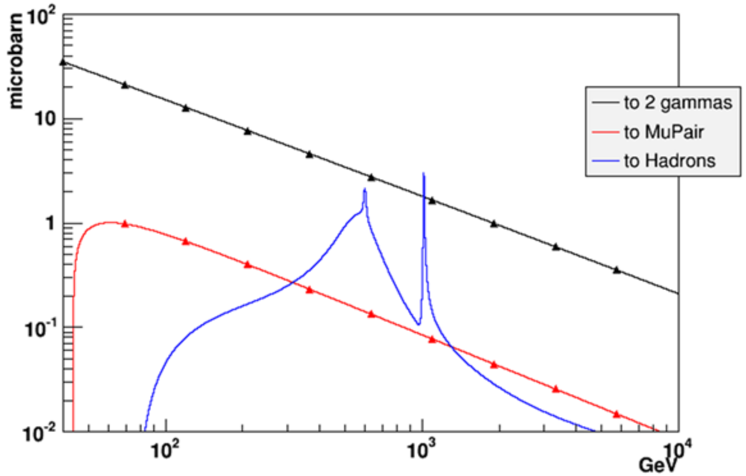
Linear polarisation of incoming gamma, nuclear recoil, and triplet production are taken into account

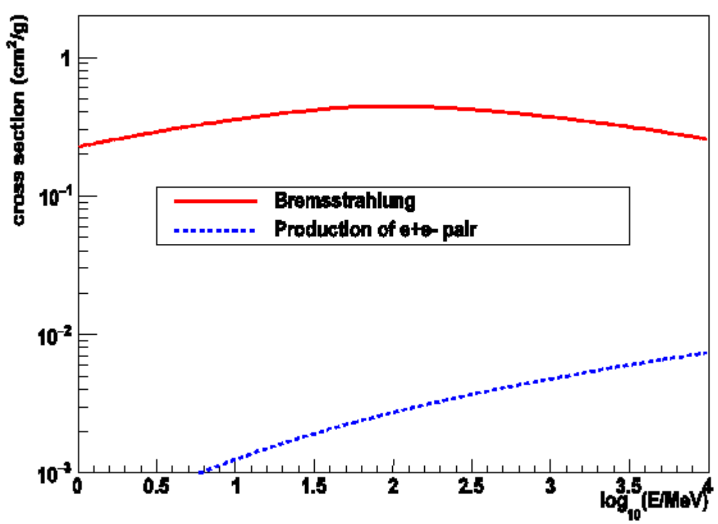
In 10.6 can be applied for full energy range from threshold and for muon pair production

- List of publications (+references inside)
  - P. Gros and D. Bernard, Astropart. Phys. 88, 60 (2017)
  - D. Bernard, Nucl. Instrum. Meth. A 899, 85 (2018)
  - V. Ivanchenko et al., EPJ Web of Conferences 214 02046 (2019)

Geant4 simulation of positron transport

- Main Geant4 positron EM interactions:
  - Ionisation
    - With nuclear form-factor corrections
  - Bremsstrahlung
    - With LPM effect
  - Two gamma annihilation
    - Optionally 3-gamma annihilation
- Rare positron processes:
  - Annihilation to $\mu+\mu-$
    - Are of concern for FCC, CLIC,
  - Annihilation to hadrons
  - e+e- pair production
    - Light dark matter search





High energy positron annihilation

- High energy positron annihilation
  - — In high energy physics, incident e^+ would annihilate with atomic e^- by the following processes[1].
  - — these processes may provide a background to the interaction region of linear collider(for example, CLIC) or to search for new physics at LHC.

Processes

e^+e^-

$\rightarrow \gamma\gamma$

$\rightarrow \mu^+\mu^-$

$\rightarrow \pi^+\pi^-$

$\rightarrow \pi^+\pi^-\pi^0$

$\rightarrow K^+K^-$

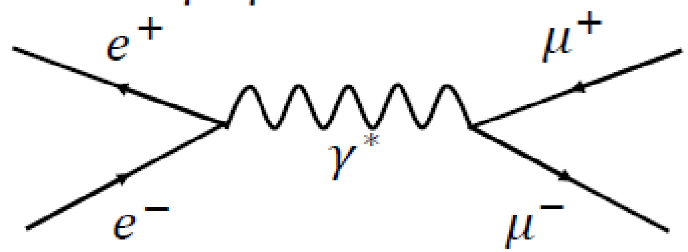
$\rightarrow K_L K_S$

$\rightarrow \eta\gamma$

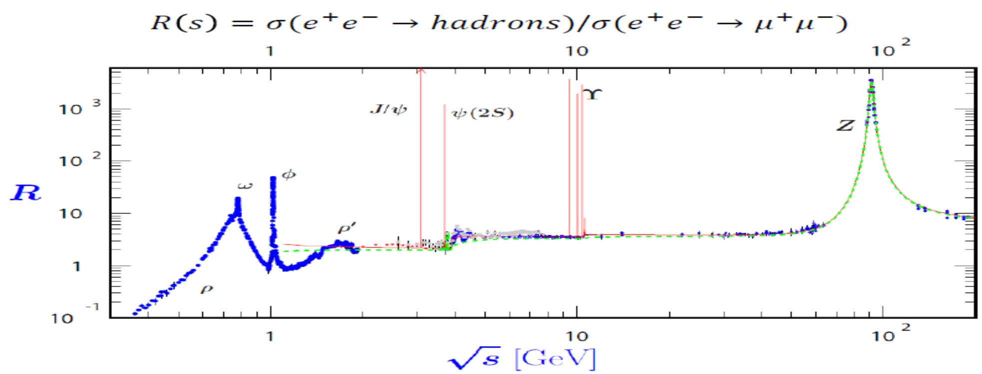
$\rightarrow \pi^0\gamma$

J. Phys: Conf. Ser. 664: 072021, 2015.

ex) $e^+e^- \rightarrow \mu^+\mu^-$



PDG data



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 (EMY) with simplified multiple scattering and other options
  - The alternative Opt4 (EMZ) physics is 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
- 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 or more G4Region(s)
    - This feature is used already by ALICE and CMS

Hadronic physics

Main recent developments:

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

Geant4 hadronic physics

- Cross section sub-library
  - Decoupled from models and processes
  - There is an interface allowing to add alternative cross section
- Hadronic processes
  - Elastic
  - Inelastic
  - Stopping
  - Fission
- Models follow the same interface for all type of processes
  - Nuclear de-excitation module may be reused between models
  - Radioactive decay module reuses nuclear de-excitation
- Several data sets used by Geant4 hadronics
  - Nuclear levels
  - Nuclear transitions
  - Radioactive decay parameters
  - Hadron cross sections
  - Neutron cross sections
- A user can add modifications replacing/adding a data file

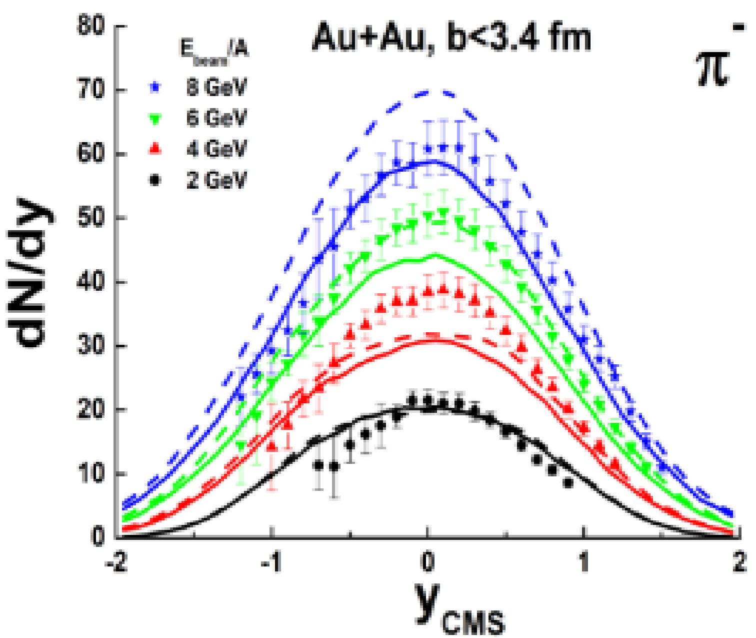
String Models Developments

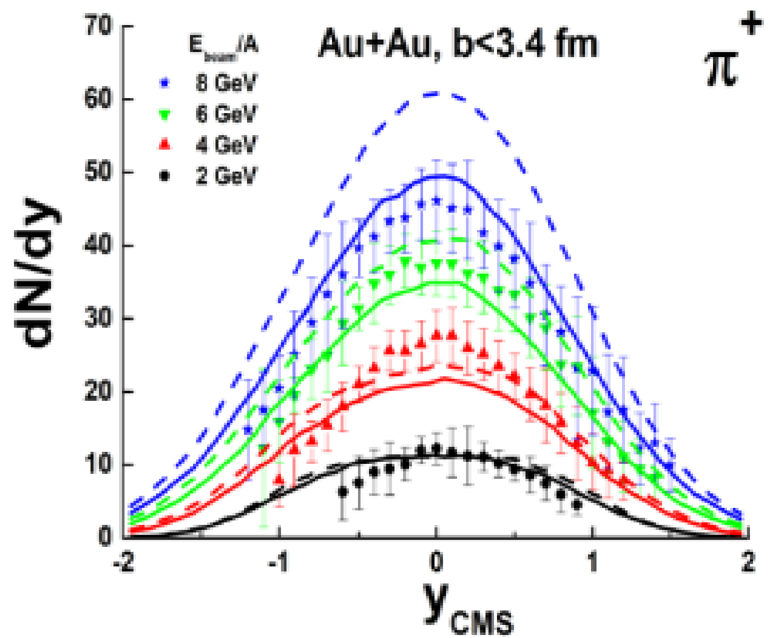
- Since 10.5 development versions of FTF and QGS are merged to the production release
  - Between 10.1 and 10.4 we tried to keep stability for simulation of Run-2 for LHC experiments
- FTF improved for
  - thin target benchmarks
  - Introduced rotating strings and smearing of resonance masses
  - Interactions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

FTF string model improvement for pion production

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,





Dashed lines are previous calculations, solid ones – current results.

Results become better for high energies, T > 6 GeV.

Interface to Fortran EPOS

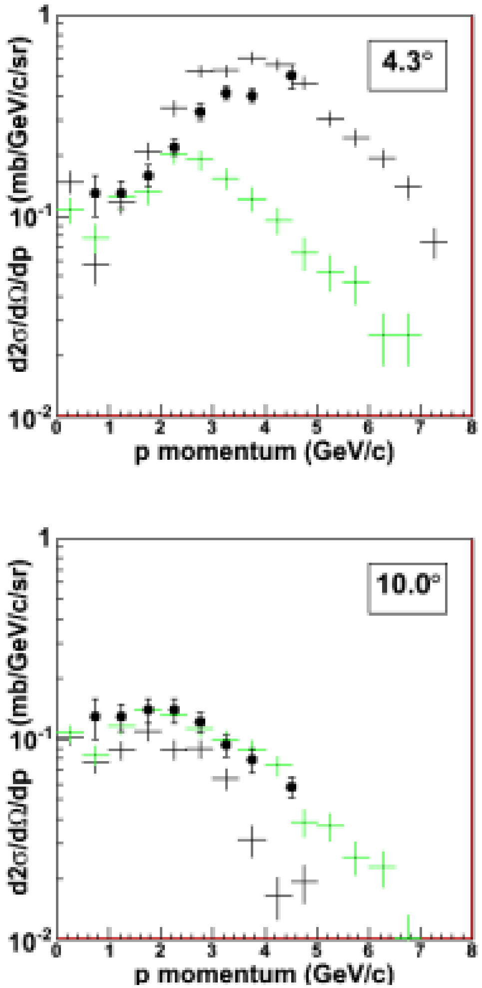
- The hadronic extended example **Hadr02** in G4 **10.5** includes an interface to **CRMC** (Cosmic Ray Monte Carlo) – which offers the possibility to use generators like **EPOS** for final-state hadron-nucleus (and nucleus-nucleus) inelastic collisions at very high energies – and created a (local) physics list which uses this interface
  - The Physics List is called CRMC_FTFP_BERT and the transition between CRMC and FTFP is currently set to be [100, 110] GeV
  - Main interest for **FCC**, to simulate **jets above ~ 10 TeV**
    - Hadron-nucleus interactions up to at least ~ 1 TeV (projectile kinetic energy in the Lab frame) are expected to be well described by the Geant4 string models (FTF & QGS); above this, missing gluon-jet production
  - Currently under testing in the context of FCC
    - At model-level we see fewer and more energetic secondaries in G4 FTF & QGS with respect to EPOS due to the lack of gluon-jet emissions
  - Needs a special version of CRMC adapted for Geant4 use...

Cascade models in 10.6

- The main production cascade model is the Bertini cascade
  - Phase space decay generator – improved multibody final state generation
- Main developments for INCLXX was for 10.5:
  - Improved strangeness production
  - Provide the best description of d, t, He3, He4 production
  - New dataset INCL1.0
- Only few bug fixes in the Binary cascade
  - Transition energy with the Bertini cascade 1-1.5 GeV
  - The Binary cascade is the most accurate for neutron production at low energy

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

Pre-compound model and de-excitation module

- Established set of model parameters for PRECO and DEEX and user interface to these parameters
- Renewed internal data structure for nuclear levels
  - 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
- It was completed in general for Geant4 10.4
  - However, some fixes and improvements will be introduced in 10.6

Fermi-BreakUp model

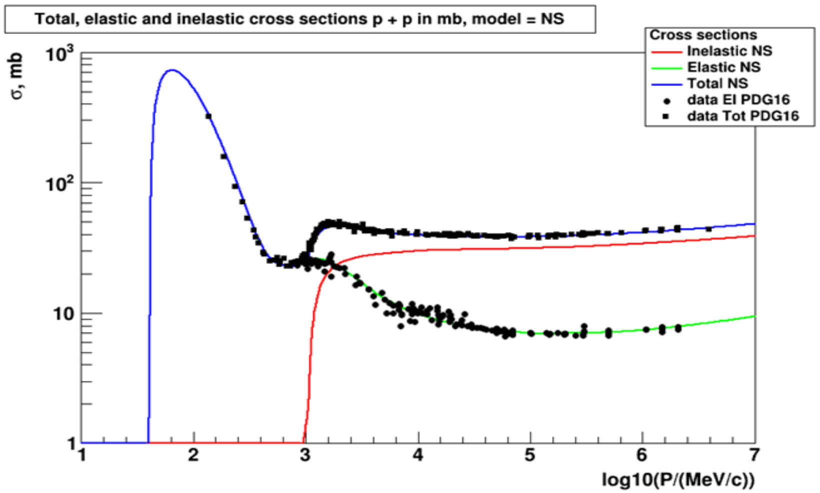
- Old G4FermiBreakUp model was based on hard-coded data
  - A pool of 112 states, Z < 9, A < 17
  - Precomputed probabilities of decay of each state from this pool into 2-, 3-, 4- body final state from this pool
- New G4FermiBreakUpVI model fully based on data of G4GAMMALEVELDATA
  - A pool of 260 states from data files and 399 reactions, Z < 9, A < 17 (10.4)
  - A pool of 380 states from data files and 991 reactions, Z < 9, A < 17 (10.5)
    - Maximal excitation energy 20 MeV
  - Only binary decay chains are considered
    - A standard Coulomb barrier computation is used
  - Probability of the first decay is computed on fly if initial excitation of the primary fragment is not equal to one of known levels
    - The second and others decay probabilities are precomputed
  - Final product is always a list of states from the main pool, which has no Fermi decay channel
    - may have gamma transition

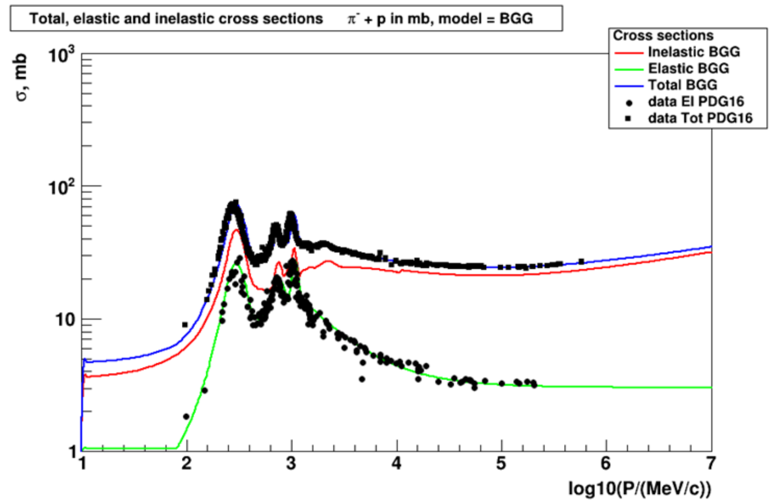
Hadronic Cross Sections

Main recent developments:

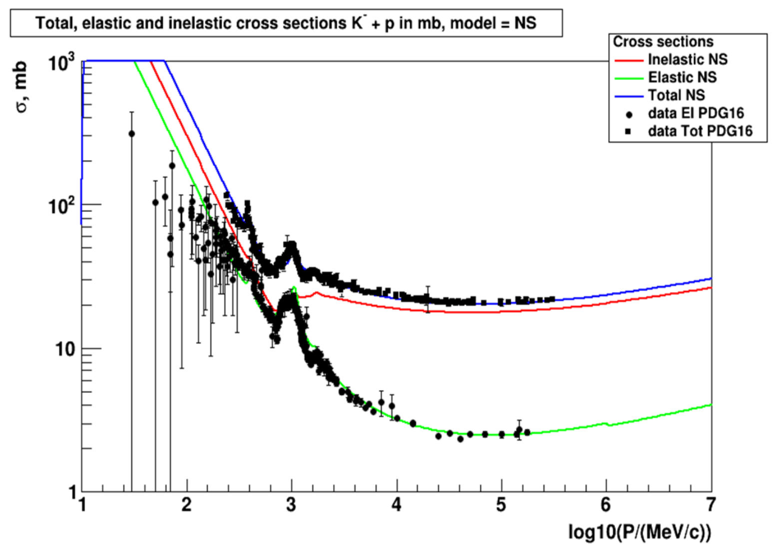
- improved elementary cross section parameterisations
- Glauber approach for hadron-nucleus and ion-nucleus cross sections
- high precision (HP) data driven cross sections

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, B- and C- mesons and baryons



Geant4 hadronic cross sections

NIM A 835 (2016) 186-225

- In Geant4 10.6 the Glauber-Gribov model will the main for all particle at any energy:

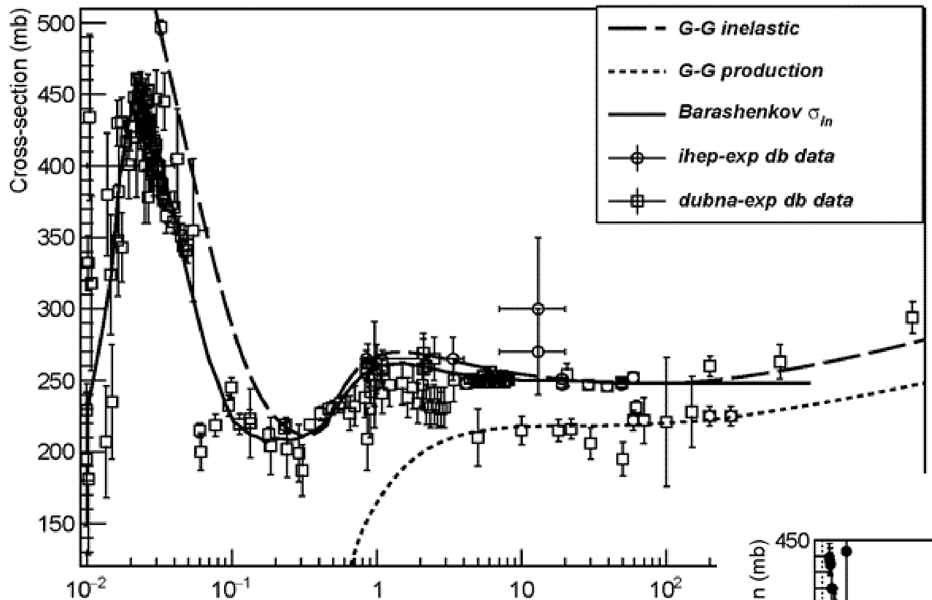
$$\sigma_{tot}^{hA} = 2\pi R^2 \ln\left[1 + \frac{A\sigma_{tot}^{hN}}{2\pi R^2}\right], \quad \sigma_{in}^{hA} = \pi R^2 \ln\left[1 + \frac{A\sigma_{tot}^{hN}}{\pi R^2}\right],$$

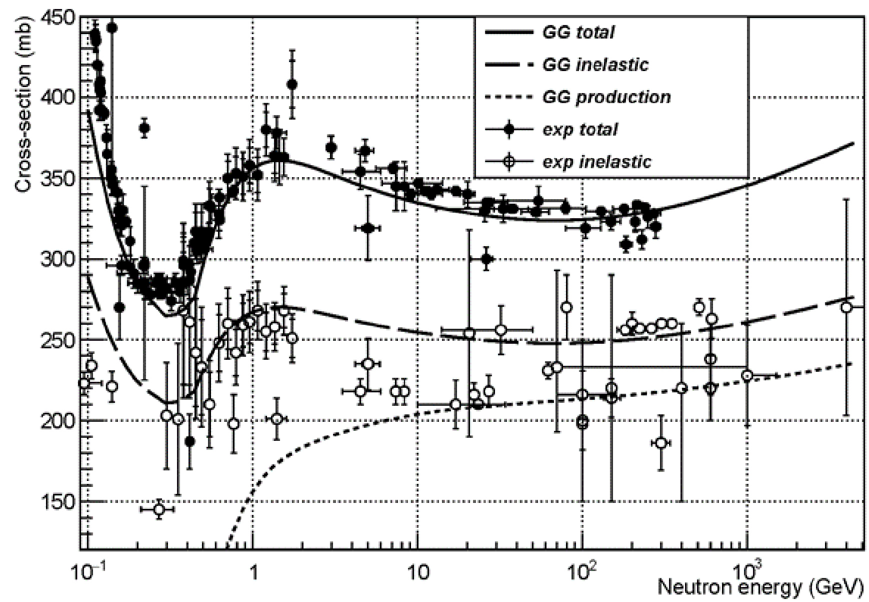
$$\sigma_{prod}^{hA} = \pi R^2 \ln\left[1 + \frac{A\sigma_{in}^{hN}}{\pi R^2}\right], \quad \sigma_{el}^{hA} = \sigma_{tot}^{hA} - \sigma_{in}^{hA}, \quad \sigma_{qe}^{hA} = \sigma_{in}^{hA} - \sigma_{prod}^{hA},$$

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

- 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-
  - Coulomb barrier for positively changed
  - Similar formulas for nuclear-nuclear cross sections
- The accuracy for hadron-nuclear and nuclear-nuclear cross sections may be estimated on level 5-10%
  - Limited by lack of data and data accuracy

Proton and neutron cross sections off Carbon

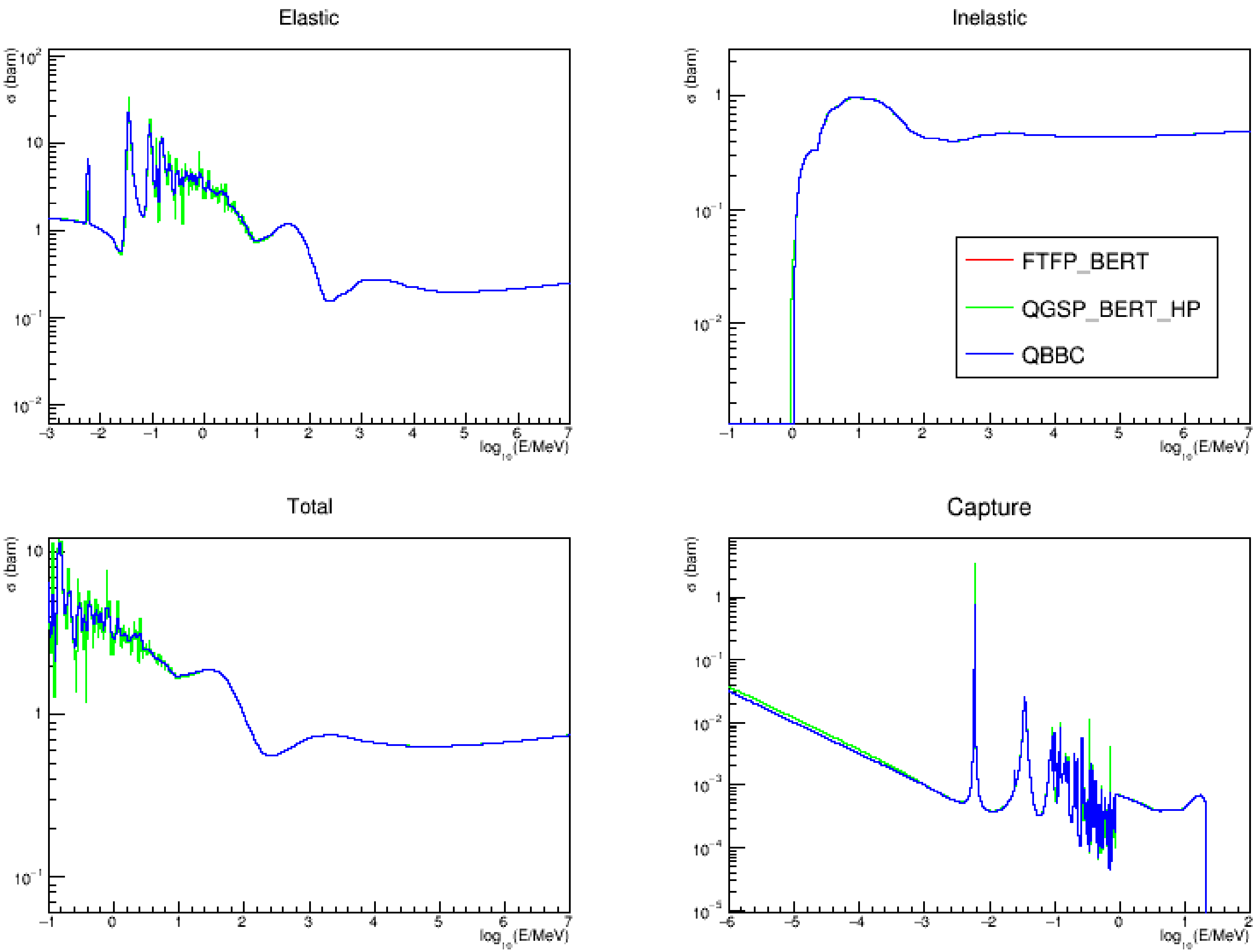




G4PARTICLEXS2.1 – Geant4 10.6

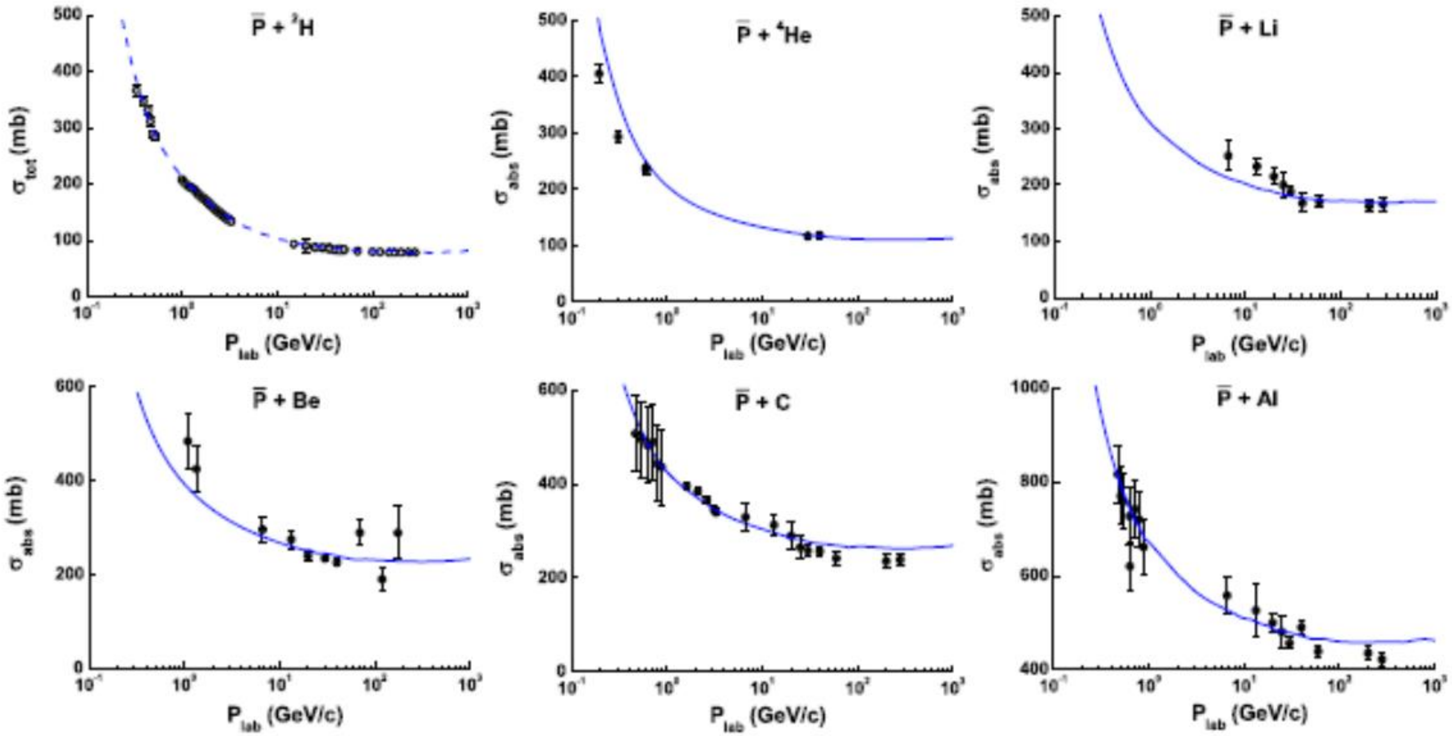
- The new data set shared between threads
  - Separate directories for n, p, d, t, he3, he4 cross sections
  - Element x-sections from threshold to max hadronic energy (100 TeV)
    - Low-energy cross sections extracted from ParticleHP
      - G4NDL4.5
    - Glauber Gribov cross section above 20 GeV for p and n
    - Glauber Gribov cross sections above 20 MeV for , d, t, he3, he4
- Added extra isotope data for 11 more elements (was 17 before)
  - Ne, Mg, S, Cl, K, Sc, Ti, Ga, Pd, In, Pt
  - Limit on isotope abundance is reduced to 0.001 (was 0.01)
- Isotope data are used only for E <= 20 MeV
  - Isotope selection according to isotope cross section
- Element cross sections for E > 20 MeV
  - Isotope abundances are used for isotope selection

Neutron x-sections in Aluminum



HP and non-HP cross sections are similar

Anti-particle cross sections



- A special parameterisation for anti-particles has been developed:
  - V. Uzhinsky et al., Phys Lett B 705 (2011) 235
  - Fit to existing anti-proton data
- Applicable for anti-proton, anti-neutron, anti-deuteron, anti-triton, anti-He3, anti-He4
  - There is no Coulomb barrier, so applicable to full energy range

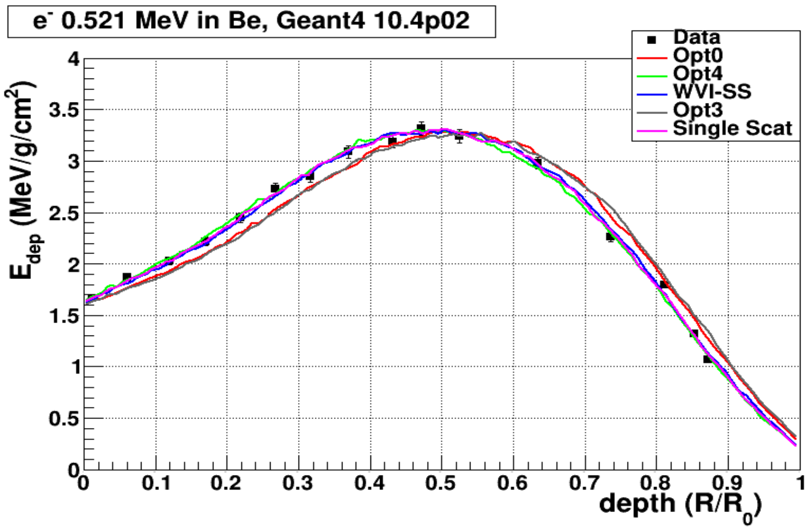
Summary

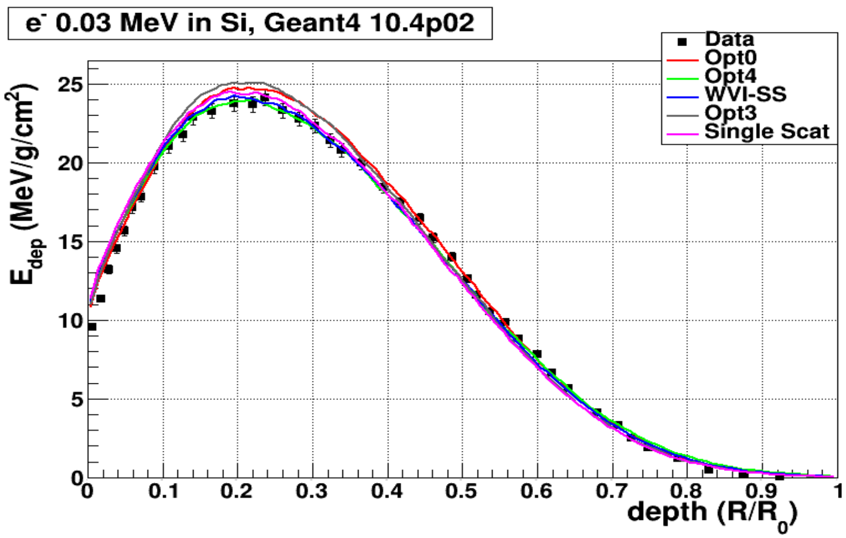
- A new version Geant4 10.6 will be available in December
  - It is likely the last release of the 10 series
  - It will include all updates of EM and hadronic physics
  - Assumed to be used for Run-3 simulations
- Several EM physics models were enhanced
  - New 5D model for gamma conversion
  - 3-gamma annihilation
- Substantial progress in hadronic models
  - FTF and QGS string models
  - Consistent used of nuclear data in the de-excitation module and radioactive decay
  - Nuclear data updated
  - Glauber cross sections are used in all Physics Lists except HP cross sections below 20 MeV

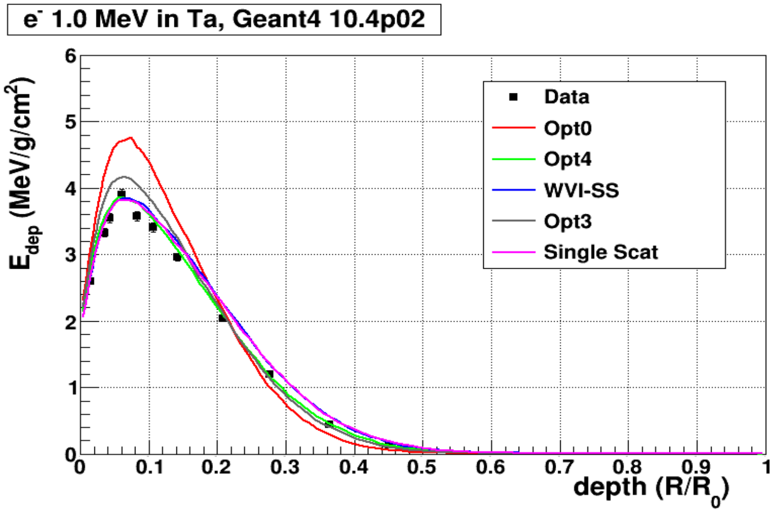
Backup

Energy deposition in semi-infinite media

SANDIA REPORT SAND79-0414.UC-34a







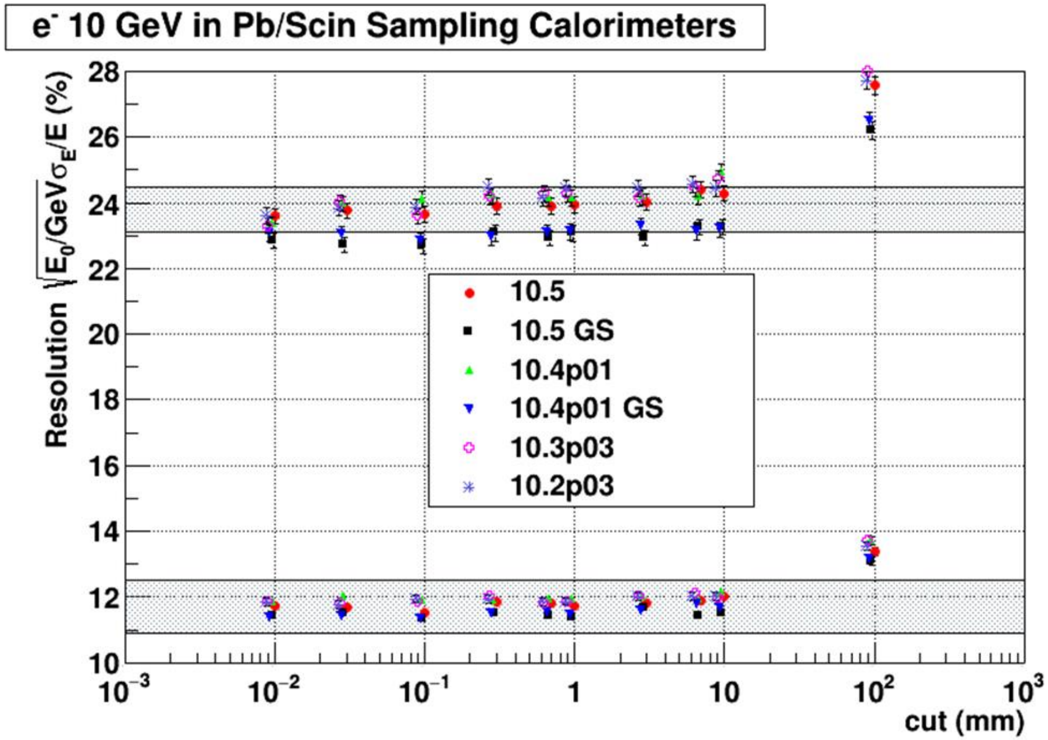
- Recent GS model now describes data for both low and high density media
- Opt0 (default) is not so accurate but is fast
- Opt4 (EMZ) is recommended as an alternative if increased precision is needed but is slower

NIEL Calculator For Radiative Background Studies

- In old Geant4 user should correctly combine tracking cuts and production thresholds in EM physics definition
  - In that case NIEL will be available from the G4Step
  - This method seems to be much more complicate and less obvious to a user
- We introduced G4NIELCalculator helper class in 10.6
  - This class calculate 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 – G4ICRU49NuclearStoppingModel

Resolution of Pb/Sc calorimeters

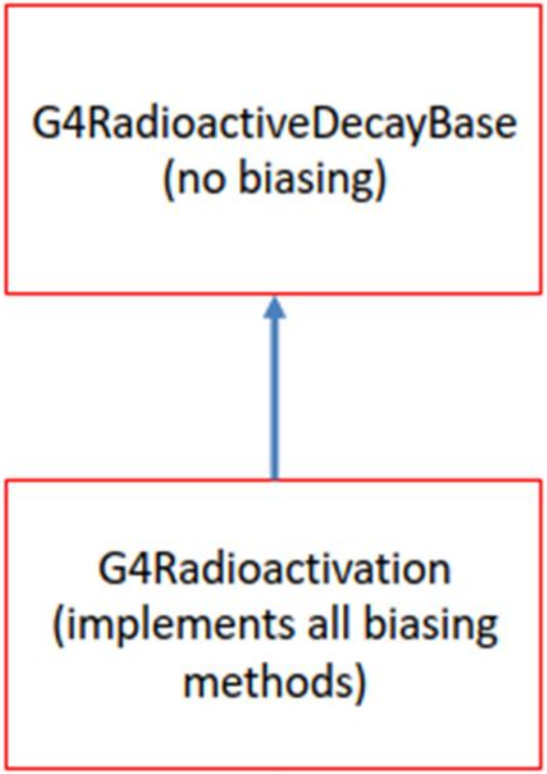
Bernardi E. et al. 1987 Nucl. Instrum. Meth. A 262, 229



- Resolution for 10.5 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

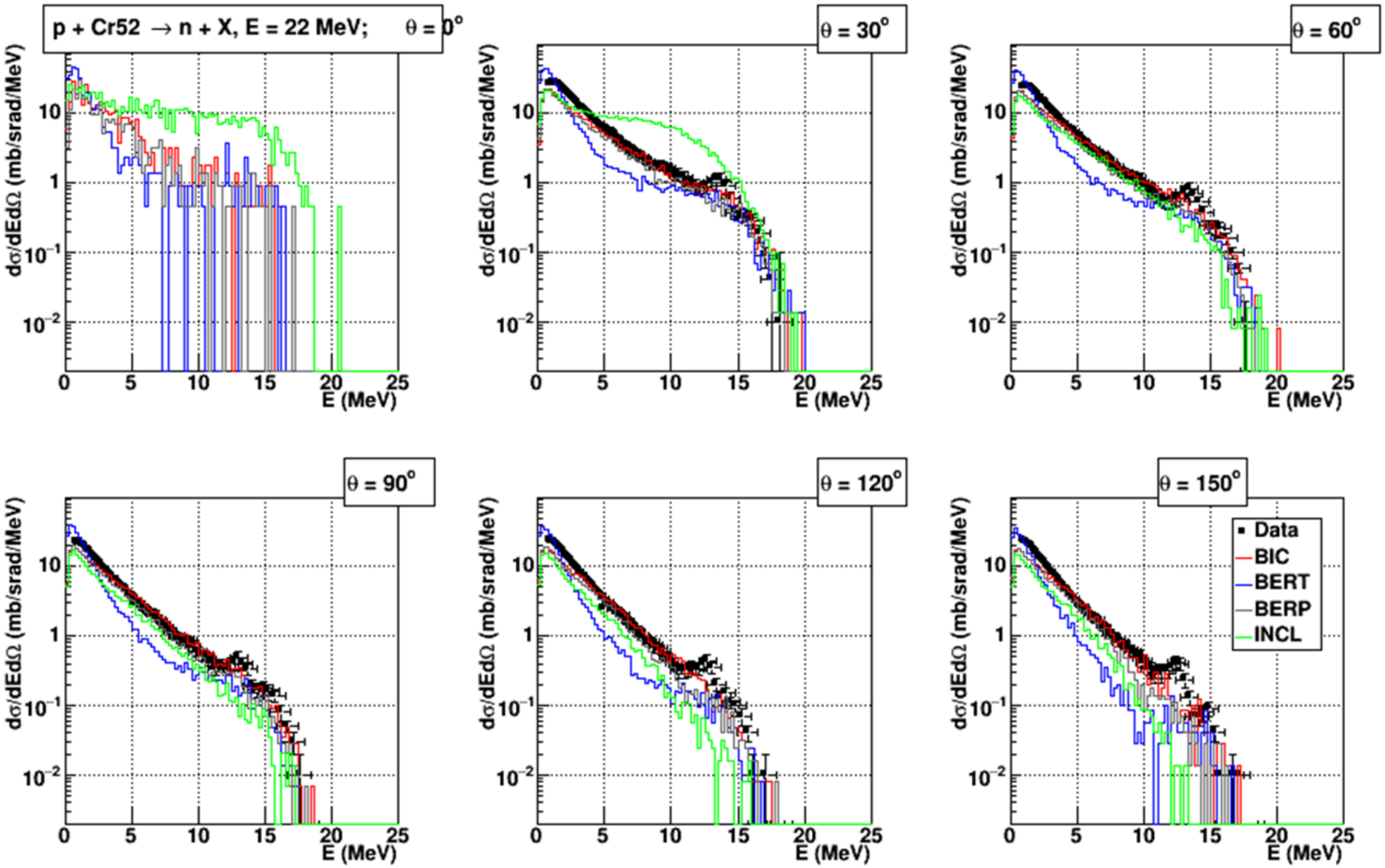
Radioactive Decay Refactoring Completed

- Remove all radioactive decay biasing methods from G4RadioactiveDecay
  - better CPU performance for those not using biasing
  - cleaner code
  - new class name: G4RadioactiveDecayBase
  - rename as G4RadioactiveDecay for major release
- Put all biasing functionality in derived class
  - use for activation studies
  - new class name: G4Radioactivation



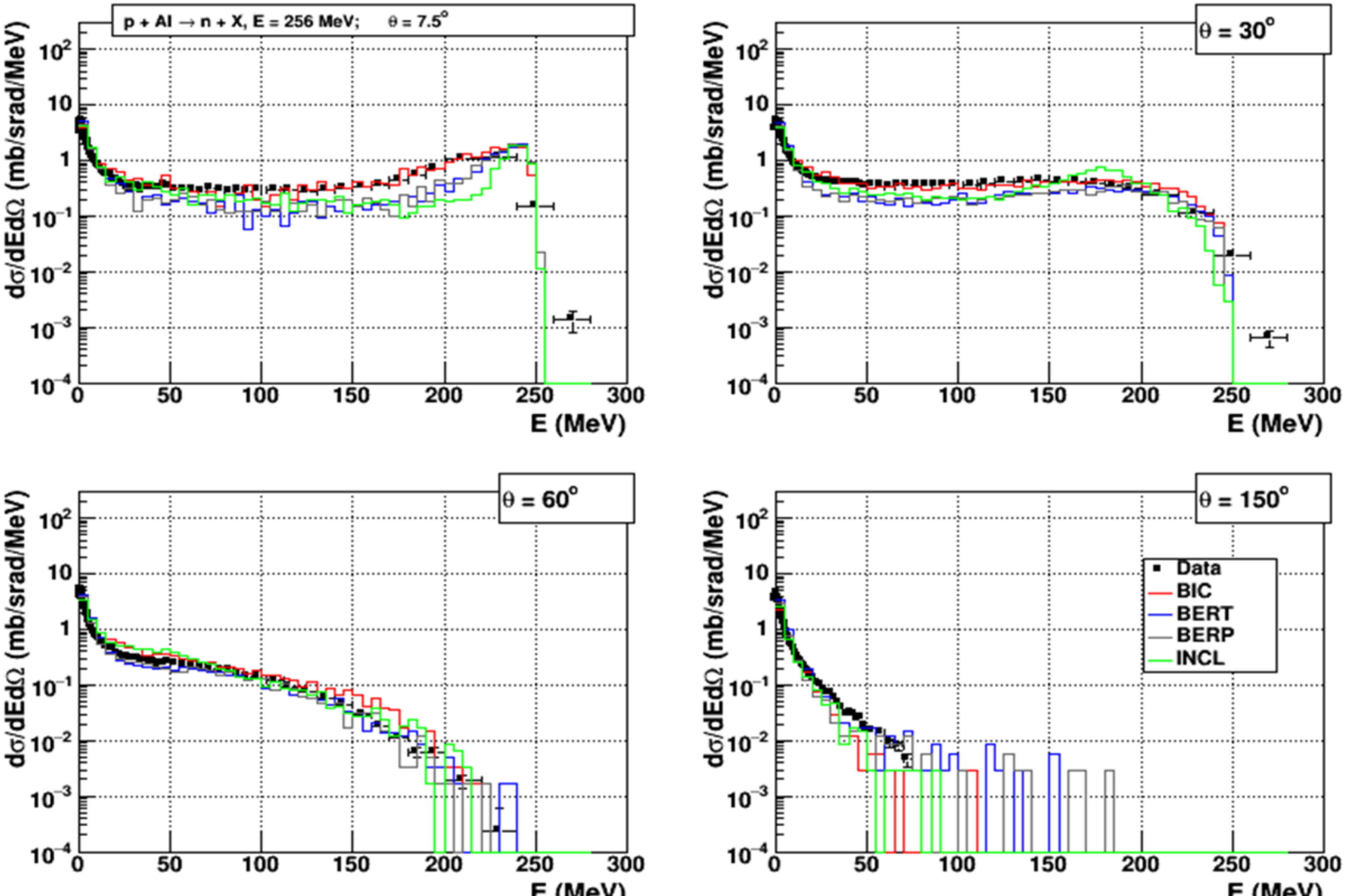
Double differential neutron production cross section for 22 MeV protons in ^{52}Cr target

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



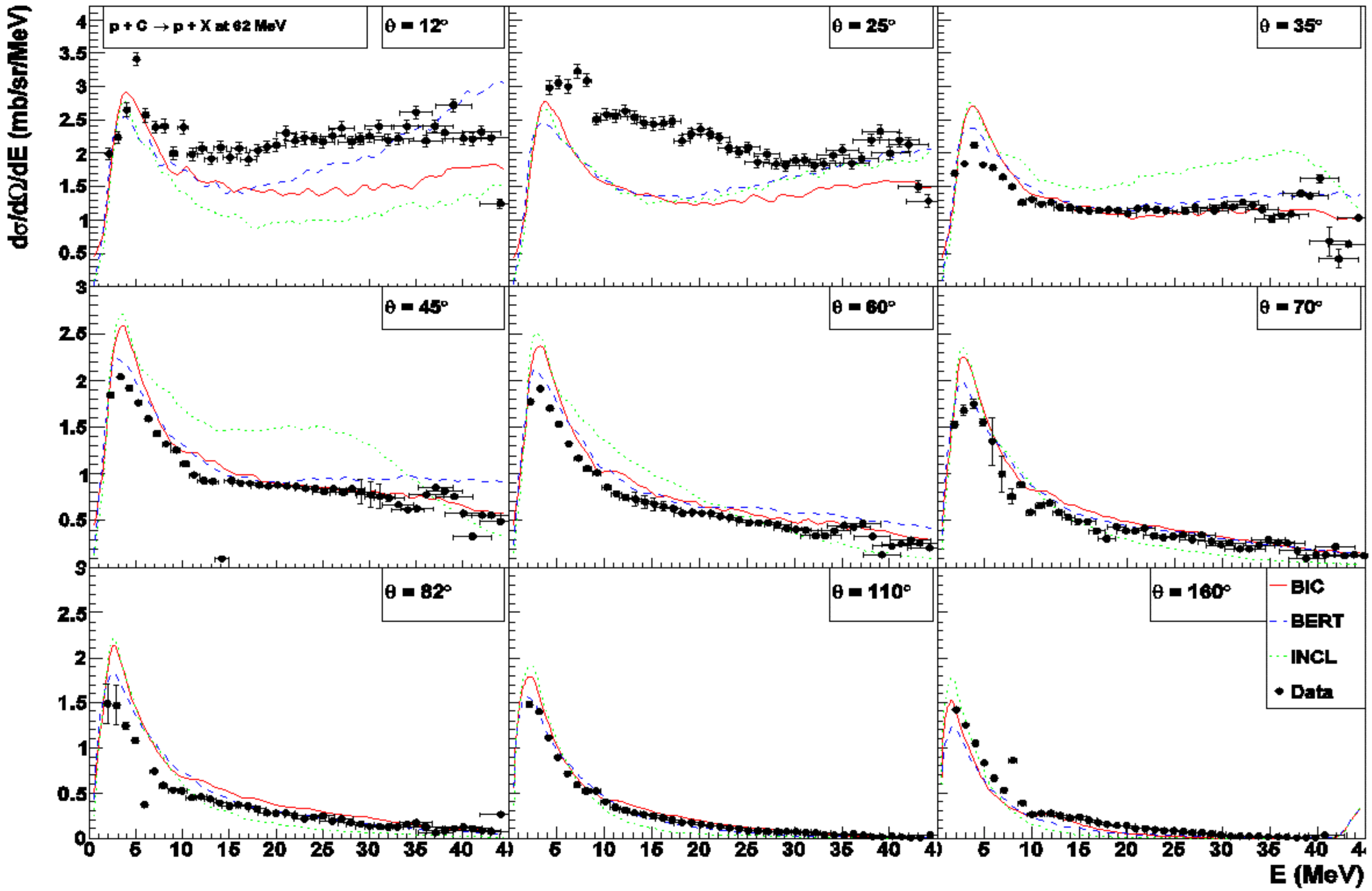
Double differential neutron production cross section for 256 MeV protons in Al target

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



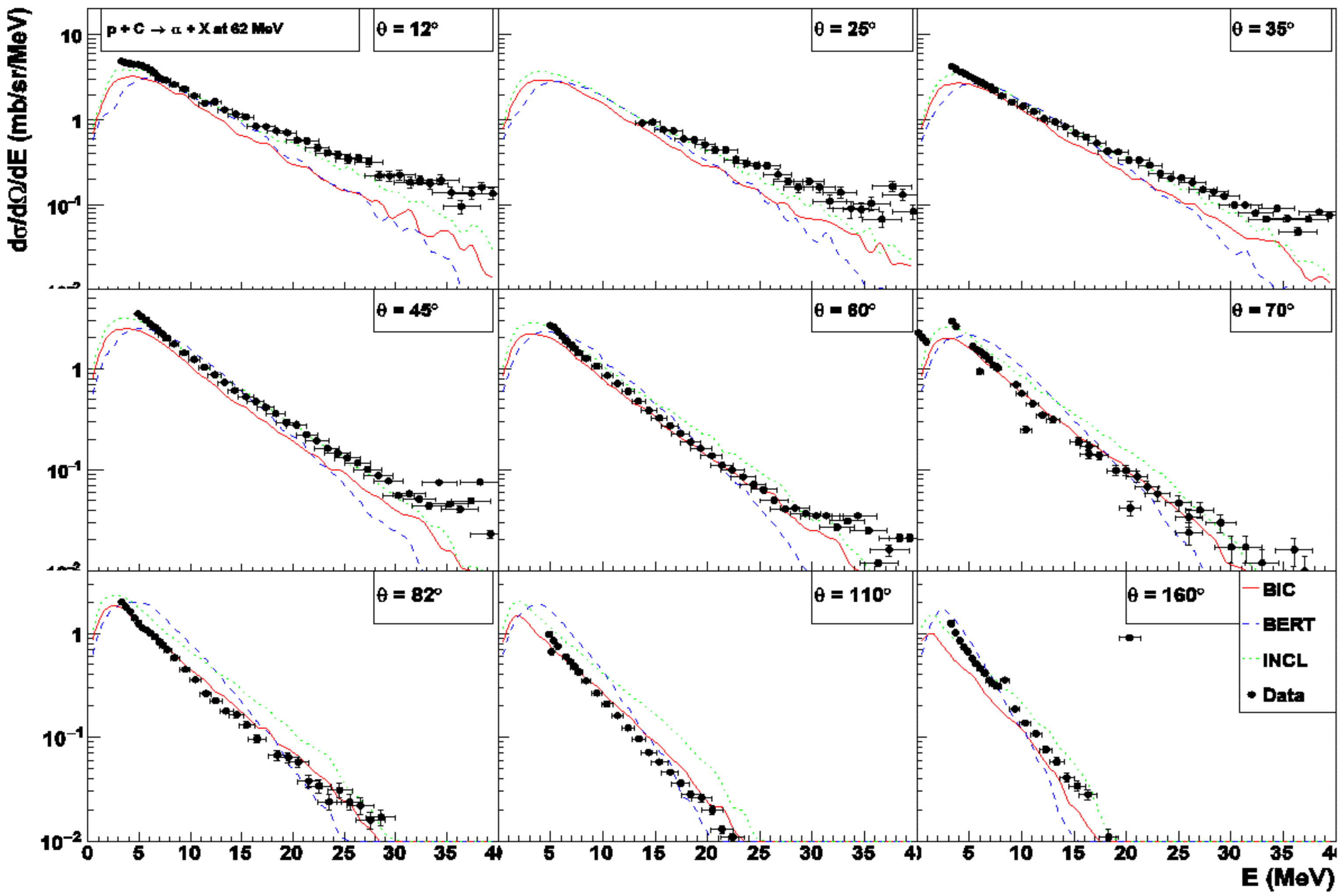
Double differential proton production cross section for 62 MeV protons in carbon target

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



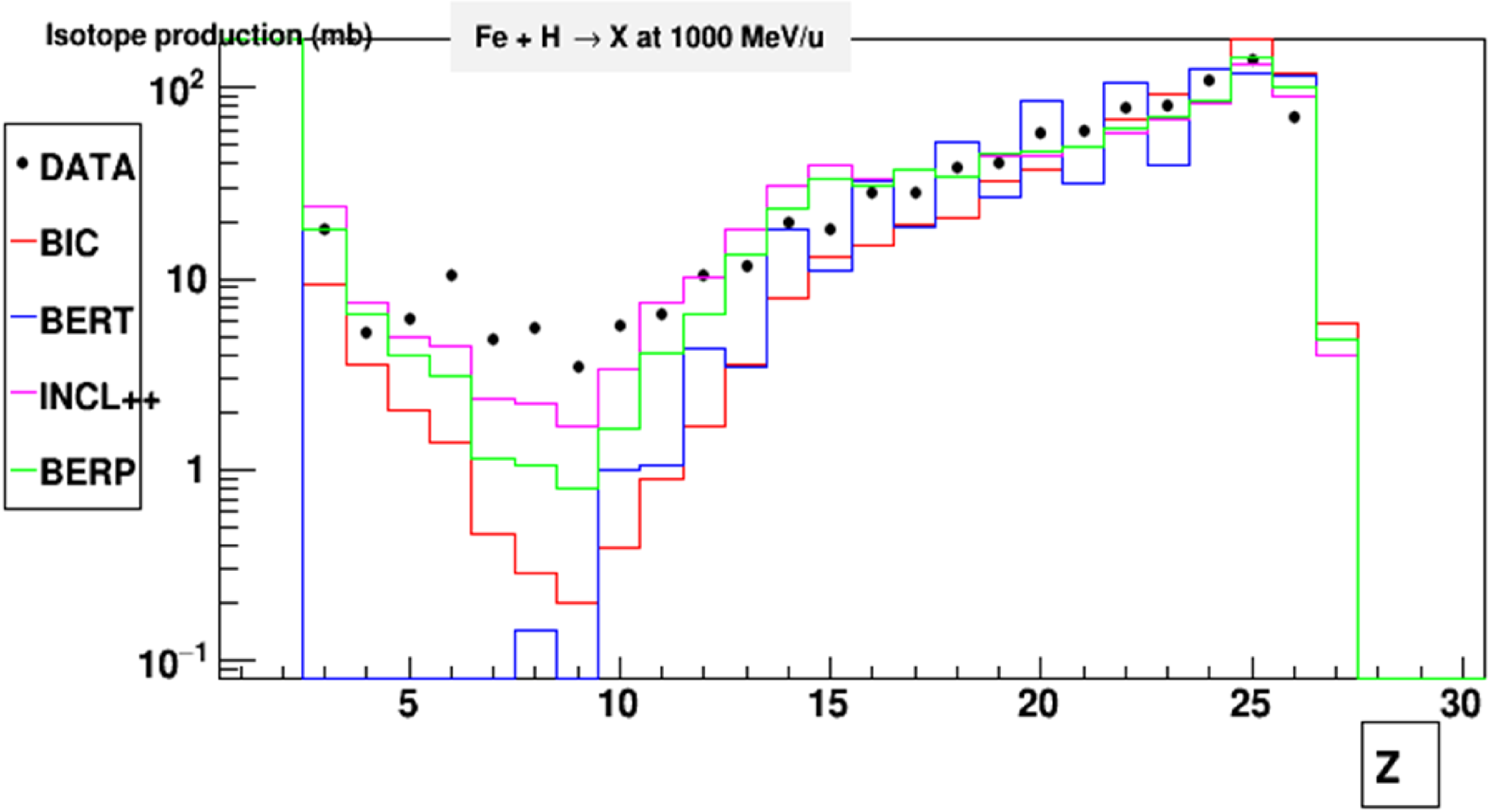
Double differential alpha production cross section for 62 MeV protons in carbon target

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