# Hadronic Aspects in Geant4

## relevant for medical applications

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# Overview

- Hadronic physics in Geant4
  - Hadronic processes: cross sections & models
  - Elastic processes
    - Cross sections
    - Models
  - Inelastic processes
    - Cross sections
    - Models: *Geant4 Hadronic Zoo*
      - Intranuclear cascade
      - Pre-equilibrium
      - De-excitation
  - Dedicated low energy treatments (use of evaluated data)
  - Physics lists
- Hadronic tests of the benchmark for medical applications
- Issue & recommendation: yieds from proton beams

# What is Geant4  Hadronic Physics?

- Interactions with atomic nuclei
- Projectile and/or produced secondary particles are hadrons
- Energy range from zero up to 100 TeV

# Hadronic Processes

- **Pure hadronic** (0 – ~TeV)
  - Elastic.
  - Inelastic.
  - Capture.
  - Fission.
- **Radioactive decay**
- **Photo-nuclear** (~10 MeV – ~TeV)
  - Gamma-induced nuclear reactions.
- **Lepto-nuclear** (~10 MeV – ~TeV).
  - e+, e- induced nuclear reactions.
  - Muon induced nuclear reactions.

# Pure hadronic processes: cross sections and models

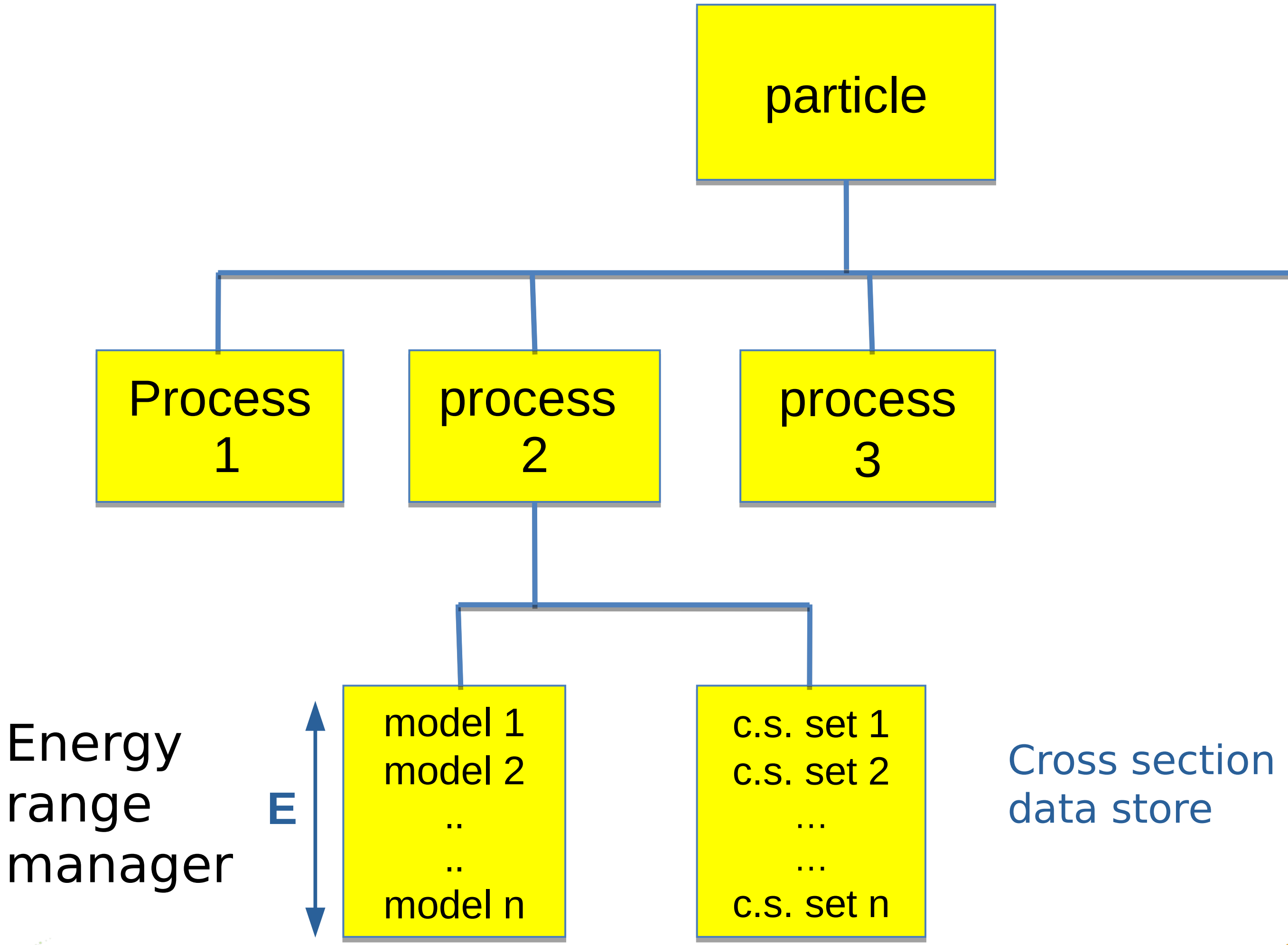
- In Geant4 physics interactions between a particle and material occur through processes

**Processes** $\left\{ \begin{array}{l} \textbf{Cross sections} \\ \text{to calculate mean free path} \\ + \\ \textbf{Models} \\ \text{to calculate final states} \end{array} \right.$

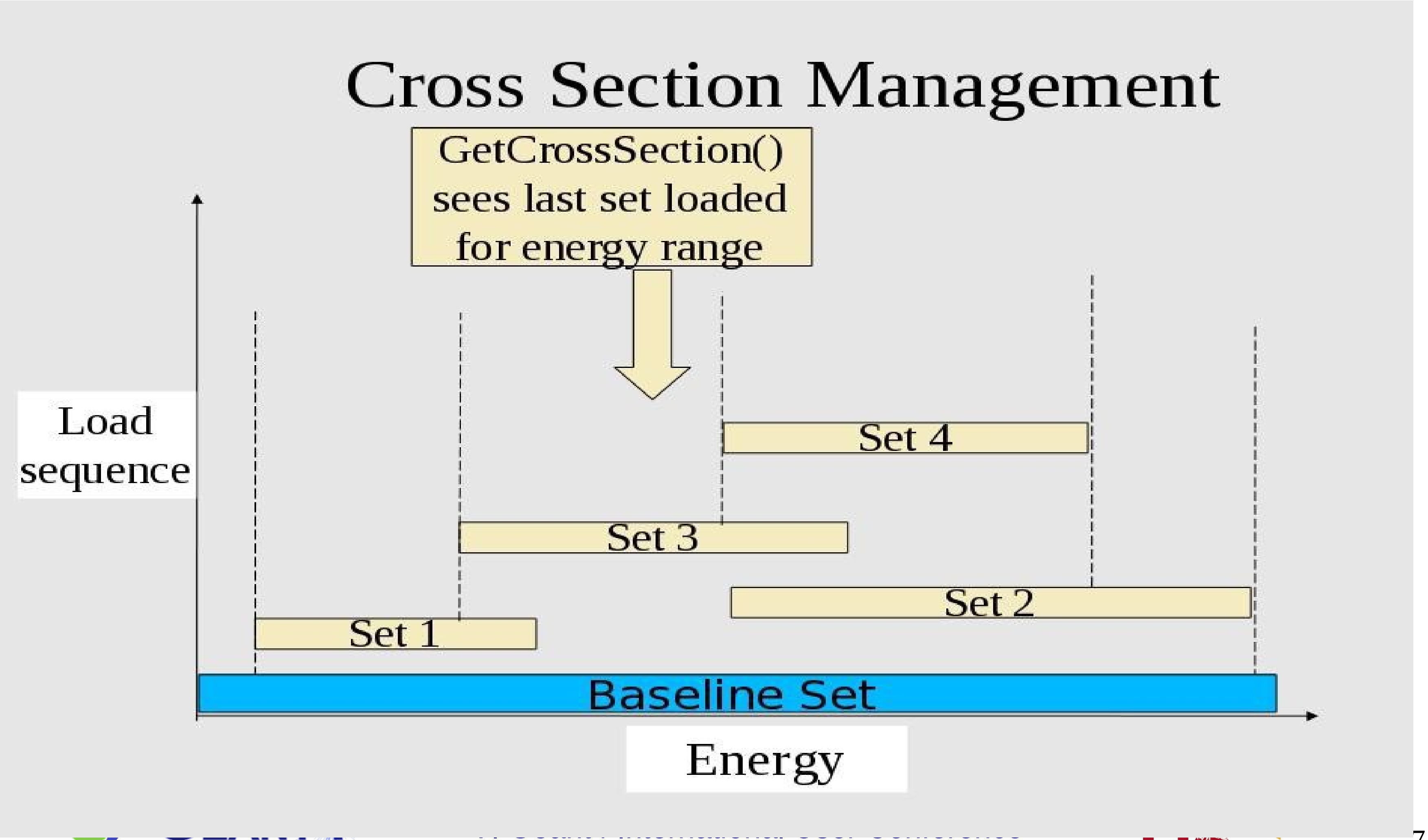
- In **Geant4 EM physics**:
  1 process ➡ 1 model + 1 cross section

- In **Geant4 Hadronic physics: the user must choose**
  1 process ➡ many possible models & cross sections

# The hadronic framework: processes, cross sections and models



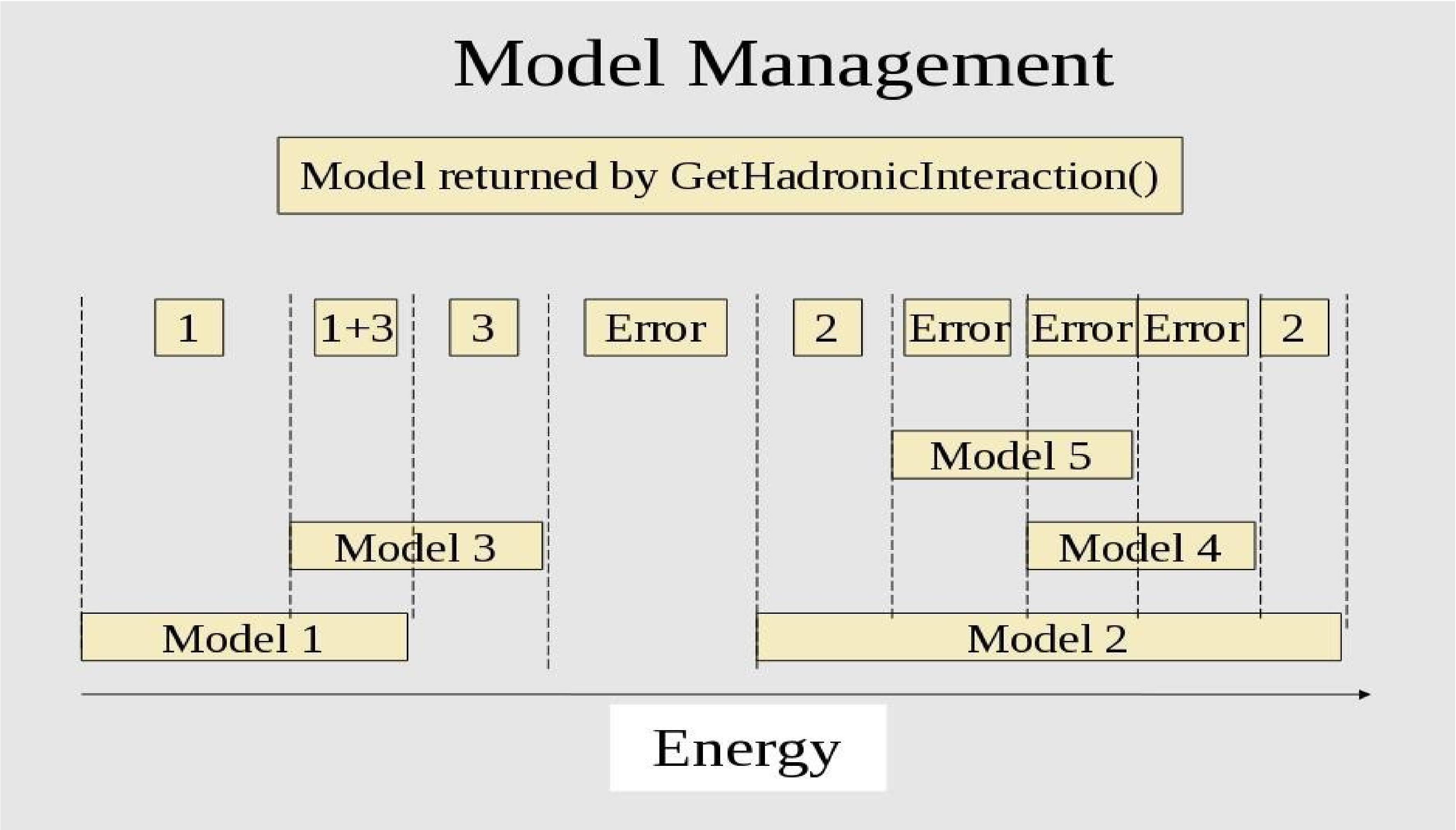
## Hadronic processes should have sets of cross sections covering the required energy range



# Hadronic Models Validity Ranges

- Processes may have one or more models registered to them
- Each model has an associated energy range.
- For each process, whole energy range (zero to “infinity”) must be covered by models
  - Model ranges may overlap at ends
  - Ranges must not be “enclosed” (duplicated)
  - No “energy gaps” are allowed
- Overlaps are “interpolated” with linear random selection at each interaction

# Hadronic processes should have sets of models covering the required energy range



# Elastic cross sections

- For **protons, π+ and π-**, **Barashenkov parameterization** (below 91 GeV) and its extension Glauber-Gribov (above 91 GeV).

- For **neutrons** from **G4PARTICLEXSDATA** data set, which below 20 MeV includes *simplified* and *smoothed evaluated* cross section data from the **Geant4 Neutron Data Library (G4NDL)**, based on the ENDF/B-VII.1 evaluated library

- When the **G4NeutronHP** physics package is activated (suffix **_HP** in the physics lists), **for neutrons below 20 MeV**, it uses *detailed evaluated* cross sections from G4NDL.

- When the **G4ParticleHP** physics package is activated (suffix **_AllHP** in the physics lists), it encompasses the G4NeutronHP physics whereas **for protons** it uses *evaluated* cross sections also from **ENDF/B-VII.1** (**up to 150 MeV**) when available , otherwise it uses **TENDL** database (with data **up to 200 MeV**)

- For **light clusters with A<5**, modified **Glauber-Gribov** cross sections

- For **nuclei with A>4**, **elastic scattering is ignored** since the screening of the atomic electrons leads to a small-angle scattering.

# Elastic Models

- The elastic scattering of **neutrons and protons** is modelled by default by the **G4ChipsElasticModel (Chiral Phase Space Invariant Phase Space)** in the full energy range.
- when **G4NeutronHP** or **G4ParticleHP** physics package are activated , evaluated elastic angular distributions are used from the same evaluated library and energy ranges as for the cross sections.
- **Light clusters (from deuteron to alpha), $\pi^+$ and $\pi^-$** use upto 1 GeV the **G4HadronElastic** model, which is a two-exponential momentum transfer model updated from Geant3 (Gheisha).

# Inelastic cross sections

- For **protons and pions** , the **Barashenkov-Glauber-Gribov parameterization** is used.

- As in the elastic case, **neutron** cross sections are extracted by default from the **G4PARTICLEXSDATA** data set

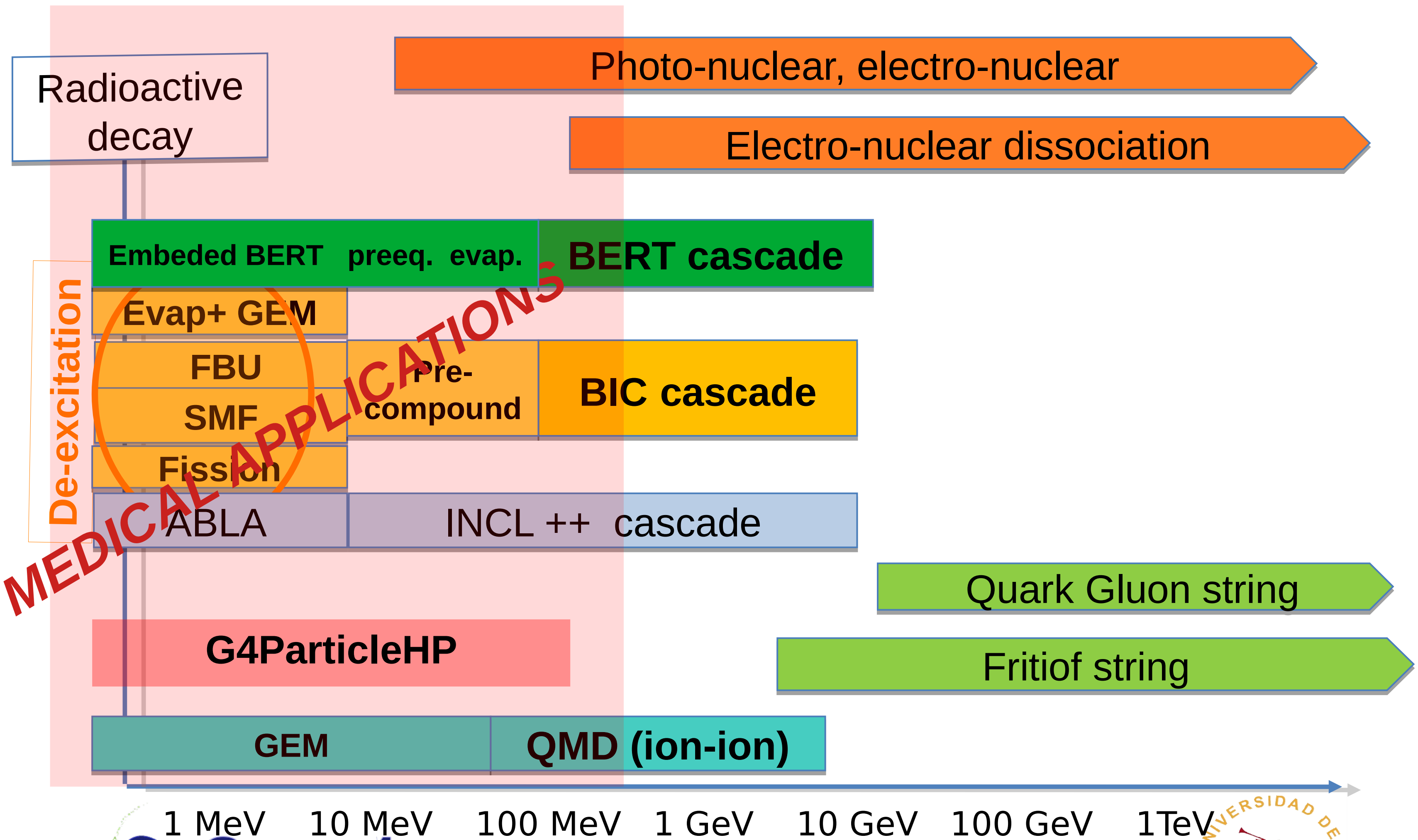
- When **G4NeutronHP** or **G4ParticleHP** physics package are activated, the same as in the elastic case holds for the neutron (below 20 MeV) and proton (below 150 or 200 MeV) inelastic cross sections.

- For **light clusters** (deuterons up to alphas), the **modified Glauber-Gribov cross section** is used for all energies.

- For **nucleus-nucleus** cross sections, in Geant4 **a variety of prescriptions are available** for the energy range of interest (below 1 GeV). At present, the **modified Glauber-Gribov** cross section is used in the hadronic physics list recommended for medical applications (**QGSP BIC_HP**, see below).

- Neutron capture cross sections are extracted from the evaluated **G4PARTICLEXSDATA** data set for energies below 20 MeV and are set to zero above this limit.
  - When **G4NeutronHP** or **G4ParticleHP** physics package are activated, neutron capture cross sections are extracted from **G4NDL** data library (up to 20 MeV).

# Inelastic models: the Geant4 hadronic “zoo”



# Intranuclear Cascade models (I)

- Description of interactions in terms of particle-particle collisions on the basis that the de Broglie wavelength  of the incident particle in nuclear collisions is, above a given threshold, comparable(or shorter) than the average inter-nucleon distance.
- The cascade begins when an incident particle strikes a nucleon in the target nucleus and produces secondaries.
- The secondaries may in turn escape, be absorbed or interact with other nucleons abiding by the Pauli blocking
- The exciton number is updated at each step
- At the end of the cascade the remnant is trasferred as an excited nuclear fragment to the pre-equilibrium model or directly to de-excitation
- Relativistic kinematics is applied throughout the cascade

# Intranuclear Cascade models (II)

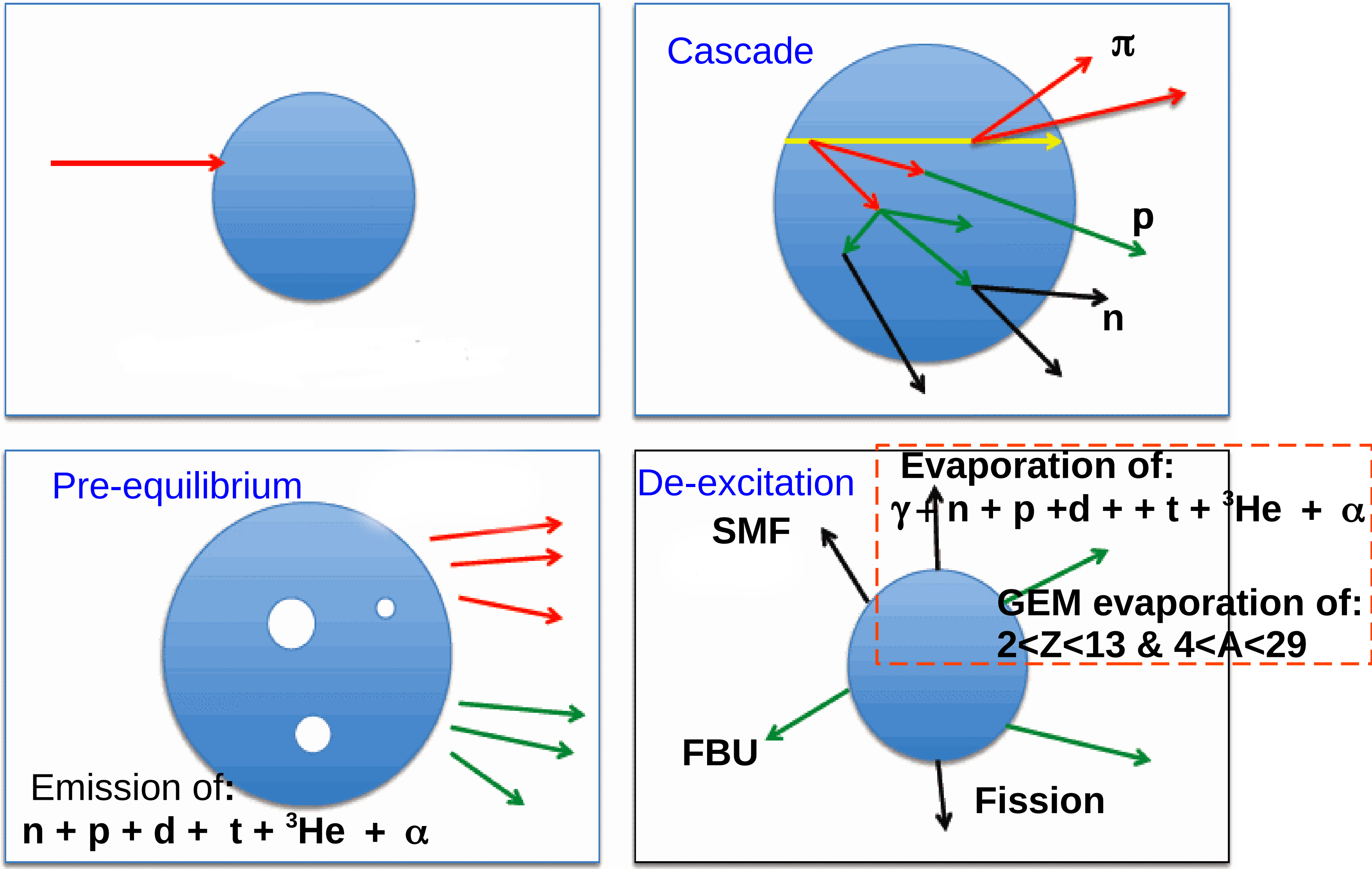
- Bertini cascade (BERT)
  - p, n, π, and strange particles with 0<Ekin<15 GeV

**Recommended for Medical applications (*) & talk by S. Guatelly**

- Binary cascade (BIC) *Native Geant4*
  - **p** and n-induced cascades Ekin< 10 GeV, and
  - π-induced Ekin<1.3 GeV
  - For light nucleus-nucleus collisions an extension is available
- Liege cascade (fully redesigned as INCL++)
  - p, n, π with 0<Ekin<3 GeV
  - -Extended to handle reactions induced by light ions with A < 19
- Quantum Molecular Dynamics (QMD)
  - More detailed tratment but **CPU demanding!**
  - **Nucleus-nucleus** reactions 100 MeV/nucleon<Ekin< 10 GeV/nucleon.

(*) P. Arce et al., "Report on G4-Med, a Geant4 benchmarking system for medical physics applications developed by the Geant4 Medical Simulation Benchmarking Group," Medical Physics, vol. 1, no. 48, pp. 19–56, 2021.

# Binary Cascade model



# G4BinaryCascade (BIC)

- Each participating **nucleon is seen as a gaussian wave packet**
- The Hamiltonian is calculated using simple time independent **nuclear optical potential** (unlike QMD), 3 dimensional model of the nucleus constructed from A and Z. Nucleon distribution follows
  - A>16 Woods-Saxon model
  - Light nuclei harmonic-oscillator shell model
  - Nucleon momenta are sampled from 0 to Fermi momentum and sum of these momenta is set to 0
- Total wave function of the nucleus is assumed to be direct product of these. (no **anti-symmetrization**)
- The centroid of this wave packet follows the **classical Hamilton equations**, which can be solved numerically.
- Remnant excited fragment (with a set of excited particle-hole states) is passed to Geant4 native preequilibrium model: G4PreCompoundModel

# G4PreCompoundModel (Exciton Model)

- It describes the post-cascade evolution until the nuclear system reaches equilibrium (*but still excited*)
- Transitions to states with different number of exciton compete with particle emissions (n + p + d + t + $^{3}$He + $\alpha$).
- The transition probabilities are calculated semimicroscopically, whereas the emission probabilities make use of the inverse reaction cross sections, which, via the reciprocity theorem.
- Transition to the state of statistical equilibrium is characterized by an equilibrium number of excitons (when transitions for increasing or decreasing the exciton number are equiprobable)
- Finally , the residual nucleus is assumed to be in a statistical equilibrium state in which the excitation energy is shared by the entire nuclear system.

# G4ExcitationHandler
## (equilibrium de-excitation)

- Manages several alternative/competitor semi-classical models, which are invoked (in order of precedence):
  - **Fermi break-up** for $Z < 9$ and $A < 17$. Includes Pauli blocking and all possible decay channels in stable and long lived fragments.
  - **Evaporation** of:
    - $n + p + d + t + {}^{3}He + \alpha$ by the standard Weisskopf-Ewing model
    - $Z \leq 12$ and $A \leq 28$, by the Generalized EvaporationModel (GEM)
  - **Evaporation of photons**:
    - discrete gammas according to tabulated E1, M1 and E2 transition probabilities taken from the Evaluated Nuclear Structure Data File (ENSDF) to create final state products including Internal Conversion electrons
    - continuous, according to GDR strenght distribution
  - **Statistical multifragmentation**, for excitation energies $E\,x > 3$ MeV .
  - **Fission**, based on Bohr-Wheeler semi-classical model

# Dedicated low energy treatments (I)

- **G4NeutronHP** model for **neutrons** with $E_{kin}$<20MeV which uses ENDF/B-VII.1 **evaluated** library
  - includes radiative capture
- **G4ParticleHP** generelises it for **protons** using TENDL-2019 data library, which includes
  - the **ENDF/B-VII.1 (*) data for 46 key isotopes** (**covering ~ all medical applications**) for Ekin<150 MeV
  - otherwise purely nuclear models (TALYS) calculated data are used (~2800 isotopes!) for Ekin<200 MeV .
  - Deuteron, triton, He3, $\alpha$ for only very few isotopes and reduced ranges of energies
- Energy-momentum and barion number are not conserved event by event, but they do on average

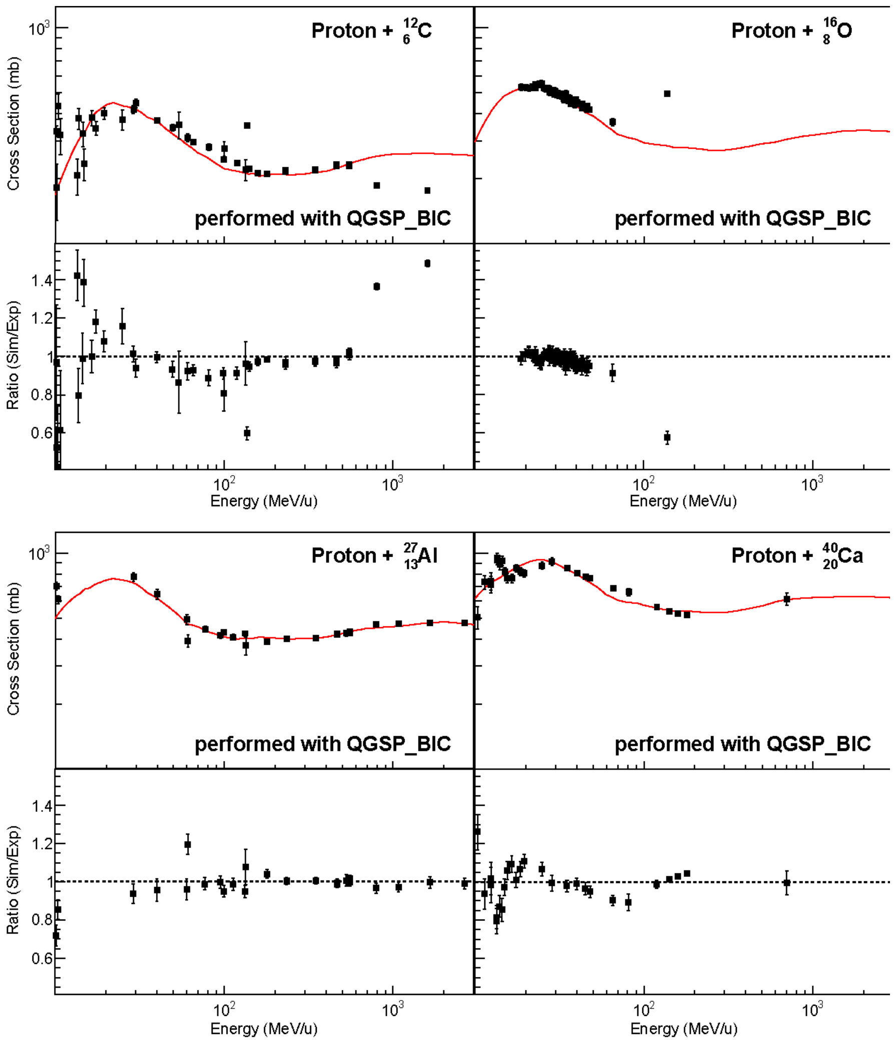
# Physics List

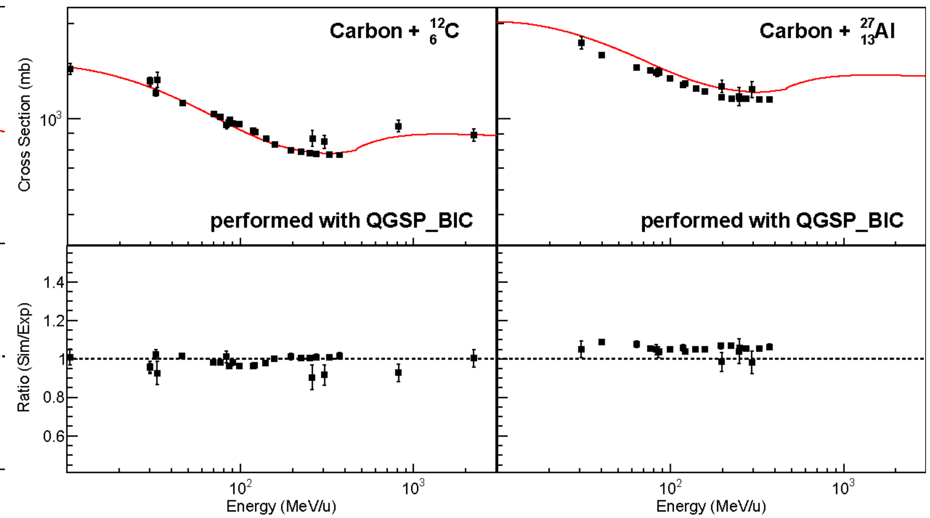
- One of the three mandatory user classes of the Geant4 toolkit
- Refer to classes which provide the means to collect and organize , for a particular application,  the
  - particle types
  - physics models
  - cross sections required
- Allow physics processes to be registered to the run manager which in turn attaches them to tracks so that they may interact properly with the simulation geometry
- The **reference physics lists** are specialized to provide standard behavior in various application domains (e.g medical applications)

## RESULTS for medical applications

## Geant4 benchmark for medical physics applications: P. Arce et al, Med. Phys. 48 (1), January 2021

# Test of nucleus–nucleus hadronic inelastic scattering cross sections



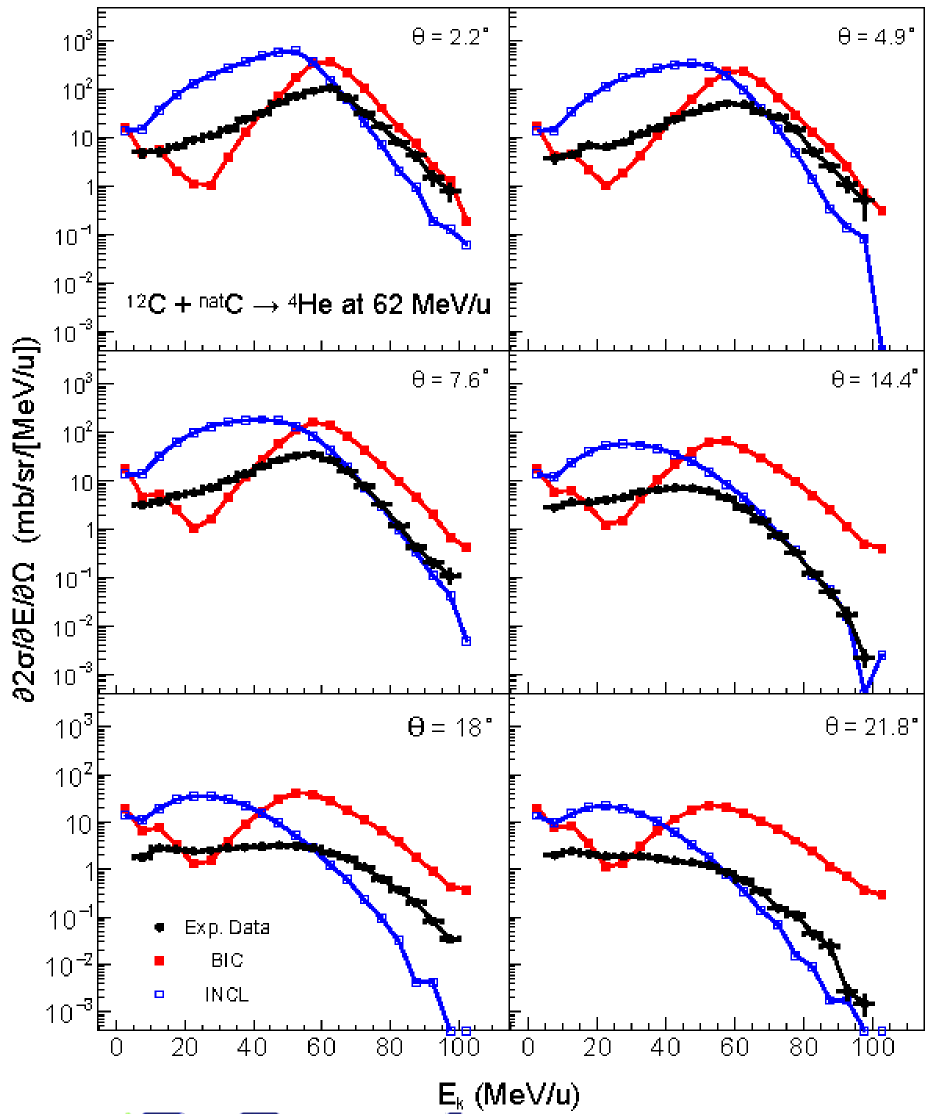




Total hadronic inelastic scattering cross sections as a function of the kinetic energy of the projectile, calculated by means of the QGSP_BIC physics list.

Red curve: Geant4 cross section; data points: EXFOR reference experimental data

Test performed by D. Sakata (Osaka University), E. Simpson (Australian National University), S. Guatelli (University of Wollongong).

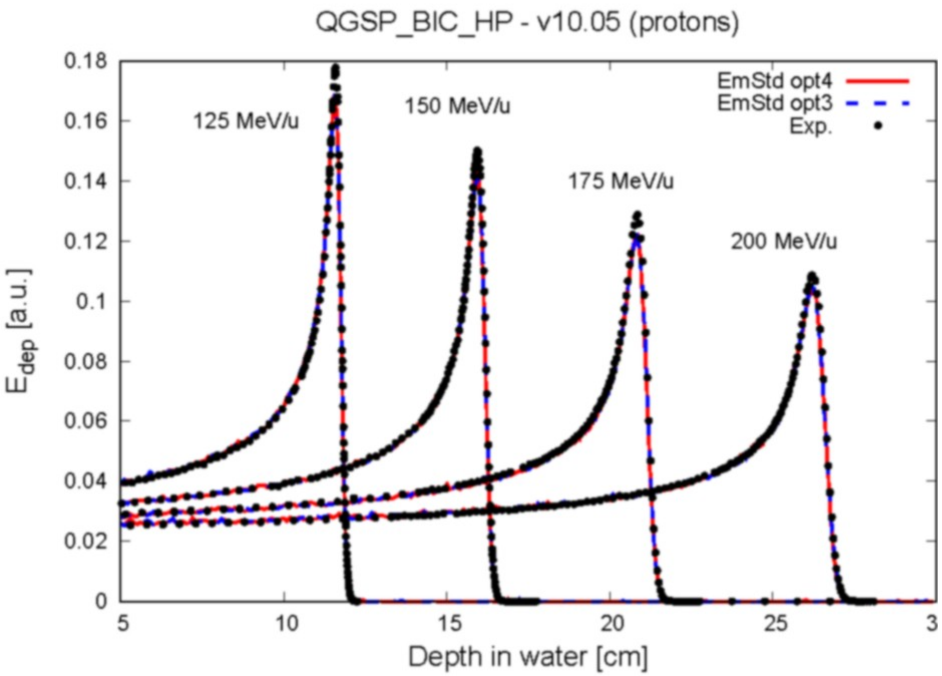
# 62 MeV/u 12C fragmentation test

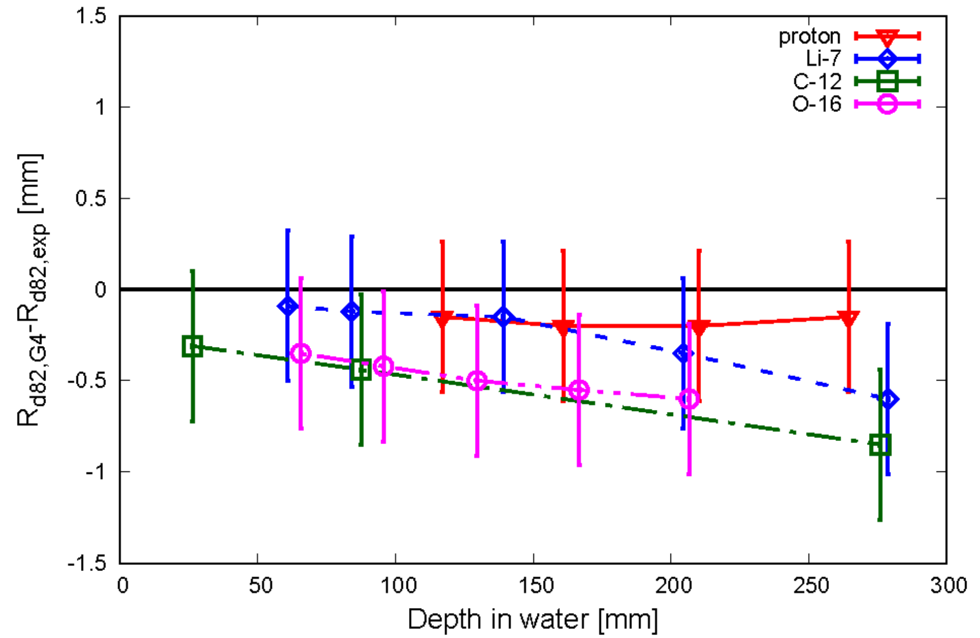



Double-differential cross sections measured at different angles of α-particle production in the 12 C interaction with a thin C target at 62 MeV/u as a function of the α-particle kinetic energy. Experimental data are compared with the two models available in Geant4 for ion interac-tions at this energy, namely INCL (in blue) and BIC (in red) extensions for light ions.

Test performed by C. Mancini (University La Sapienza)

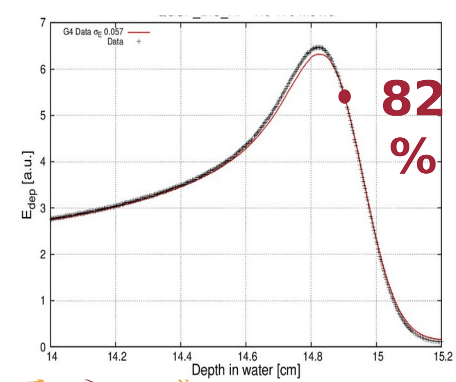
# Light ion Bragg Peak test



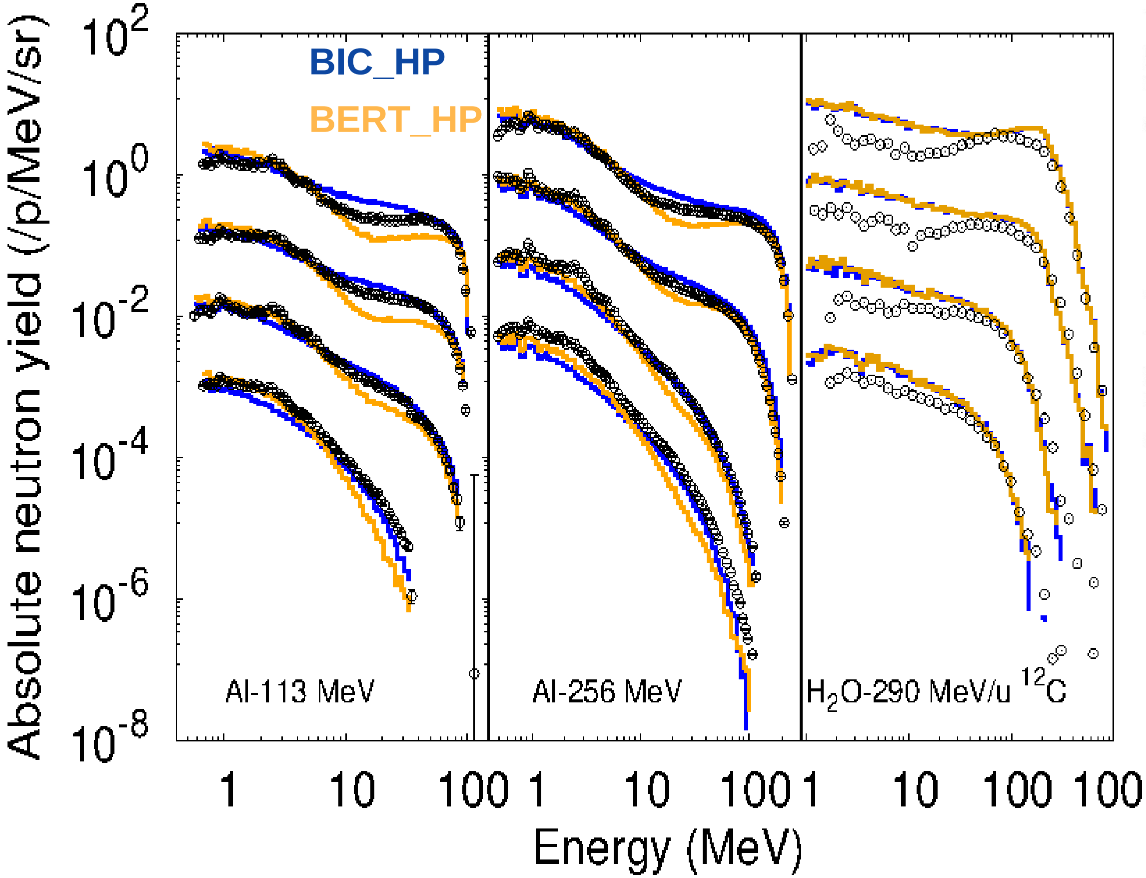



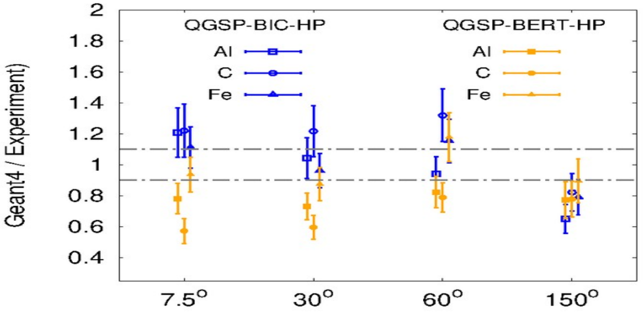

- **LightIonBraggPeak** test (G4Med) (M.A. Cortés-Giraldo, A. Perales, J.M. Quesada).
- **Exp. data** by D. Schardt et al. (GSI, 2007)

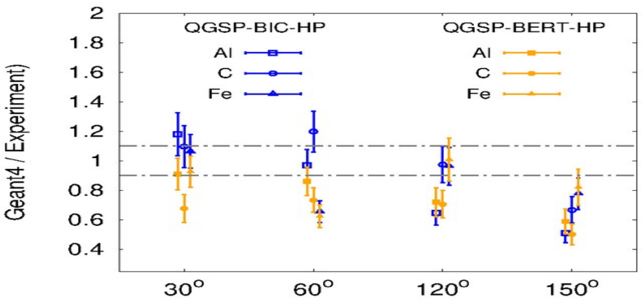
***R*$_{d82}$** values defined by the depth of 82% **distal** dose level

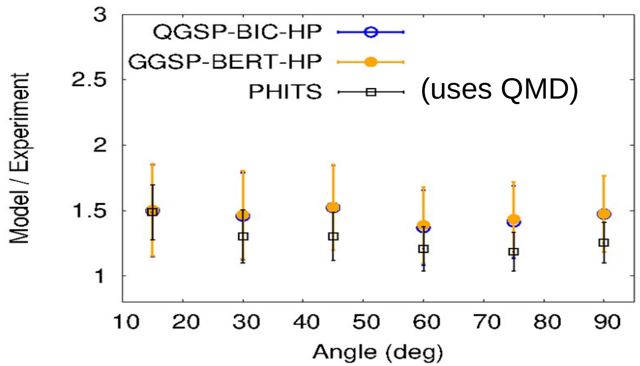


# Neutron yield of protons with energies 113 and 256 MeV and carbon ions at 290 MeV/u



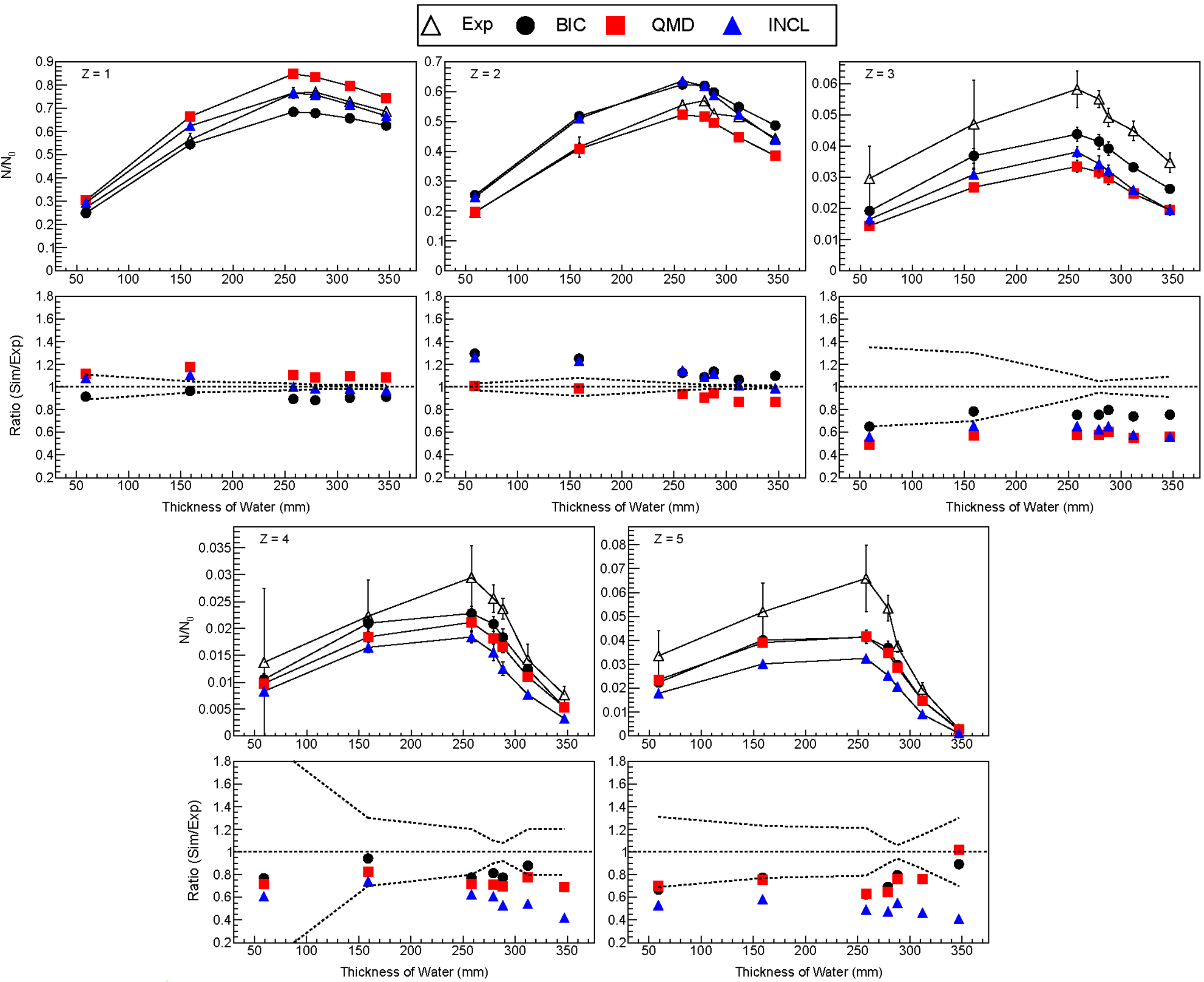




Absolute neutron yield (top left) for protons of 113 and 256 MeV impinging an aluminum target and 290 MeV/u carbon ions in a water phantom. Geant4 calculation using QGSP_BIC_HP is shown with blue solid line, whereas results with QGSP_BERT_HP is shown with orange solid lines. Experimental data are shown with empty markers.
Test performed by B. Faddegon & José Ramos-Mendez (University of California UCSF)

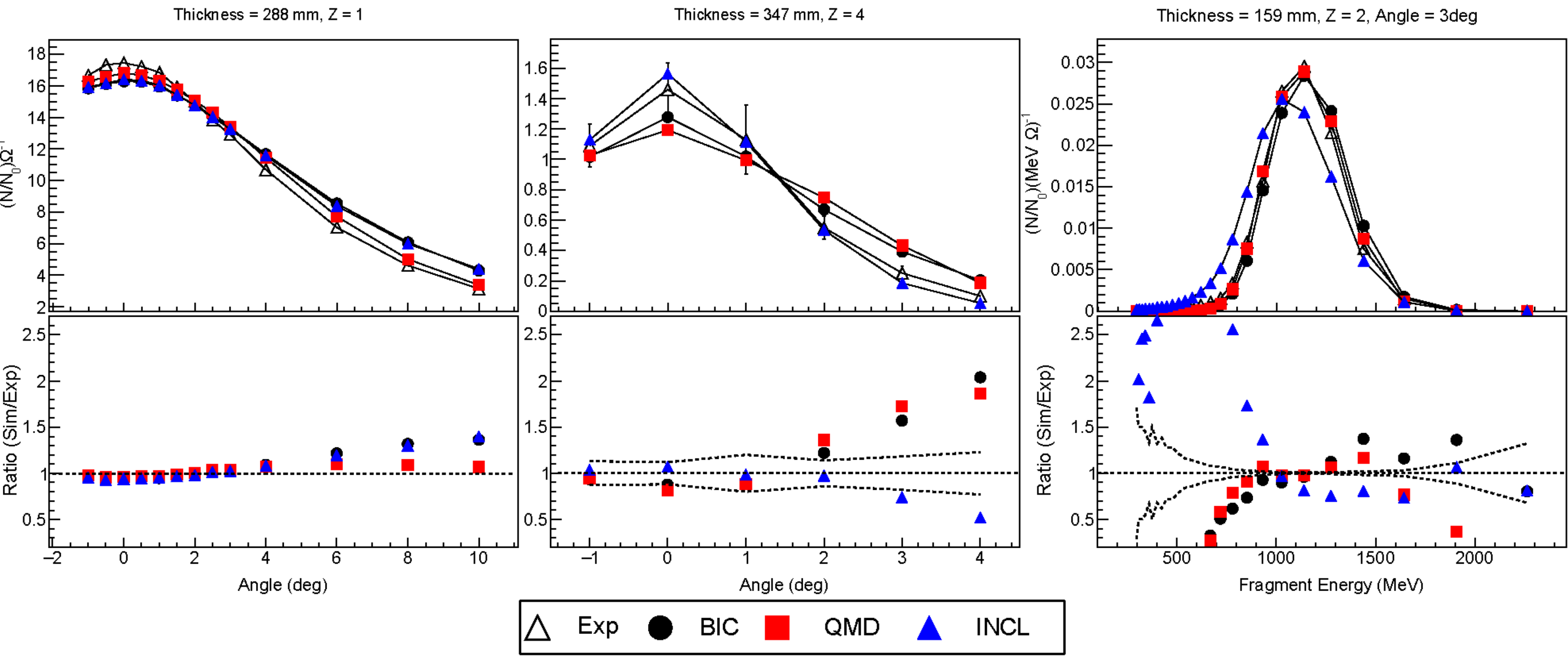
# Fragmentation of a 400 MeV/u 12 C ion beam in water (I)




The fragment yields, N , produced from $N_0$ mono-energetic 400 MeV/u 12C ions incident upon different thicknesses of water. The fragments were scored within a forward angle of 10° from the centre of the water targets. Experimental measurements of fragments with different atomic number ranging from 1 to 5 are compared against alternative models available in Geant4. The dashed lines on the bottom ratio plots indicate the experimental uncertainty.

Test performed by D. Bolst and S. Guatelli (University of Wollongong)

# Fragmentation of a 400 MeV/u 12 C ion beam in water (II)




Fragment distributions comparing experimental measurements against alternative models available in Geant4 for a 400 MeV/u mono-energetic 12 C ion incident upon water. Left and Middle: Angular distribution of H (left) and Be (middle) produced from water thickness of 288 mm and 347 mm, respectively. Right: An example energy distribution of He fragments recorded at an angle of 3º from the centre of the 12C ion beam when incident upon 159 mm of water. The dashed lines on the bottom ratio plots indicate the experimental uncertainty.
Test performed by D. Bolst and S. Guatelli (University of Wollongong)

# Recommendation for medical applications

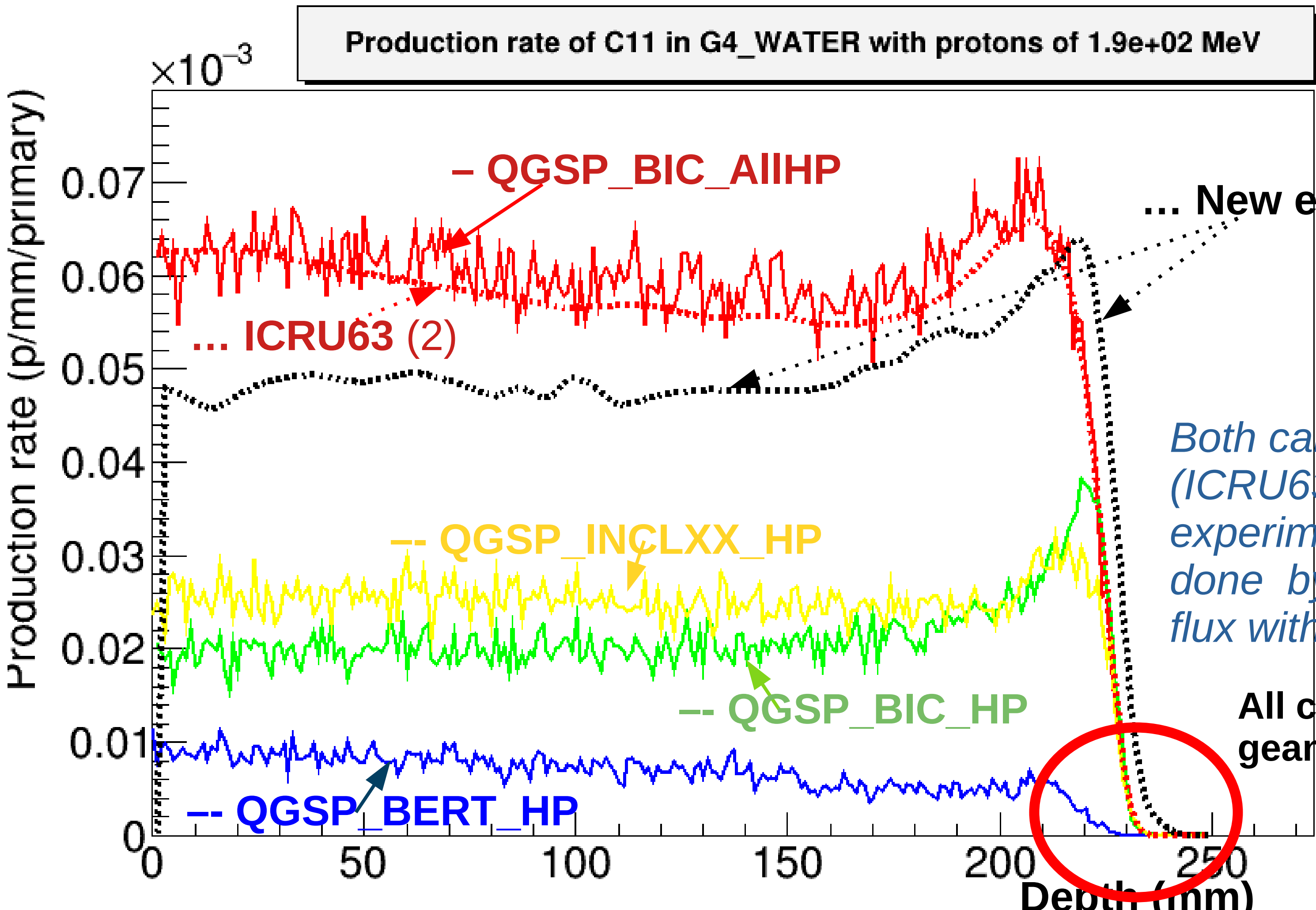
The hadronic benchmark (*) showed that **QGSP_BIC_HP** physics list (which models EM interactions with Opt4 in Geant4 10.5) provides an overall adequate description of the physics involved in  hadron therapy, including proton and carbon ion therapy.

(See talk by S. Guatelli)

(*) P. Arce et al, “Geant4 benchmark for medical physics applications: ,  Med. Phys. 48 , January 2021

**but ..**

# Yields of β+ emitters with proton beams




*Both calculations (ICRU63 and new experimental) were done by folding proton flux with production XS*

**All calculations with geant4.10.07.p03**

***(1) Production of 11 C, 13 N and 15 O in proton-induced nuclear reactions up to 200 MeV***
T. Rodríguez-González, submitted to Nuclear Data SheetsI
(2) **ICRU Report 63 (2000)**, Nuclear Data for Neutron and Proton Radiotherapy and for Radiation Protection.

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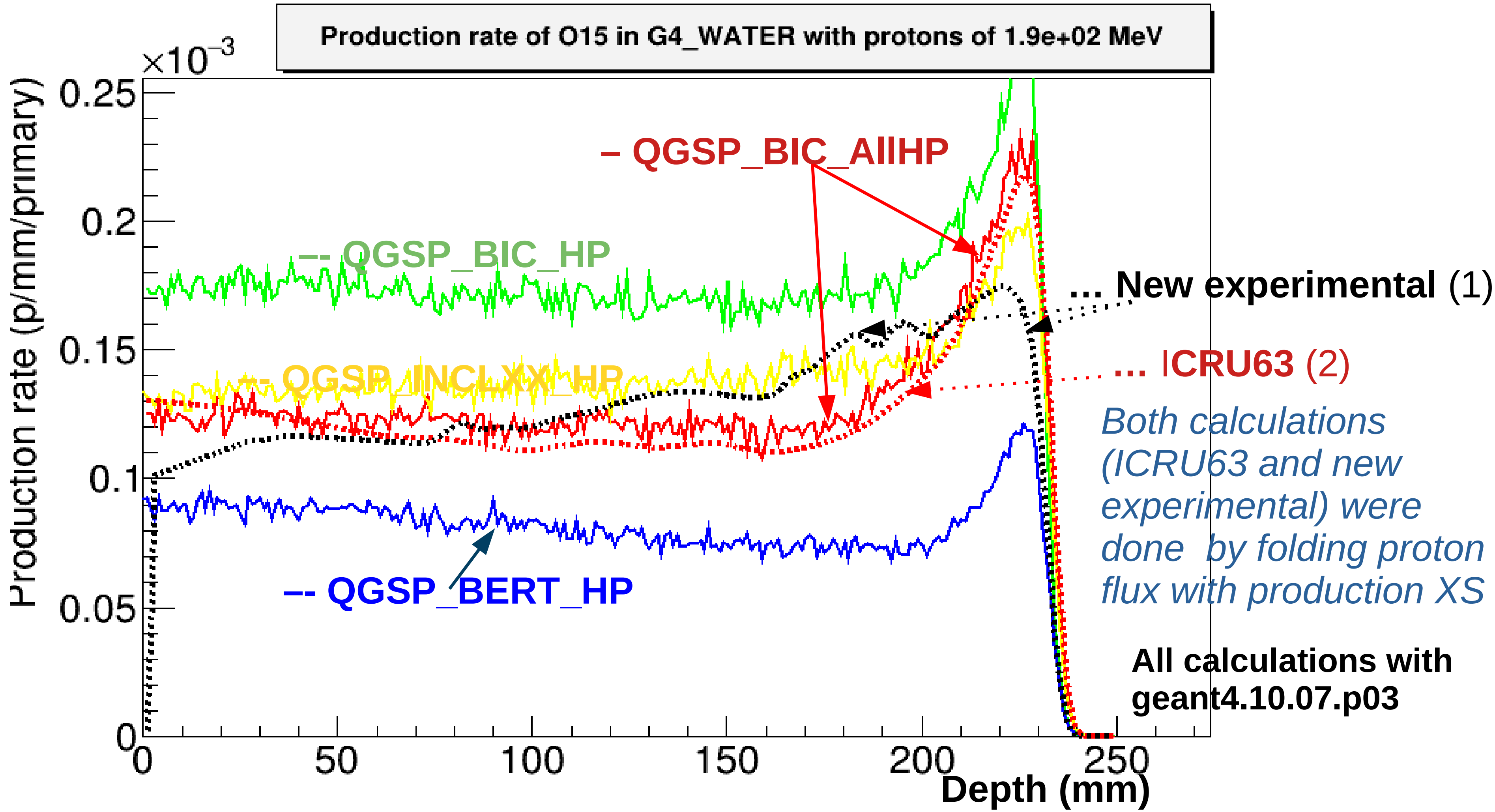


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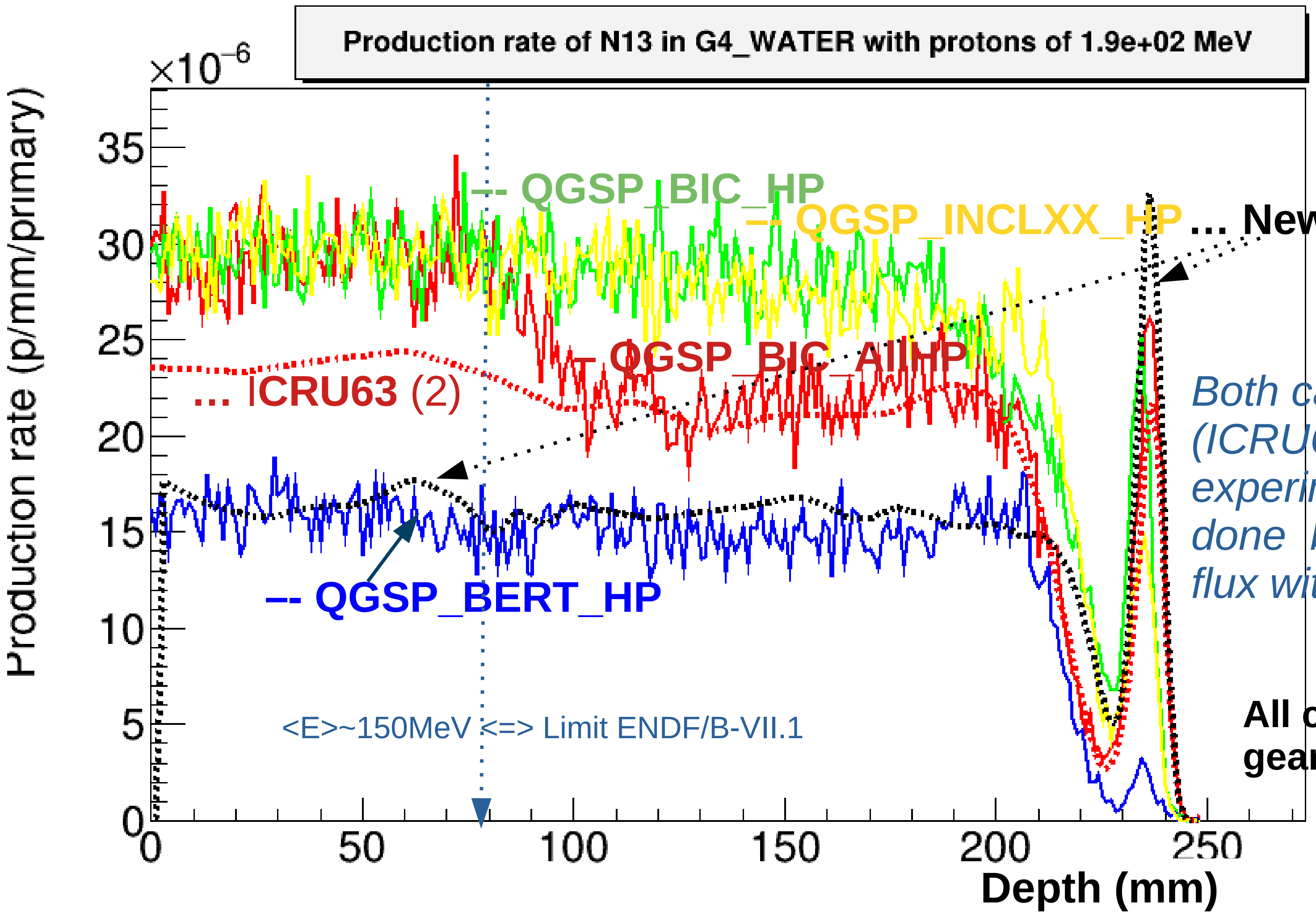


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# Hadronic recommendation for medical appplications (my personal guess ..)

- In general (dosimetric calculations, yields in heavy ion therapy, etc ..):
  - **QGSP_BIC_HP**

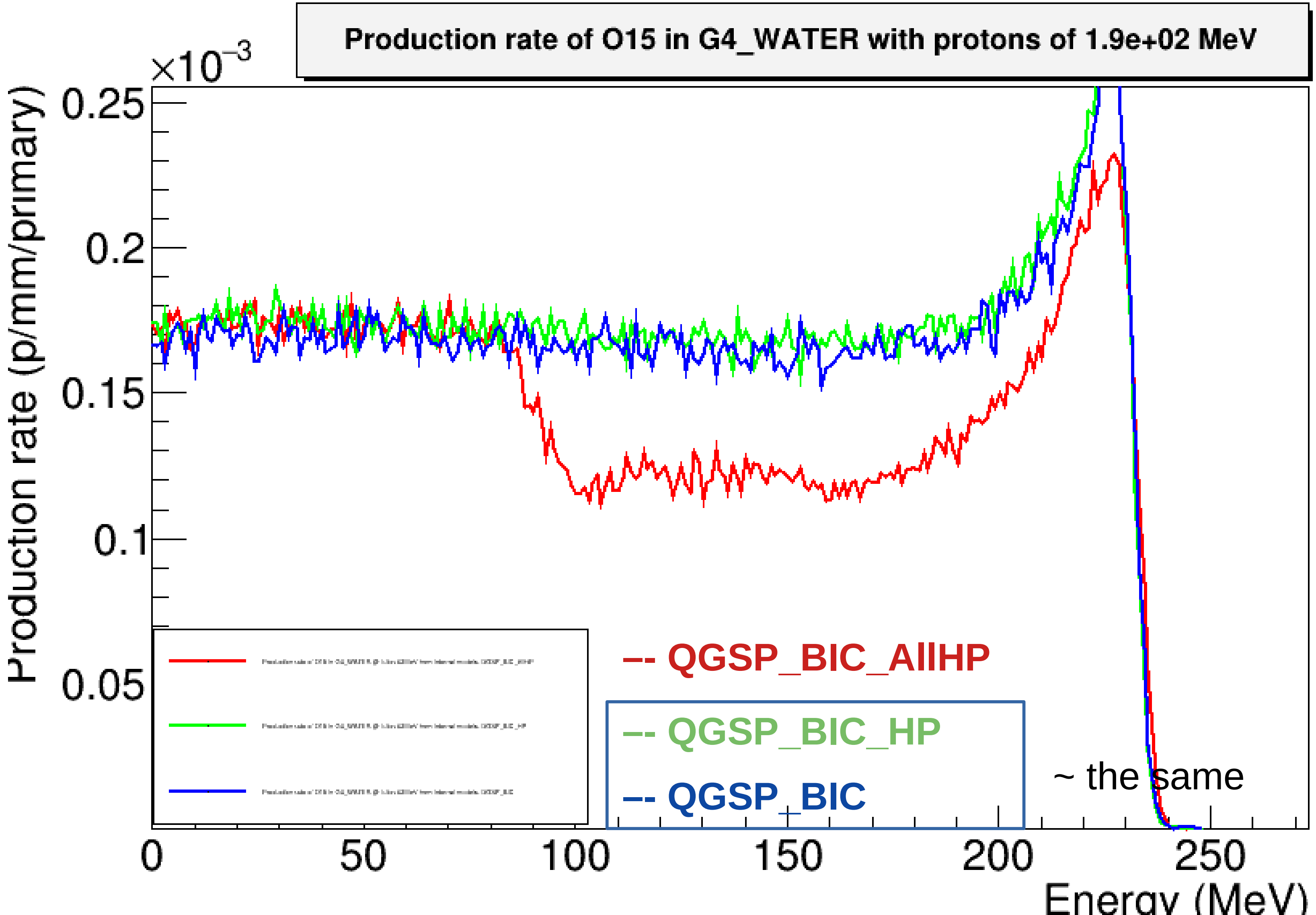
- For the calculation of yields *with proton beams*
  - **QGSP_BIC_AllHP**
  - Folding with **ICRU63** cross sections or more recent experimental data (**faster**)

Grazie per vostra attenzione

Thanks for your attention

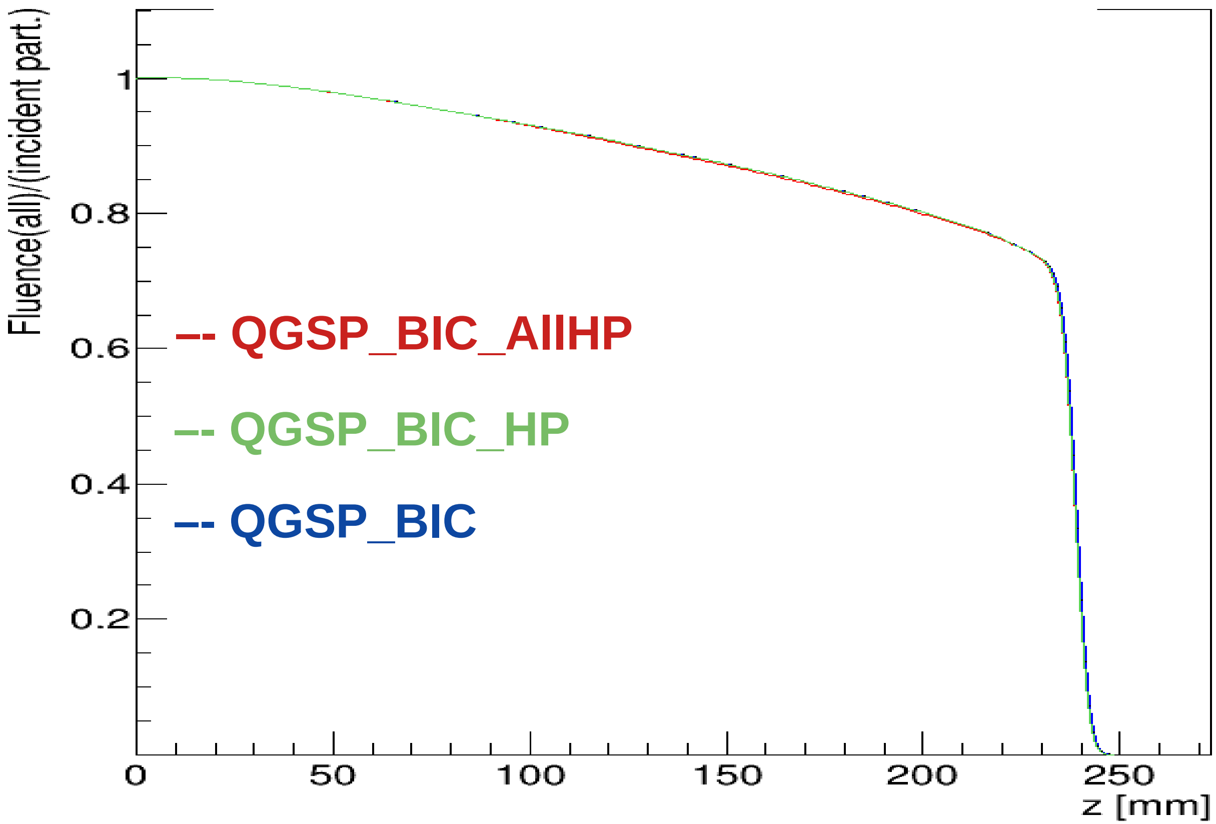
# Backup slides

# BIC & BIC_HP ~ same results for yields



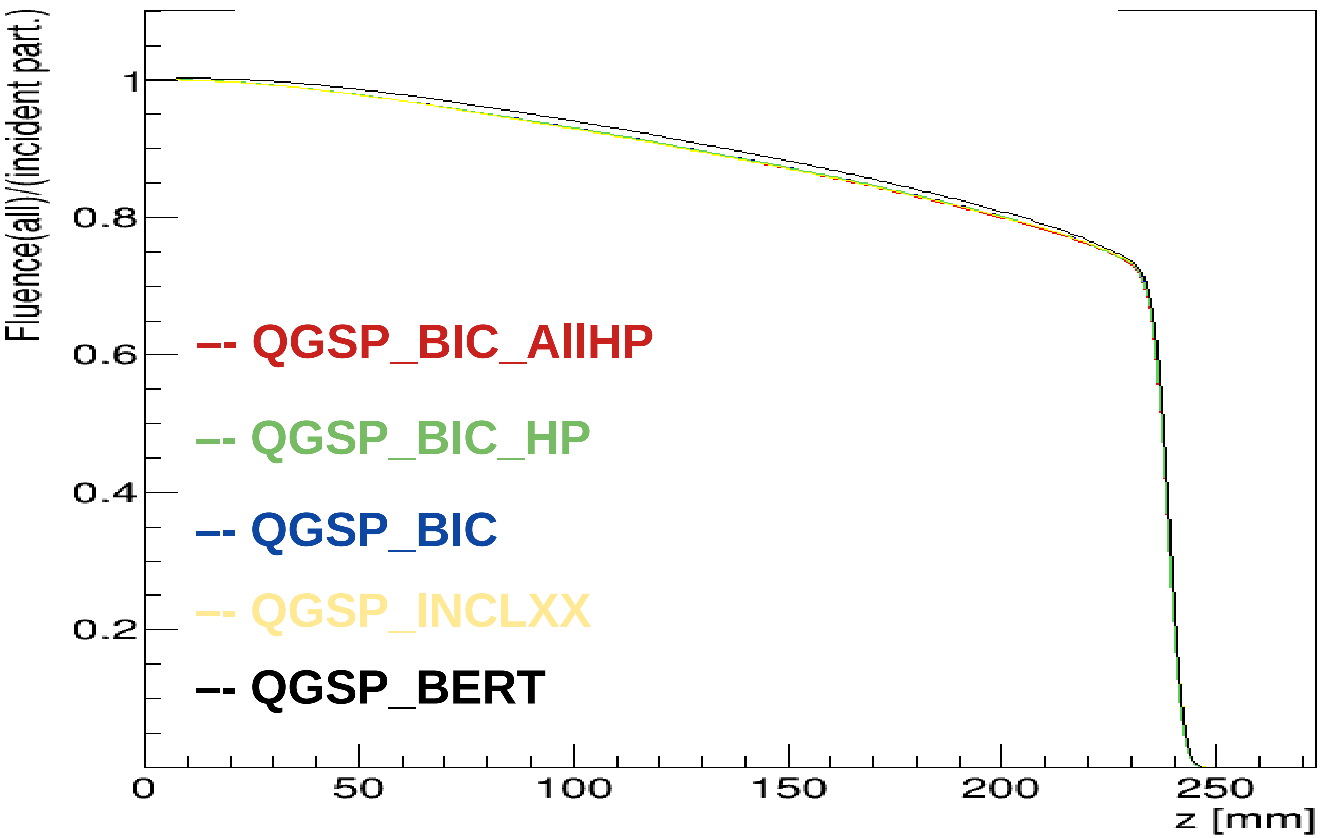
# Proton fluence in WATER Ep=190 MeV

**Indistinguishable results from BIC PL's!** → For folding with external library **use the faster (BIC)**



# Proton fluence in WATER Ep=190 MeV

**Indistinguishable results  from BIC and INCLXX PL's!**
**Only BERT deviates**



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