Recent developments in Geant4 pre-compound and deexcitation modules

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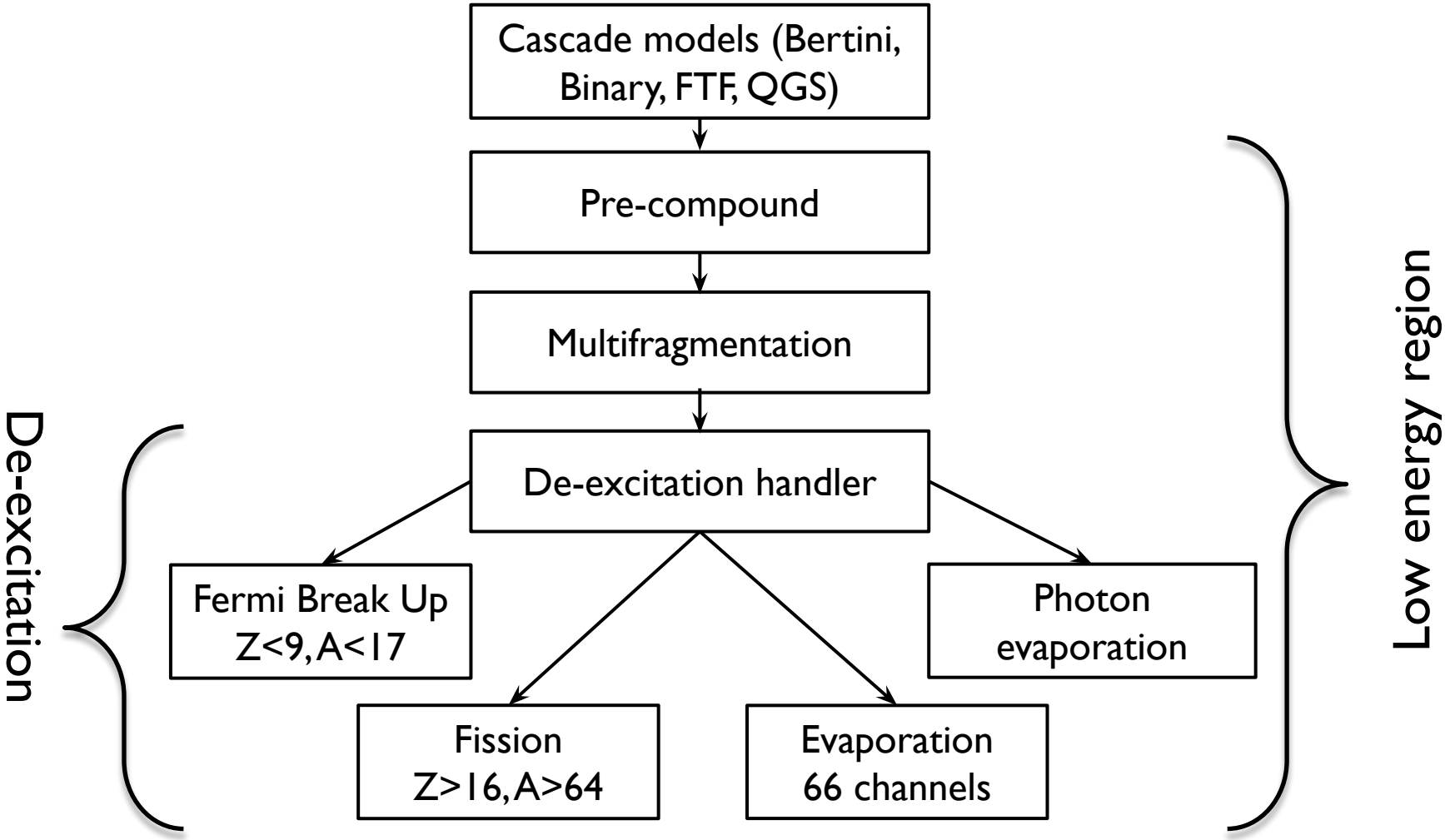
Contents

Introduction

- We report latest changes to de-excitation and pre-compound modules in Geant4 Toolkit for the simulation of passage particle through matter.
- Our motivation is improve simulations of low energy processes with hadrons and ions in high energy physics experiments (LHC, NICA) and other applications
- Geant4 version 11.4beta (released 28 June).

The study was carried out within the framework of the state assignment of the Ministry of Science and Higher Education of the Russian Federation (project No. FSWM-2025-0023)

Low energy models



Pre-compound model

- The pre-compound model [1] in Geant4 process residual nuclear fragments and simulate the emission of neutrons, protons, and light ions, which ensures the transition of an excited nucleus to an equilibrium state.
- We implemented new criteria of transition to equilibrium state [2]:
  - $A < 5$
  - $Z < 2$
  - $U < 0.1 \cdot A$ [MeV] – excitation energy
- These limitations preclude the application of the pre-compound model to states for which its physical premises are no longer relevant.

[1] K.K. Gudima, et al. *Nucl. Phys. A* 401, 329-361 (1983).

[2] N.A. Chalyi, V.N. Ivanchenko. *Russ. Phys. J* 67, 1962-1968 (2024).

Evaporation

The evaporation model is a key component of the nuclear relaxation module, responsible for the generation of most final fragments in a nuclear decay [3].

Probability: $$P_j(E_x, \varepsilon)d\varepsilon = g_j \sigma_{\text{inv}}(\varepsilon) \frac{\rho_d(E_x - \varepsilon)}{\rho_i(E_x)} \varepsilon d\varepsilon,$$

Level density: $$\rho(E) = C \exp\left(2\sqrt{aE'}\right),$$

We changed description of $E' = \max(E_x - \delta, 0)$,

where δ is the pairing energy correction of the daughter nucleus, and *a* is the level density parameter.

[3] I. Dostrovsky, et al. *Physical Review* 116(3), 683–702 (1959).

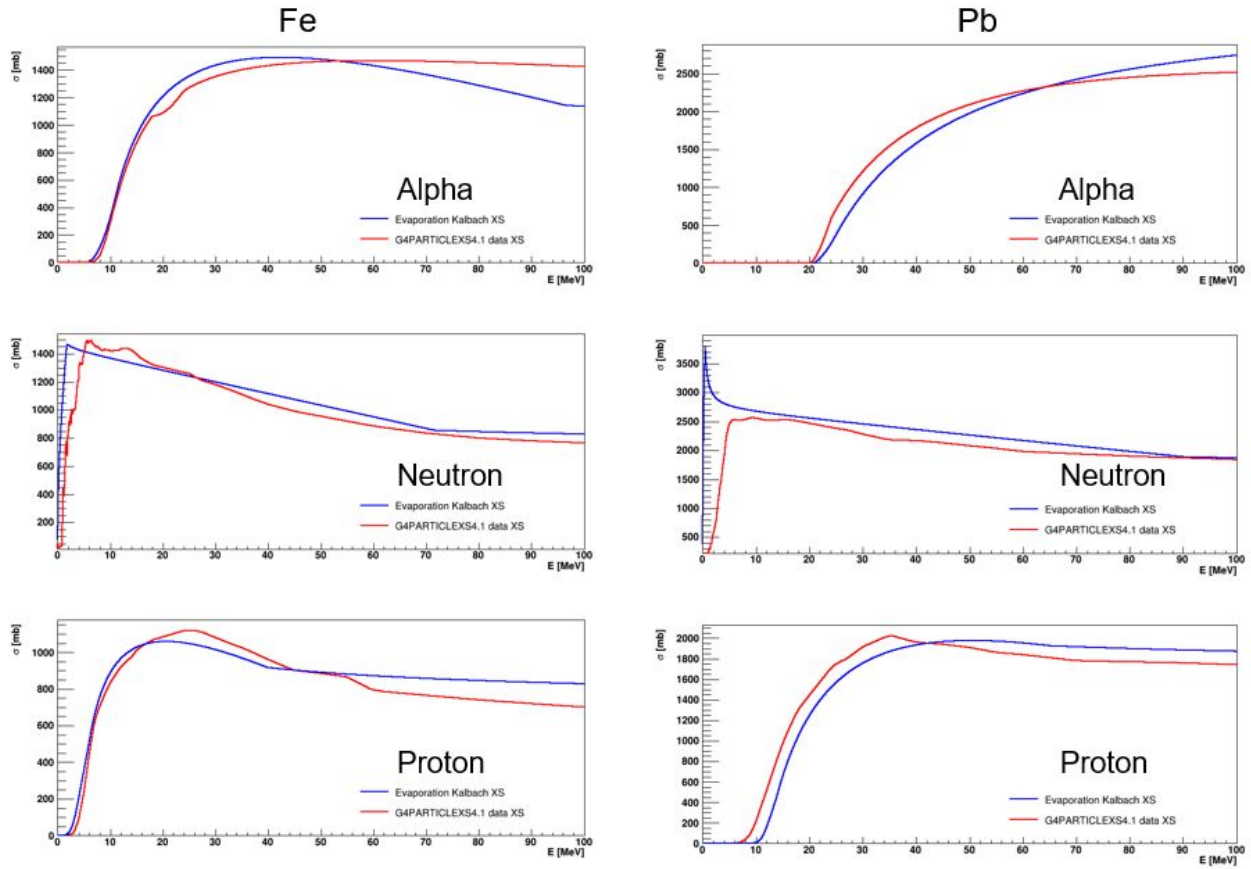
G4InterfaceToXS

- The inverse reaction cross section $\sigma_{\mathrm{inv}}(E)$ is traditionally described by the empirical Kalbach parameterization [4].
- We proposed an alternative approach using data from the G4PARTICLEXSDATA database via the *G4InterfaceToXS* interface class.
- The choice of method (parameterization or data) can be specified at the Geant4 initialization stage.
- This module implemented as an option for the Evaporation model and also can be easily accessed from anywhere.

[4] C. Kalbach, *Z Physik* A 287, 319–322 (1987)

G4InterfaceToXS

Comparison of default Kalbach parameterization (blue lines) for cross sections VS G4PARTICLEXSDATA (red lines) for Iron and Lead



G4VSIntegration

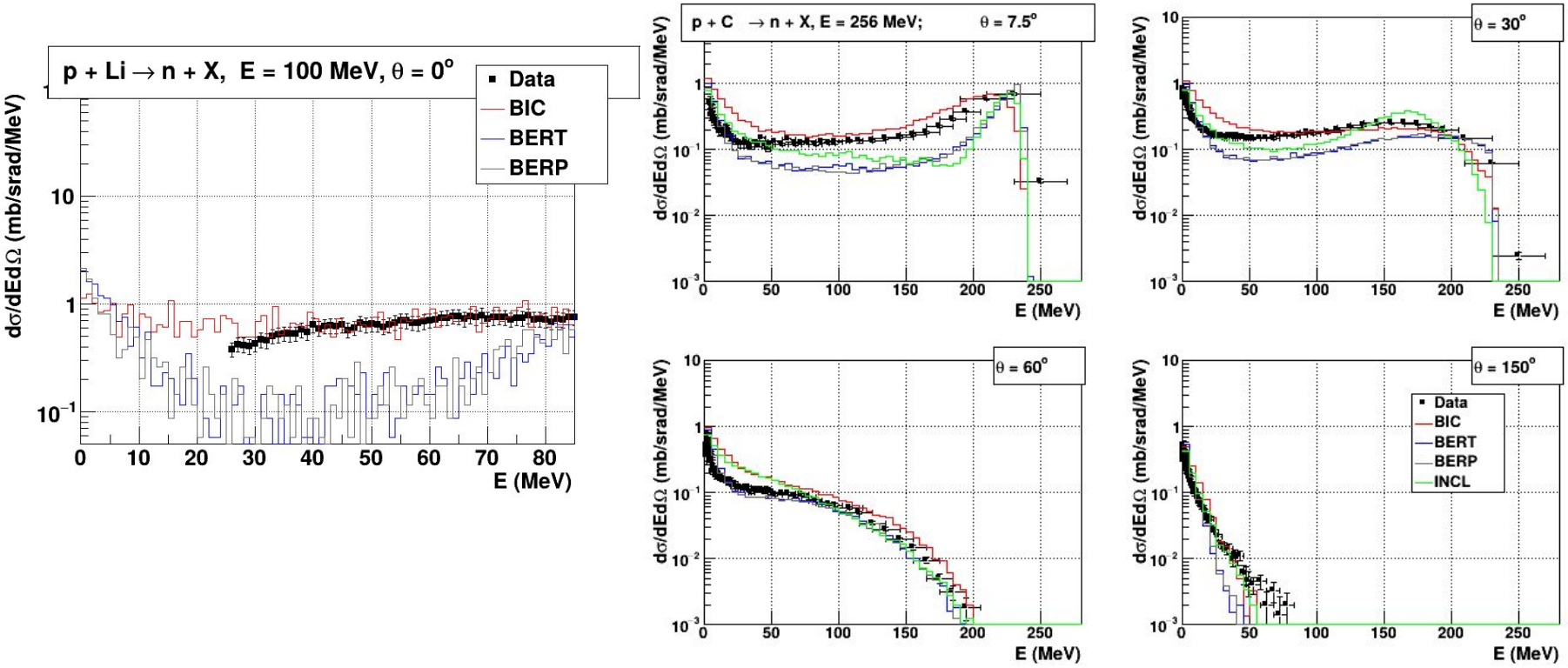
We implemented new method *G4VSIntegration*, which provides functionality for calculating integrals over a given energy range and sampling distributions of random variables for arbitrary one-dimensional final-state probability density functions. Key methods of the class include:

- *InitialiseIntegrator(...)*
- *ComputeIntegral(Emin, Emax)*
- *SampleValue()*

To implement the method, the user class must contain the *ProbabilityDensityFunction(E)* method, which returns the probability density value for energy E.

Validation

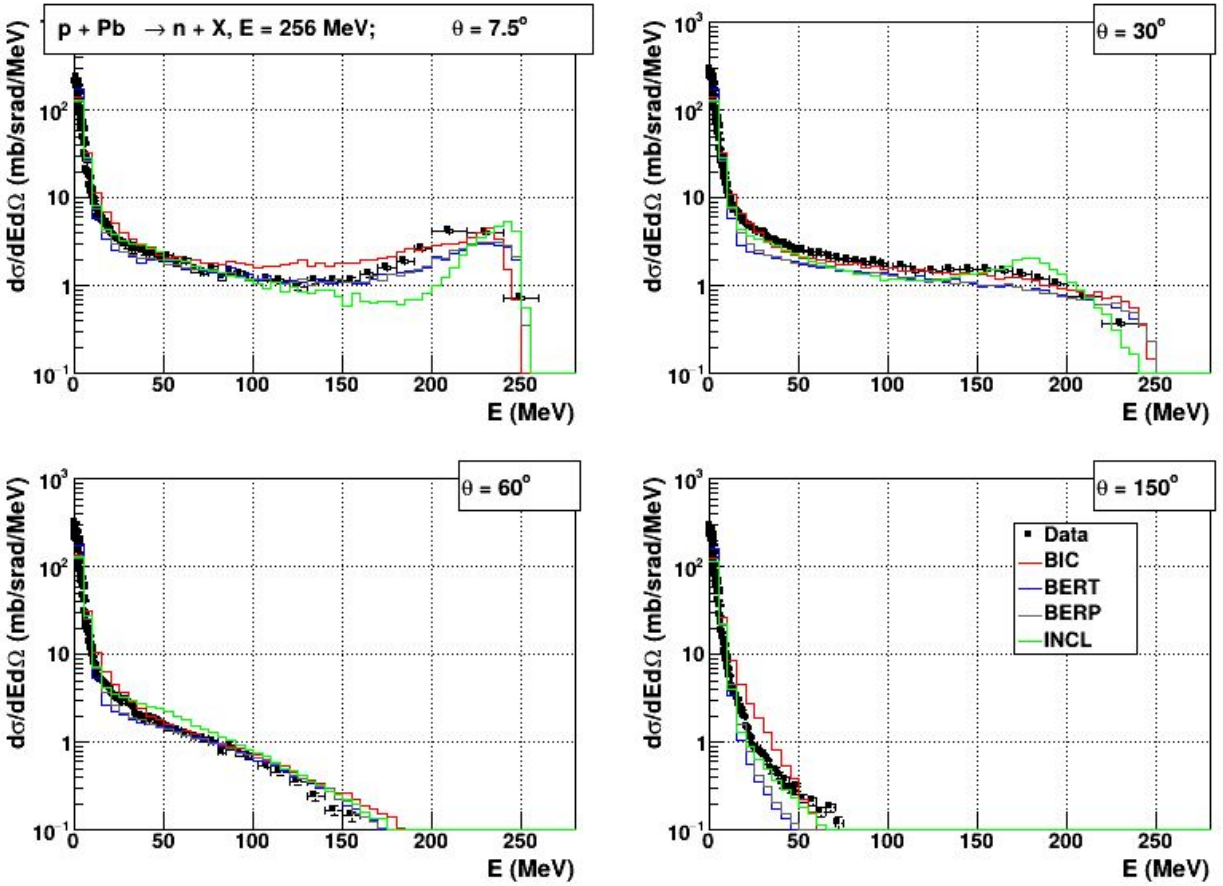
Neutron double differential cross sections in p+Li and p+C



Data taken from EXFOR database

Validation

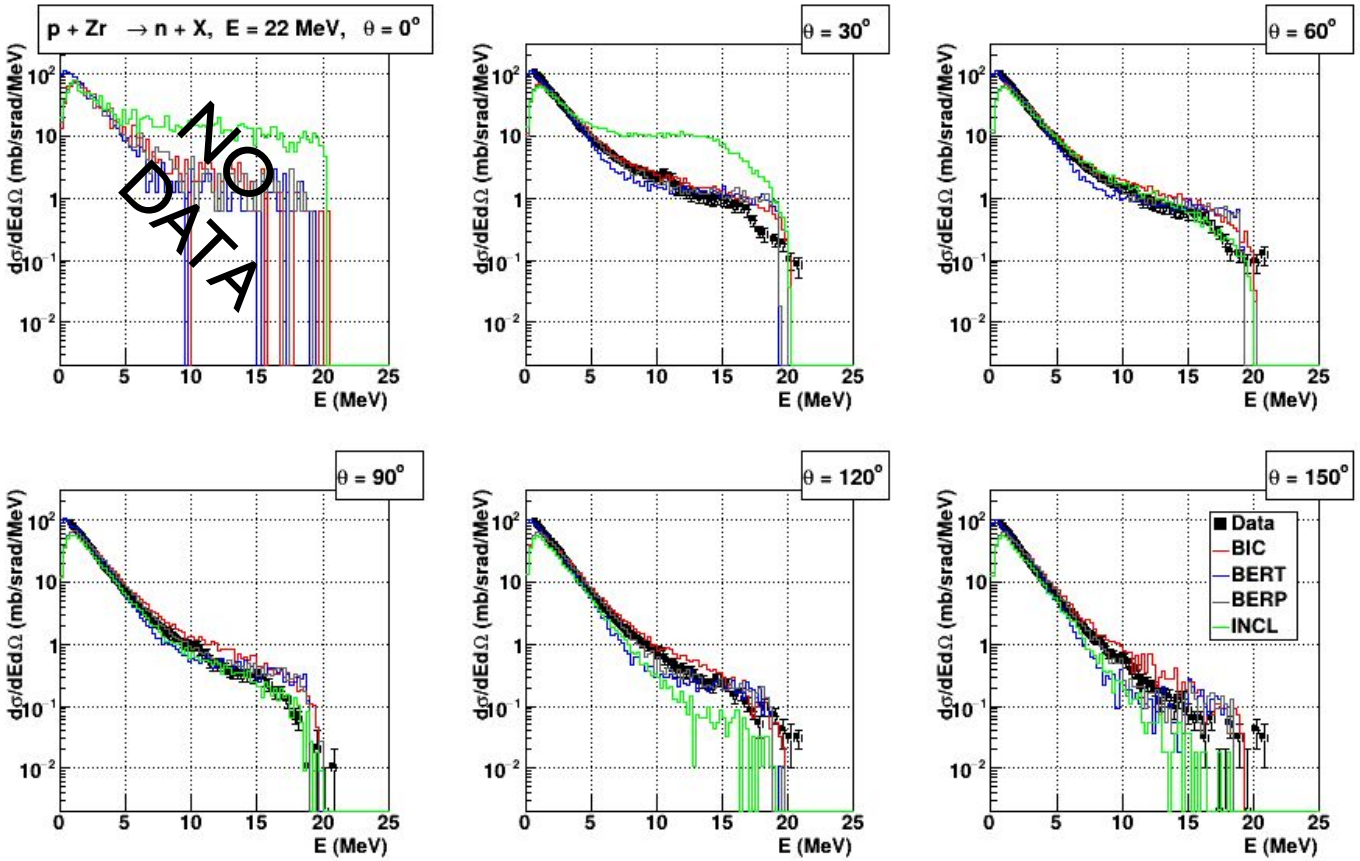
Neutron double differential cross sections in p+Pb



Data taken from EXFOR database

Validation

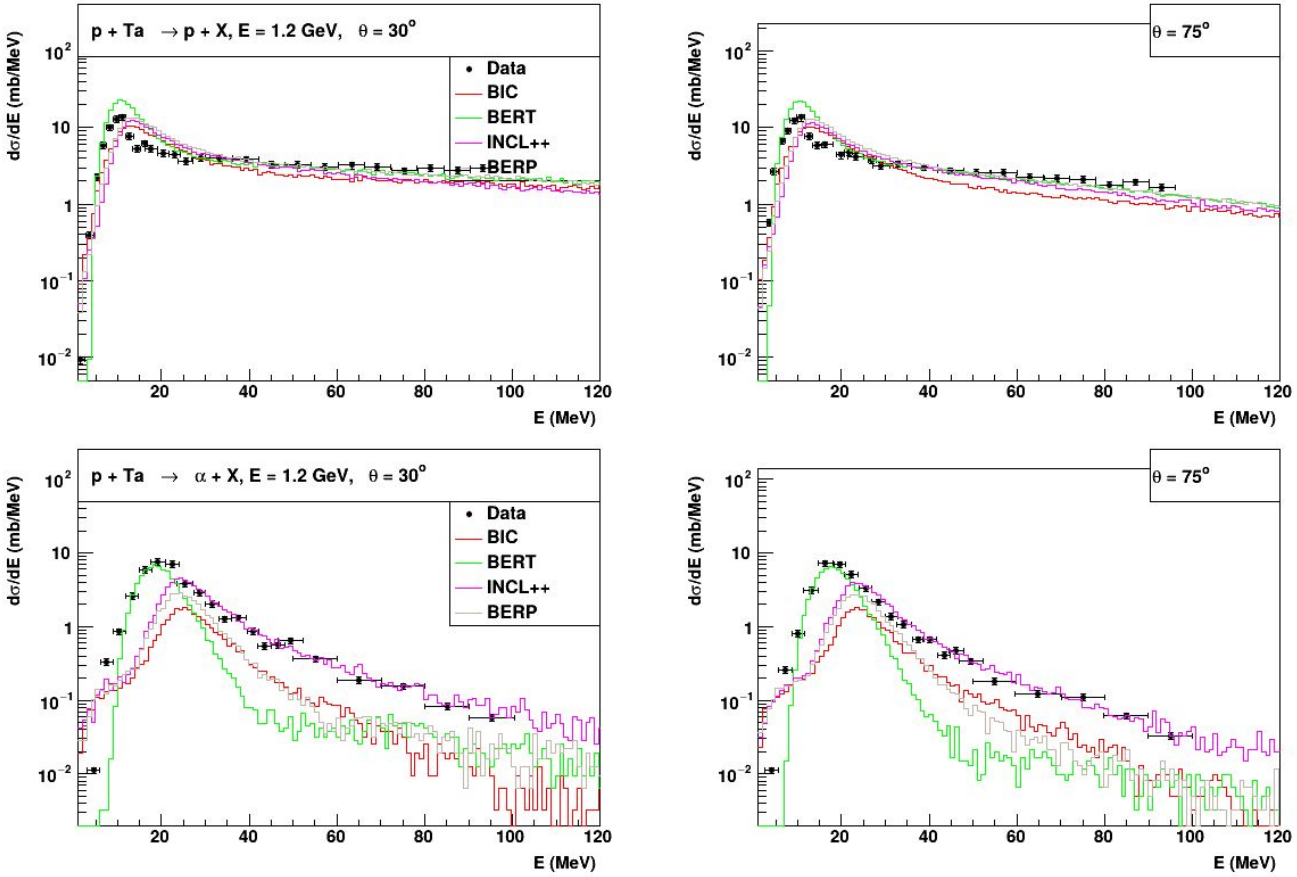
Neutron double differential cross sections in p+Zr



Data taken from EXFOR database

Validation

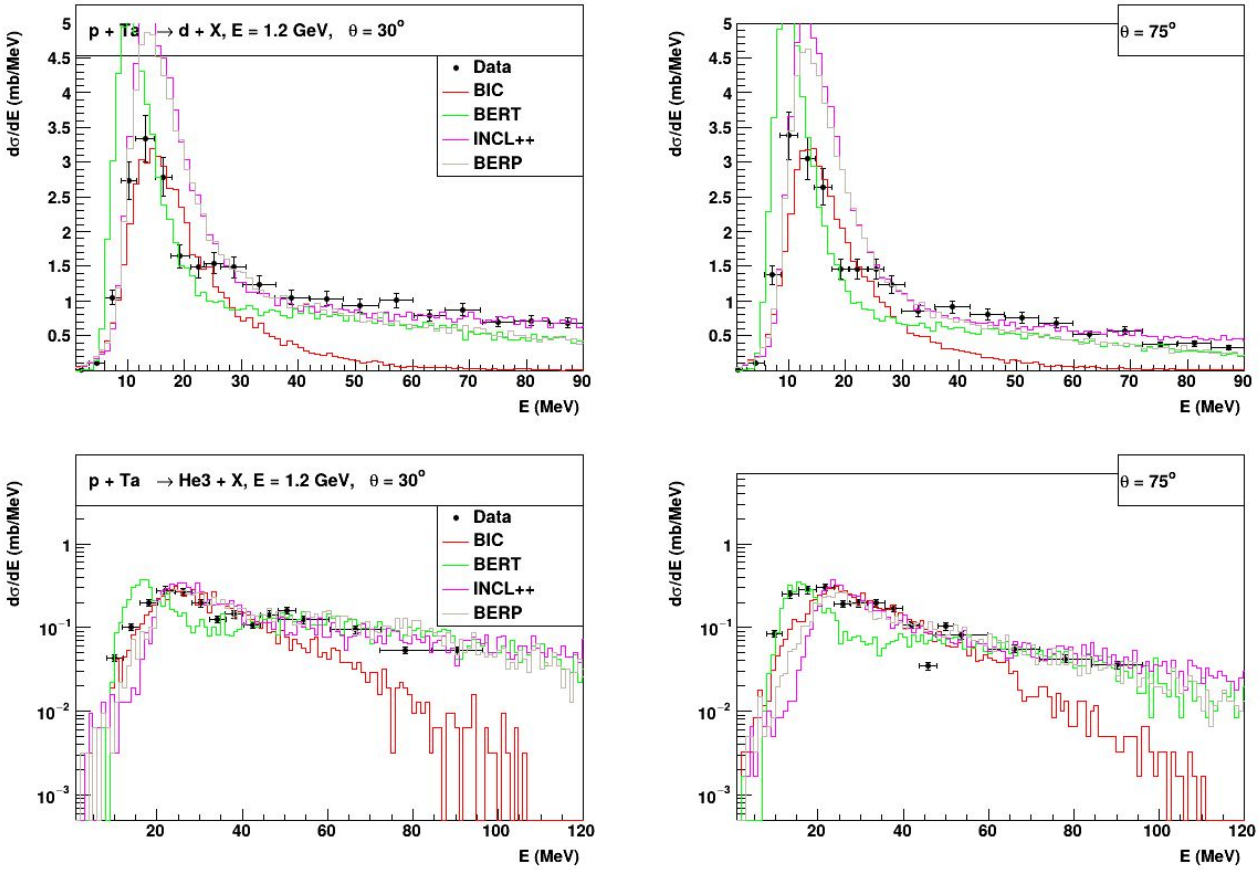
Proton and alpha double differential cross sections in p+Ta



Data taken from EXFOR database

Validation

Deuteron and He3 double differential cross sections in p+Ta



Data taken from EXFOR database

Conclusion

- In this work, the existing low-energy hadron physics models for describing the pre-compound state and nuclear evaporation in the were improved and implemented in Geant4 11.4beta.
- Two new methods for general improvement of modeling in Geant4:
  - G4InterfaceToXS — for simplifying and accelerating data loading from databases
  - G4VSIntegration — containing algorithms for integrating and sampling the values of dynamic probability density functions, instead of separate algorithms for each individual model.

Future plans

- Optimize pre-compound model parameters.
  - Change the order of model: set multifragmentation model before pre-compound (right now multifragmentation is suppressed by default).
  - Optimize transfer from pre-compound to de-excitation modules.
- Expand Evaporation from 66 to 81 channels.
- We are also working on a web service in TSU that will:
  - allow external non-experienced users to do some basic simulation (close to standart Geant4 examples)
  - present validation results of different versions of Geant4.

Thank you for your attention!

Looking for feedback and suggestions!
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