# Geant4 simulation of nuclear spallation reactions

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**Abstract**. Geant4 has contributed to the IAEA nuclear spallation reactions benchmark with simulation results for all mandatory sets of data, including neutron production, light charged particle production, isotope production, excitation functions up to 3GeV, and pion production. Two hadronic multi-staged intra-nuclear cascade models were used in calculations: the Binary cascade and the Bertini intra-nuclear cascade. The Chiral Invariant Phase Space model was also used for nuclear de-excitation and isotope production. Short descriptions of the models and results of the benchmark are presented and discussed.

## 1. Introduction

Geant4 is a powerful toolkit for the simulation of the passage of particles through matter [1, 2]. The primary focus of Geant4 was on preparation of experiments for the Large Hadron Collider [1, 2]. At the same time its areas of applications are growing and include high energy, nuclear and accelerator physics, studies in hadron therapy, tomography, space dosimetry, and others. Geant4 physics includes different models for simulation of interactions of hadrons with nuclei [2, 3]. For the simulation of spallation reactions, both the Bertini-style cascade (BERT) [3, 4] and the Binary cascade (BIC) [5, 6] were selected. These cascades are used in many Geant4 applications and are applicable within the energy range of the benchmark 20MeV-3GeV. Recently the Chiral Invariant Phase Space (CHIPS) generator [6-9] has been extended to the proton-nuclear and neutron-nuclear reactions. It is also used in the benchmark.

## 2. Bertini Cascade

The Geant4 Bertini-style model is a classical intra-nuclear cascade. It is based on the FORTRAN INUCL code [10] which in turn is based on a combination of the original Dubna and Bertini cascades [11]. The INUCL code was re-engineered into C++ and upgraded to include several features not found in the original code, such as Coulomb barriers and kaon-induced interactions.

The model simulates interactions in three stages: intra-nuclear cascade, pre-equilibrium de-excitation of the residual nucleus, and evaporation. The pre-equilibrium phase consists of the Griffin exciton model [12], a simple nucleus explosion model and a fission model. The evaporation modulus is based on that of Dostrovsky [13]. If a light nucleus is highly excited, the Fermi break-up model is executed. Also, fission is performed if that channel is opened. The emission of particles is computed until the excitation energy falls below 0.1 MeV.

The target nucleus is represented by a set of constant density three-dimensional shells which approximate the density distribution of nuclear matter. All interactions within the nucleus are based on the free-space hadron-nucleon cross sections, which are effectively modified by Pauli blocking. Also included is the reduction of nuclear density due to the ejection of nucleons during the cascade. Relativistic kinematics is applied throughout the cascade. The cascade is stopped when all the particles which can escape the nucleus, have done so. Then conformity with energy conservation is checked.

## 3. Binary Cascade

The model proceeds in three stages: intra-nuclear cascade, pre-equilibrium decay and evaporation. The Binary cascade is native to Geant4 and introduces a new approach to cascade calculations [5]. It is a time-dependent model in which the interaction is modelled exclusively on binary scattering between reaction participants and nucleons. Propagation of the particles in the nuclear field is done by numerically solving the equation of motion.

The nucleus is described by a detailed three-dimensional model with a Woods-Saxon density distribution. Collisions within the nucleus proceed according to free-space cross sections and are modified by Pauli blocking. In the Binary model, resonances can be formed after the initial collision. The resonance may then scatter or decay. The cascade terminates when both the average and maximum energy of all particles within the nuclear boundary are below a given threshold. Coulomb barriers, relativistic kinematics and energy conservation are all included.

The pre-equilibrium stage is an exciton model which follows Gudima et al. [14]. Some refinements have been introduced, namely more realistic inverse cross section parameterizations [15, 16] and combinatorial factors for particle emission. The pre-equilibrium terminates when transition probabilities for increasing and decreasing the exciton number become equal. At the end of the pre-equilibrium stage, the residual nucleus is supposed to be left in an equilibrium state, in which the excitation energy is shared by the whole nuclear system. Such an equilibrated compound nucleus is characterized by its mass, charge and excitation energy with no further memory of the steps which led to its formation.

The Geant4 equilibrium de-excitation models are invoked by a specific handler class which manages the competition among the corresponding processes. Three of them have been considered in the present validation: statistical multifragmentation [17], fission [18, 19] and particle evaporation.

The Geant4 fission model is able to predict final excited fragments as result of nuclear de-excitation by symmetric or asymmetric fission. The fission process ($A > 65$) is considered as a competitor to the evaporation process, when the nucleus transits from an excited state to the ground state.

The Geant4 evaporation model follows the method of Dostrovsky [13], but includes also an improved set of inverse reaction cross sections [15, 16]. It is capable of predicting final states as a result of evaporative break-up of an excited nucleus with atomic number more than 16. The evaporation of neutrons, protons, deuterons, tritons, $He^3$ and alpha particles are taken into account. It implements a version of the Weisskopf-Ewing model for particle evaporation [20].

## 4. CHIPS

CHIPS is a quark-level event generator for the fragmentation of hadronic systems into hadrons [3, 6]. In contrast to most other models CHIPS is non-perturbative and three-dimensional. It is based on the Chiral Invariant Phase Space model [7-9] which employs a 3D quark-level SU(3) approach. Thus Chiral Invariant Phase Space refers to the phase space of mass less partons and hence only light (u, d, s) quarks can be considered. It has been recently improved in terms of light ion interactions with nuclei and added to the spallation reactions benchmarking. A parameterization within CHIPS is also used for the simulation of elastic scattering of protons and neutrons.

## 5. Results and discussion

Results for the IAEA benchmark were produced using the Geant4 release 9.2patch01, which can be downloaded from the official Web page [21]. Additional computations were done for the CHIPS generator using newest 9.3beta release.

In order to produce the benchmark results, a special application was designed based on an approach developed for the Geant4 hadronic validation suites [22]. In this application a beam particle is forced to interact with the target nucleus. Secondary particles are scored in 3D histograms versus kinetic energy and polar angle. For the normalisation of these histograms Geant4 hadronic interaction cross sections are used. For the *(p,xp)* and *(n,xn)* reactions additional simulation of hadron elastic scattering (ELAST) was performed.

Neutron production from proton and neutron bombardment *(see Fig.1-2)* is an essential test of hadronic models. From the comparison of model predictions with experimental data we came to the conclusion that BIC and BERT models do a good job of simulating *(p,xn)* and *(n,xn)* double differential cross sections. This was already demonstrated by a number of test suite and benchmark runs [4, 22]. Similar successful results were obtained for pion production double differential cross sections using proton beams *(see Fig.3)*.

Light charged particle production is an innovation for the Geant4 hadronic models *(see Fig.4-5)*. We found that α and proton data on double differential cross sections are in qualitative agreement with Geant4 simulation. Other particle production cross sections need to be improved.

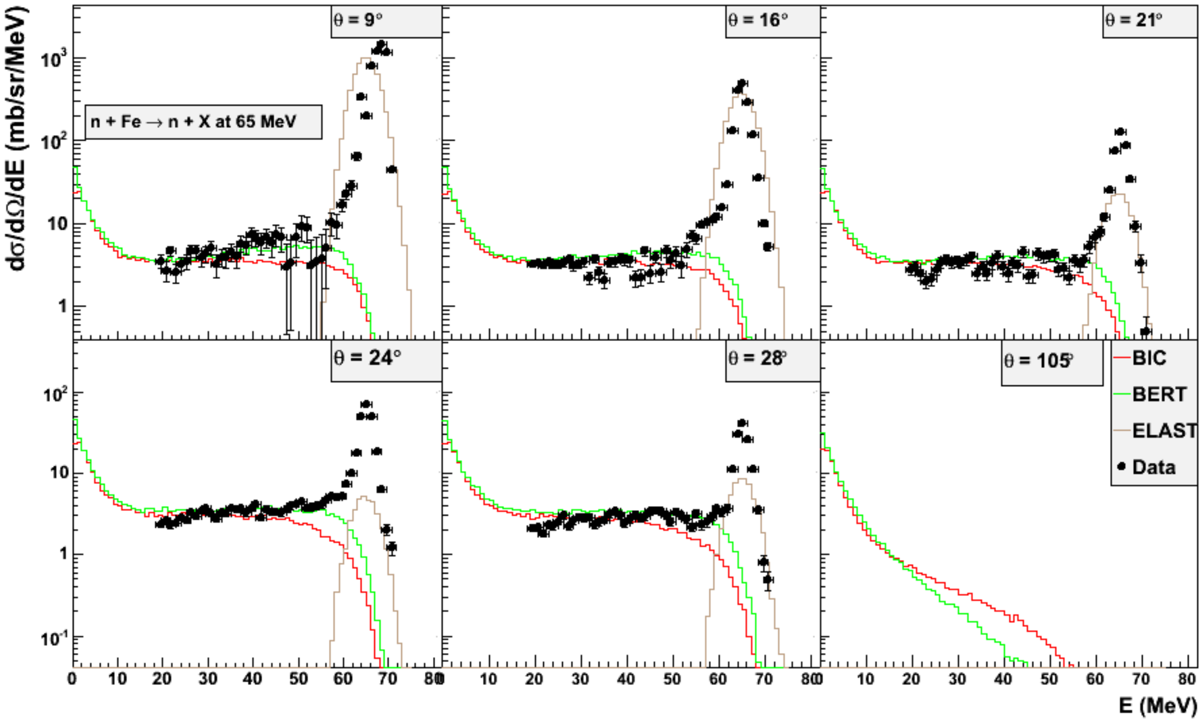

*FIG. 1. Spallation (n,n) reaction on Fe at 65MeV. Data points [23], histograms: Geant4 simulation.*

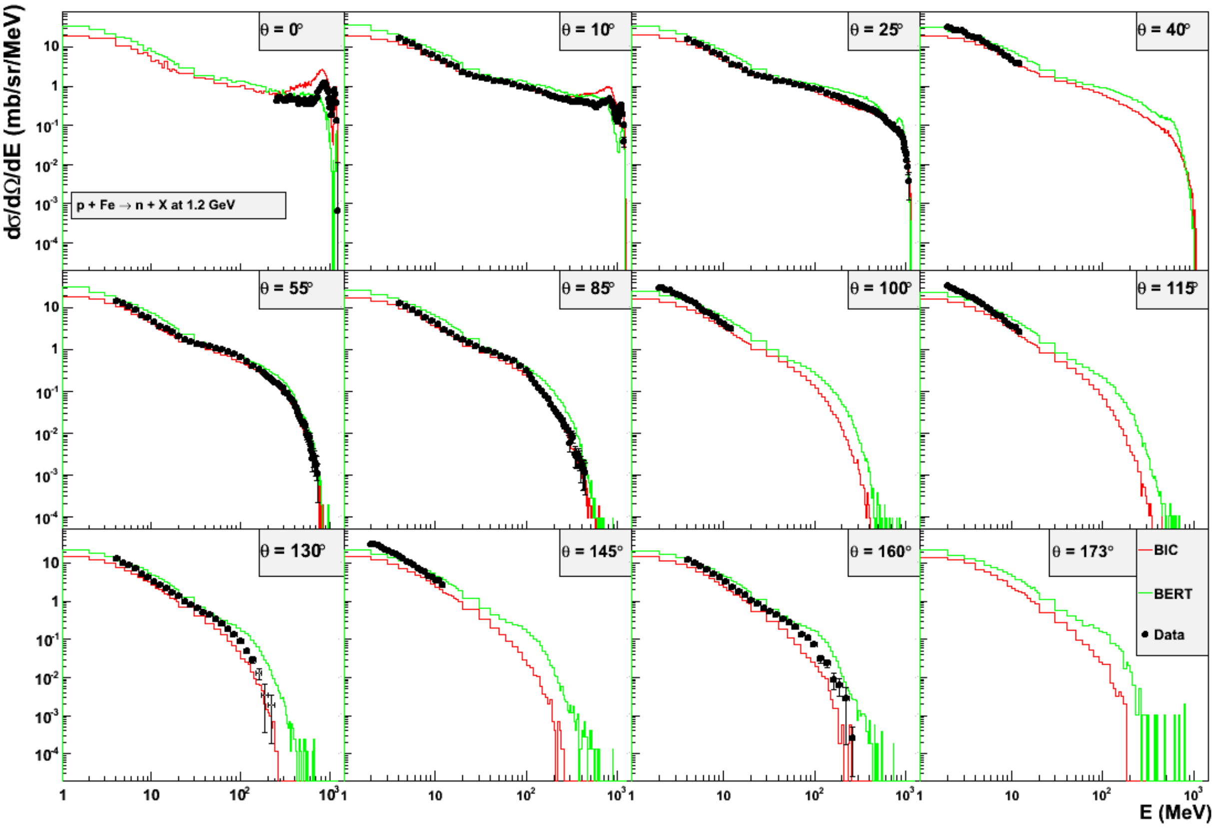

*FIG. 2. Spallation (p,n) reaction on Fe at 1200MeV. Data points Saturne [24], histograms - Geant4 simulation.*

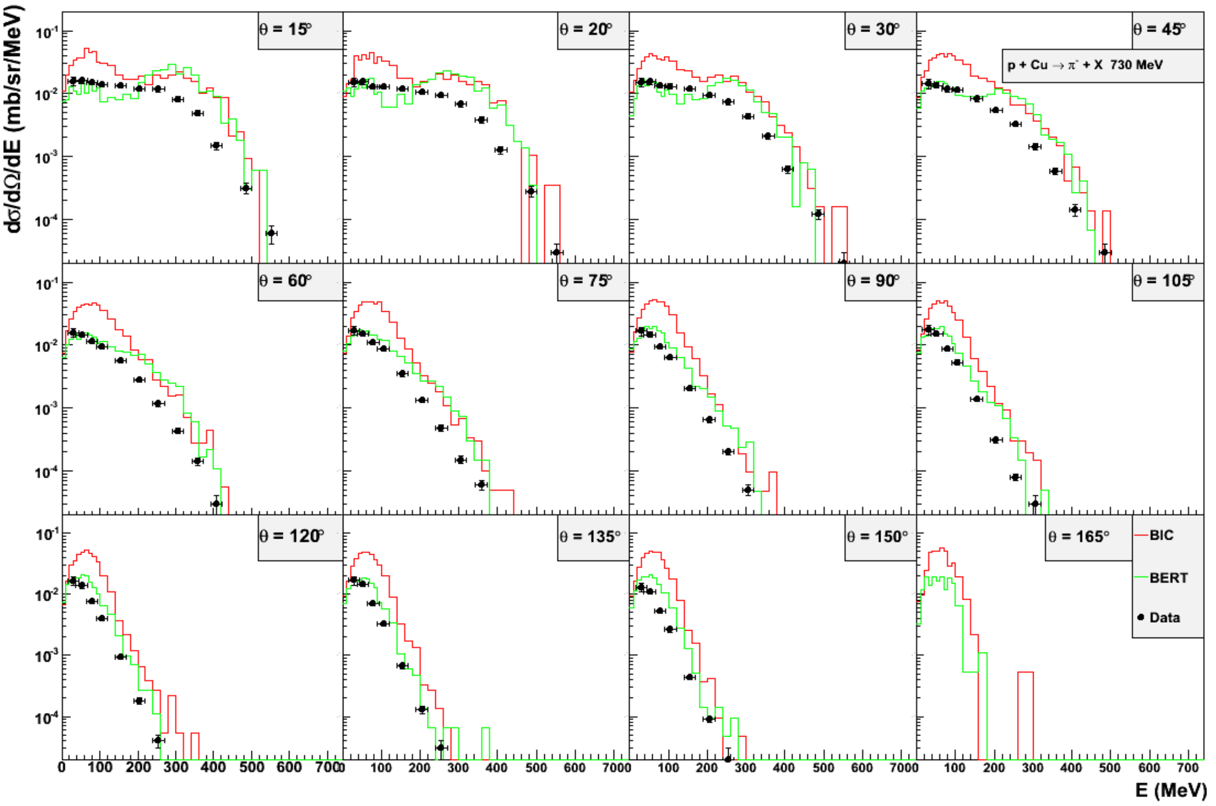

*FIG. 3. Spallation $(p,\pi^-)$ reaction on Cu at 730MeV, data points [25], histograms - Geant4 simulation.*

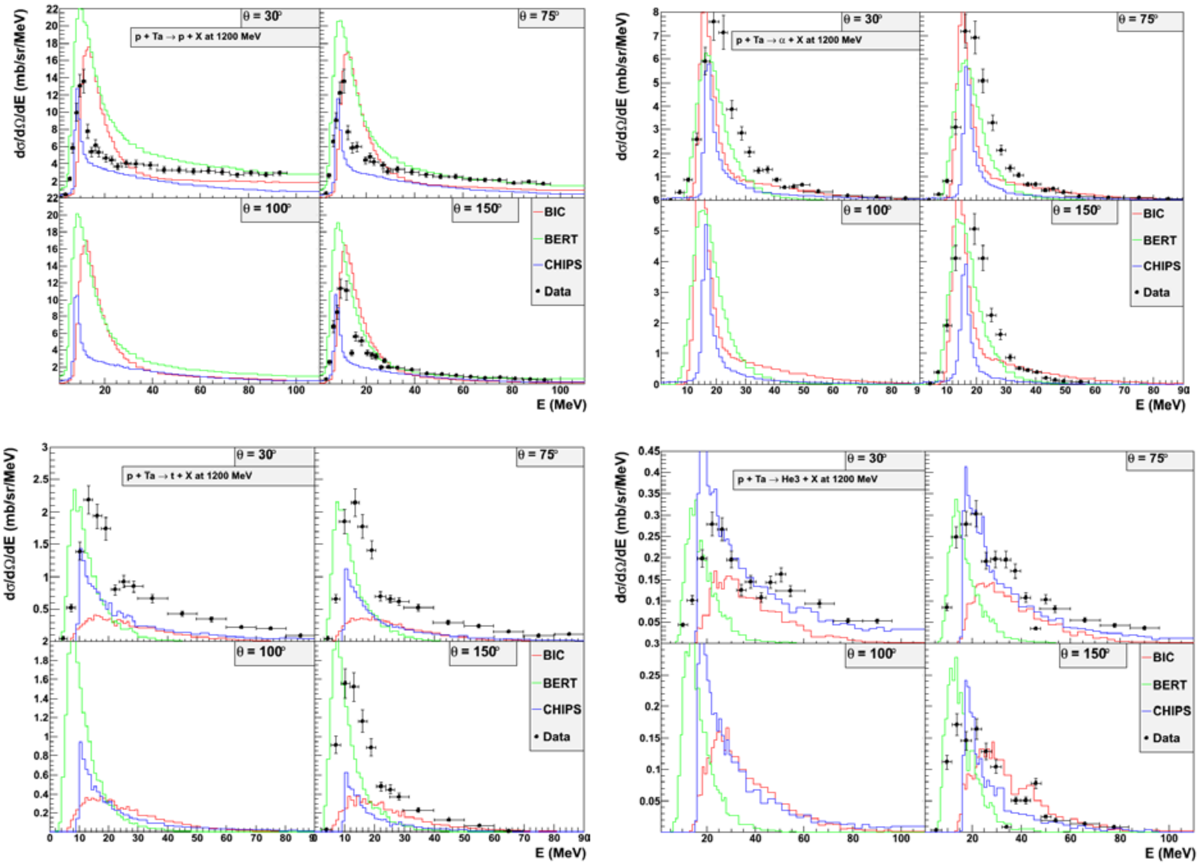

*FIG. 4. Spallation (p,p), (p,α), (p,t), and (p,He$^3$) reactions on Ta at 1200MeV. Data points COSY [26], histograms - Geant4 simulation.*

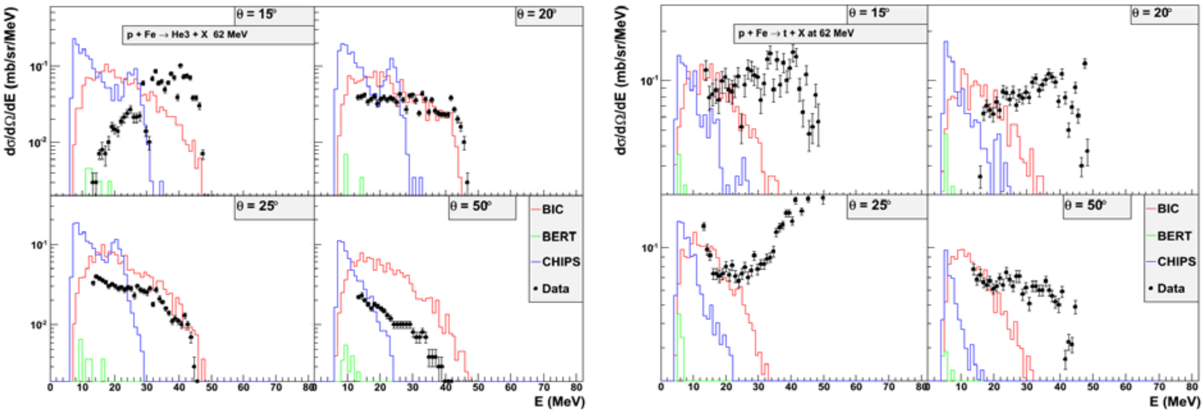

*FIG.5. Spallation (p,He$^3$) and (p,t) reactions on Fe at 62MeV. Data points [29], histograms - Geant4 simulation.*

Isotopic distribution cross sections with inverse kinematics (GSI experiment, Germany) were done using all three models *(see Fig.6-7)*. It should be pointed out that CHIPS in this case is a better model for low-Z isotope production.

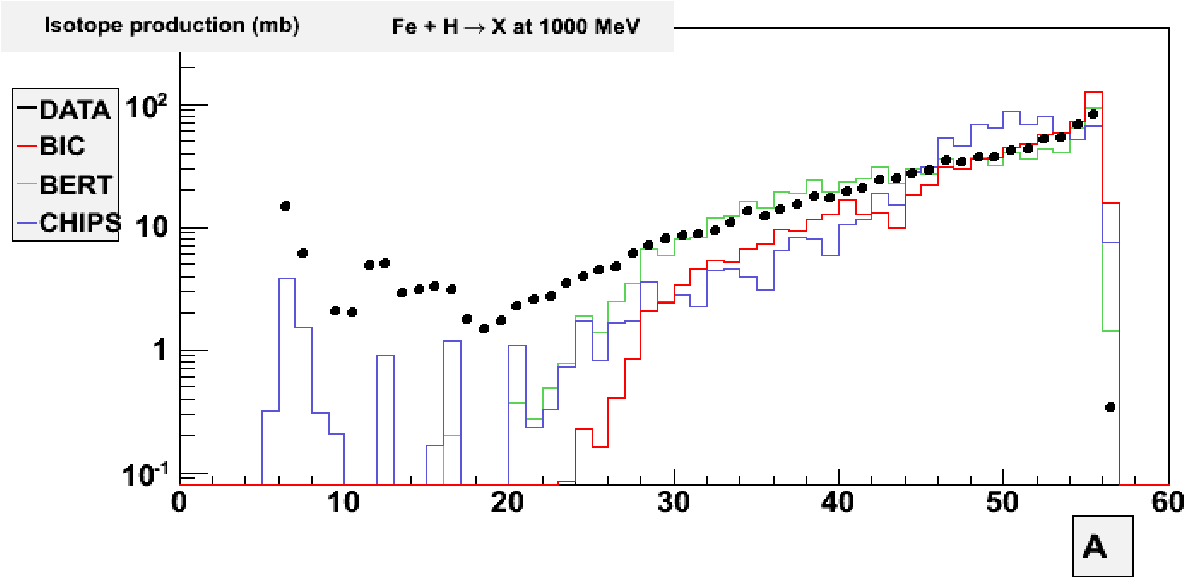

*FIG.7. Isotopic distribution cross sections with inverse kinematics. Data points GSI [27], histograms - Geant4 simulation.*

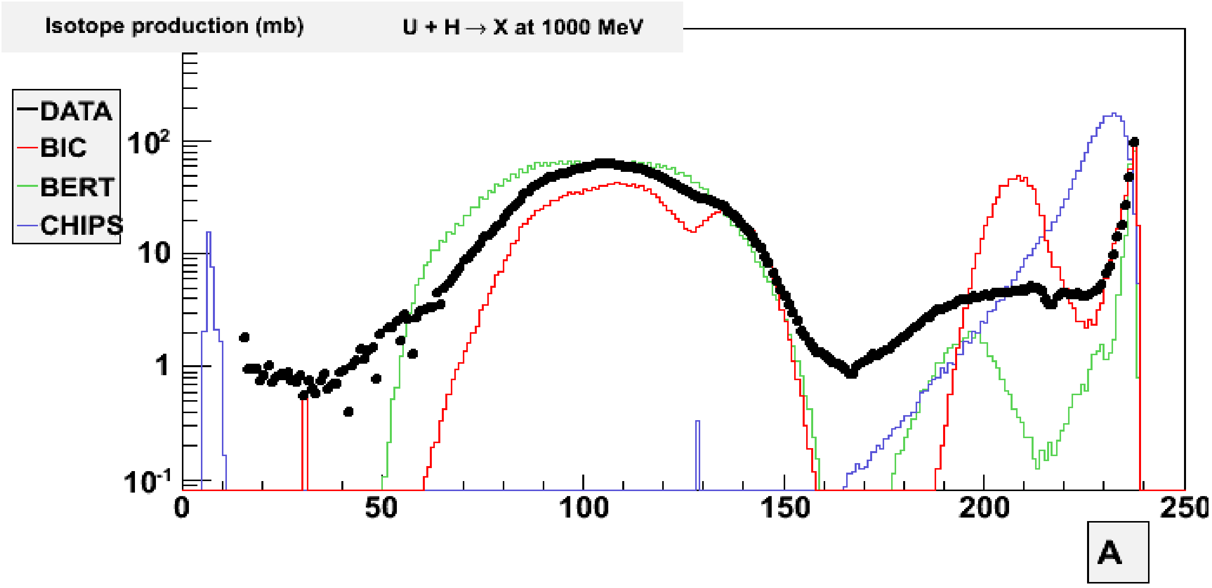

*FIG.8. Isotopic distribution cross sections with inverse kinematics. Data points: GSI [28], histograms - Geant4 simulation.*

## 6. Conclusion

Geant4 participated in the IAEA hadronic Spallation benchmark by submitting predictions from three hadronic models: Bertini, Binary Cascade and CHIPS. The intra-nuclear cascade models reproduce the spallation data fairly well in most cases, with Bertini performing better under some circumstances and Binary Cascade performing better under other circumstances. Isotope production with inverse kinematics can be simulated by all three models. Some obvious problems exist in reproducing the minima for the U + H reaction, but the qualitative features are reproduced. Some complications exist for light ion production from various targets. In Bertini and Binary, these problems are due to the lack of clusterization within the target nucleus as well as the absence of coalescence methods.

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