A Geant4 physics list for spallation and related nuclear physics applications based on INCL and ABLA models

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Abstract. A new Geant4 physics list is prepared for nuclear physics applications in the domain dominated by spallation. The C++ translation of original Fortran INCL intra-nuclear cascade and ABLA fission/de-excitation codes are used in the physics list. The INCL model prepared is well established for targets heavier than Aluminium and projectile energies from $\sim$ 150 MeV up to 2.5 GeV $\sim$ 3 GeV. Validity of the new Geant4 physics list is demonstrated, and the neutron double differential cross sections and residual nuclei production discussed. Foreseen improvements of the physics models for the treatment of light targets (Carbon - Oxygen) and light ion beams (up to Carbon) are discussed.

1. Introduction

This paper is focused on issues relevant to Geant4 [1] simulation of nuclear physics applications, modelling of spallation reactions, and validating neutron production and fragmentation.

Our motivation is to develop Geant4 simalation tools for European Isotope Separation On-Line Radioactive Ion Beam Facility (EURISOL project) [2] and Accelerator Drive Systems (ADSs) [3]. The goal of accelerator driven sub-critical reactor development is to provide safer and more effective methods of nuclear power production.

The most important benefits of this new type of reactor include improved safety. In case of an emergency the accelerator can be shut down which in turn shuts down the reactor. Another important safety benefit is that the system transmutes nuclear waste to less harmful isotopes.

To this aim we present a new Geant4 physics list, based on INCL [4] intra-nuclear cascade model and ABLA model [5, 6, 7] in Geant4 9.2. This physics list can be used to simulate the main components of an ADS system: accelerator, spallation target and sub-critical core.

This paper is organized as follows. Section 2 briefly summarise the concept of Geant4 physics list. Geant4 9.2 models intra-nuclear cascade INCL or Liege cascade, and ABLA evaporation-fission model applied in this work are introduced in Section 3, while Section 4 documents the details of physics list implementation. Physics performance is demonstrated in Section 5, and status of carbon projectiles is given Section 6. Section 7 concludes with outline of future developments.

2. Geant4 physics lists

A unique feature of Geant4 is to decouple physics models, cross sections, and processes using abstract interfaces, and manage the usage of different options with so-called the physics lists:

- Concept provides transparent access to various physics models.
- The Geant4 physics system can be easily extended with physics lists.
- Physics lists allow users to find a good balance between various goals (e.g. CPU time requirements vs. accuracy of results).

Often an optional models are available with specific strengths and limitations, so physics lists concept is used to provide optimal set of functionality for specific use case.

3. INCL and ABLA models in Geant4

INCL and ABLA models are casted into independent Fortran based Monte Carlo codes INCL4.2 [4] and ABLA v3 [5]. Recently these implementations have been translated into C++ and codes distributed as part of Geant4 toolkit [9]. First beta release of INCL 4.2 and ABLA v3 was in Geant4 9.1 (December 2007) [8]. Currently new versions of INCL and ABLA versions in Geant4 are relatively straightforward and stable Fortran to C++ translations. Table 1 summarise the key features of these models.

Table 1. Summary of key features of INCL and ABLA models in Geant4 [9].

INCL4.2	
Projectiles	INCL/ABLA for protons, neutrons, pions (π^-, π^-, π^+)
	D, T, ^{3}He, α
Energy range	~150 MeV – ~3GeV
Target nuclei	Carbon – Uranium
Model features	Stand alone mode with built in random number generation
	No ad hoc parameters
	Woods-Saxon nuclear potential
	Coulomb barrier
	Pauli blocking
	non-uniform time step
	π and Δ production cross sections
	Δ decay
ABLA v3	
Supported input	Exited nuclei
Model features	Fission
	Evaporation of p, n, and α
Output particles	Fission products, residual nuclei, p, n, α

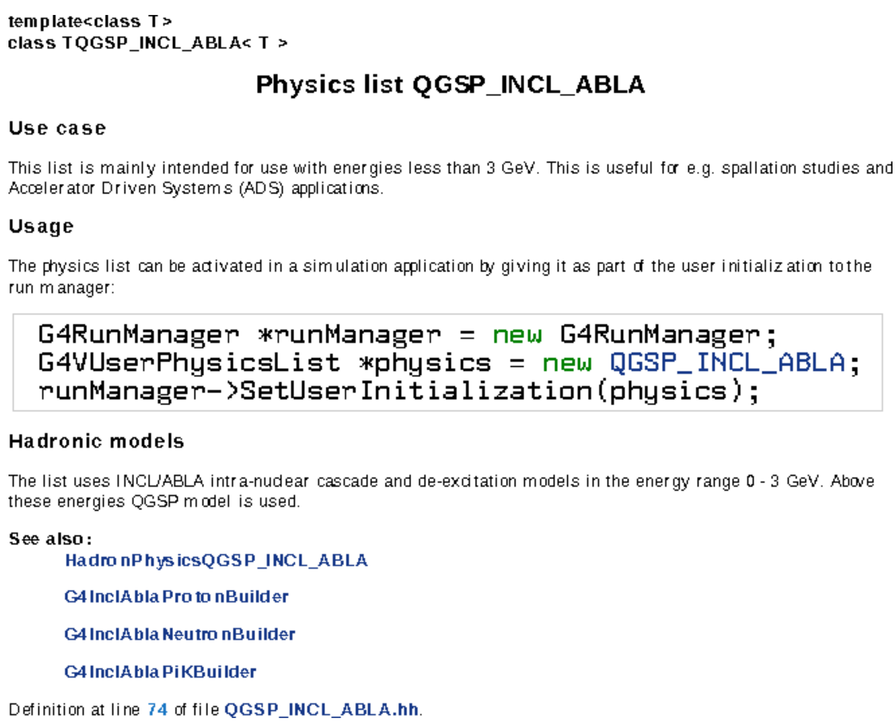
4. A new Geant4 physics list `QGSP_INCL_ABLA`

We have implemented a new physics list called `QGSP_INCL_ABLA` with spallation physics in mind. The list is based on widely used `QGSP_BERT` physics list. The new physics list uses INCL and ABLA models for proton, neutron and pion inelastic interactions in the energy range 0 - 3 GeV. Above 3 GeV threshold Geant4 QGSP model is used, since this list is intended for spallation and ADS applications we have not optimized the physics performance for energies higher than 3 GeV. Key features of `QGSP_BERT` physics list are summarised in Table 2.

Table 2. Summary of `QGSP_INCL_ABLA` physics list [9].

Models	Description
Electromagnetic physics	Geant4 standard EM
Spallation modelling	INCL cascade with ABLA fission and evaporation (E<3 GeV)
High energy model	QGSP (E>3 GeV)
Use-cases	
	Spallation studies
	Accelerator driven systems
	Fragment production
	Neutron production

The class reference documentation of the INCL/ABLA models is produced using Doxygen [10] documentation generator (see Fig. 4). It allows us to produce full documentation of the class structure complete with usage instructions, class diagrams, detailed descriptions of all methods and code listings.


template<class T>
class TQGSP_INCL_ABLA< T >

Physics list QGSP_INCL_ABLA

Use case

This list is mainly intended for use with energies less than 3 GeV. This is useful for e.g. spallation studies and Accelerator Driven Systems (ADS) applications.

Usage

The physics list can be activated in a simulation application by giving it as part of the user initialization to the run manager:

```
G4RunManager *runManager = new G4RunManager;
G4VUserPhysicsList *physics = new QGSP_INCL_ABLA;
runManager->SetUserInitialization(physics);
```

Hadronic models

The list uses INCL/ABLA intra-nuclear cascade and de-excitation models in the energy range 0 - 3 GeV. Above these energies QGSP model is used.

See also:
HadronPhysicsQGSP_INCL_ABLA
G4InclAblaProtonBuilder
G4InclAblaNeutronBuilder
G4InclAblaPiKBuilder

Definition at line 74 of file QGSP_INCL_ABLA.hh.

Figure 1. Doxygen documentation of Geant4 `QGSP_INCL_ABLA` physics list is provided.

5. Physics performance

Extensive validation has been performed to ensure the quality of INCL and ABLA models and correctness of Fortran to C+ translation. Particularly fragmentation of C - Pb targets bombarded with 0.8 - 1.6 GeV protons has been investigated with simulations and results compared with GSI data [11]. In addition to mass number distributions neutron production double differentials have been compared with accurate data from [13].

We have introduced a cut to choose between ABLA and Fermi break-up for light targets. So, INCL can now be used with the Geant4 Fermi break-up model. Currently, INCL interface provides Fermi break-up [12] for remnant nuclei lighter than A = 13 and ABLA for heavier elements.

For example, comparison of the fragment production results for reaction p(1.0 GeV) + C calculated using INCL and ABLA, INCL with Fermi break-up and Geant4 Bertini cascade are shown in Fig. 2. Table 3 summarises the validations reported in this paper.

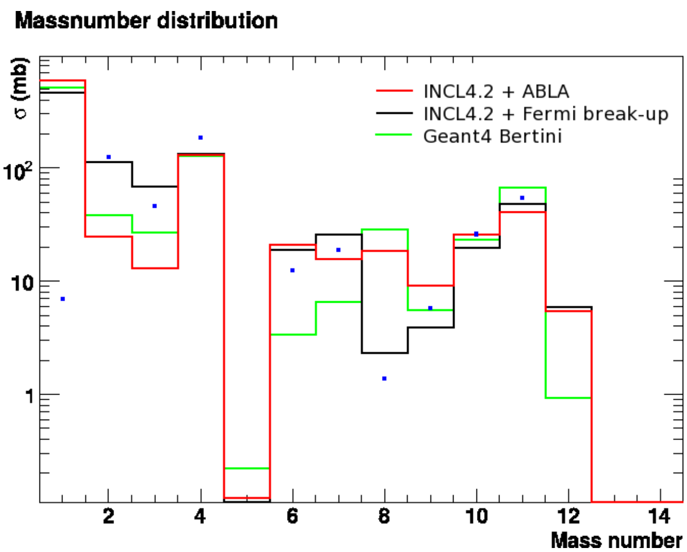


Figure 2. Comparison of massnumber distributions from p(1.0 GeV) + C reaction, given INCL4.2 cascade with ABLA evaporation and with standard Geant4 Fermi break up model against data from [11]. Also, results from Geant4 Bertini cascade with internal fragmentation model are shown.

Table 3. Summary of Geant4 INCL ABLA validations.

Validation	Configuration	Figure
Fragmentation		
	p(1.0 GeV) + C	Fig. 2
	p(1.0 GeV) + ^{208}Pb	Figs. 3 and 4
Neutron production		
	p(1.2 GeV) + Al → n + X	Fig. 5
	p(0.8 GeV) + Fe → n + X	Fig. 6
	p(1.6 GeV) + Fe → n + X	Fig. 7

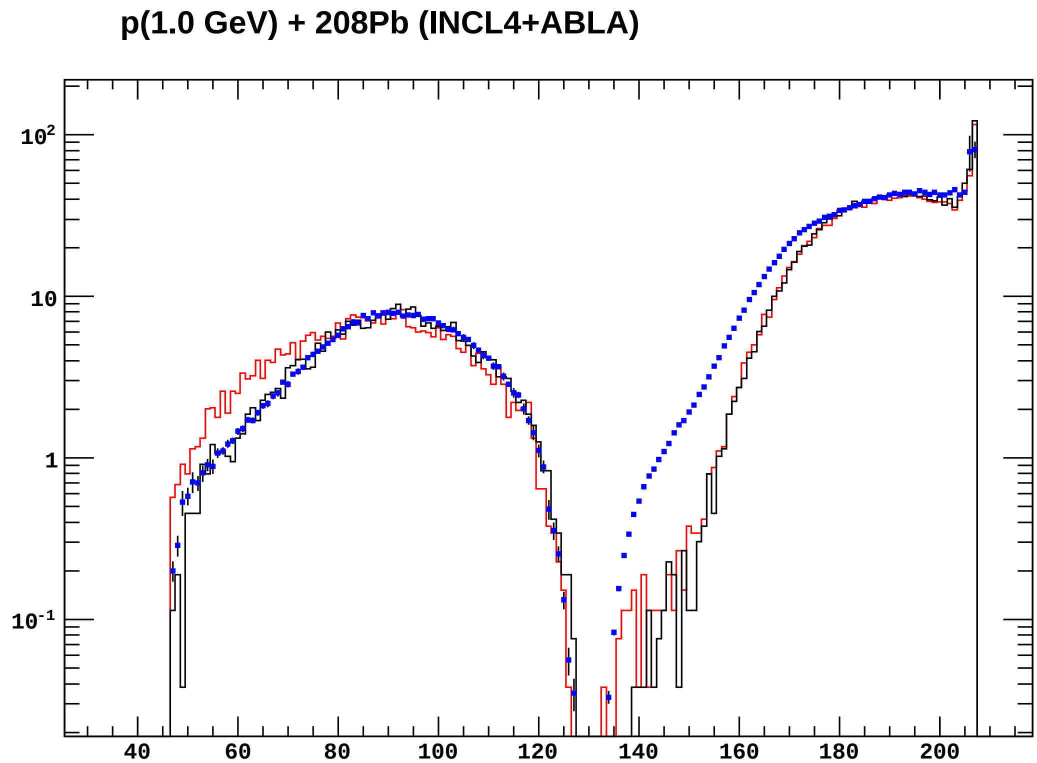


Figure 3. Mass distribution of fragments for p(1.0 GeV) + ^{208}Pb interaction using the INCL and ABLA models. Histograms are the results from the original FORTRAN version (black) and new C++ implementation (red). Data is from Ref. [11].

6. Carbon projectiles

The INCL4.2 method of handling composite projectiles is a simple extension of the single projectile particle case. Instead of shooting a single projectile particle an ion that consists of protons and neutrons is used. Standard INCL4.2 implementation in Geant4 9.2 contains support for light ion projectiles up to α particle.

Carbon beams are of particular interest for medical applications of Geant4, and the method of composite projectiles has been used to extended INCL model to include carbon ions. This functionality is already provided in Geant4 9.2 for interested test users, but more validation is need to be done before the formal release.

7. Conclusion

The new Geant4 physics list `QGSP_INCL_ABLA` for spallation studies provides powerful Geant4 machinery for ADS studies, enabling in an integrated fashion such diverse tasks as simulations of radioactive beams, electromagnetic interactions, and shielding studies. The power of this physics list comes from recent Geant4 implementations of dedicated Fortran codes INCL4.2 and ABLA v3, providing detailed modelling of spallation, fission, and evaporation.

Ongoing work is improve of the physics models for the treatment of light ion beams. In future releases the physics list `QGSP_INCL_ABLA` will be further optimised. For high energy applications the physics list need to be modified so that additional model is added between QGSP and INCL/ABLA to treat interactions in 3-9 GeV energy range. Further, our goal is to completely

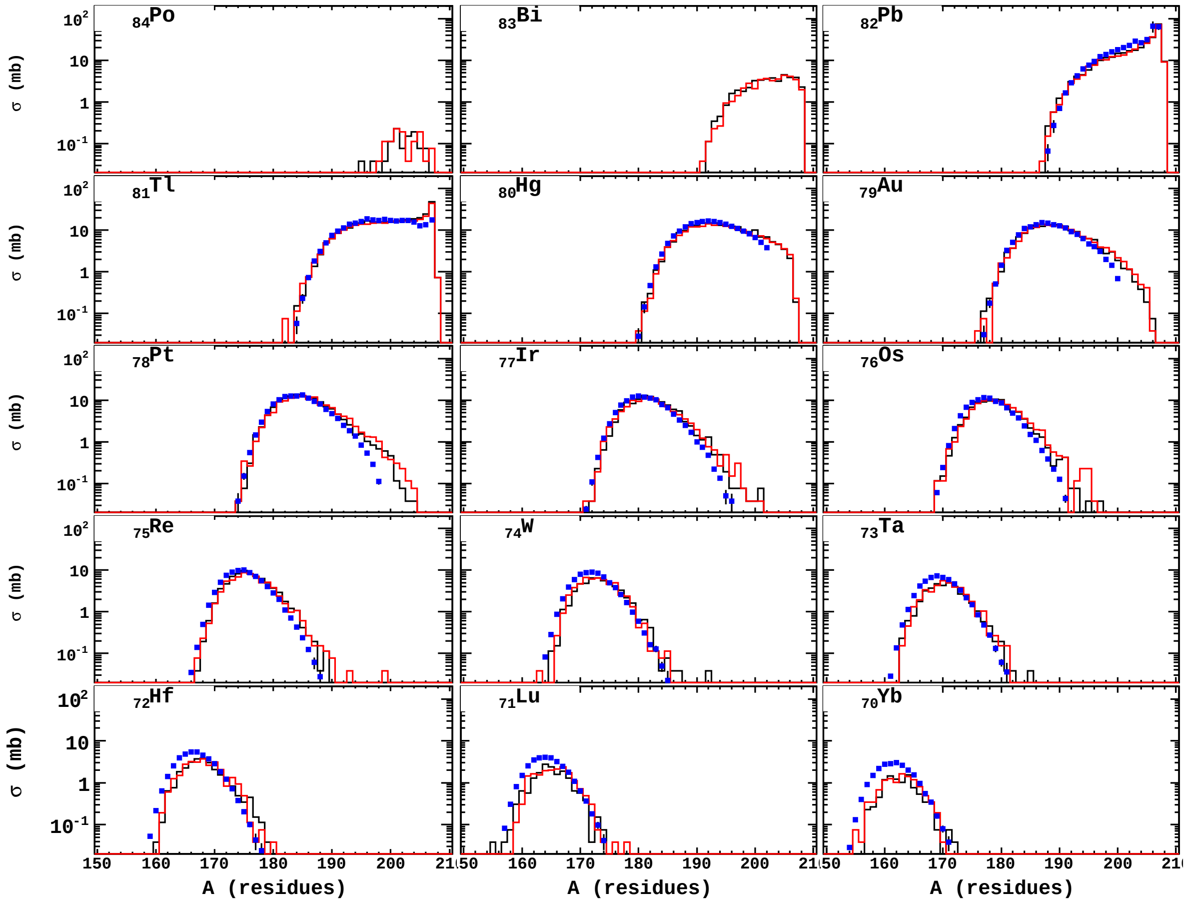


Figure 4. Fragment production of the INCL and ABLA models for p(1.0 GeV) + ^{208}Pb interaction. Histograms are the results from the original FORTRAN version (black) and new C++ implementation (red). Data is from Ref.[11].

redesign the INCL cascade code using modern object-oriented techniques.

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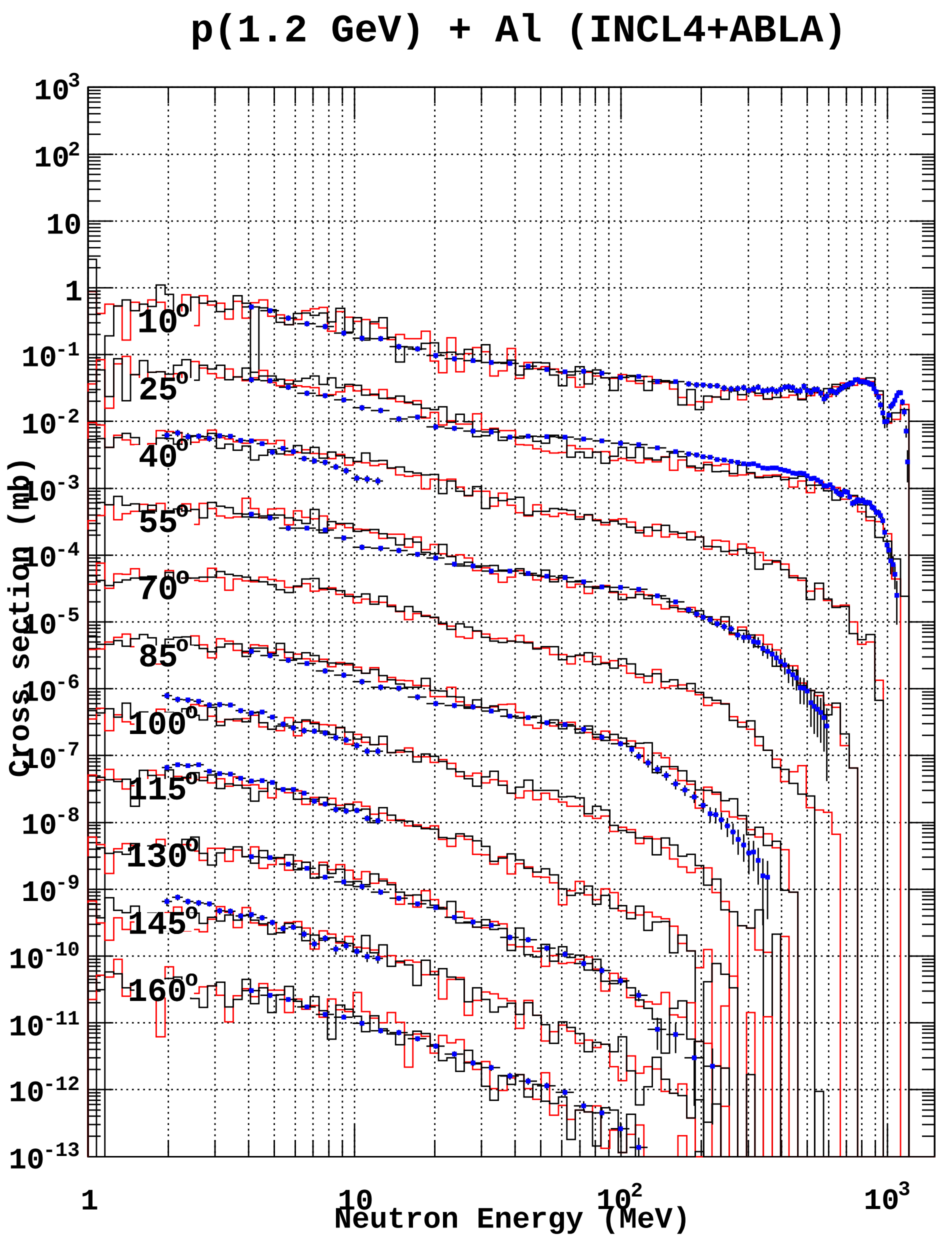

Figure 5. Double-differential for neutron production cross section from Geant4 INCL and ABLA models in p(1.2 GeV) + Al → n + X reaction. Histograms are the results from the original FORTRAN version (black) and new C++ implementation (red), respectively. Neutron evaporation from ABLA model is shown below E ≃ 20 MeV. Data is from Ref. [13].

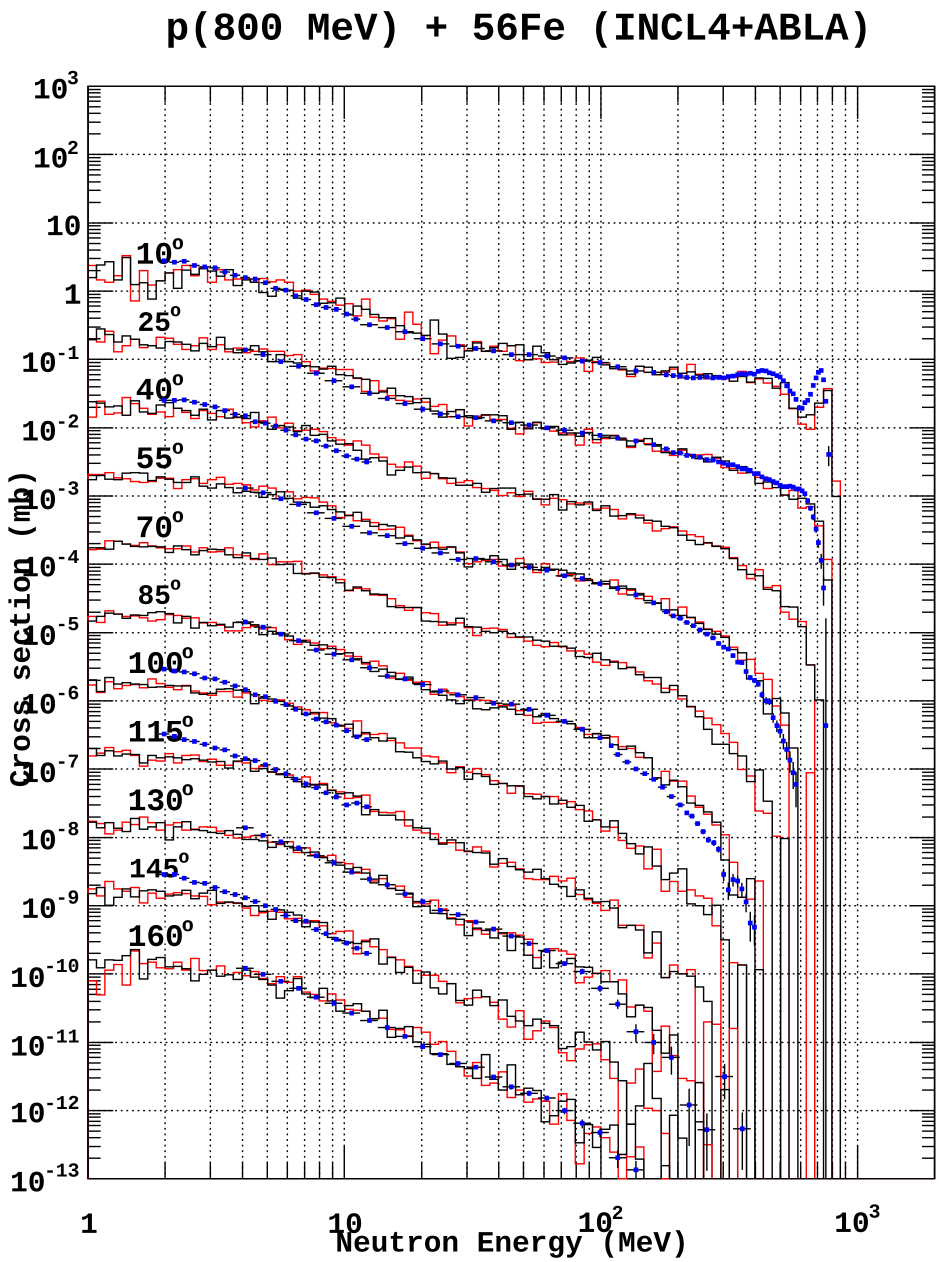

Figure 6. Neutron production from p(0.8 GeV) + Fe → n + X. Data is from Ref. [13].

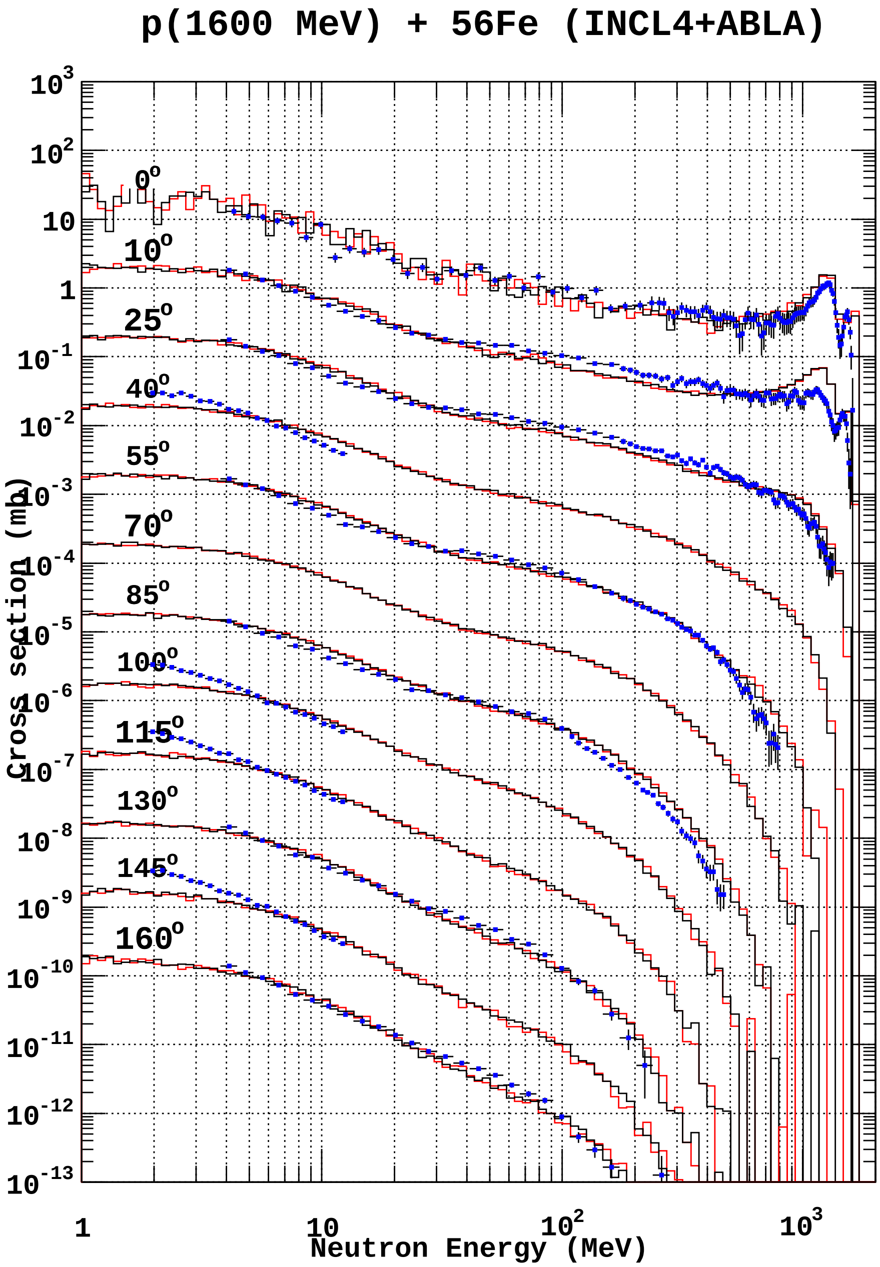

Figure 7. Double-differential for neutron production cross section from Geant4 INCL and ABLA models in p(1.6 GeV) + Fe → n + X reaction. Data is from Ref. [13].

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