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 150 MeV up to 2.5 GeV - 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 simulation tools for European Isotope Separation On-Line Radioactive Ion Beam Facility (EURISOL project) [2] and Accelerator Driven Systems (ADSs) [3]. The main goal of accelerator driven sub-critical reactor development is to provide a facility dedicated to the transmutation of long lived isotopes issued from the nuclear industry (mainly nuclear wastes from nuclear power plants). Spallation is also used for the production of intense neutron sources of wide energy spectra which are useful for material study and fundamental measurements.

To this aim we present a new Geant4 physics list, based on INCL [4] intra-nuclear cascade model and ABLA de-excitation 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.

2. Geant4 physics lists

In Geant4 hadronic physics different aspects of the calculation are separated using abstract interfaces. In this scheme:

- **Cross section** determines when a reaction will take place.
- **Physics model** calculates the final state of the reaction.
• Process combines the model and the cross section to create a description of how particles interact with matter.

In a Geant4 application the needed physics processes, cross sections, models and model options (such as energy limits) must be explicitly assigned to the particles used in the application. This configuration is managed by using so-called physics lists. The decoupling offers several advantages:

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

Often in Geant4 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
Fortran based Monte Carlo codes INCL4.2 [4] and ABLA v3 [5] are implementations of corresponding INCL and ABLA models. Recently these implementations have been translated into C++ and distributed as part of the Geant4 toolkit [8]. The first beta release of INCL4.2 and ABLA v3 was in Geant4 9.1 (December 2007) [9]. Currently the INCL and ABLA versions in Geant4 9.2 and upcoming 9.3 are straightforward Fortran to C++ translations [10]. Table 1 summarises the key features of these models.

| Table 1. Summary of key features of INCL and ABLA models in Geant4 9.2 [8, 9]. |
|-----------------------------------|
| **INCL4.2**                      |
| Projectiles                      | Protons, neutrons, pions ($\pi^-$, $\pi^0$, $\pi^+$), d, t, $^3$He, $\alpha$ |
| Energy range                     | $\sim$150 MeV – $\sim$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 |
|                                  | $\pi$ and $\Delta$ production cross sections |
|                                  | $\Delta$ decay |
| **ABLA v3**                      |
| Supported input                  | Exited nuclei |
| Model features                   | Fission |
|                                  | Evaporation of p, n, and $\alpha$ |
| Output particles                 | Fission products, residual nuclei, p, n, $\alpha$ |

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 the widely used QGSP_BERT physics list. The new physics list uses INCL and ABLA models for proton, neutron, pion, deuteron, triton, $^3$He, and $\alpha$ inelastic interactions in the energy range 0 – 3 GeV. Above 3 GeV threshold Geant4 Bertini cascade model [11] is
used, and above 10 GeV the parametrized LEP model. With energies higher than 15 GeV the QGSP high energy model is used. However, 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-INCL-ABLA physics list are summarised in Table 2. This physics list will be included in the December 2009 Geant4 9.3 release.

| Models | Description |
|--------|-------------|
| Electromagnetic physics | Geant4 standard EM |
| Spallation modelling | INCL cascade with ABLA fission and evaporation (E < 3 GeV) |
| High energy models | Bertini cascade (3 GeV < E < 10 GeV) |
| | LEP parametrized model (10 GeV < E < 15 GeV) |
| | QGSP (E > 15 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 [12] documentation generator. It allows us to generate full documentation of the class structure, complete with usage instructions, class diagrams, and detailed descriptions of all methods and code listings.

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 double-differential neutron production cross sections of Al - Pb targets bombarded by 0.8 - 1.6 GeV protons have been investigated with simulations and comparison with accurate experimental data from [13]. Validation results for proton beams of different energies and on different targets are reported in the Figs. 4-7. In addition to neutron production also fragment production has been compared against data from Refs. [14, 15].

In case of light cascade remnant nuclei de-excitation Fermi break-up, model is more appropriate choice than ABLA. We have made this functionality available through the INCL Geant4 interface. Currently, INCL interface uses Geant4 Fermi break-up [16] for remnant nuclei lighter than A = 13 and ABLA for heavier elements.

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. 1. Table 3 summarises the validations reported in this paper.

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
Figure 1. Comparison of mass number distributions from $p(1.0 \text{ GeV}) + C$ reaction, given by INCL4.2 cascade with ABLA v3 evaporation and with standard Geant4 Fermi break up model against data from [15]. Also, results from Geant4 Bertini cascade with internal fragmentation model are shown.

Table 3. Summary of Geant4 INCL4.2 / ABLA v3 validations.

| Validation                      | Configuration                  | Figure       |
|---------------------------------|--------------------------------|--------------|
| Fragmentation                   | $p(1.0 \text{ GeV}) + C$      | Fig. 1       |
|                                 | $p(1.0 \text{ GeV}) + ^{208}\text{Pb}$ | Figs. 2 and 3 |
| Neutron production              | $p(1.2 \text{ GeV}) + \text{Al} \rightarrow n + X$ | Fig. 4       |
|                                 | $p(0.8 \text{ GeV}) + \text{Fe} \rightarrow n + X$ | Fig. 5       |
|                                 | $p(1.6 \text{ GeV}) + \text{Fe} \rightarrow n + X$ | Fig. 6       |
|                                 | $p(1.6 \text{ GeV}) + \text{Pb} \rightarrow n + X$ | Fig. 7       |

of protons and neutrons is used. Standard INCL4.2 implementation in Geant4 9.2 contains support for light ion projectiles up to $\alpha$ particle.

Carbon beams are of particular interest for medical applications of Geant4, and the method of composite projectiles has been used to extend the INCL model to support carbon ions. This functionality is already provided for interested test users, but more validation is needed 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.

The reason for the difference between the C++ and Fortran versions seen in Fig. 2 is under investigation and improvement of the physics models for the treatment of light ion beams is underway. In future releases the physics list QGSP_INCL_ABLA will be further optimised. For low energy applications the physics list need to be modified, so that additional model is added below INCL/ABLA validity region to treat interactions of low energy particles. Further, our goal is to completely redesign the INCL cascade code using modern object-oriented techniques and taking benefit of the most recent INCL version [17].
Figure 2. Mass distribution of fragments for $p(1.0 \text{ GeV}) + ^{208}\text{Pb}$ 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. [14].

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References
[1] Geant4 collaboration, *Geant4 - a simulation toolkit*, Nucl. Instr. and Meth. A, 506, 2003, 250–303
[2] J.Cornell (ed.), *The EURISOL Report, A feasibility study for a European isotope-separation-on-line radioactive ion beam facility*, European Commission contract No. HPRI-CT-1999-50001, December 2003
[3] C. D. Bowman, *Accelerator-driven systems for nuclear waste transmutation*, Annual Review of Nuclear and Particle Science Vol. 48: 505-556, December, 1998, doi:10.1146/annurev.nucl.48.1.505
[4] A. Boudard et al., *Intra-nuclear cascade model for a comprehensive description of spallation reaction data*, Phys. Rev. C66 (2002) 044615
[5] J. Benlliure et al., *Calculated nuclide production yields in relativistic collisions of fissile nuclei*, Nuc. Phys. A628 (1998) 458
[6] J. J. Gaimard et al., Nuc. Phys. A628 (1998) 458
[7] A. R. Junghans et al., Nuc. Phys. A629 (1998) 635
[8] A. Heikkinen, P. Kaitaniemi, and A. Boudard, *Implementation of INCL$^4$ cascade and ABLA evaporation codes in Geant4*, Journal of Physics: Conference Series 119 (2008) 032024, doi:10.1088/1742-6596-119/3/032024
[9] Geant4 collaboration, http://cern.ch/geant4
[10] A. Heikkinen, N. Stepanov, and J. P. Wellisch, *Bertini intra-nuclear cascade implementation in Geant4*, arXiv:nucl-th/0306008, SLAC-R-636 (2003)
[11] Doxygen source code documentation generator tool v1.5.9 (2009)
Figure 3. Fragment production of the INCL and ABLA models for $p(1.0 \text{ GeV}) + ^{208}\text{Pb}$ interaction. Histograms are the results from the original Fortran version (black) and new C++ implementation (red). Data is from Ref. [14].

[13] S. Leray et al., Spallation Neutron Production by 0.8, 1.2, and 1.6 GeV Protons on Various Targets Phys. Rev. C65 044621 (1999)
[14] T. Enqvist et al., Nucl. Phys. A686 (2001) 481
[15] D.L. Olson et al., Factorization of fragment-production cross sections in relativistic heavy-ion collisions, Phys. Rev. C28, 1602 (1983), doi:10.1103/PhysRevC.28.1602
[16] Geant4 collaboration, Geant4 9.2 Physics Reference Manual: Fermi Break-up Model
[17] A. Boudard and J. Cugnon et al., Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions, p 29, ICTP Trieste, February 2008
Figure 4. Double-differential for neutron production cross section from Geant4 9.2 INCL and ABLA models in $p(1.2\text{ GeV}) + \text{Al} \rightarrow n + X$ reaction. Histograms are the results from the original Fortran version (black) and new C++ implementation (red). Data is from Ref. [13].
Figure 5. Neutron production from $p(0.8 \text{ GeV}) + \text{Fe} \rightarrow n + X$. Data is from Ref. [13].
Figure 6. Double-differential for neutron production cross section from Geant4 9.2 INCL and ABLA models in $p(1.6 \text{ GeV}) + \text{Fe} \rightarrow n + X$ reaction. Data is from Ref. [13].
**Figure 7.** Double-differential for neutron production cross section from Geant4 9.2 INCL and ABLA models in $p(1.6 \text{ GeV}) + \text{Pb} \rightarrow \text{n} + X$ reaction. Data is from Ref. [13].