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Implementation of INCL cascade and ABLA evaporation codes in GEANT4

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Abstract. We introduce a new implementation of the Liège cascade INCL4.2 and of the evaporation/fission code ABLA V3 in GEANT4. INCL treats the cascade of hadron, deuterium, tritium, and helium projectiles of energies up to 3 GeV, while ABLA, based on evaporation and fission, provides a treatment of the excited nucleus produced at the end of the cascade. Details of the implementation of INCL and ABLA in the GEANT4 9.1 release are presented and C++ performance is compared with the original FORTRAN implementation. A test suite for validating the code translation is based on ROOT software, and we report on advanced features of our testing environment, including scripting and automatic documentation. In addition, we introduce a GEANT4 application using INCL and ABLA models, demonstrating the physics performance and enabling comparisons against another GEANT4 intermediate energy hadronic model, the Bertini cascade. Finally we outline the future development of the Liège cascade, INCL5, in the context of the GEANT4 hadronic physics framework.

1. Introduction

GEANT4 is a general detector simulation toolkit [1] providing an extensive set of hadronic physics models to meet user requirements in areas such as precision studies of LHC hadronic calorimetry shower shapes, shielding studies in space applications, and spallation studies in nuclear physics. A single hadronic model is not able to support all GEANT4 user requirements in these areas which cover evaporation, intranuclear cascade and intermediate energies of up to 10-15 GeV. In these regions GEANT4 provides alternative models.

The need to develop a additional microscopic intranuclear codes is a GEANT4 user requirement. More accurate models are particularly important in detailed hadronic calorimeter studies, since standard parametrized models based on GEANT3 GEISHA code [2] have trouble reproducing shower shapes accurately enough [3]

Thus we have set a goal to complement theory-driven GEANT4 models in this regime (the Binary and Bertini cascades are currently most widely used) with the inclusion of the INCL code, also known as the Liège cascade. Since INCL is often used with the independent evaporation/fission code ABLA, we decided to incorporate ABLA as well into GEANT4. These codes are actively developed and validated against recent data. Typical users are from the nuclear physics community studying spallation processes, for example. With the inclusion of INCL/ABLA, GEANT4 can respond to the growing list of user requirements from nuclear physics community. We have cast these FORTRAN-based codes into C++, and will proceed now to a redesign of the model structure. The main objective of the redesign project is to facilitate easier development of future physics features with a clearly structured codebase. This can be done by focusing on the design of proper data structures that represent the physics incorporated into INCL and ABLA in the most natural way possible. The next step in redesign will be to prepare well-defined data structures with access methods supporting fully the interfaces defined in the Geant4 hadronic physics framework [4] This will improve the code quality and make development and debugging work easier. We believe that C++ releases of stand-alone INCL and ABLA codes will benefit the nuclear and particle physics simulation communities in general, since currently Geant4 is one of the few major C++ -based detector simulation tools available. Future releases of C++ -based INCL and ABLA codes hopefully show a general trend in our community to support and adopt contemporary programming paradigms for physics modelling.

The outline of this paper is as follows: in section 2 we summarize the features of INCL and ABLA codes. For detailed discussions on INCL and ABLA models we refer to publications listed in table 1. In section 3 the design of the first implementation of INC4.2 and ABLA v3 is presented. Section 4 describes validation between the FORTRAN and C++ versions. Finally, section 5 discusses the future plans of our project.

2. Modeling intra-nuclear cascade and evaporation with INCL and ABLA codes

INCL is an intra-nuclear cascade code, which is largely free of parameters. It has been carefully validated against recent spallation data together with the ABLA evaporation/fission model. From the Geant4 perspective, INCL provides particularly interesting models because of its continuing development and up-to-date validation program.

The key features of INCL4.2 and ABLA v3 are summarized in table 1, together with key references to detailed descriptions of specific model features.

Table 1. Summary of key features available in INCL and ABLA codes. For detailed discussions of models we refer to publications listed in this table.

INCL4.2	Key references [5, 6, 7, 8]
Projectiles	p, n, pions (π^+, π^0, π^-)
	d, t, ^{3}He, α
Energy range	$\sim$ 200 MeV - 3 GeV
Target nuclei	Carbon - Uranium
Models	
	Woods-Saxon nuclear potential
	Coulomb barrier
	Non-uniform time-step
	Pion and delta production cross sections
	Delta decay
	Pauli blocking
	Utility functions making INCL an independent code
ABLA v3	Key references [9, 10]
Supported input	Excited nuclei
Models	Evaporation of p, n, and α
	Fission
Output particles	p, n, α, fission products, and residual nuclei

3. Implementing INCL and ABLA for GEANT4 release

We have translated INCL4.2 and ABLA v3 codes from FORTRAN to C++ and interfaced these models to the GEANT4 9.1 hadronic physics framework using standard interfaces. Figure 1 provides a UML diagram describing key classes prepared for the first release. The first release included in GEANT4 9.1 contain a simple and straightforward translation following closely the original code structure, data flow, and algorithms.

Users of these cascade or evaporation codes can build their GEANT4 physics list by using the interface classes `G4InclCascadeInterface`, `G4InclLightIonInterface`, or `G4AblaEvaporation`. Documentation and example code is provided to clarify the details.

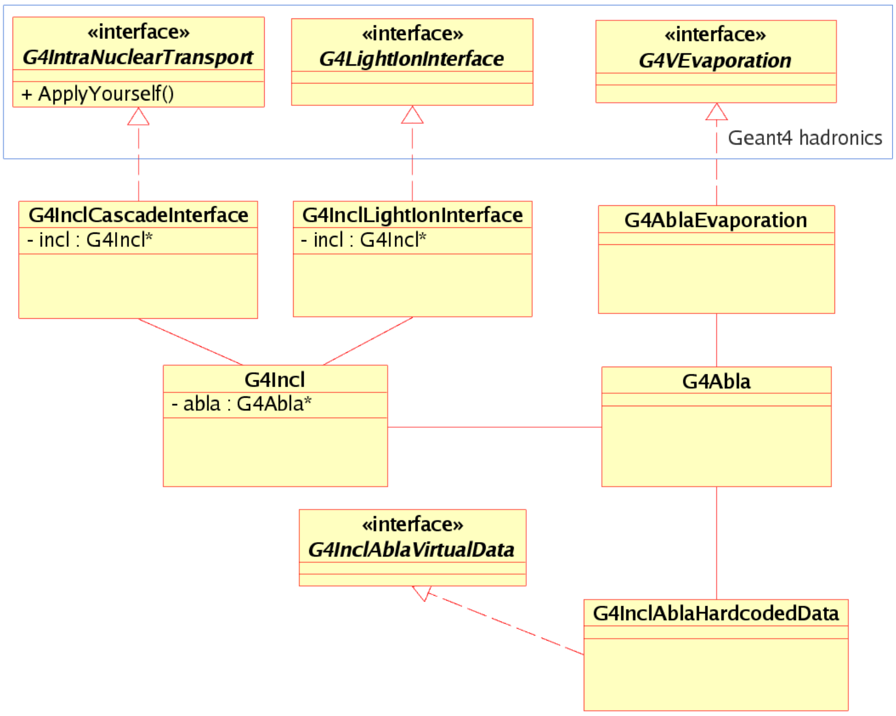


Figure 1. Main components of the first C++ implementation of INCL4.2 and ABLA v3 in GEANT4 9.1. This first iteration of the class design, visualized with Unified Modeling Language UML, follows closely the organization of the original FORTRAN code, thus simplifying the casting to C++.

To document the new implementations of INCL and ABLA we have used the DOXYGEN documentation system together with the advanced introspection features provided by the ROOT programming environment [11]. This system generates HTML pages and graphics that can be uploaded to the web and viewed by any standards-compliant web browser. Figure 2 shows an example of a DOXYGEN call graph for the `G4InclLightIonInterface::ApplyYourself()` -method and figure 3 demonstrates LaTeX support available in DOXYGEN.

4. Validating INCL and ABLA models in GEANT4

The first implementations of the INCL and ABLA codes in the GEANT4 framework were direct translations, in which each FORTRAN function was mapped simply to a corresponding C++ method. We have been able to validate in detail the quality of the translation.

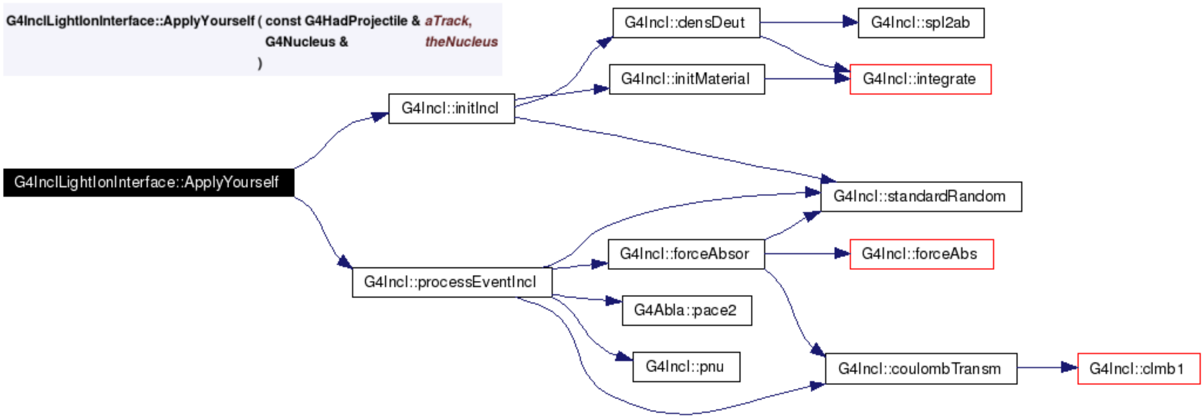
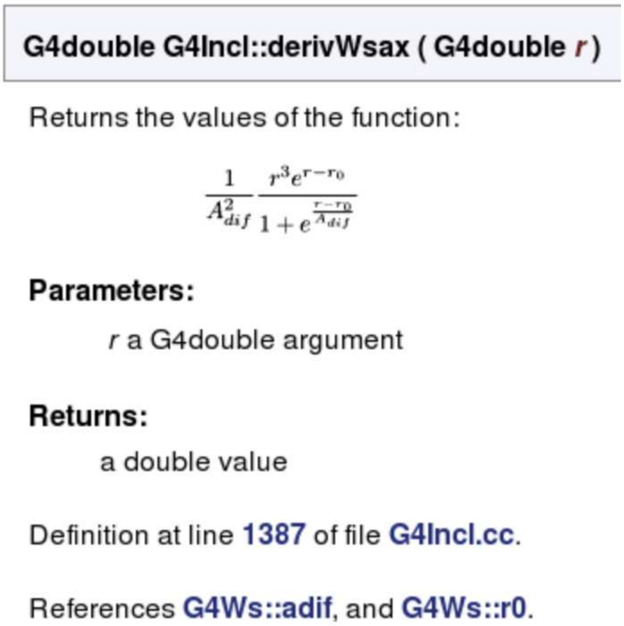


Figure 2. DOXYGEN based HTML documentation for the INCL interface. A call graph for the `G4InclLightIonInterface::ApplyYourself` function is shown. For users, the on-line class browser generated by DOXYGEN provides a quick way to understand the structure of the code.



G4double G4Incl::derivWsax (G4double *r*)

Returns the values of the function:

$$\frac{1}{A_{dif}^2} \frac{r^3 e^{r-r_0}}{1+e^{\frac{r-r_0}{A_{dif}}}}$$

Parameters:

r a G4double argument

Returns:

a double value

Definition at line 1387 of file G4Incl.cc.

References G4Ws::adif, and G4Ws::r0.

Figure 3. Woods-Saxon nuclear potential in GEANT4 9.1 INCL release. This on-line documentation is produced by DOXYGEN HTML-generation.

The test suite for the validation of the translation is based on ROOT software [11]. ROOT provides a C++ scripting system that has proven to be a good environment for software development. In addition to ROOT scripting for hybrid FORTRAN – C++ comparisons, we used automatic documentation features to systematize unit testing. Histograms resulting from ROOT scripts were included recursively back to related HTML-documents. This functionality is made available and enforced with the reflectivity extension, enabling introspection of data structures.

Figure 4 shows a comparison between C++ and FORTRAN versions. Close to the target mass, the cross sections agree reasonably well if we consider that the random number generators are not the same. The further the mass is from the target one the larger is the deviation between the code versions. This indicates a possible incompatibility between the FORTRAN and the C++ version of the de-excitation (ABLA part). This conclusion is confirmed if we look at the neutron spectra produced from protons of 1.2 GeV on Lead in Figure 8. Above 20 MeV the neutrons are purely produced by the cascade stage and we can note a perfect agreement in energy and angle between the two versions. Below 20 MeV the spectrum is dominated by evaporation, we conclude that there are some remaining problems in the C++ translation of ABLA.

Figure 5 extends the verification by comparing INCL/ABLA performance against another model, the Bertini cascade, available in GEANT4.

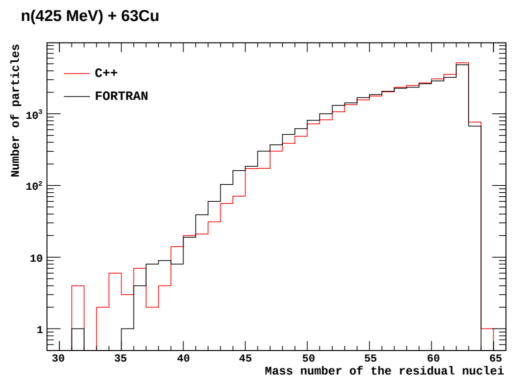


Figure 4. Validating FORTRAN to C++ translation of INCL and ABLA models. Residual nuclei mass number distribution is shown for collisions initiated by 425 MeV neutrons colliding with a ^{63}Cu target. Some amount of fluctuation in the histograms is expected, since the random number generators are different in both versions.

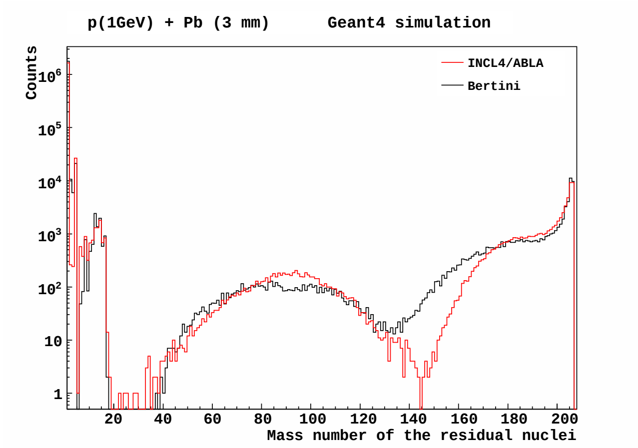


Figure 5. INCL/ABLA model performance in GEANT4 compared with the Bertini model which contains an internal treatment for evaporation and fission [12]. This kind of comparison provides a starting point for preparing an optimal physics list for a specific physics use case.

Figures 6 and 7 demonstrate an example application prepared for utilizing new models. Visualization of inelastic scattering produced by INCL and ABLA models is supported with the ability to collect simulated data into histograms.

5. Conclusion and future plans

We have published INCL4.2 and ABLA V3 in the December 2006 release of GEANT4 9.1. After this first release we will proceed to re-design the codes. This step will be particularly sensitive since INCL4.2 and the upcoming INCL5 C++ versions need to be released also as independent codes. Recently there has been great interest coming from the medical physics community to simulate treatment facilities utilizing Carbon beams. Thus, we continue to develop and validate these models and support our users in particle, nuclear, and medical physics communities alike.

6. Acknowledgements

We are grateful to INCL developers Joseph Cugnon (University of Liége, Belgium) and Y. Yariv (SphN-DAPNIA, CEA-Saclay and Soreq, Israël) for supporting this project, and contributing to two INCL/ABLA-GEANT4 mini-workshops organized in 2006. The ABLA group kindly

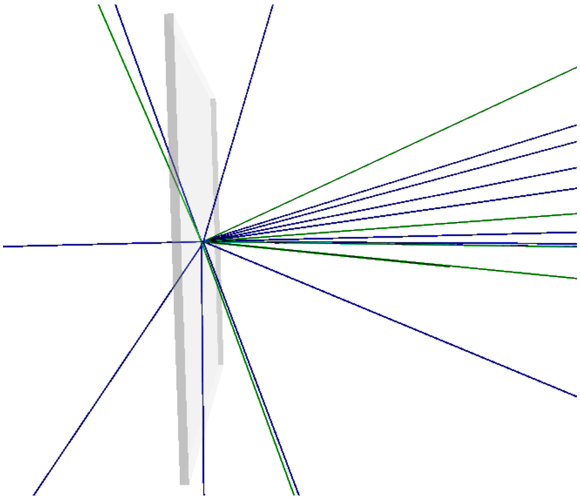


Figure 6. An example GEANT4 9.1 application utilizing INCL4.2 cascade model. Proton projectiles with 500 MeV energy are incident upon a 2 mm Pb target. A visualization of 100 events is shown.

```
INCL4 4.2 C++ thin-target calculation:

Run setup:
Bullet:
        Type: 1
        Energy: 500 MeV
Target:
        A: 208
        Z: 82
Events: 100

Calculation output in ROOT file: ../data/Pb208Proton500MeV100Events.root

Output information:
Total number of events:
        Asked by the user: 99
        Transparent: 47
        Proper cascades: 52
Maximum impact parameter: 10.9878
Geometrical cross-section: 3792.89 mb
Total reaction cross section: 1992.23 mb
```

Figure 7. Log from example application associated with Figure 6.

provided code for the GEANT4 translation project. Special thanks to Christelle Schmidt (IPNL) for providing a C++ translation of the fission part of ABLA. Thanks to Alexander Howard and Alberto Ribon from CERN for acting as GEANT4 testers for the interfaces we provided using C++ wrapped FORTRAN-based INCL and ABLA. and validating physics against TARC data. Finally, we acknowledge Dennis Wright from SLAC for kindly reading the manuscript and providing his feedback.

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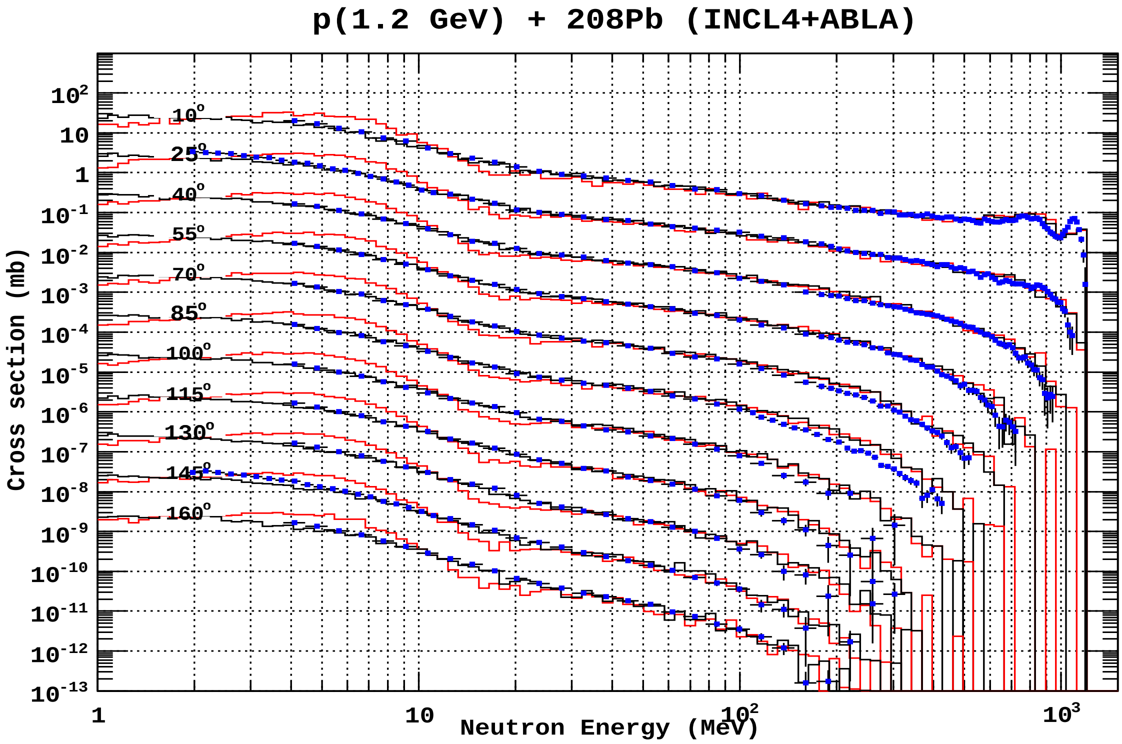

Figure 8. Example of first implementation of INCL4.2 together with ABLA v3 in GEANT4 9.1. Neutron double differential cross section for 1.2 GeV proton-induced reactions on Pb is compared with the experimental data from Reference [8] The red histogram is produced by the C++ version and the black histogram by the FORTRAN version. There is some discrepancy between the two versions for energies below 20 MeV. This indicates that the GEANT4 version of the ABLA still need to be improved.