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IMPLEMENTATION OF NUCLEAR-NUCLEAR PHYSICS IN THE GEANT4 RADIATION TRANSPORT TOOLKIT FOR INTERPLANETARY SPACE MISSIONS

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ABSTRACT

Future manned missions to Mars being planned by the European Space Agency will involve long-duration interplanetary transit and activity on the surface, with mission durations potentially lasting three years. The additional risk to the crews from the ionising radiation environment is a particular concern to mission planners. To date the majority of our experience of radiobiological effects in the space environment comes from low Earth orbit missions, whereas in the interplanetary environment there is greater influence on the radiobiological dose from cosmic ray and solar particle ions heavier than protons, and no option of rapid return to Earth in the case of an emergency. Spacecraft and planetary habitat structures should be optimised to attenuate these sources with minimum production of secondary particles, particularly secondary neutrons which are an important contributor to the total radiobiological dose. It is therefore essential that accurate models are available to mission planners and designers to simulate radiation transport, including the treatment energetic nuclear-nuclear interactions. This paper describes a programme of work undertaken to implement abrasion-ablation and electromagnetic dissociation physics into the Geant4 radiation transport toolkit in order to improve the simulation of nuclear fragment production from nuclear-nuclear collisions. The abrasion model is shown to be in good agreement with experimental data (often providing better than factor-of-two agreement for nuclear fragment yields), whilst results from the electromagnetic dissociation model are shown to be within 5 and 42% of the experimental data.

Key Words: nuclear-nuclear models, abrasion, ablation, electromagnetic dissociation

1 INTRODUCTION

Lunar and interplanetary manned missions planned for the next decades may carry a significant risk of long-term, and in some cases acute, radiobiological effects to the crews. To date, much of the experience for manned missions has been for the near-Earth environment which is better protected by the geomagnetic field, and there is the option for a rapid return to Earth in the event of an emergency. In contrast, the radiobiological risk to crews of interplanetary missions will arise from the long-term exposure (over approximately one to three years based on missions currently being considered) to galactic cosmic radiation (GCR) and solar particle radiation, and secondary particles which often can account for a greater fraction of the radiobiological dose due to particle multiplicities and their greater stopping powers (for charged particles).

Even on the Martian surface, the risk is not significantly reduced. Earth's atmosphere provides the equivalent of ≈1,000 g/cm^2 of shielding, so that secondary particle production maximises at approximately 20km (the so-called Pfotzer maximum) and is then attenuated significantly before reaching the Earth's surface. Mars' tenuous atmosphere provides only 16-30 g/cm^2 of shielding (depending upon the season) and therefore the secondary particle production maximises just beneath the surface of the planet.

Shielding strategies to minimise radiation dose can vary significantly depending upon the species, energy spectrum and temporal nature of the source. The relatively softer spectrum of the solar particle source means there is greater benefit from shielding against these particles, and the duration of the events means that increased shielding is required during the event, achieved, for example, by restricting crew activities to specific habitat or vehicle locations, and deploying large water-filled bags or other temporary shielding structures in the vicinity. GCRs constitute a continuous background with a hard energy spectrum, and whilst slowing these particles down generally increases their stopping powers (and therefore ionisation rates), for some ion species there will be benefits from particle attenuation through nuclear interactions, and the increased risk of cell-death instead of cell damage and potential mutation. In either case it is essential to minimise the production of secondary particles through the careful selection of spacecraft materials.

In order to assist spacecraft design and mission planning, accurate prediction of radiation propagation in the structure and shielding materials is required. Several radiation transport simulation tools exist to perform detailed modelling of energetic particles in complex 3D geometries, allowing treatment of ionising and nuclear interactions. One such code is Geant4 [1,2] which has been developed by an international collaboration of (amongst others) high-energy physics groups, nuclear physicists, medical physics groups and the space radiation effects community. However, in order to be applicable to Mars missions, it must be able to treat energetic nuclear interactions of ions from energies of ≈10MeV/nucleon to ≈10GeV/nucleon, and for species up to iron.

This paper describes work undertaken to extend the existing physics models within Geant4 to more accurately treat nuclear-nuclear interactions, and some of the results from the new physics implementations.

2 THE GEANT4 RADIATION SIMULATION TOOLKIT

2.1 General Description and Physics Implemented

Geant4 is a software toolkit for the comprehensive simulation of energetic particles in 3D geometries [1,2]. It is the result of the collaboration of approximately 100 scientists from over 40 institutes world-wide. The code was first made available publicly in December 1998, and the version of the code used to generate the results described here is Geant4 v6.1, released in March 2004.

The toolkit currently comprises approximately one million lines of source code written in C++ describing 2000 classes, and continues to evolve in order to meet the needs of its growing user community. Indeed the rigorous object-oriented design of the software with a clear hierarchical structure and unidirectional flow of dependencies provides a clear and intuitive understanding of the system, and easy extension of the software through class inheritance.

A variety of new physics models has been implemented in Geant4, but the toolkit also includes versions of physics models from codes such as the intranuclear cascade code, INUCL, and the parameterised hadron-nuclear code, GHEISHA, that have been re-engineered in C++. Figure 1, which summarises the hadronic physics models implemented in or currently being developed for Geant4, highlights the range of particles and physics which can be simulated by the code. The last column identifies the relevance of these models to the analysis of space radiation effects. Processes that are based on theory can typically be applied to any material. Those that utilise databases, such as the low-energy neutron transport and photo-evaporation are limited by the availability of data for specific materials. However, the database used for <20 MeV neutron transport has been drawn from many sources to provide a wide range of elastic and inelastic cross-sections. These data include commonly used spacecraft materials. The data used to model discrete photo-evaporation are derived from the Evaluated Nuclear Structure Data File (ENSDF) [3,4], and is considered the most comprehensive source for information of this type.

The Geant4 electromagnetic physics classes treat electron, positron, photon and muon interactions, as well as the electromagnetic interactions of hadrons and ions. Ionisation induced by ions is calculated using stopping power formulae published by Ziegler [5,6] or issued in the ICRU-49 report [7] for protons and α-particles, and scaled by the effective charge and mass of the projectile. Multiple scattering is based on the work of Lewis [8], and ion electromagnetic interactions includes the generation and transport of δ-ray "knock-on" electrons above the material-dependent cut-off (taken as twice the mean ionisation energy of the material).

2.2 Hadron Models for Nuclear-Nuclear Interactions

The principal theory-based models available within Geant4 for hadron-nuclear interactions are:

- The Classical Cascade (CC) model from the University of Helsinki, which is based on a re-engineering of INUCL. This implements the Bertini intranuclear cascade (INC) model and has been tested against experimental data for kinetic energies from 100MeV to 5GeV (it is advisable not to use this model for energies above ≈10GeV).
- The Binary Cascade (BC) model developed by members of the collaboration at CERN and INFN, and applicable over the energy range from 70MeV to 10GeV. Below 70 MeV,

the Binary Cascade model selects the Pre-compound model to treat the nuclear interaction using pre-equilibrium physics.

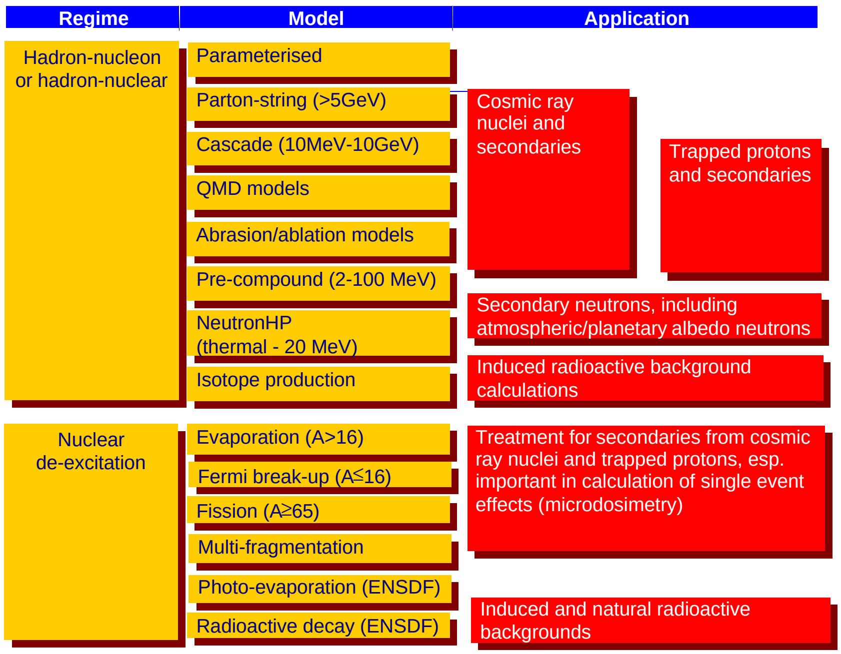

Figure 1. High-energy physical processes in or being developed for Geant4 and their application to space radiation studies.

A recent improvement to the Binary Cascade model has been its extension to treat nuclear-nuclear interactions, which has so far been tested for light nuclear projectiles. Similar modification is being undertaken for the Classical Cascade model.

An interface between an existing quantum molecular dynamics (called the Jaeri QMD model or JQMD) and Geant4 has also been developed by Koi at SLAC [9]. During the period of software development described in this paper, the JQMD model was only able to treat nuclear-nuclear interactions from several 10's MeV/nucl to ≈1 GeV/nuc – the upper limit being set by the omission of treatment for the Δ resonances. The key drawback of this model , however, is its limited simulation speed compared with Binary Cascade.

For energies above ≈10GeV/nuc, quark-gluon-string models (QGSM) are available for the simulation of hadron-nuclear interactions, and members of the collaboration at CERN are currently extending this model to simulate nuclear-nuclear interactions for >10 GeV/nuc.

At the other extreme, the Pre-compound model is the best basis for the treatment of nuclear-nuclear collisions below ≈100MeV/nuc, but currently the angular momentum of the projectile-target system is omitted in the Geant4 implementation (*i.e.* it is still only applicable to light/hadron projectiles or targets).

3 DESCRIPTION OF NEW NUCLEAR-NUCLEAR INTERACTION MODELS IMPLEMENTED

3.1 Abrasion-Ablation Models

The existing models for nuclear-nuclear interactions, and those being developed, treat the interaction process at the "microscopic level" in that they simulate at least to the hadron-nucleon level collisions for each of the interacting nucleons in the projectile and target, as well as secondary nucleons and mesons. An alternative approach based on "macroscopic" abrasion-ablation physics has been used by Townsend *et al* and Wilson *et al* in NASA's HZEFRG1 and NUCFRG2 codes [10,11]. Their model for abrasion is based on a number of simple assumptions:[1]

- The projectile and target nuclei are assumed to have well defined radii, which are functions of their respective nucleon numbers only. At radii less than the nuclear radius, the nucleon density is constant, or otherwise zero outside.
- Geometric arguments are used to determine the overlap region of the incident projectile and target nuclei. Nucleons within the overlap region are considered to be participants in the interaction whilst those outside are spectators that form the nuclear pre-fragment. (In the implementation in HZEFRG2 and Geant4, a correction is made to the impact parameter to account for the Coulomb force acting between the two nuclei as they approach each other.)
- The mean-free-path for nucleons of the projectile within the overlap region of the target is energy-dependent but independent of the position inside the nucleus.
- The number of nucleons abraded, and the excitation of the nuclei from nucleon-nucleon scattering, are determined from the mean-free-path, the chord-length in the interaction region for the maximum probability of interaction, and the fraction of the projectile geometric cross-section in the interaction region.
- Additional excitation of the pre-fragments is assumed to result from the excess surface area of the pre-fragment (i.e. the degree of asphericity) following abrasion.

In the implementation of Wilson *et al*, the projectile pre-fragment is treated by an ablation model in which nucleons and other light nuclear-fragments (deuterons, tritons, ^{3}He nuclei and α-particles) are ejected from the pre-fragment. Again, this process is based on relatively simple principles:

- The energy required to liberate one nucleon is 10MeV, independent of the nucleon and proton numbers of the initial and final nucleus. From the A of the pre-fragment and excitation energy, it is therefore possible to determine the nucleon number of the final fragment.
- The proton number of the fragment is sampled from the Rudstam equation, allowing the change in A and Z (ΔA and ΔZ) to be determined.
- Given the ΔA and ΔZ, α-particles are assumed to be emitted preferentially from the pre-fragment, since these have the highest binding energy, followed by other nuclear fragments in order of decreasing binding energy.

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[1] The reader is also referred to references [12] and [13] at [14] for a full quantitative description of the models implemented.

The basis principles of the NUCFRG2 model have been implemented in Geant4 to complement the detailed models already within the toolkit, or under development by other Geant4 collaborators. In particular, it was anticipated that the new models would better treat the nuclear fragment production due to the inclusion of the excitation from pre-fragment asphericity, currently omitted in the Binary Cascade model. For the Geant4 implementation, the pre-fragments of *both the projectile and target nuclei* are treated by the `G4WilsonAbrasionModel` C++ class. De-excitation for both pre-fragments can be simulated by the standard nuclear de-excitation models within Geant4 which treat pre-equilibrium, evaporation, Fermi break-up (for pre-fragments with $A \leq 12$ and $Z \leq 6$), and multi-fragmentation. Alternatively, the ablation model is implemented in the C++ class `G4WilsonAblationModel`, which uses the selection rules described above to determine the species of the particles emitted, but also applies aspects of Geant4's evaporation model to determine the kinematics of the particle emission and recoil.

3.2 Electromagnetic Dissociation

Electromagnetic dissociation (ED) is the emission of nucleons or light nuclear fragments from one nucleus as a result of the electromagnetic force (rather than the strong force) as the nucleus passes the electric field of another nucleus at relativistic speeds. The contribution of this source to the total inelastic cross-section becomes important for higher-Z target materials or projectiles, due to the Z^2 dependence of the virtual photon spectrum produced. Jilany [15] reports on the percentage of electromagnetic dissociation from relativistic ions in NIKFI-BR-2 nuclear emulsion[2], and finds for light- to medium- mass relativistic nuclei such as ^{7}Li to ^{28}Si, the number of ED interactions can be ~5-11% of the number of nuclear interactions, depending upon the projectile species and energy. The percentage of ED events for 200 MeV/nucleon ^{32}S projectiles in the nuclear emulsion is stated as being 22% of the nuclear interaction events. Obviously the composition of the nuclear emulsion, which includes bromine and silver, is also important in producing this relatively high probability of ED events, and for lower-Z elements in the emulsion (carbon, nitrogen and oxygen) the interaction rate will be lower. In the case of common space applications where, for example a relativistic cosmic-ray ^{56}Fe is incident upon an ^{56}Fe target, the probability of ED interaction compared with strong nuclear interaction is ~6%. However, high-Z materials will still be used on interplanetary missions, whether for specialised equipment such as radiation monitors, mass balance, and fissionable materials if nuclear power/propulsion is used.

The implementation of ED interactions by Wilson *et al* in HZEFRG1 and NUCFRG2 treats the emission of nucleons only through the E1 and E2 components of the virtual photon spectrum [11]. The energy transferred in the process is assumed to correspond to the energies of the giant dipole resonance (GDR) and giant quadrupole resonance (GQR) of the nucleus undergoing dissociation, and the photo-nuclear cross section, determined for these energies by relatively simple formulae developed by Bertulani and Baur [16].

The algorithm used by Wilson *et al* [11] was implemented into Geant4 as the C++ classes `G4EMDissociation`, `G4EMDissociationCrossSection`, and `G4EMDissociationSpectrum`. As with the abrasion model, ED of the target in the field of the projectile is considered as well as the ED of the projectile in the field of the target.

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[2] NIKFI-BR-2 nuclear emulsion comprises ^{1}H, ^{12}C, ^{14}N, ^{16}O, ^{32}S, ^{80}Br, ^{108}Ag, ^{127}I.

3.3 Total Cross-Section Models for Nuclear-Nuclear Interactions

Hadronic physics in Geant4 often utilises two types of model to treat collisions:

- Total cross-section models, which often are in the form of parametric fits to experimental data. These are used to provide rapid calculation of particle mean-free-paths during particle tracking to determine where an interaction occurs.
- Interaction models (such as described in sections 3.1 and 3.2 above) which are applied when it has been determined that an interaction has occurred at the current particle step, and the final state must be determined.

In addition to the new final-state models (*i.e.* abrasion-ablation and electromagnetic dissociation), improvements were made to estimate more accurately total inelastic cross-sections for nuclear-nuclear in which one of the participants has nucleon number, $A \leq 4$. The model used to calculate the total inelastic cross section in this regime is Tripathi *et al*'s algorithm for "light systems" [17]. Furthermore, it is recommended that this model for total inelastic cross-sections should be used for proton interactions with nuclei that have $A<12$, since it provides better performance for light-targets compared with Wellisch and Axen's algorithm implemented in Geant4 [18]. For heavier nuclear-nuclear interactions (*i.e.* where both the target and projectile nucleon numbers are greater than four) the general algorithm of Tripathi *et al* is more applicable and has previously been implemented in Geant4 in the class `G4TripathiCrossSection` [19].

4 PERFORMANCE OF NEW MODELS

4.1 Treatment of abrasion-ablation interactions

Figures 2 to 4 compare the predicted projectile final fragment species (following abrasion and evaporation/multi-fragmentation) from `G4WilsonAbrasionModel`, NUCFRG2, and experimental data reported in [11]. The results from `G4WilsonAbrasionModel` generally follow the same trend in the experimental data, and approximately 50% of the time are within a factor of two of the reported experimental result. There are a few cases where the output from the Geant4-based model is closer to experiment than NUCFRG2, and usually `G4WilsonAbrasionModel` provides a more accurate prediction for cases where the mass of the final nuclear fragment is close to that of the projectile. Overall though, NUCFRG2 is on average more accurate in its prediction of the yields.

An interesting artifact is apparent in the `G4WilsonAbrasionModel` results in protions of Figures 3 and 4. The cross-section of the final fragment appears to be highly dependent upon whether the nucleon or proton numbers of the fragment are odd or even, presumably due to spin pairing. However, the fluctuations between adjacent odd and even Z products is a factor of four, whereas the experimental data suggests that in reality there is a much lower dependence. This odd-even dependence appears to be an artifact of the Geant4 evaporation model, and using the ablation model does result in significant improvement in the accuracy, and removal of the large fluctuations with A and Z (for example, see Figures 3 and 4 for 600MeV/nuc and 1570MeV/nuc ^{56}Fe on C, and 2100MeV/nuc ^{16}O on Cu).

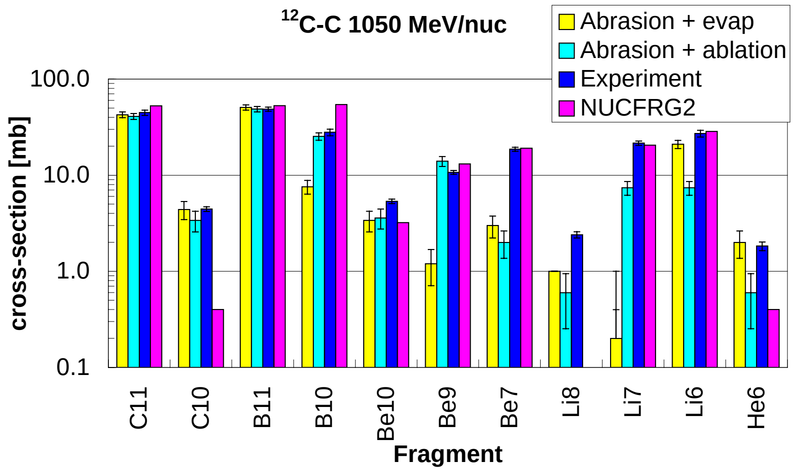

Figure 2. Comparison of cross-sections for 1050 MeV/nuc ^{12}C on carbon. Note that NUCFRG2 predicts the cross-section for ^{8}Li production as 0.1 mb.

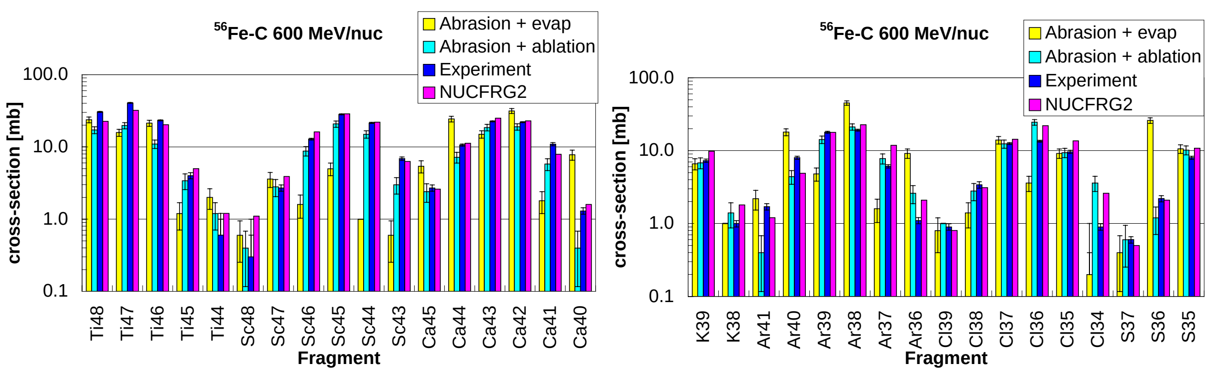

Figure 3. Comparison of cross-sections for 600 MeV/nuc ^{56}Fe on carbon.

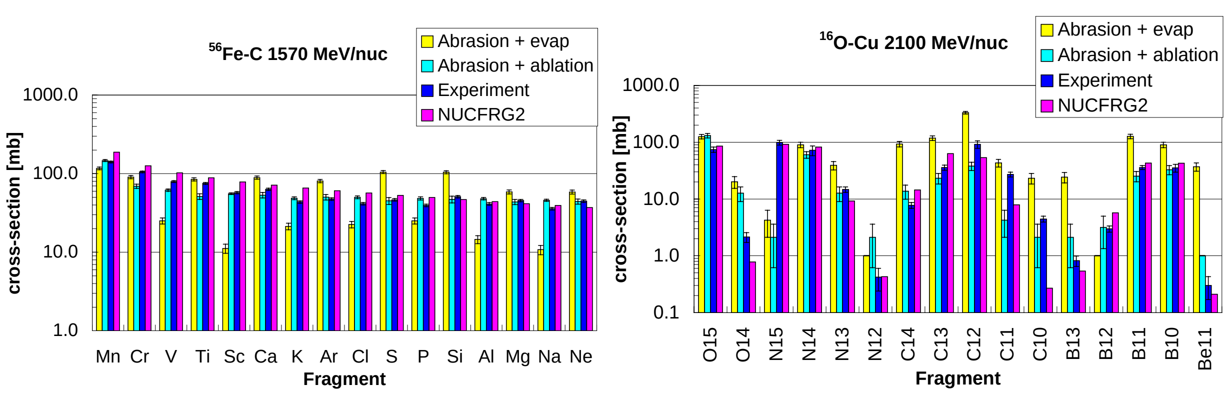

Figure 4. Comparison of cross-sections for 1570 MeV/nuc ^{56}Fe on carbon (left) and 2100 MeV/nuc ^{16}O on copper.

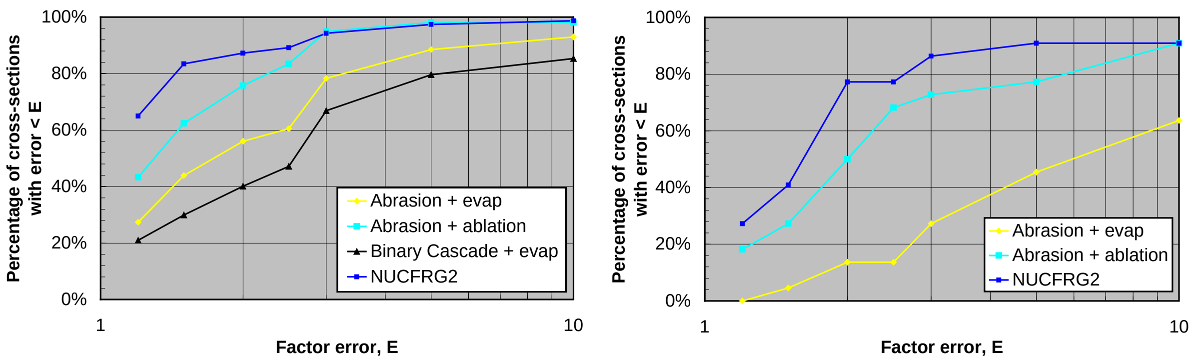

Figure 5. Comparison of the percentage of times the predicted cross-section for fragment production is within a factor of E of the experimental value, for various projectile nuclei on carbon target (left) and 2100 GeV/nuc ^{16}O nuclei on copper target (right).

Figure 5 summarises the performance of the new Geant4 classes in predicting the production cross-section for a range of nuclear-nuclear interactions [20]. The figures show the percentage of times the predicted cross-section was within a factor E of the experimental value, expressed as a function of E from 1 to 10, and confirm that using `G4WilsonAbrasionModel` with `G4WilsonAblationModel` is more accurate than if the former is used with Geant4's standard de-excitation physics. For the case of nuclei incident upon carbon, the cross-section predicted using the Geant4-based abrasion-ablation approach is within a factor-of-two over 75% of the time, compared with 85% of the time for NUCFRG2. Ambiguities in some of the details of the algorithm implemented by Wilson *et al* [11] have resulted in some differences between the Geant4 Monte Carlo results and the NUCFRG2 data. Note also that in Figure 5 the predicted nuclear production cross-sections from the Binary Cascade model (implemented in the `G4BinaryLightIonReaction` class) have the largest errors compared with experiment and other models.

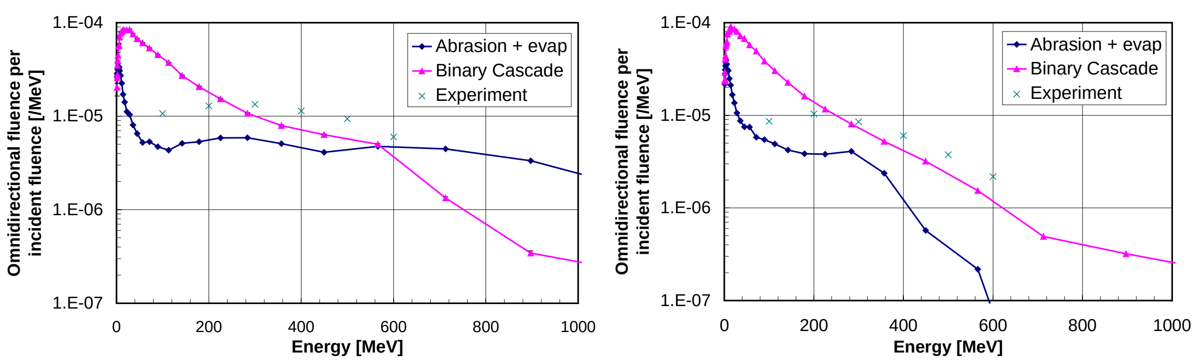

Figure 6. Comparison of secondary proton spectrum predicted by abrasion and binary cascade models, and experimental data for 800MeV/nuc ^{20}Ne incident on ^{20}Ne [21] (protons leaving at ~30^{o} (left) and ~40^{o} (right)).

The abrasion model does less well in predicting the secondary nucleon fluxes from nuclear-nuclear interactions compared with `G4BinaryLightIonReaction`. This, however, is not surprising since the macroscopic model approach used in the abrasion model avoids detailed simulation of nucleon-nucleon collisions required to specify their kinematics inside or outside of the nucleus. Figure 6 shows the secondary proton fluence (per unit incident particle fluence per steradian) for 800 MeV/nuc ^{20}Ne incident on ^{20}Ne. For proton energies above approximately 200 MeV, the results of the Binary Cascade simulation does appear to more accurately follow the experimental data, whilst the abrasion model (with or without ablation) consistently underestimates the differential proton spectrum, typically by a factor 2-4, but with much higher discrepancies at high energies and large angles (note that experimental and Poisson errors are smaller than the dimensions of the markers). At proton energies less than 200MeV, `G4BinaryLightIonReaction` does underestimate the measured spectra, an observation also reported by Yariv and Fraenkel from the results of their VEGAS code extended to treat nuclear-nuclear interactions of ^{20}Ne-^{20}Ne [21]. Analysis of ^{40}Ar-^{40}Ar collisions [19] confirms that in gross terms, the predicted secondary nucleon spectrum *from the two models* differ by a factor of two to four, but can be much higher for nucleons emitted at large angles.

`G4BinaryLightIonReaction` would therefore appear to be a better choice to treating the secondary nucleon spectrum, whilst `G4WilsonAbrasionModel` and `G4WilsonAblationModel` are more appropriate for simulating the production of the nuclear fragment from nuclear-nuclear interactions.

4.2 Treatment of electromagnetic dissociation

Table I provides a comparison of the predicted ED cross-section based on the model implemented in `G4EMDissociation` and experimental data reported by Jilany [15]. The simulation results are generally consistent with experiment, with errors typically between 5 and 42%, or 0.5 to 2 standard deviations of the experimental data. The largest difference is observed for 14.5 GeV/nuc ^{28}Si on silver, in which `G4EMDissociation` appears to overestimate one of the measured cross-section values by 70% (2.6 standard deviations), but it is also acknowledged that there is noticeable variability in the measurement and the prediction is 42% higher than the *weighted mean*.

Table I. Comparison of cross-sections for ED interactions in silver in which projectile produces a single proton. Experimental data are as reported by Jilany [15].

Projectile	Energy [GeV/nuc]	Product from ED	G4EMDissociation [mbarn]	Experiment [mbarn]
Mg-24	3.7	Na-23 + p	124 ± 2	154 ± 31
Si-28	3.7	Al-27 + p	107 ± 1	186 ± 56
	14.5	Al-27 + p	216 ± 2	165 ± 24 128 ± 33
O-16	200	N-15 + p	331 ± 2	293 ± 39 342 ± 22

5 CONCLUSIONS

Several new models have been implemented in the Geant4 radiation transport toolkit to treat nuclear-nuclear interactions:

- An abrasion nuclear-nuclear interaction model to simulate in a macroscopic approach the production of the two nuclear pre-fragments from the collision.
- An version of the ablation model, which treats de-excitation by nucleon and light nuclear fragment emission based on the principles of the Wilson model, together with the Geant4 evaporation classes to sample the momenta of the emitted particles.
- An electromagnetic dissociation model (ED) to simulate the ejection of protons and neutrons from a nucleus as a result of the virtual photons created as the nucleus travels at relativistic speeds in the field of a second nucleus.

In addition, enhancements have been made to the treatment of total inelastic cross-section (used to calculate distances to the next particle interaction in geometry tracking) to improve the simulation of interactions in which one of the nuclei is light (A≤4).

These models complement new hadronic physics which has been developed (or is currently under development) by other members of the collaboration, such as `G4BinaryLightIonReaction`, JQMD, and QGSM for nuclear-nuclear collisions.

The abrasion model provides a more accurate prediction of nuclear fragment production than Geant4's Binary Cascade model, especially when used in conjunction with the ablation model to treat de-excitation physics. For the case of nuclei incident upon carbon, the cross-section predicted using the Geant4-based abrasion-ablation approach is within a factor-of-two over 75% of the time, compared with 85% of the time for NUCFRG2, and 40% for `G4BinaryLightIonReaction`. However, the abrasion model is less accurate in predicting the secondary nucleon spectrum, and in the example presented here for 800 MeV/nuc ^{20}Ne incident upon ^{20}Ne, predicts secondary proton flux levels typically between factors of 2-4 lower than measured, but for high-energy protons at large scattering angles, can differ by more than an order of magnitude. For accurate treatment of secondary nucleon levels using Geant4, it is recommended that the binary cascade models be used, which performs better for proton energies >200MeV for the ^{20}Ne-^{20}Ne reaction.

The simulation results from the new electromagnetic dissociation model are generally consistent with experiment, with errors typically between 5 and 42%, or 0.5 to 2 standard deviations of the experimental data.

Future work should address ED of larger nuclear fragments, as well as angular momentum effects on the Geant4 pre-equilibrium model when applied to general nuclear-nuclear interactions in <100MeV/nuc.

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