GRAS: A General-Purpose 3-D Modular Simulation Tool for Space Environment Effects Analysis

Giovanni Santin, Vladimir Ivanchenko, Hugh Evans, Petteri Nieminen, and Eamonn Daly

***Abstract*—Geant4 Radiation Analysis for Space (GRAS) is a modular, extendable tool for space environment effects simulation. Analyses include cumulative ionizing and NIEL doses, effects to humans, charging, fluence and transient effects in three-dimensional geometry models.**

***Index Terms*—Aerospace biophysics, aerospace industry, aerospace simulation, biological effects of radiation, dosimetry, Monte Carlo methods, radiation effects, simulation software, software tools.**

I. Introduction

KNOWLEDGE of the potential impact of the radiation environment on evolving space borne devices relies on precise analysis tools for the understanding and the prediction of the basic effects of the particle environment on new technologies. In addition to cumulative effects such as dose, single event effects (SEE) in modern microelectronics are often a major cause of spacecraft failures or anomalies [1], [2].

Simulation can play a major role in the understanding of the underlying phenomena of the interaction of the particle radiation with the spacecraft devices. It is recognized, for missions flying commercial off-the-shelf (COTS) technology and sensitive detectors, that engineering design margins are a crucial issue. A complete space qualification ground test procedure for all new components makes costs higher, without being able to cover, in energy and species, the entire range of the particle radiation population in space. The availability of reliable simulation tools could lower costs by complementing a more limited set of experimental tests, while still giving enough confidence on the component behavior in space. New requirements for the analysis of the radiation biological effects are also arising in the context of increased interest in human exploration initiatives.

Particle transport tools based on a look-up table approach (such as SHIELDOSE-2 [3]), which are often integrated in 3-D ray tracing applications for sector analysis, are widely used in the space domain and are much faster than full Monte Carlo simulations, but have limited applicability in complex geometries and give imprecise description of the secondary particle emission. Well-established Monte Carlo tools include codes as EGS4 [4], FLUKA [5] and MCNPX [6]. Other codes, such as the analytic code HZETRN [7] and NOVICE [8], have also shown good performance but are not widely available.

Geant4 [9] is an open source object-oriented simulation toolkit that offers a wide set of electromagnetic and hadronic physics models, a good performance of the particle transport in complex geometry models and the possibility of interfacing to external packages such as simulation engines and visualization or analysis tools. The European Space Agency (ESA) has recently been strongly focused on making Geant4 readily accessible to a variety of engineering applications and WWW-based radiation effects studies through the development of easy-to-use interfaces, advanced models, and auxiliary software. MULASSIS [10], [11] is a successful example of a ready-to-use 1.5D tool with a user-friendly interface. However, there is still need for new tools to address the issues left open, such as the modularity of the analysis, support of more complex geometry models, and flexibility of the design.

II. Description of the Main GRAS Features

GRAS has been designed to enable an easy implementation of the analysis of many radiation environment effects. A modular approach has been followed for most of the essential components such as geometry model, physics description and the extraction of the radiation effects data.

The simulation is entirely driven via user interface (UI) scripting commands (interactively and via macro files). This includes the selection of the geometry model, the physics, the insertion of analysis modules, and for each module the definition of the relevant parameters, such as the volumes in which the analysis has to be performed, or the units for the result printout.

A. Geometry

The user can select the input format for the geometry model via UI commands. The present standard format is the geometry description markup language (GDML) [12] through which it is possible to define materials and a volume tree from all the Geant4 shape primitives. An example showing an approximated but complex model of the JWST NIRSpec instrument is given in Fig. 1.

A layered geometry model (similar to MULASSIS) has been included into the GRAS tool and is available through the User Interface. In case neither the GDML nor the layered geometry is selected, a simple geometry model (hard coded in C++) is loaded as a default. This model can be used for test purposes,

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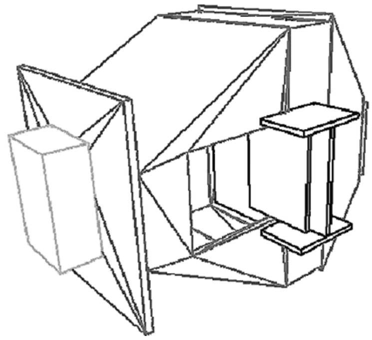

Fig. 1. Example of a 3-D geometry in GRAS: the shielding design for the JWST near infrared spectrometer (NIRSpec). The detector in the focal plane array (FPA) is protected by a silicon carbide (SiC) camera on one side (with structural elements and mirrors) and a molybdenum-titanium back shielding on the other. The shielding thickness in the various detector elements is being optimized with respect to cumulative doses and secondary particle production, while respecting the rigid mass budget imposed by the launch.

and is available also when the GDML libraries are not available for the complete GRAS installation.

B. Physics

Space radiation sources range from very low to very high energy, and their interactions with the spacecraft sensitive devices and the shielding structures include both electromagnetic and hadronic processes. The GRAS tool includes therefore a very large subset of the physics models available within Geant4, with the aim of giving an almost complete coverage of the main interaction mechanisms for trapped, solar and cosmic radiation in the spacecraft materials.

Thanks to a modular design, the user can select between the "standard" and "low-energy" electromagnetic packages, and can include the hadronic models for low, mid and high-energy particles. The low and mid energy hadronic models available are the Binary intra-nuclear cascade model, which describes the nuclear interactions of protons and neutrons with energy up to 10 GeV and pions up to 1 GeV, and the alternative Bertini cascade model, which describes proton, neutron and pion and kaon interactions up to 10 GeV. The quark gluon string (QGS) model, valid up to 100 TeV, covers higher energies and allows the simulation of a significant part of the protons in the wide Cosmic Ray spectrum.

A recent extension of the binary cascade model to light ions with energy below 10 GeV/nucleon is also included. However, its use for ions of higher atomic number and weight is not recommended. As an alternative, the recent Geant4 implementation [13] of the abration/ablation models [14], [15] is available. For higher energies, an extension of the QGS model to ions [16] is under development within the Geant4 collaboration and will be included as soon as it becomes public, due to its relevance to both SEE studies and estimates of the radiation effects on manned space flight.

C. Analysis Modules

The core part of the analysis is constituted by the "analysis modules," which can be inserted by the user via UI commands to perform the individual analysis tasks. The modular approach keeps analysis types independent and isolates each complete analysis inside one class. This makes both the development and the debugging easier, as it offers a clear view of the analysis mechanisms, from the initialization to the printout of the results. Advanced users can easily add new module types by extending or implementing analysis models not existing yet in GRAS: a new analysis class can inherit the functionalities of an existing (object-oriented) GRAS class to quickly add features as a new module type.

Existing analysis types include cumulative effects such as total ionizing dose (TID) or non-ionizing energy loss (NIEL) dose, to study performance degradation in scientific detectors, commercial payload components or service elements such as solar arrays. TID estimates can be output in several output units, including rad and Gy (the required detector mass is in this case automatically obtained from the geometry model). NIEL analysis modules offer a choice among several NIEL coefficient tables, obtained from the literature for different semiconductor technologies. Data selected from the CERN-RD48 (ROSE) collaboration for protons, neutrons, electrons and pions are included, providing NIEL coefficients for particle interaction in silicon. Curves for damage estimates in several semiconductor materials (including Si, GaAs, InP) from [17] are also included. A new collection of NIEL curves computed for typical device materials for protons and neutrons [18] have been implemented and tested. At present the microscopic NIEL calculation is not possible, but a new implementation of the Geant4 Coulomb elastic scattering of the particles on atomic nuclei is expected to become publicly available providing this functionality, in addition to the present look-up table approach.

Specific modules have been developed for the evaluation of the effects of radiation to humans: "dose equivalent" analysis, based on LET quality factors (QF); and "equivalent dose" based on the incident particle weights are available in GRAS, with a choice among several factor functions from existing protocols in the literature. The "dose equivalent" calculation takes into account the relative biological effectiveness (RBE) of radiation as a function of particle type and energy through the use of QF. The Q(L) relationship between the QF and the LET has been implemented in GRAS based on the ICRP 60 recommendations [19]. The "equivalent dose" estimate makes use of radiation weighting factors (w_R): the user has the choice between the values adopted in [19] or the re-appraisal of the factors given in ICRP 92 [20]. A special technique has been developed in the GRAS application to ensure the correct weighting factor is applied to the dose deposited by the particles (the primaries and the generated secondary products) according to the "incident" particle type: once a weight w_R is assigned to a particle, it is then propagated to all its secondary interaction products. The definition of "incident particle" is also not restricted to the primary particle: the user can define as "incident" particles that cross a selected boundary. This is crucial for dosimetry applications in which the primary radiation interacts with a shielding structure before reaching the sensitive target: in this case there is a clear difference between the particles that are "incident" onto the target (astronauts, dosimeters, etc.), which consist of slowed-down primaries and secondary particles, and the primary particle. The user can select the boundary that defines a particle as "incident" module by module, so that analyses can be performed in parallel during the same simulation run on different sensitive target volumes.

The same mechanism is applied to all cumulative effect analyses. As an example, it is used in the "dose modules," to distinguish the contribution to the TID from different "incident" particle types, as opposed to different "local" types of radiation depositing a dose at a point. The usefulness of this method is apparent when analyzing shielding effectiveness from the separate effects of charged and neutral particles, as the latter only deposit energy locally through the charged products after interaction. Typical applications are the separate contributions after shielding given by input electrons and generated Bremsstrahlung photons, or by spallation neutrons produced from hadronic interactions.

Fluence of primary or secondary particles is tallied in the Fluence modules. In addition to the total integrated fluence by particle, individual energy spectra are recorded for user defined particle types.

Specific modules implementing single event effects models available in the literature have been developed. Transient effects are addressed at present by pulse height and LET spectra, included in the dose modules, a threshold model and a "track length" analysis.

All analyses can be applied to any user defined set of volumes or surfaces, chosen among those present in the geometry model. Results are saved as histograms or "tuples" (tabular data for later analysis), while basic summary quantities are also output in simple text format. Users also have the choice of the units for the result output.

D. GRAS and Existing Geant4 Applications

There are several cases in which the user might desire to benefit from the GRAS analysis modules, still preserving some work from the development of a previous standalone Geant4 application. In case a geometry model had already been implemented in C++, this can be integrated into GRAS. In case a significant portion of code had been written for the analysis of the simulation output, GRAS can be integrated into the previous application through a dedicated simulation manager class that, during the simulation, executes both the user and the GRAS analysis. In this case the combined application will produce results from the old code and GRAS in parallel, as shown in Fig. 2.

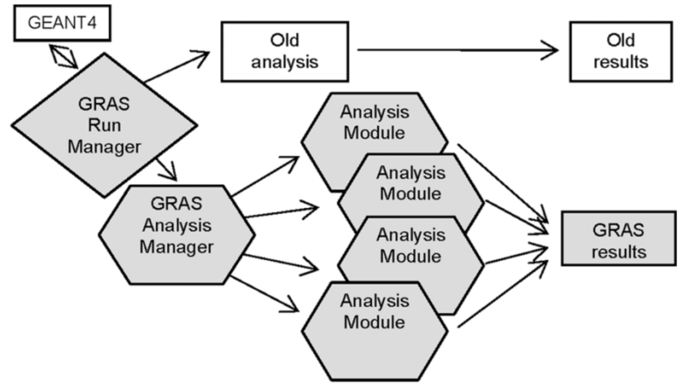

Fig. 2. Diagram of an example user application in which GRAS is inserted as analysis tool (through the GRAS run manager) to extract from the GEANT4 simulation the user results and the GRAS ones in parallel.

TABLE I
TOTAL IONISING DOSE IN THE JWST NIRSPEC FPA DETECTOR

Tool, Model	*Dose [krad] (11 mm equiv. Al)*	*Dose [krad] (18 mm equiv. Al)*
SHIELDOSE-2, Spherical shell	3.9	1.9
GRAS, Spherical shell	3.5 +/- 0.2	2.3 +/- 0.2
GRAS, Realistic model	2.2 +/- 0.1	1.1 +/- 0.1

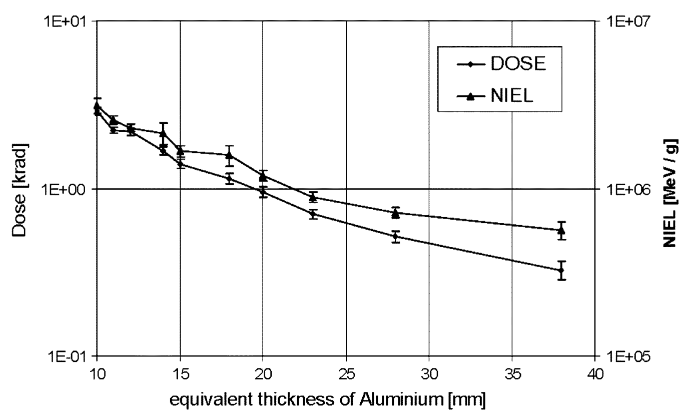

Fig. 3. Analysis of the cumulative degradation effects to the JWST NIRSpec detector. TID and NIEL as a function of the shielding thickness in units of mm of equivalent thickness of aluminum. Real thickness depends on material density. Incident protons follow the ESP spectrum (see text).

III. APPLICATION EXAMPLES

GRAS has been used in three examples discussed below. The first shows the advantages for employing GRAS in a space project. The second is a terrestrial application that is extended to act as an experimental verification of Geant4 secondary particle production at an accelerator. The final example demonstrates an analysis to understand the source of glitches observed in a space platform and refinements for a follow-on instrument.

A. Radiation Effects to the JWST NIRSpec Detector

Effects to components that are shielded by nonisotropic spacecraft structures are correctly described by 3-D models, as in the case of the JWST NIRSpec focal plane array (FPA), whose geometry model is shown in Fig. 1. Table I shows results for cumulative TID analysis for the three cases of SHIELDOSE-2 (spherical shell), GRAS (spherical shell) and GRAS with a 3-D realistic configuration (with a front silicon-carbide compartment, and a Mo/Ti back shielding). The results illustrate the importance of a representative, albeit approximated, 3-D model of the geometry for a correct estimate of the radiation effects. Fig. 3 shows TID and NIEL for the realistic geometry as a function of the shielding thickness, which is set for each material (SiC for the camera, Mo and Ti for the back shielding) according to its density and is plotted in units of equivalent thickness of aluminum. The spectrum used for the TID estimate

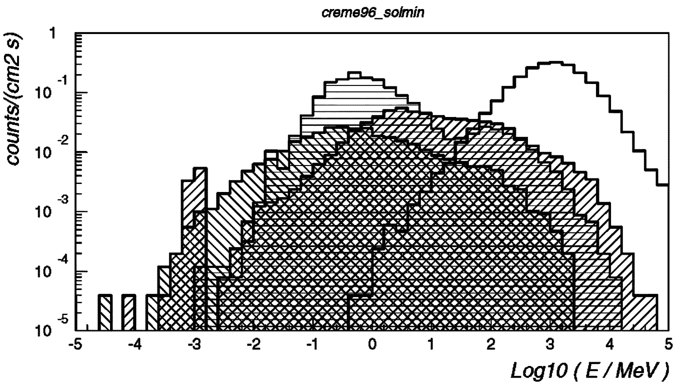

Fig. 4. JWST NIRSpec analysis of secondary particle emission: the incident source is given by protons with CRÈME'96 solar minimum spectrum. The spectrum of primary protons reaching the detector (empty histogram) is superimposed to the spectra of gammas (horizontal stripes), electrons (left stripes), and neutrons (right stripes). The integrated gamma flux is of the same order of magnitude of the proton one.

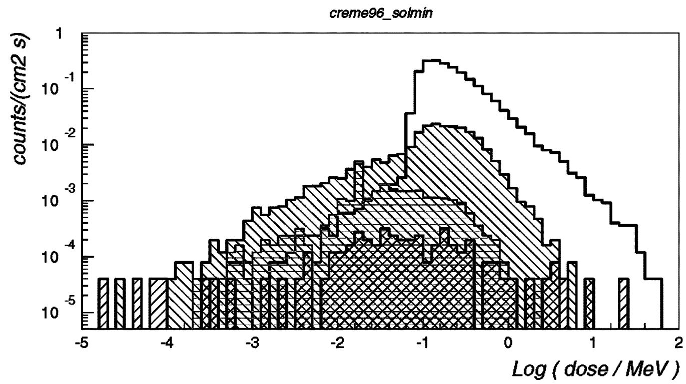

Fig. 5. JWST NIRSpec: effect of the secondary emission on the NIRSpec observation strategy. The spectrum of the energy deposited in the detector by protons (black, empty histogram) is superimposed to the one for gammas (horizontal stripes), electrons (left stripes), and neutrons (right stripes).

is obtained with the emission of solar protons (ESP) model [21] for five active years and a 95% confidence level (CL).

An advantage of using GRAS instead of 1-D shielding assessment tools is the possibility of having realistic 3-D isotropic sources impinging onto the complex geometry model. This avoids approximate assumptions on the combination of several, independent simulations with different shielding hypotheses. Moreover, the secondary particle spectra produced in the spacecraft structure can only be correctly transported to the sensitive devices in a realistic 3-D geometry model. Fig. 4 shows the energy spectrum of primary and secondary particles at the surface of the JWST NIRSpec detector. The effect of these particles on the detector performance is linked to the spectrum of the energy deposit inside the detector, which is shown in Fig. 5.

B. Neutron Time of Flight Measurements

Secondary neutron experimental energy spectra are often derived from time of flight (TOF) measurement with scintillator detectors. Fig. 6 shows the simulation results obtained with GRAS from a simple model describing a beam test made at PSI, Switzerland.

Protons of 70 MeV (kinetic energy) impinging on a 1 mm silicon target undergo elastic and inelastic collisions producing, amongst others, neutrons and gammas which are detected in a liquid scintillator (NE213). From TOF measurements and particle identification techniques the neutron spectrum can be obtained at various angles. The protons, which are dominating the simulated distribution, are stopped, in the real experimental setup, by a thick slab put in front of the detector. The discrimination of gammas from protons is critical as the time spectra for the two particle types partially overlap, as seen in Fig. 6, and is experimentally provided through pulse-shape analysis.

The experimental results will eventually be used as an validation of the Geant4 secondary particle production hadronic models, which are often used to assess the shielding effectiveness in mission design, as described in the previous paragraphs.

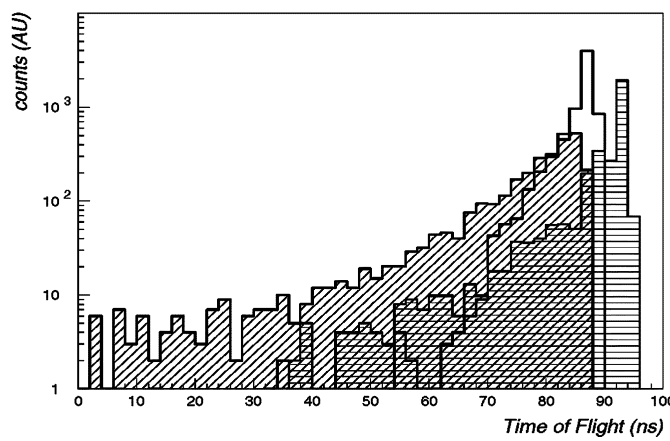

Fig. 6. TOF measurement simulation at PSI for the determination of the spectra of secondary neutrons produced by proton interaction in silicon targets. Protons (black empty histogram) from elastic scattering are dominating the TOF distribution but are actually prevented to reach the detector in the real setup. Gamma (horizontal stripes)—neutron (right stripes) discrimination is later performed with pulse-shape analysis.

C. Cosmic-Ray Glitch Rate Testing for Herschel PACS

Past experience with the photoconductor technology onboard the ESA infrared space observatory (ISO) mission [22] showed that the interaction of highly energetic particles within the sensitive volumes may induce glitches, which can affect the extraction of the infrared signal. The design of the Herschel PACS Photoconductor detector, based on a similar technology, is taking this into account, and ground tests of the sensitive devices under proton irradiation are being performed [23]. The plot in Fig. 7 shows the application of GRAS to the simulation of the test setup. The initial proton (kinetic) energy is 70 MeV, with a spread of 100 keV. In order to modulate the energy of the protons impinging onto the detector, three different experimental conditions were set up, with: no energy degrader, 1 and 2 energy plastic (polyethylene) degraders. The results of the simulation studies show that the proton LET, which in turn depends on the presence of the degraders, strongly influences the energy deposition in the detector. A detailed refinement of the setup modeling has been required to take the proton energy

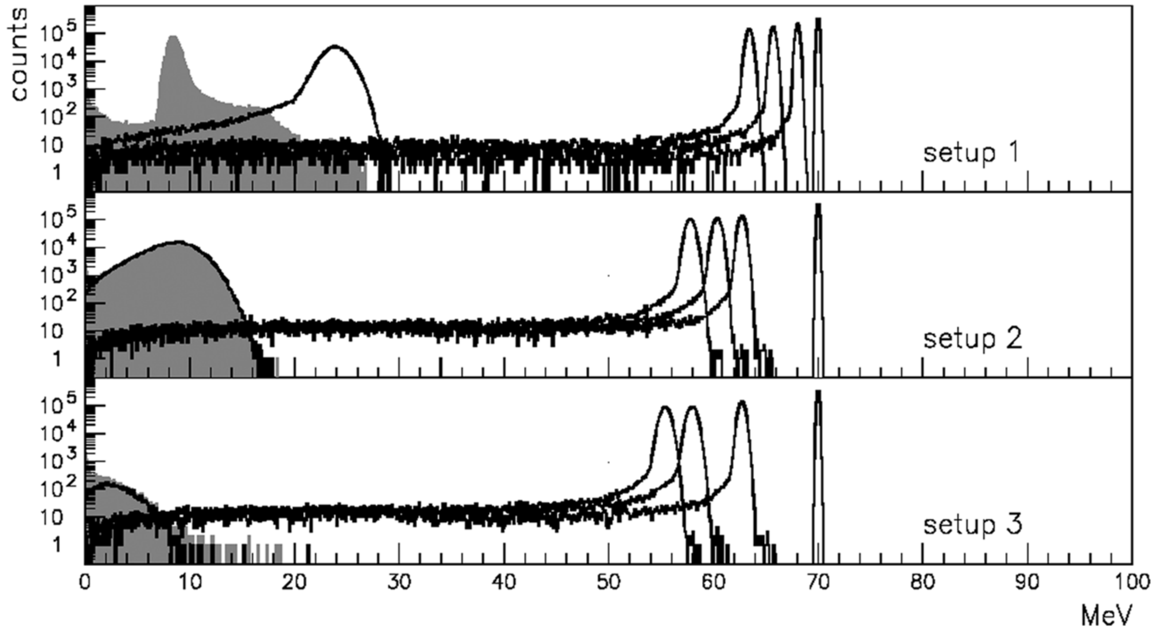

Fig. 7. HERSCHEL PACS photoconductor ground proton beam test. From top to bottom, proton fluence histograms for three setups, which correspond to no energy degrader, 1 and 2 energy degraders. The initial proton (kinetic) energy is 70 MeV, with a spread of 100 keV. In each plot, in black, from right to left, the histograms represent the proton fluence spectrum sampled at the source, after the first and the second degrader, at the entry of the test Dewar and at the entry of the photoconductor crystal, obtained with GRAS fluence modules. The red filled histogram represents the energy deposit spectrum (pulse height) in the crystal, obtained with a dose module.

losses precisely into account along the beam line and inside the cryogenic detector (in the Dewar and the PACS structure).

The energy deposit pattern in the filled histograms, in particular in the upper plot in Fig. 7, can be explained as the superposition of different primary and secondary particles arriving at the crystals. Low energy secondaries (mainly from hadronic interactions) populate the very left part of the spectrum; primary protons passing through the crystals are the main source of the peak, while the right most part is given by lower energy protons, passing though or stopping protons, whose Bragg peak is contained in the crystals. Presently simulation results are being compared against glitch shape and rate.

IV. Conclusion

A new Geant4-based simulation tool has been developed for the analysis of the space radiation environment effects. Thanks to the wide set of Geant4 physics models and to a modular design in all its components, GRAS is already covering most basic space analyses, and is open to new developments.

The tool has been applied in several occasions to spacecraft design process, and will be the main tool for a deeper understanding of safety margin procedures, with detailed comparisons of simple procedures such as sector analyses, against the full Monte Carlo approach.

The 3-D analyses of energy deposition patterns will offer in the near future the possibility of direct accurate estimates of the SEE rates directly, without making unnecessary assumptions on the geometrical model of the sensitive devices in modern microelectronics.

A web interface inside the Space Environment Information System (SPENVIS) [24] is under development.

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