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HIERRAS – HUMAN INTERPLANETARY EXPLORATION RADIATION RISK ASSESSMENT SYSTEM

EXECUTIVE SUMMARY REPORT

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Acronyms and Abbreviations

ACE	Advanced Composition Explorer
API	Application Programming Interface
AU	Astronomical Unit
CIRSOS	Collaborative Iterative Radiation Shielding Optimisation System project
CIRVis	CIRSOS Visualisation software (to interactively view GDML files)
CL	Command Line, Confidence Limit or Confidence Level
CLI	Command Line Interface
CREME96	1996 version of the Comic Ray Effects on Micro-Electronics model
CSDA	Continuous Slowing Down Approximation
DLR	Deutsches Zentrum für Luft- and Raumfahrt
EPAM	Electron Proton Alpha Monitor
ERNE	Energetic and Relativistic Nuclei and Electron instrument on SOHO
ESA	European Space Agency
ESHIEM	Energetic Solar Heavy Ion Environment Models
ESP	Energetic Storm Particle
ESSR	European Space Software Repository
ESTEC	European Space Research and Technology Centre
GCR	Galactic Cosmic Radiation or Galactic Cosmic Ray
GDML	Geometry Definition Mark-up Language
GLE	Ground Level Enhancement
GOES	Geostationary Operational Environmental Satellite
GRAPPA	Geant4 Radiation Analysis for Planets, Planetary-satellites and Asteroids
GRAS	Geant4 Radiation Analysis for Space
GUI	Graphical User Interface
HAPI	Heliophysics Application Programmer's Interface
HEPAD	High Energy Proton and Alpha Detector
HIERRAS	Human Interplanetary Exploration Radiation Risk Assessment System
HMI	Human-Machine Interface
HTML	HyperText Markup Language
ICRP	International Commission on Radiological Protection
IRENE	International Radiation Environment Near Earth (AE9/AP9/SPM)
IRPP	Integral Rectangular ParallelePiped
ISO	International Organization for Standardization
ISS	International Space Station
JSON	JavaScript Object Notation
LEO	Low Earth Orbit
LET	Linear Energy Transfer
LRO	Lunar Reconnaissance Orbiter
MSM	Magnetosphere Shielding Model
MULASSIS	MUlti-LAyered Shielding SImulation Software
NAIF	NASA's Navigation and Ancillary Information Facility
NASA	National Aeronautics and Space Administration
NCEI	National Centers for Environmental Information
NoM	Network of Models
ODI	Open Data Interface
RD	Reference Document
RDS	Reference Data Set (SEPEM)

SAPPHIRE	Solar Accumulated and Peak Proton and Heavy Ion Radiation Environment
SAPPHIRE-HEX	SAPPHIRE High Energy eXtension
SAPRE	SAtellite PREdiction
SEE	Single Event Effect
SEP	Solar Energetic Particle(s)
SEPEM	Solar Energetic Particle Environment Modelling system
SEU	Single Event Upset
SHIELDOSE-2/2Q	(SD2/SD2Q) NIST 1D shield simulation software for protons and electrons (SHIELDOSE-2Q is QinetiQ-modified version to treat additional shield and target materials)
SOHO	SOlar and Heliospheric Observatory
SPARC	Space Applications & Research Consultancy
SPE	Solar Particle Event
SPECTIRES	Spectra and Effects Comparison Toolkit for Ionising Radiation Environments in Space
SPENVIS	Space ENVironment Information System
SPENVIS-NG	Next Generation Space ENVironment Information System
SPICE	NASA NAIF Observation Geometry System for Space Science missions
SSAT	(Geant4-based) Sector Shielding Analysis Tool
TAS	Thales Alenia Space
TID	Total Ionising Dose
TNID	Total Non-Ionising Dose
VRML	Virtual Reality Modelling Language

1 INTRODUCTION

This document is the Executive Summary Report for ESA Project *HIERRAS—Human Interplanetary Exploration Radiation Risk Assessment*, ESA Contract 4000127129/19/NL/HK. In the framework of this contract, a new, comprehensive system of tools was developed to permit accurate and easier calculation of radiobiological and equipment radiation effects for future human interplanetary missions within helio-radii 0.9 to 1.6 AU. A more detailed description of the work can be found in the Contract Final Report [RD 1] and the documents referenced therein.

The work was performed by the following consortium:

- DH Consultancy BV (Leuven, Belgium; Prime Contractor): D. Heynderickx
- Kallisto Consultancy Ltd (Farnborough, UK): P. Truscott
- RadMod Research Ltd (Camberley, UK): F. Lei
- Deutsches Zentrum für Luft- und Raumfahrt (DLR, Cologne, Germany): D. Matthiä and T. Berger
- Department of Physics and Astronomy, University of Turku (Finland): O. Raukunen and R. Vainio.

In addition, A. Tsigkanos and I. Sandberg of Space Applications & Research Consultancy (SPARC, Athens, Greece) consulted on the construction of the updated SEPEM Reference DataSet (RDS).

During the contract, a group of expert stakeholders was formed to provide feedback on the work throughout the contract: W. Atwell, E. Daly, L. Dartnell, A. Fogtman, M. Giraudo, P. Gonçalvez, C. Lobascio, S. McKenna-Lawlor, A. McSweeney, L. Narici, G. Reitz, G. Santin, R.C. Singleterry, U. Straube. Their contributions are greatly appreciated.

This Executive Summary Report summarizes the new model and software developments and describes the modelling and implementation approach, the software system design and development, the various user interfaces and the software verification and validation:

- Requirements definition (Section 2)
- System level architecture, models and user interfaces (Section 3)
- Verification and validation (Section 4)
- Update of the SAPPHIRE SEP model (Section 5)

2 HIERRAS REQUIREMENTS DEFINITION

2.1 DESCRIPTION OF GENERAL CALCULATION PROCESS

The general calculation processes which HIERRAS needs to treat are identified as boxes A, B, and D to F in Figure 1. The user is assumed to have as inputs a definition of a complete mission or part of a mission (trajectory, start and end datetimes for each phase) and details of the 3D or 1D shielding afforded to the astronauts and systems by the spacecraft and/or habitat structures, including equipment items such as EVA suits. Using HIERRAS, the user should then be able to:

A. Apply one or more environment models for each phase of the mission.
B. Define a surface environment, together with atmosphere and local magnetic field (in the case of Mars), and perform simulations for particle propagation.
D. Define a local geometry behind or within which the modified radiation environment and radiation doses are to be determined—a simple 1D shield or full 3D geometric representation of a vehicle or surface habitat. Using either deterministic or Monte Carlo radiation transport simulations, the particle fluence spectra and/or doses at locations within the geometry are then calculated.
E. Based on the radiation shielding calculations, calculate radiobiological exposure quantities such as Effective dose equivalent H_E and Gray-equivalent (Gy-Eq) dose in tissue/organ, G_T. The basis of these calculations are

fluence-to-dose conversion coefficients from ICRP-123, or absorbed dose in an ICRP anthropomorphic phantom.

F. Determine standard equipment radiation effects quantities: total ionising and non-ionising doses, LET spectra, upset rates and solar-cell degradation.

The functions depicted by box G in Figure 1, (radiation hardness assurance and failure analysis) are outside of the scope of the HIERRAS System, and the radiation protection limits are assumed to be defined as part of the mission definition, based on ICRP-123 and/or ECSS documents. Also, the radiobiological and system effects of man-made radiation sources (box C) have not been treated within HIERRAS.

2.2 User Characteristics

To help define the System requirements, it was assumed that the user community for HIERRAS comprised the following classes:

- A designer of the interplanetary mission spacecraft system/subsystem who wishes to use HIERRAS to calculate radiation exposure to astronauts and systems.
- A mission planner who uses HIERRAS to quantify the relative radiation exposure and risk for different mission scenarios, including the effectiveness of emergency protocols (e.g., for different magnitude solar particle events and early event warning sensors).
- HIERRAS can be used by scientists to interpret results obtained from sensors during the mission or post-flight in order to help interpret the results and improve environment and effects models as well as improve detector designs.

HIERRAS can be used by general spacecraft engineers as well as radiation effects experts by allowing advanced users greater control over some of the key functions/parameters.

3 System Level Architecture, Models and User Interfaces

3.1 System Architecture

The HIERRAS System is divided into several distinct functional modules identified in the top-level software architecture diagram shown in Figure 2 [RD 3].

3.1.1 System Front Ends

The front end of the system is the Graphical User Interface (GUI) which:

- Defines a set of interactive webpages for the user.
- Collects user inputs from the webpages, packages them in JSON request structures and sends these to the Listener module.
- Receives JSON status structures from the Listener and updates the web pages accordingly.
- Provides a set of context sensitive and background information help pages.

The Command Line Interface (CLI) provides direct interaction with the Listener module in a similar manner to the GUI [RD 4]. Requests can be sent using cURL, for instance, and responses could be captured in a custom-built Python notebook application.

3.1.2 Listener Module

This module treats the requests received on a separate host IP port from clients inside and outside of the firewall. Each request is received as a JSON stream from the GUI/CLI and spawns a separate HIERRAS Application (App) process. The (JSON formatted) response generated by the App is returned to the calling application.

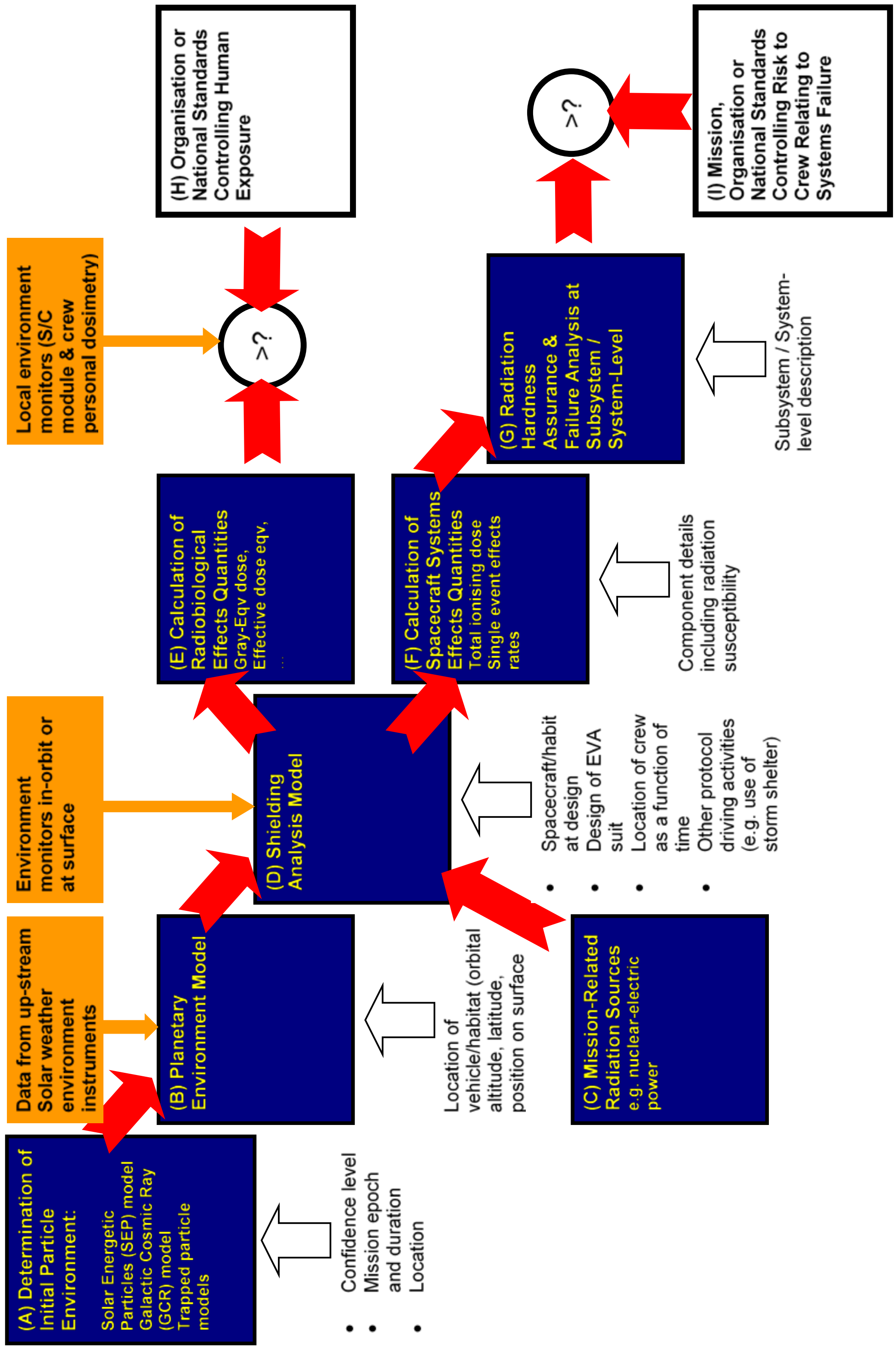

Figure 1: Process flow for assessment of radiation exposure of crew and equipment (adapted from [RD 2])

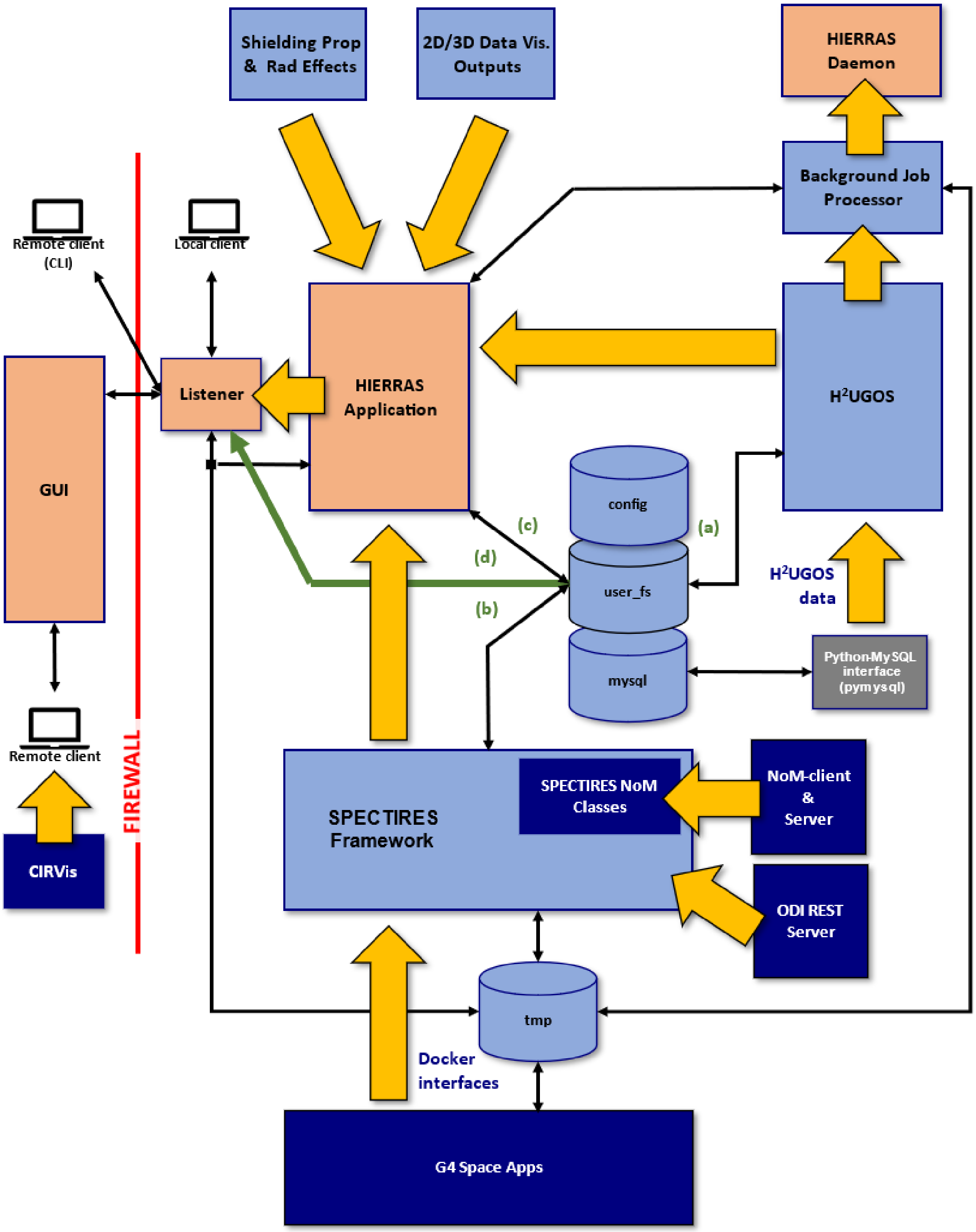

Figure 2. HIERRAS System Top-Level Architecture. The light-orange boxes represent Python-based code modules which one or more executable scripts (i.e., to run a top-level application). Light blue boxes represent Python code modules which provide classes and functions to perform tasks required by the other modules, e.g., to instantiate and run an environment or effects analysis model.

3.1.3 HIERRAS Application (App)

This application is responsible for controlling the high-level functions of the system. It performs request/response handshaking communication with the GUI/CLI through the Listener module of the commands sent from the user. Its primary function is to interpret the requests received and control processes performed using other HIERRAS modules that undertake functions such as:

- Authenticating the user at login and subsequent requests with a rolling authentication key.
- Changing the user's current working directory and group under which they are performing tasks.
- Environment and effects model runs using the SPECTIRES Framework, Shielding Propagation and Radiation Effects modules, and generating plots using intrinsic SPECTIRES facilities as well as functions in a separate 2D/3D data visualization module. And saving files to the user file system area.
- Registering in the H^2UGOS database Geant4 background run submissions by the user. Also process the run requests subsequently submitted to it by the Background Processor in HIERRAS Daemon.
- Directory and file handling processes and standard housekeeping functions, such as updating the user password.

3.1.4 HIERRAS Handler for Users, Groups, and Object Storage (H^2UGOS) Module

H^2UGOS is an independent module introduced to treat the bookkeeping functions of HIERRAS and manage data persistence through the use of an SQL database. Its principal functions are to:

- Register and manage users and groups.
- Maintain a record of all files in the user area and maintain information on input/output file dependencies.
- Register requests from and responses to the GUI/CLI and association with any files generated.
- Control information about submitted, ongoing and completed background jobs.
- Record HIERRAS System broadcast messages.

3.1.5 SPECTIRES Framework

The SPECTIRES Framework comprises a toolkit and a series of model wrappers to perform the necessary radiation environment and effects predictions. The Toolkit provides the lower-level functionality for managing quantities relevant to the calculations, such as coordinates, trajectories, spectra, effects quantities and response functions as well as metadata associated with these objects.

Models exist within the Toolkit covering:

- trajectory propagation;
- GCR, solar particle and trapped radiation environments;
- planetary radiation environments;
- shielding transport models;
- component or systems effects analysis models (including solar cell damage and single event effects).

The Toolkit includes interfaces to the ODI HAPI REST server which can be used to extract time-dependent SEP spectra for events from the SEPEM Reference Dataset [RD 5][RD 6].

As part of the HIERRAS activity, new SPECTIRES classes have been introduced to interface with ESA's Network of Models (NoM) servers, providing alternative implementations of many of these models. A full list of the models available in HIERRAS through SPECTIRES and NoM is provided in Section 3.2.

3.1.6 Shielding Propagation and Radiation Effects Module

The Shielding Propagation and Radiation Effects module in Figure 2 refers to an additional module developed specifically to cover aspects of the shield and effects analysis not fully treated by the tools within SPECTIRES, including [RD 7]:

- The conversion of JSON-formatted requests, submitted to the App, into Geant4 macro files.

- Calculation of radiobiological effects quantities from shielded particle fluxes.
- Integrating sector shielding analysis results with dose-versus-depth curves to estimate radiation dose quantities.
- Application of response functions generated from MULASSIS and GRAS to allow rapid calculation of fluxes and dose rates as well as cumulative fluence and dose as a function of time.
- Perform 2-stage GRAS simulations, where an initial Monte Carlo run is performed for a larger geometry, and the calculated residual primary and secondary particle fluxes at the surface of a smaller volume are used as the source of the second stage simulation.

3.1.7 G4 Space Apps Docker

Several docker build scripts have been created by the HIERRAS Project which construct a Ubuntu docker image with a full Geant4 v10.7 installation, and then install upon this the ESA applications MULASSIS, SSAT, GRAS, CIRVis, and GRAPPA. As part of this process, the ESA C++ codes were updated, verified and validated to ensure they operated correctly with G4 v10.7.

The resulting docker image, referred to as g4_space_apps, contains all the Geant4 data libraries, while the docker build is performed directly from source code and data held on ESA and CERN repositories. As such, this provides a greatly simplified and reliable method of creating and distributing the ESA Geant4 applications which had previously been complicated/error-prone processes.

3.1.8 HIERRAS Daemon

This is a separate application to the App which monitors requests for long execution runs and submits these for processing depending upon the available "worker processes". Once a job is submitted, the user can interrogate its status through the GUI/CLI and, if necessary, abort the run.

3.1.9 2D/3D Data Visualisation

SPECTIRES already includes a series of classes which can be used to generate spectra, flux maps, trajectory and dose-versus-depth plots. Additional graphics classes or routines are provided in a separate 2D/3D data visualisation module to generate plots more relevant to radiological dose information and radiation heat maps for both particle flux/fluence and dose. Figure 3 – Figure 8 show examples from this module and from SPECTIRES.

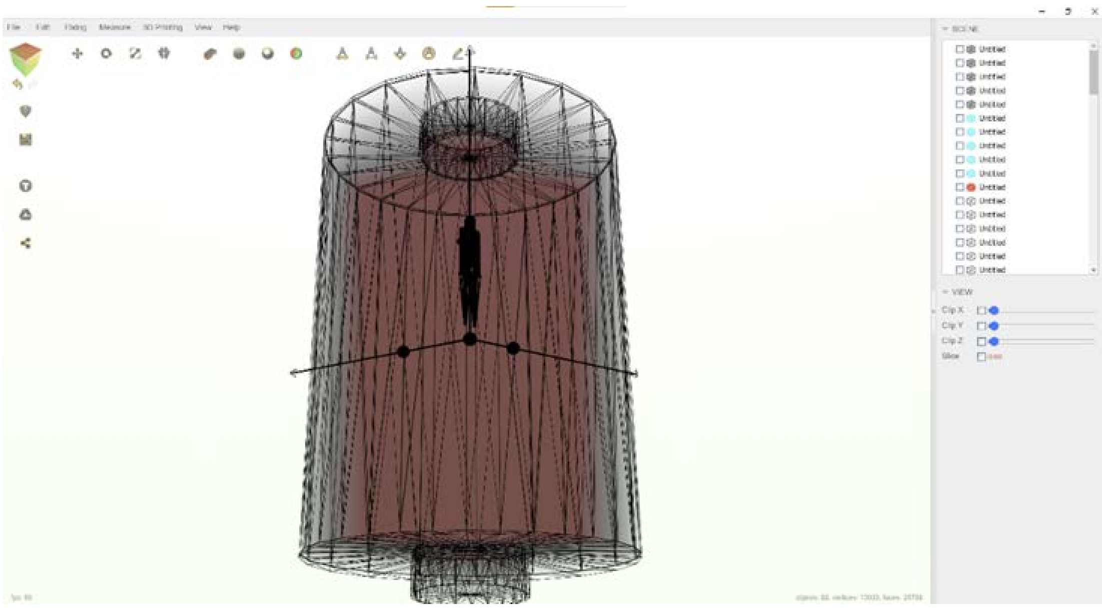

Figure 3 Sample simulation geometry setup exported in VRML format

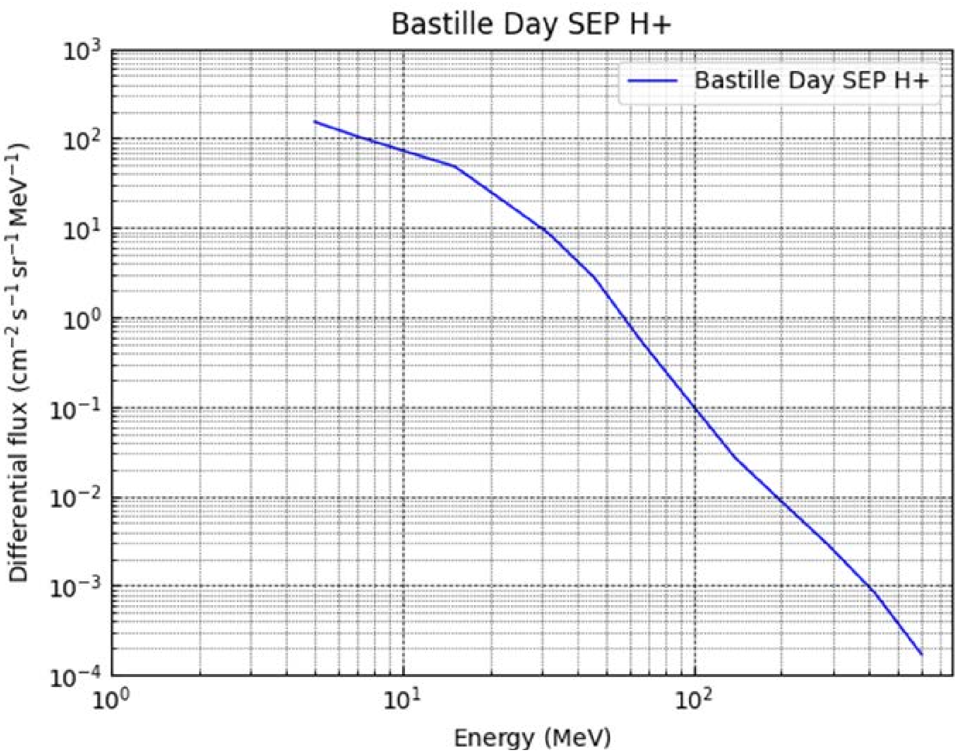

Figure 4 Sample SEP event fluence spectrum plot

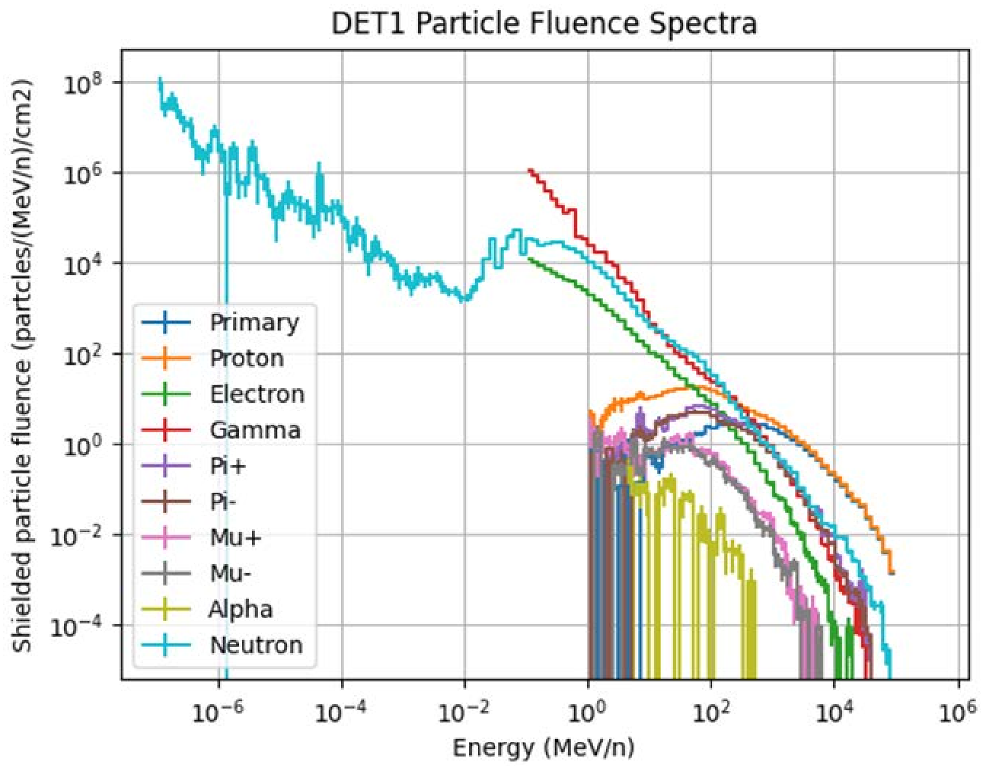

Figure 5 Sample plot of detector tallied fluence spectra from a GRAS simulation

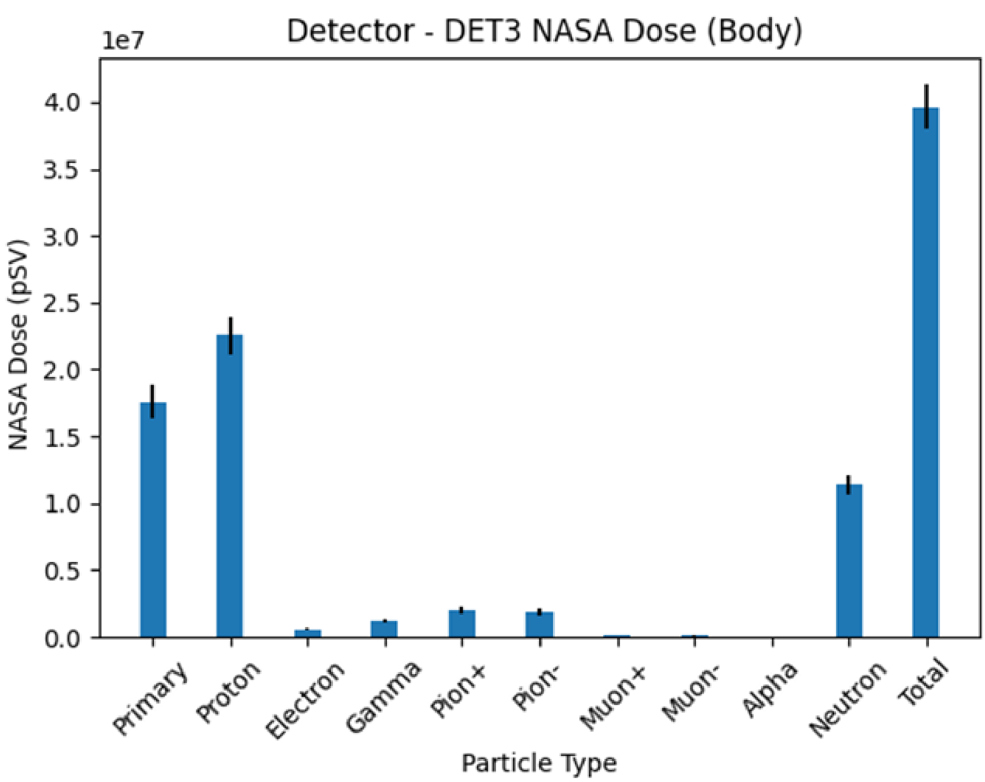

Figure 6 Sample bar plot of radiobiological doses from a GRAS simulation

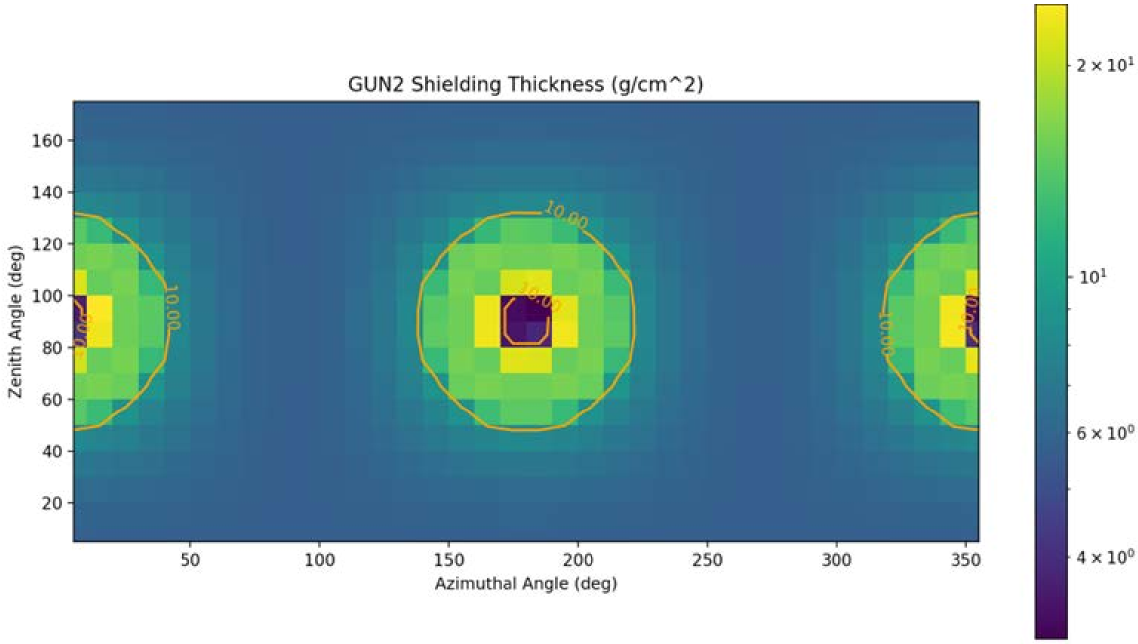

Figure 7 Sample 2D shielding map plot

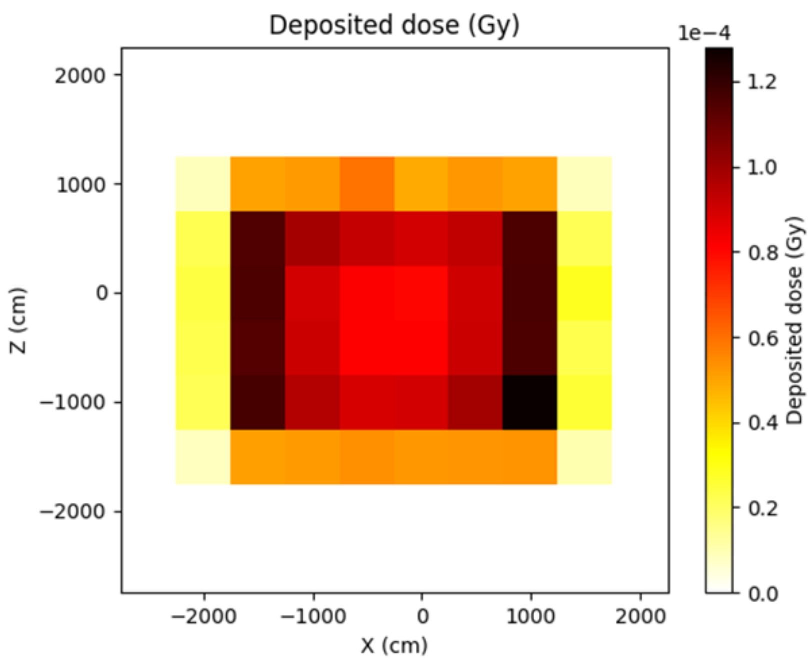

Figure 8 Sample 2D dose heat map plot

3.2 Simulation Models and Methods in HIERRAS

In this section, we briefly summarise the models, data sources and calculation approaches used in HIERRAS. Table 1 identifies the SPECTIRES Python-based as well as wrapped (Fortran/C++) models and also the NoM models available through SPECTIRES; here the following should be noted:

- SAPPHIRE and SAPPHIRE-HEX are the standard SEP environment prediction models available to the user. The user may also select from a range of time-dependent spectra available online through SPECTIRES from the HAPI server. Table 2 lists the historical ESP events defined in HIERRAS.
- The GCR and SAPPHIRE models in NoM can be run either with or without magnetic shielding, i.e., they include intrinsic geomagnetic shielding models.
- The Geant4-based models (MULASSIS, GRAS, SSAT and GRAPPA) are executed using the g4_space_apps docker implementation, installed directly as part of HIERRAS and also available on the NoM Server.
- The total ionising dose (TID), total non-ionising dose (TNID) and solar cell damage calculations are performed only for trajectory-integrated quantities. The SEE models allow both instantaneous rates (such as SEU rates) to be calculated as well as time-integrated quantities.
- The input file formats treated by the models are:
    - OEM for trajectory files.
    - Geant4 macro files for MULASSIS, GRAS, SSAT and GRAPPA, to bypass macro files generated by the Shielding Propagation and Radiation Effects Analysis module.
    - GDML geometry definitions, e.g., for 3D representations of the spacecraft or habitat.

  Otherwise, HIERRAS uses a native, comprehensive JSON file format for input and output of quantities such as trajectories, spectra, effects quantities and response functions generated by multiple GRAS and MULASSIS runs. Further information on this format is available in [RD 8].

Table 1 Standard models available in SPECTIRES including NoM models executed through SPECTIRES

Category	Subcategory	NoM Models Available Through SPECTIRES	SPECTIRES Intrinsic & Wrapped Models	Model References
Trajectory	Simple Propagator	NAIF SPICE-based (“GREET” traj. model)	NAIF SPICE-based	[RD 9]
	Detailed propagator	SAPRE	(None)	
Environment	GCR	ISO 15390 DLR CREME-96	ISO 15390 DLR	[RD 10] [RD 11] [RD 12]
	SEP (Model)	SAPPHIRE SAPPHIRE-HEX	SAPPHIRE SAPPHIRE-HEX	[RD 13] [RD 14]
	SEP (Past event data)	(None)	ODI HAPI	[RD 5]
	Trapped particles	AP8/AE8 IRENE	AP8/AE8 IRENE LARB	[RD 15] [RD 16] [RD 17] [RD 18] [RD 19]
Geomagnetic shielding		(Not used)	PyMSM	[RD 20]
Geant4-based		GRAS MULASSIS SSAT GRAPPA	GRAS MULASSIS SSAT GRAPPA	[RD 21] [RD 22] [RD 23] [RD 24]
TID		SHIELDOSE-2 SHIELDOSE-2Q	SHIELDOSE-2 SHIELDOSE-2Q	[RD 25] [RD 26]
TNID		SPENVIS NIEL tool	(None)	[RD 27]
Solar cell		EQFLUX	EQFLUX-like model	[RD 28]

Category	Subcategory	NoM Models Available Through SPECTIRES	SPECTIRES Intrinsic & Wrapped Models	Model References
SEE	Trajectory-average	BIRA long-term BIRA short-term	First order and IRPP models (nuclear and direct ionization)	[RD 29]
	Time-dependent	BIRA time-series		

Table 2 Default historic solar particle event data available in HIERRAS

Index	Designation	Start Datetime	End Datetime
1	Apr 1984	1984-04-25 00:00:00	1984-05-06 20:00:00
2	Oct 1989	1989-10-19 00:00:00	1989-11-10 00:00:00
3	Mar 1991	1991-03-23 00:00:00	1991-03-31 20:00:00
4	Bastille Day	2000-07-12 20:00:00	2000-07-24 00:00:00
5	Nov 2000	2000-11-08 23:00:00	2000-11-16 00:00:00
6	Guy Fawkes	2001-11-04 16:00:00	2001-11-13 00:00:00
7	Halloween	2003-10-26 17:00:00	2003-11-09 00:00:00
8	GLE 69	2005-01-15 08:00:00	2005-01-23 20:00:00
9	Dec 2006	2006-12-05 17:00:00	2006-12-17 00:00:00
10	Jan 2012	2012-01-20 11:00:00	2012-02-03 10:00:00

To determine biological doses, the Shielding Propagation and Radiation Effects module performs the following types of calculation:

- **Simulations without anthropomorphic phantoms** – Here, published fluence-to-dose conversion coefficients are used to determine dose from particle fluences calculated in HIERRAS using GRAS and MULASSIS:
  - *Organ dose equivalent and effective dose equivalent, H_E* – The absorbed dose per unit fluence, D_T/Φ, coefficients tabulated in ICRP-123 [RD 30] are integrated over the predicted particle spectra to determine the tissue-dependent absorbed doses, D_T, due to isotropically incident ions (Z=1 to 28) and their secondaries, i.e. neutrons and $\pi^{\pm}$ particles. These are combined with quality factors, Q_T, tabulated in ICRP-123, to convert D_T to dose equivalent in the organ/tissue and then multiplied with tissue weighting factors, w_T, published in ICRP-103 [RD 31] and summed over relevant organs/tissues.
  - *Effective dose, E* – To calculate this quantity, effective dose per unit fluence conversion coefficients tabulated in ICRP-116 [RD 32] are integrated over the predicted particle spectra. The coefficients treat protons, neutrons, photons, $e^{\pm}$, $\mu^{\pm}$, $\pi^{\pm}$, and α-particles, and in the HIERRAS implementation the calculation can be performed for isotropic, anteroposterior, or posteroanterior particle fields incident upon the body.

  NOTE: In this report, we define effective dose, *E*, strictly according to the ICRP definition, i.e. calculated using radiation weighting factors rather than quality factors, in order to differentiate it from the NASA effective dose.
  - *Gray-equivalent dose, G_T* – This dose quantity is determined from the values for absorbed dose, D_T, (calculated from D_T/Φ coefficients) and RBE coefficients for deterministic effects published in ICRP-92 [RD 33]. Gray-equivalent doses and corresponding exposure limits are organ/tissue specific.

- **Simulations using anthropomorphic phantoms** – In this case, the Shielding Propagation and Radiation Effects module uses the dose equivalent and equivalent dose ($H_{T,Q}$ and H_T) simulated by GRAS for each of the phantom's organs. These are used with ICRP-103 tissue weighting factors, w_T, to determine organ/tissue specific effective dose equivalent and effective dose, respectively. The GRAS-calculated absorbed doses in relevant phantom organs are also collected from the Monte Carlo simulation as functions of radiation type and weighted by ICRP-103 RBE values to calculate gray-equivalent doses.

The radiobiological dose quantities are calculated by the Shielding Propagation and Radiation Effects module for results from single GRAS or MULASSIS runs to multiple Monte Carlo runs used to build response function databases as a function of spectrum interval or (for MULASSIS) layer in a 1D shield. As part of the post-processing of the results from the Geant4 applications, the module also stores the processed data in JSON format to allow easier use by subsequent models.

3.3 The Graphical User Interface

The HIERRAS App can be accessed in two ways:

- By importing the App and related codes into a Python script to be run on a command line; this is the way how, for instance, the App test codes operate.
- By sending JSON requests to the Listener (using, for instance, cURL, or through the GUI) which in turn calls the App as in the first method.

The Graphical User Interface is implemented as a Python Flask application using a Bootstrap layout, as shown in the screen shot figures in the following sections. The landing (home) page is shown in Figure 9. The horizontal menu bar at the top of the page (and all GUI application pages) provides links to:

- Home: the home (landing) page (Figure 9),
- HIERRAS: the application pages (Section 3.3.1),
- Gallery: the gallery page,
- Documentation: the documentation pages (Section 3.3.2), which open in a new browser tab using the same Flask application as the application pages.

The menu also has a user login and registration menu on the right-hand side, and displays the current selected mission in the middle once a user is logged in.

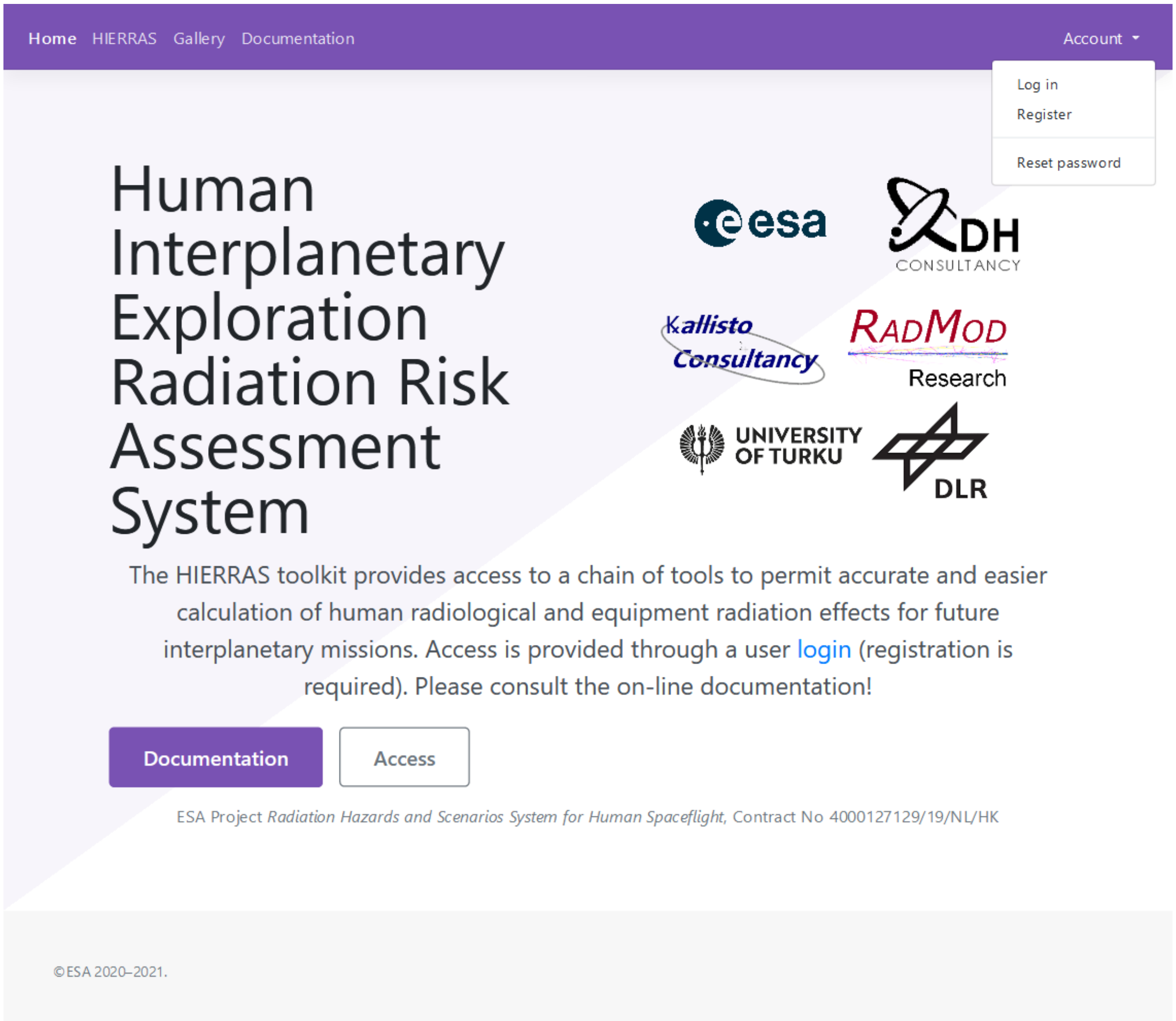

Figure 9 Landing page of the HIERRAS GUI

3.3.1 Application Web Pages

The left-hand menu on the application pages provides access to the various models and tools available on the application server: definition of missions and trajectories, environment models (SEP, GCR, …), radiation effects, geometry definition, etc (as an example, Figure 10 shows the input page for defining a location on the surface of Mars). The menu item for the active page is rendered with bold highlighting. Note that as long as no mission has been selected or created, only the Mission, Geometry and Results page links are shown in the left-hand menu. The icon in the top right-hand corner of the application pages provides a link to the relevant context sensitive documentation page.

When a direct run request is submitted, the response is displayed in a Bootstrap modal displaying a list of output files with download links, plus a zip archive download link. In case the request returned an error, the error code and message are displayed in the modal window. A success or failure message is also displayed in a green or red message bar at the top of the request page. For background process runs, a submit request message is displayed in the message bar with the process run id and no modal is created. Progress of background processes can be monitored on the `Results` page.

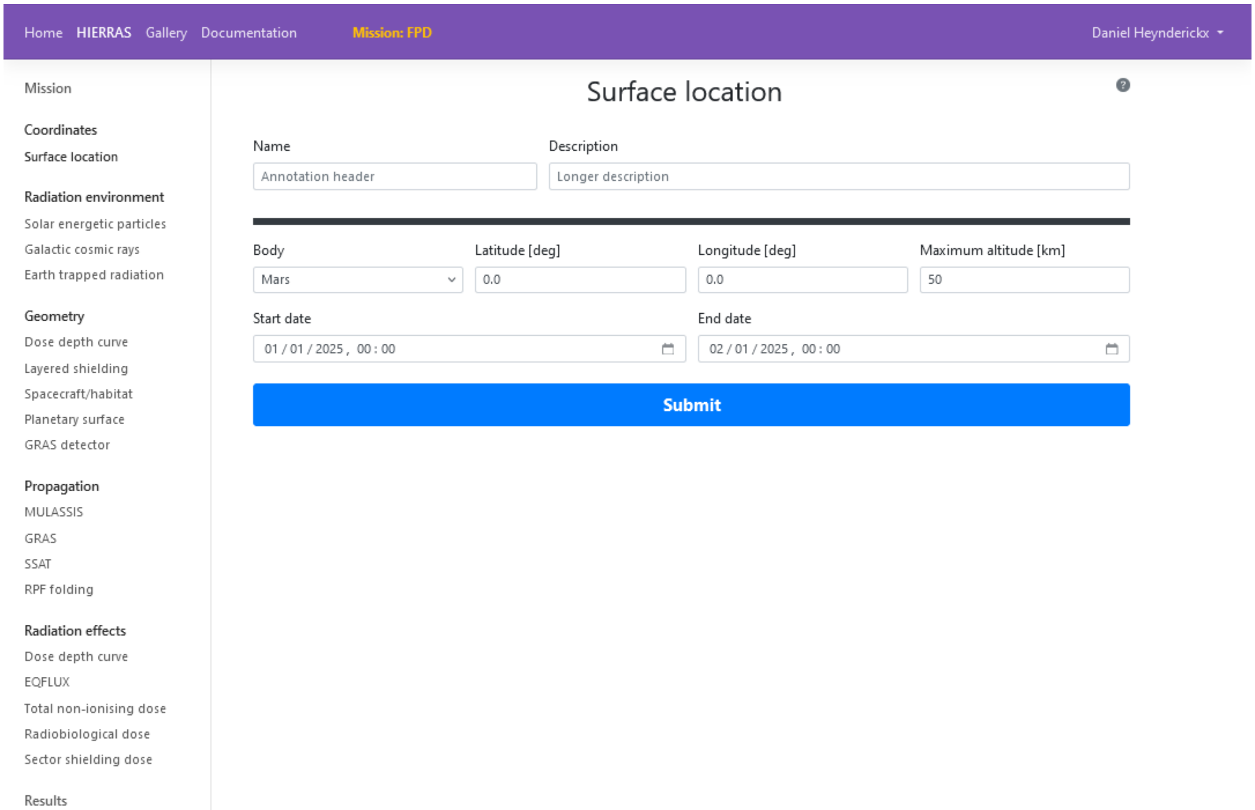

Figure 10 GUI input page for a planetary surface location

3.3.2 Documentation Web Pages

Although the documentation web pages are static pages (in the sense that they are read-only without user inputs except for clicking links), they are rendered by the same Flask service that also renders the application web pages. This allows for the implementation of context sensitive menus.

The entry page for the documentation package is shown in Figure 11. All documentation pages consist of:

- A left-hand menu allowing to navigate between pages; the current page is highlighted in bold face in the menu.
- A right-hand menu allowing to navigate between sections in the current page using anchors.
- The main body in the middle containing the page text.

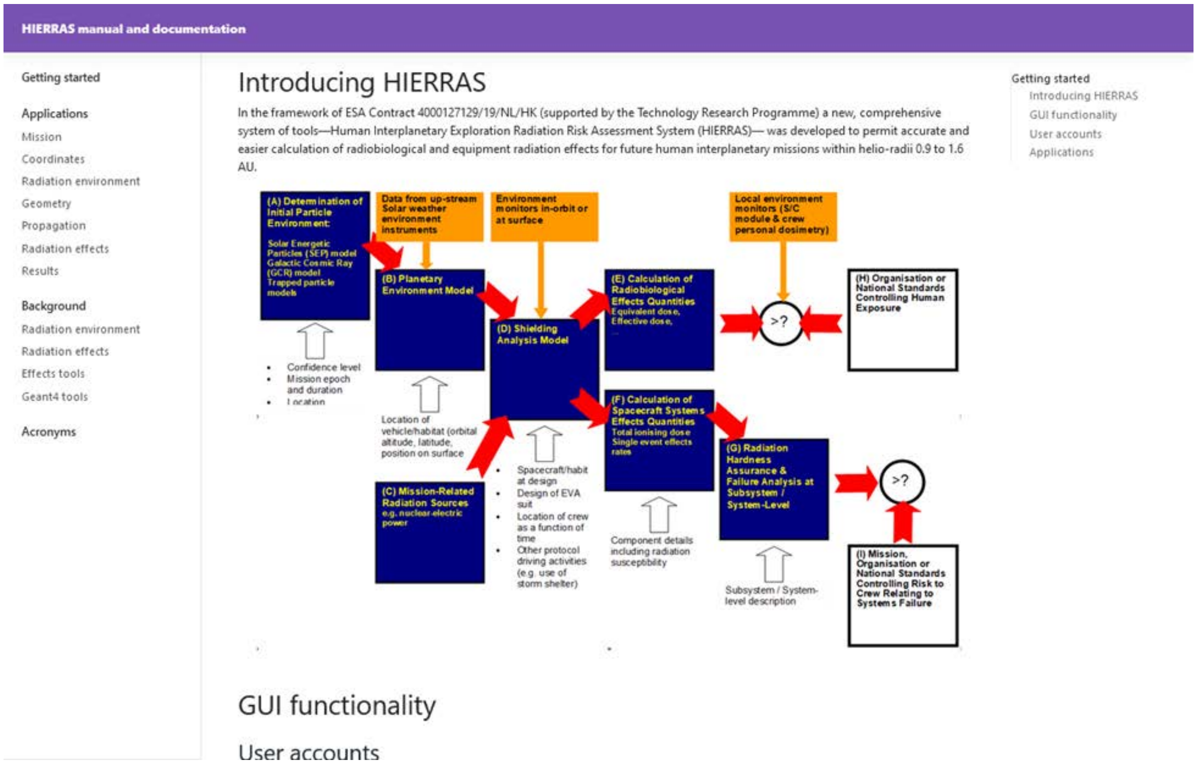

Figure 11 Entry page for the HIERRAS GUI documentation

4 Software Verification and Validation

In general, evaluation of a software system involves a series of verification and validation activities. Validation is a process to confirm the software system has been implemented correctly and completely. Verification is a process to confirm that adequate specifications and inputs exist for any activity, and that the outputs of the activities are correct and consistent with the specifications and inputs.

The software verification procedures are outlined in Section 4.1, while the system validation runs and results are described in Section 4.2. A more detailed description can be found in [RD 34].

4.1 Software Verification

Depending on the specific requirement to be tested, one or both of the following testing methods have been used:

- **Testing**: execution of test cases to demonstrate that the software under test fulfils the established requirements.
- **Review**: review of source code and documentation. This method consists of checking of the software code, design documentation and user manuals, as well as reviewing of software aspects not related to a working process, e.g., contents of the GUI menus or of specific GUI windows.

Testing is the primary method for HIERRAS. The review method was used only when the specific requirement or feature could not be tested.

The verification tests are divided into the following categories:

1. **Building and Installation testing**: specific tests to evaluate the process of installing the simulation framework, including all the third-party dependences and the building/compiling of code. The tested components are the front user interface (GUI) and the application backend (App).
2. **Unit Testing**: to test the low-level units of code for newly developed pieces of software. Unit tests were created at each module/submodule level. Unit testing is carried out as part of regular git merge request, in the GitLab CI/CD pipeline.
3. **System Verification Testing**: to verify the high-level functionality of the HIERRAS framework against the system and user requirements. The key components to be tested are the App, the Listener and the GUI. Tests are run in an automated fashion using the Python `pytest` module, which generates very advanced test reports in HTML format. `pytest` also performs regression tests with the results of the `pytest` execution against the reference output data stored in the system test folder. In addition, a comprehensive set of test scripts are provided with the App distribution. These command line scripts load the required App components and directly interact with the App routines, i.e. without using the Listener. Finally, a set of administrator test cases is provided to test the system administrator functions.

4.2 Software Validation

The software validation consists of two parts:

- Comparison of specific outputs of a number of HIERRAS runs to experimental data (Section 4.2.1).
- Comparisons of HIERRAS run outputs to ROSSINI validation results (Section 4.2.2).

4.2.1 Comparison of HIERRAS Simulation Results to Experimental Data

The validation of the system was performed using a variety of experimental data taken at different locations and representing different scenarios in spaceflight (LEO, Moon, Mars) and different sources of cosmic radiation (GCR, SAA, SPE). Table 3 gives an overview of the experimental data that were used for the validation including the data source, data format, cosmic ray source and the time and endpoint that was modelled. For DOSIS/DOSIS3D and CRaTER an extended time period is available. For the validation, suitable time periods representing solar minimum and maximum conditions for GCR and SPE conditions have been identified and modelled. Dose rates averaged over the ISS orbit were modelled and compared with the dose rate measured in the DOSIS/DOSIS3D project. The MATROSHKA data is based on measurements with passive detectors which do not allow the separation of the contributions from GCR and SAA. The system was then used to model the combination of the two sources for the validation.

Table 3 Summary of experimental data used in the software validation

Experiment	Scenario	Period	Source	Type of data/endpoint	Output	Reference
MATROSHKA	LEO/ISS	26 Feb 2004 – 18 Aug 2005	GCR+SAA	Organ absorbed dose rate	Dose rate	[RD 35] https://www.fp7-hamlet.eu/
MSL-RAD	Mars surface	Aug 2012 – Jan 2013; 15 Nov 2015 – 15 Jan 2016	GCR	Dose rate in silicon, dose equivalent rate; H-Fe spectra, E<100-300 MeV/n;	Dose and dose equivalent rate; particle intensity vs energy	[RD 36] [RD 37] [RD 38] [RD 39]
CRaTER	Moon surface	Solar max / solar min conditions	GCR/SPE	Dose rate in silicon	Dose rate vs time	[RD 40] http://crater-web.sr.unh.edu/
DOSIS/DOSIS3D	LEO/ISS	Solar max / solar min conditions	GCR/SAA	Dose rate in silicon	Dose rate vs time	[RD 41] [RD 42] [RD 43]

GLE spectra	Primary particle spectra	GLE 69: 20 Jan 2005 07:00 – 12:00	SPE/GLE	30 min averages of energy spectra	Intensity vs energy	[RD 44]

4.2.1.1 Validation Scenarios and Strategy

The validation scenarios listed in Table 4 were performed using the following workflow (Figure 12):

1. Validation scenarios were derived from experimental data (Table 3).
2. For each validation scenario one or several macro files were created which are necessary to run HIERRAS.
3. Processing scripts were created to automatically run HIERRAS using the macro files from 2.
4. ROOT scripts for the comparison with experimental data were created based on the HIERRAS output format.
5. Based on the HIERRAS output and the comparison with experimental data it was decided if changes to the system were necessary and feasible.

Table 4 Specification of software validation scenarios using experimental data. W refers to the single model parameter in the DLR GCR model.

Description	Quantity	Period	Experiment
GCR solar min (W=0) Lunar surface	Dose rate in Si	2009-12-01 – 2010-01-01	CRaTER
GCR solar min (W=0) + trapped particles ISS, COLUMBUS	Dose rate in Si	2009-12-01 – 2010-01-01	DOSIS
GCR solar max (W=80.8) BR2478, lunar surface	Dose rate in Si	2015-03-19 – 2015-04-15	CRaTER
GCR solar max (W=80.8) + trapped particles BR2478, ISS, COLUMBUS	Dose rate in Si	2015-03-19 – 2015-04-15	DOSIS3D

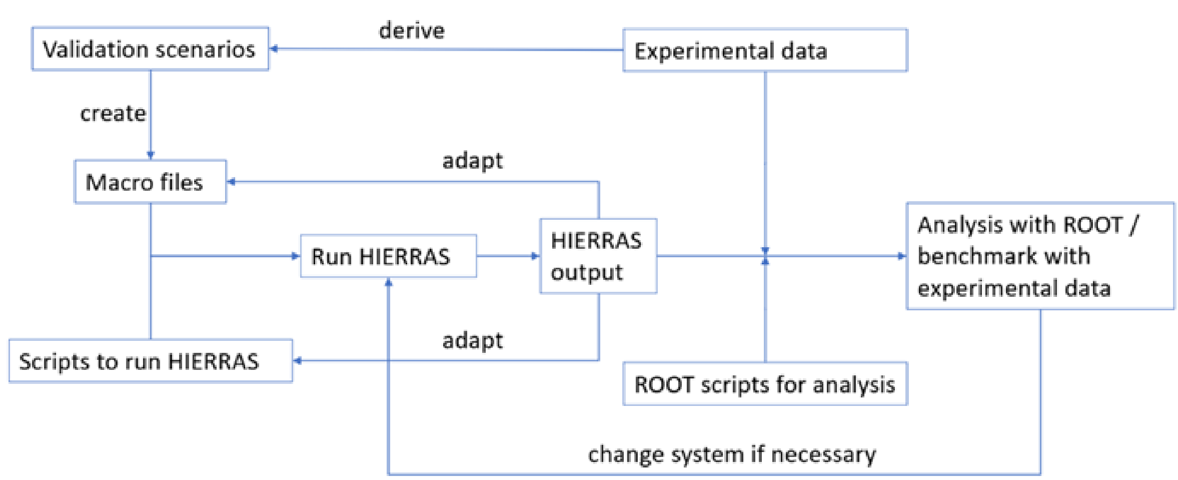

Figure 12 Validation workflow

4.2.1.2 Validation Reports

Detailed results for the four validation scenarios can be found in [RD 34]. Here, the MATROSHKA case study is discussed as an example.

The MATROSHKA scenario simulates the radiation exposure during an extravehicular activity on the ISS. The simulation of the scenario is a combination of elements of the DOSIS/DOSIS3D and the HIERRAS-ROSSINI (see Section 4.2.2) inter-comparison with a different detector position outside the cylindrical shielding. The calculation was performed as follows:

- Creation of a trajectory segment around the Earth at an altitude of 370 km above the surface, which was the approximate altitude of ISS in 2004, and a 51.6° inclination.
- Creation of the planet shadowing response and magnetic shielding function for the trajectory.
- Creation of the magnetically shielded primary GCR spectrum for primary hydrogen and helium using the DLR model and the AP-8/MIN and MAX models for trapped protons.
- Loading the GDML file and creating the cylindrical shielding geometry identical to the HIERRAS-ROSSINI inter-comparison (Section 4.2.2 and Figure 14).
- Running GRAS to calculate the particle spectra on a sphere detector with radius 30 cm, positioned outside the cylindrical shielding and surrounded by a spherical carbon shielding with a thickness of 2.3 mm and a radius of 45 cm.
- Running the BioDose module in HIERRAS calculating the organ doses and whole-body dose from the particle spectra of the previous step.

Notes: The trajectory duration for the creation of the GCR spectra was set to one day (2004-02-26); the trajectory duration was set to ten days for trapped protons for a better sampling of the trapped proton spectra inside the SAA; the organ dose from the BioDose module is the mission integral dose, which means that the result needs to be normalized to the number of days to obtain the dose rate (per day). The carbon shielding was used to simulate the carbon fiber container surrounding the phantom in the MATROSHKA experiment [RD 35]. 100 million primary particles were simulated for the trapped proton environment using AP-8/MIN and MAX, respectively. 10 million primary particles were simulated for the GCR primary hydrogen and helium, respectively.

Table 5, Table 6 and Figure 13 summarise the results of the HIERRAS simulations for the calculated dose equivalent rates from GCR hydrogen and helium and trapped protons using the BioDose module (ICRP conversion coefficients) for the whole-body dose (effective dose equivalent), red bone marrow, skin and eye lens. In Figure 13b and Table 6 the GCR dose rates are summed up together with the results of either AP-8/MIN or AP-8/MAX and compared to the experimental data [RD 35]. While the GCR model is expected to provide estimates for the defined mission time, the AP-8 model only provides solar minimum and maximum extreme values. As a consequence, it is expected that a realistic value for a given mission time lies between these extremes. The exposure during the MATROSHKA project was in 2004, after but still relatively close to the solar maximum of solar cycle 23. Figure 13b shows that the experimental results fall between the HIERRAS extreme values for the sum of GCR and AP-8 data, which is the expected behaviour. Additionally, the HIERRAS data is self-consistent, showing a steep drop in the dose rate from trapped protons for the red bone marrow, which is caused by the self-shielding of the body, and the whole-body dose, which is dominated by the inner organs with high tissue weighting factors.

Table 5 HIERRAS effective dose equivalent rates (HE) and dose equivalent rates (HT,Q) for the MATROSHKA setup per particle type

Organ	GCR H (µSv/d)	GCR He (µSv/d)	AP8 min (µSv/d)	AP8 max (µSv/d)
Body, H_E	140 ± 28	67 ± 2	618 ± 30	321 ± 14
Red bone marrow, $H_{T,Q}$	137 ± 29	67 ± 2	487 ± 22	277 ±12
Skin, $H_{T,Q}$	319 ± 34	136 ± 2	3641 ± 225	914 ± 68
Eye lens, $H_{T,Q}$	143 ± 23	65 ± 1	1329 ± 70	571 ± 31

Table 6 Sum of HIERRAS effective dose equivalent rates (H_E) and dose equivalent rates ($H_{T,Q}$) for the MATROSHKA setup and experimental dose rates from [RD 35]

Organ	GCR H+He, AP-8/MIN (µSv/d)	GCR H+He, AP-8/MAX (µSv/d)	Reitz et al., 2009
Body, H_E	826 ± 41	528 ± 32	
Red bone marrow, $H_{T,Q}$	691 ± 36	481 ± 31	
Skin, $H_{T,Q}$	4096 ± 228	1369 ± 76	1642 ± 131
Eye lens, $H_{T,Q}$	1538 ± 74	779 ± 38	966 ± 77

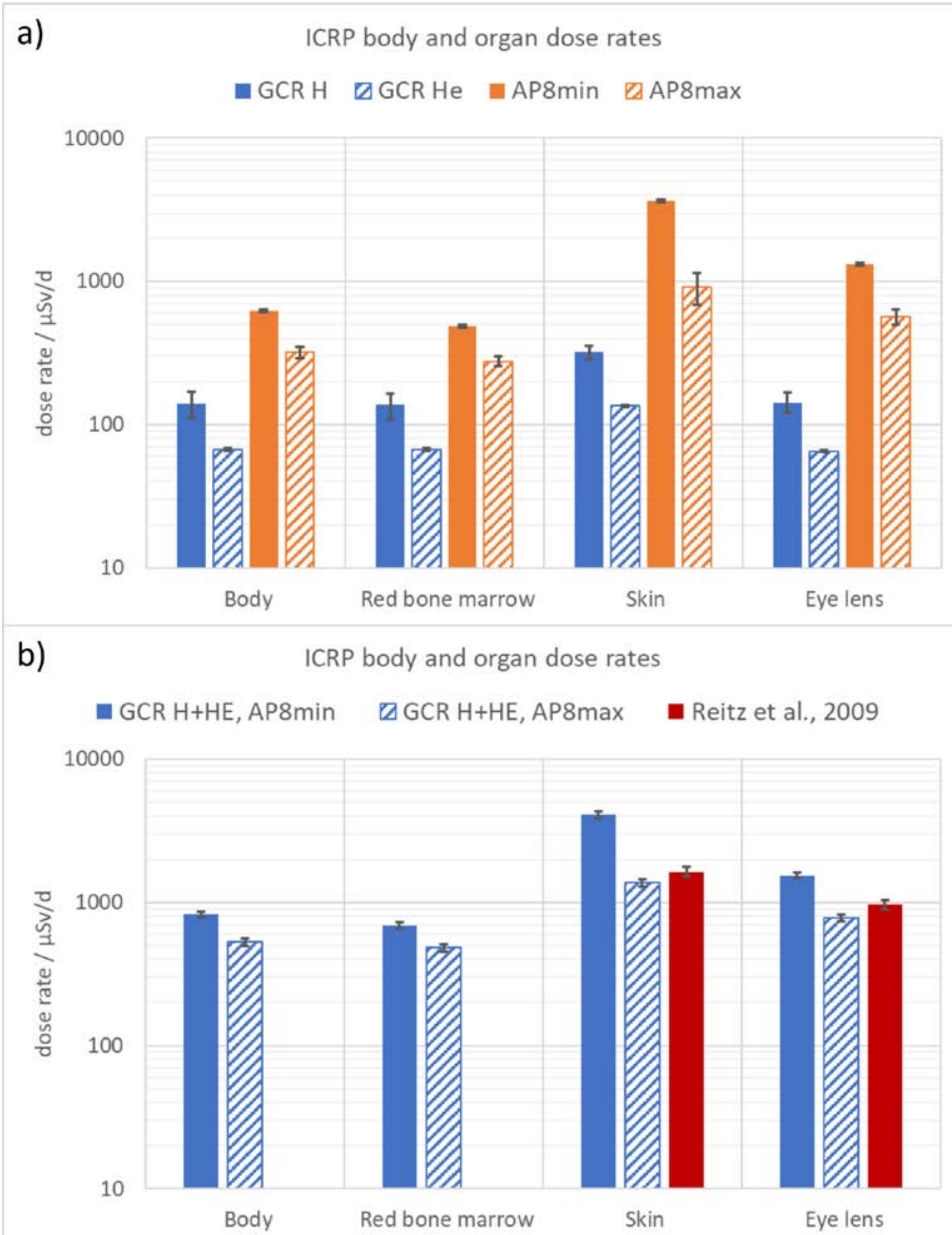

Figure 13 HIERRAS effective dose equivalent rates (H_E) and dose equivalent rates ($H_{T,Q}$) (per particle type and total dose). Total skin and eye lens dose are compared to the organ dose rates published in [RD 35].

4.2.2 Intercomparison of HIERRAS-ROSSINI Simulations

4.2.2.1 Specification

The following radiation environment spectra (used in both simulation frameworks) were generated using the DLR GCR and SAPPHIRE SEP models:

- GCR: H to Ni
- SEP: SAPPHIRE spectra for H and He, for the following conditions:

- o 1 year cumulative fluence at 95% confidence level in solar minimum
- o 1 in 1000-year event total fluence. It should be assumed that this fluence is delivered over one week.

Three geometry models, based on simple cylindrical models of the spacecraft, were provided by Thales Alenia Space (TAS), with a 1 m radius spherical detector at their centres:

- Cylindrical aluminium shielding with 10 cm walls (see Figure 14).
- Cylindrical aluminium shielding with 5 cm walls.
- Cylindrical aluminium shielding with 1.5 cm walls.

For the calculation of the dose and particle flux, the geometry with 10 cm Al walls was used.

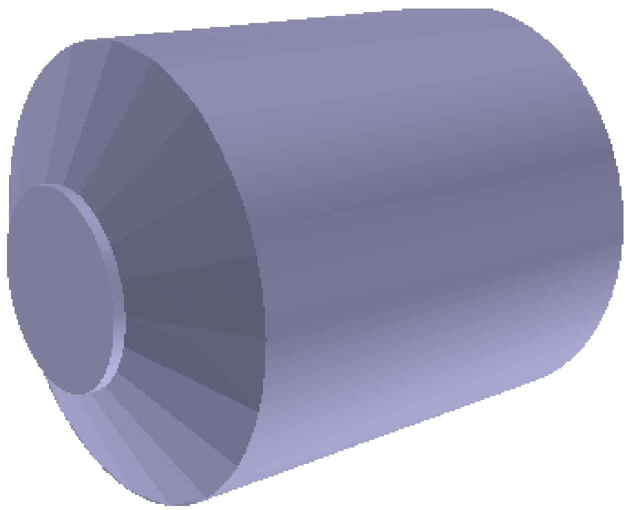

Figure 14 Visualisation of the cylindrical 10 cm thick Al geometry used for the HIERRAS-ROSSINI intercomparison

Particle fluxes entering the spherical detector centred in the geometry were tallied by both simulation frameworks. The following particles were tallied: proton, neutron, e-, e+, pi+, pi-, alpha, Li-7, Be-9, B-11, C-12, N-14, O-16, F-19, Ne-20, Na-23, Mg-24, Al-27, Si-28, P-31, S-32, Cl-35, Ar-40, K-39, Ca-40, Sc-45, Ti-48, V-51, Cr-52, Mn-55, Fe-56, Co-59, Ni-59. Doses were calculated based on particle-by-particle conversion. Within HIERRAS only, an additional comparison was made with dose derived from binned fluence. Effective dose equivalent was calculated using the ICRP-123 fluence to dose conversion coefficients for isotropic radiation.

4.2.2.2 HIERRAS Simulations and Results

The results for the HIERRAS-ROSSINI inter-comparison have been obtained using a number of Python scripts to run the HIERRAS App. The following steps are performed within the scripts:

- Definition of an interplanetary near-Earth location for the date 2010-01-01.
- Creation of the GCR primary spectra based on the ISO model.
- Creation of the 1 year cumulative event fluence and the 1 in 1,000 year event fluence with SAPPHIRE.
- Loading the GDML file and creating the cylindrical shielding geometry (Figure 14).
- Running GRAS to calculate the particle spectra on a detector sphere with radius 1 m and positioned at the centre of the cylindrical shielding.
- Running the BioDose module in HIERRAS to calculate the organ doses and whole-body dose from the particle spectra of the previous steps.

4.2.2.2.1 SAPPHIRE 1 Year Cumulative Fluence

Figure 15 shows the particle spectra inside the cylindrical shielding calculated with HIERRAS and ROSSINI for protons (left hand panel) and neutrons (right hand panel). The shielded proton spectra are additionally compared to the primary proton event fluence spectrum. The particle spectra agree in shape but differ in their absolute values, which is likely related to a missing normalization factor. The resulting total effective dose equivalent values agree well: 4.6±0.8 cSv from HIERRAS and 3.18±0.01 cSv from ROSSINI. The contributions of different particle types to the effective dose equivalent calculated by HIERRAS are shown in Figure 16.

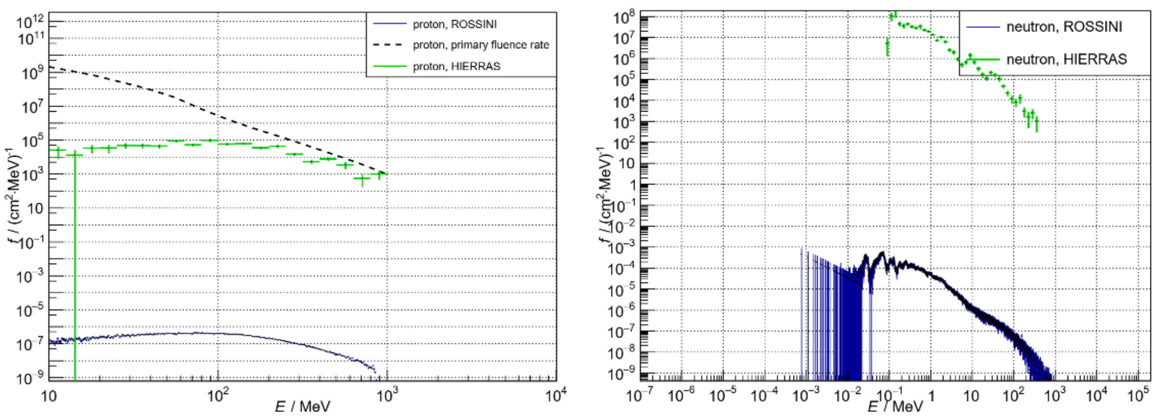

Figure 15: Proton (left hand panel) and neutron (right hand panel) spectra inside the cylindrical shielding from HIERRAS, ROSSINI and the primary proton spectra; right: neutron spectra from HIERRAS and ROSSINI.

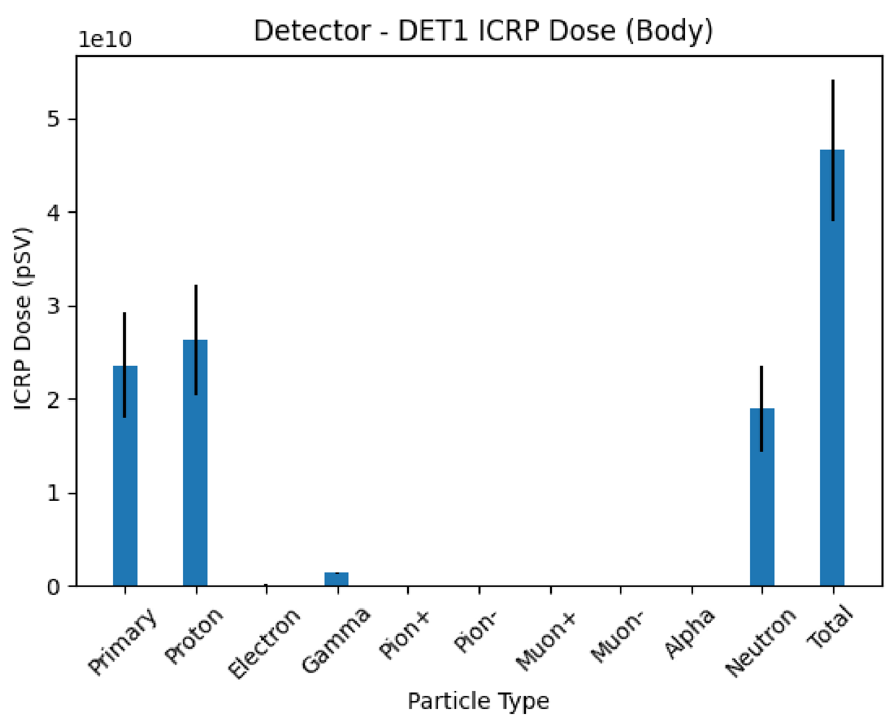

Figure 16 HIERRAS effective dose equivalents for the SAPPHIRE 1 year cumulative fluence

4.2.2.2.2 Galactic Cosmic Rays

Figure 17 shows example particle spectra inside the cylindrical shielding calculated with HIERRAS and ROSSINI from primary GCR protons: protons (top left), electrons (top right), neutrons (bottom left) and γ rays (bottom right). The primary GCR proton spectrum is also shown in the top left-hand panel for reference. The comparison shows identical shapes of the particle spectra for HIERRAS and ROSSINI. The ROSSINI particle flux tends to be lower than the HIERRAS results, which is unexpected due to the fact that the HIERRAS results were obtained from primary GCR protons only while the ROSSINI results contain contributions from heavier primary GCR ions. The proton flux spectra from HIERRAS and ROSSINI have an identical shape compared with the primary proton spectrum. The proton spectra at high energies above several GeV are about 30% to 50% lower than the primary GCR spectrum, which is reasonable and can be attributed to the shielding effect of primary particles. At low energies the proton spectra inside the shielding exceed the primary GCR proton spectra due to the production of secondary protons from interactions with the shielding.

The total effective dose equivalent for the GCR flux is 24.2±0.3 cSv/yr from HIERRAS and 50.8±0.6 cSv/yr from ROSSINI. The ROSSINI value is about a factor of two greater than the HIERRAS value. This is a reasonable result, considering the fact that only primary GCR protons have been considered in the HIERRAS calculation. It is, however, surprising, looking at the comparison of the particle spectra at the detector (Figure 17) in which the ROSSINI spectra seem to be consistently lower than the HIERRAS results. Possible explanations could be a smaller particle energy range considered in HIERRAS compared to ROSSINI or discrepancies in the number of particle types considered in the calculation of the dose. The contributions of different particle types to the effective dose equivalent calculated by HIERRAS are shown in Figure 18.

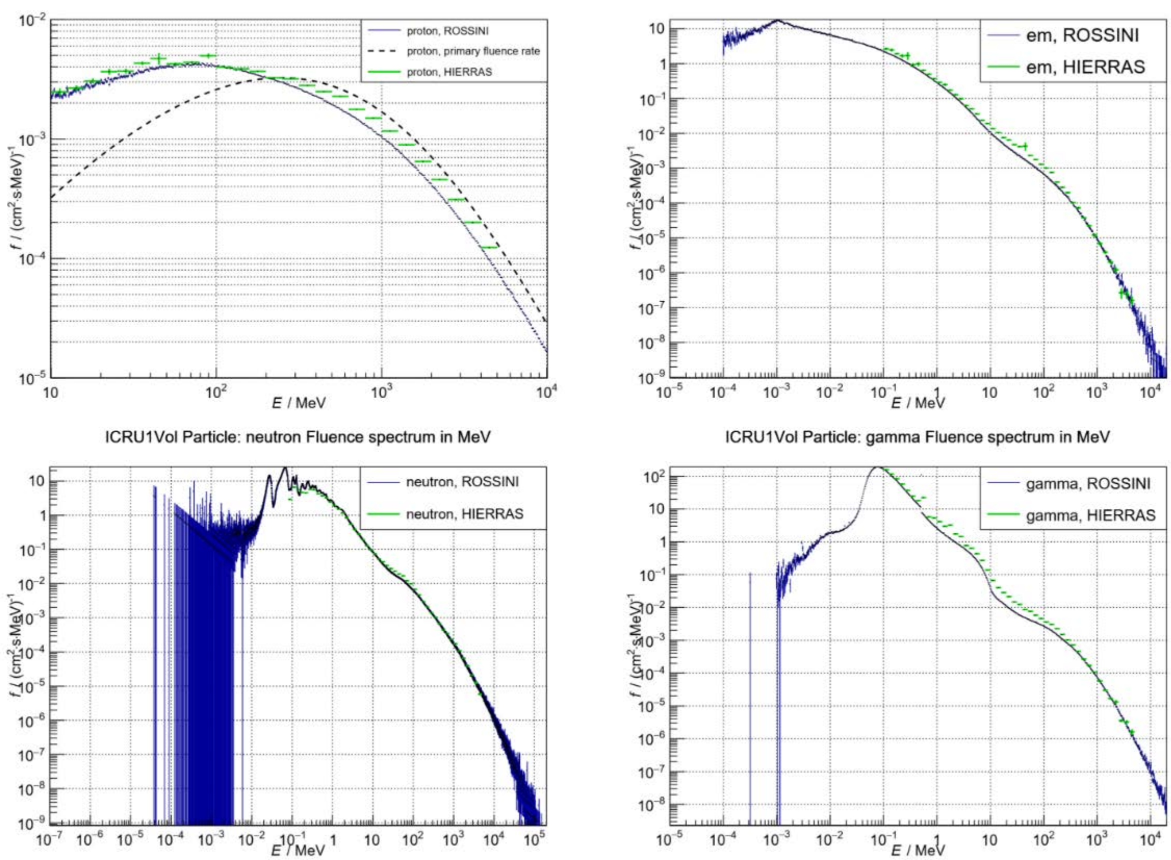

Figure 17 Particle spectra spectra inside the cylindrical shielding from HIERRAS and ROSSINI for primary GCR protons. Top left: protons, top right: electrons, bottom left: neutrons, bottom right: γ rays. The primary GCR proton spectrum is also shown in the top left-hand panel.

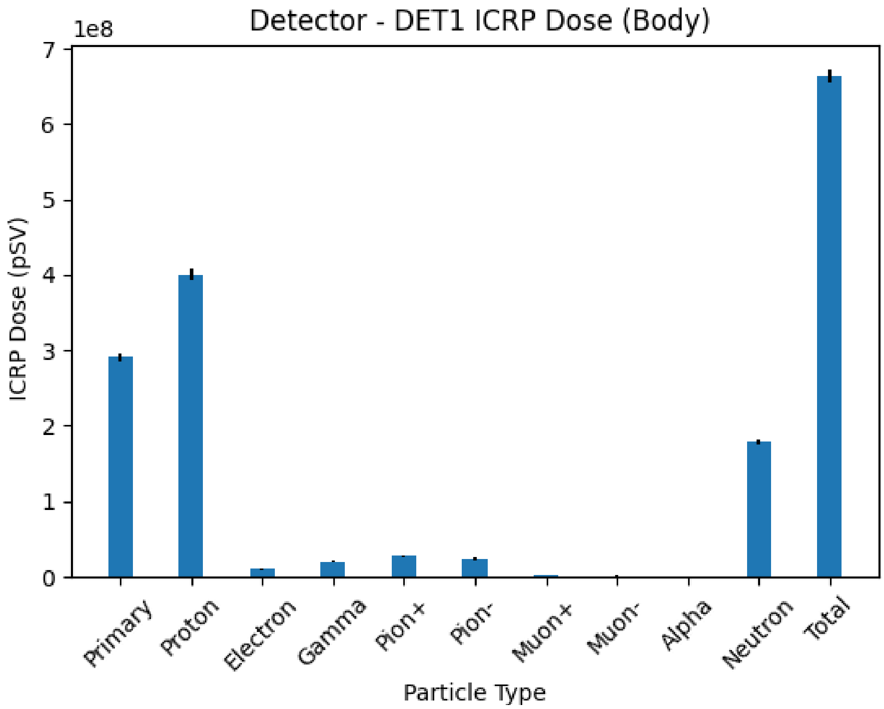

Figure 18 HIERRAS effective dose equivalents for primary GCR protons

5 UPDATE OF THE SAPPHIRE SEP MODEL

In the course of the SEPEM project [RD 45] and subsequent ESHIEM project [RD 46], a H (and He) reference dataset (RDS v2) was built using GOES energetic H data (EPS and EPEAD channels P2–P7) in the time range 1974–2017 [RD 47]. Using this dataset and the statistical methods developed and implemented during SEPEM, a new SEP H model was built, referred to as SAPPHIRE [RD 13] [RD 14].

One of the tasks of the HIERRAS project was to extend the H RDS v2 dataset to higher energies using GOES/HEPAD data, and to update the SAPPHIRE model accordingly. The HEPAD data for channels P9 and P10 were cleaned and re-calibrated and were added to the EPS/EPEAD P2–P7 channels; after performing a background identification and subtraction, the spectrum time series were interpolated to the SEPEM reference channels (extended with three high energy channels, F12–F14) to form the RDS v3 dataset (the complete channel set is listed in Table 7). The new RDS was used to update the high energy portion of the SAPPHIRE model and produce a new SAPPHIRE-HEX model. More details can be found in [RD 48].

Figure 19 shows a comparison of the output spectra of the new model and the original SAPPHIRE for cumulative fluence at solar maximum. The mission lengths and confidences of the example spectra are listed in the figure. The differences are quite small, except for the highest energies, which is expected.

Table 7 SEPEM reference energy channels (MeV)

Channel	E_l	E_u	E_c
F1	5.000	7.231	6.013
F2	7.231	10.46	8.695
F3	10.46	15.12	12.57
F4	15.12	21.87	18.18
F5	21.87	31.62	26.30
F6	31.62	45.73	38.03
F7	45.73	66.13	54.99
F8	66.13	95.64	79.53
F9	95.64	138.3	115.0
F10	138.3	200.0	166.3
F11	200.0	289.2	240.5
F12	289.2	418.3	347.8
F13	418.3	604.9	503.0
F14	604.9	874.7	727.4

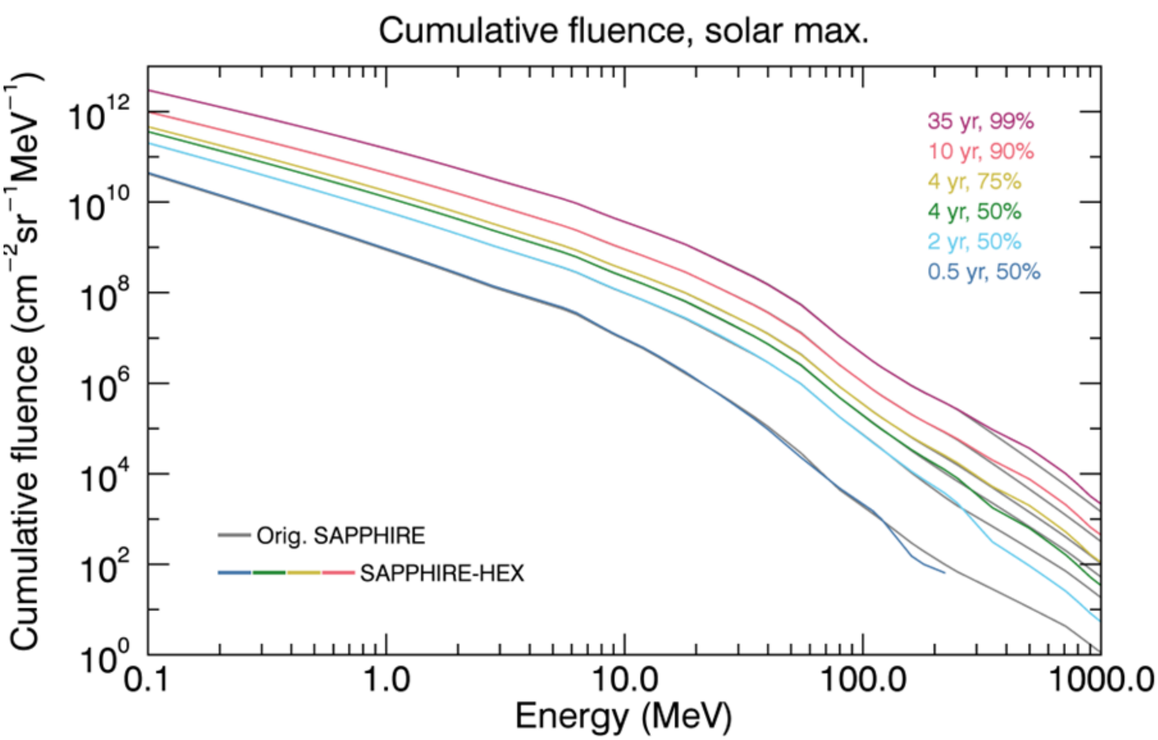

Figure 19 Example cumulative fluence spectra (coloured lines) from the new model outputs, compared to the original SAPPHIRE spectra (grey lines)

6 RECOMMENDATIONS FOR FUTURE WORK

Further analysis using HIERRAS is recommended to better understand the speed-versus-accuracy trade-off between full 3D GRAS simulations for a complete spectrum and approximate methods used at different levels of fidelity, such as energy-tabulated response functions or SSAT-integrated results from MULASSIS dose-versus depth calculations. The efficiency of some of the more intensive calculations should be reviewed with the view of potentially undertaking these using a compiled language (Fortran, C or C++) to speed up these parts of the process. HIERRAS as well as other systems of tools (such as SPENVIS) would benefit significantly from an implementation of a multithreaded version of MULASSIS.

It is further recommended that comparisons with alternative simulation tool results (such as from FLUKA, eMEREM, OLTARIS/HZETRN) be performed for further validation. In addition, more instrument data is available that could be potentially useful in further validation studies in the future.

Currently, only one phantom model is supported in HIERRAS; in the field of human radiation medicine, significantly more advanced phantoms are recommended and are being used. Additional models can be added to HIERRAS by providing GDML files and producing JSON configuration files. Also, currently the Agency does not have a geometry model for EVA suits which can be used with its radiation modelling software, such as GRAS.

The GRAPPA software should be extended to treat surface topography to support human spacecraft and uncrewed missions, particularly those which use remote sensing of high energy particles for surface assaying.

H^2UGOS is designed, in so far as possible, to be an independent service module for HIERRAS, i.e., it does not "have knowledge" of the top-level application it is providing this service to. Therefore, H^2UGOS potentially has much greater use across systems of models, including for example CIRSOS. The HIERRAS Background Processor also potentially has wider use, particularly to perform groups of runs (such as dose-versus-depth shielding calculations using MULASSIS) and allow balanced allocation of computer resources across the user groups. Indeed, its use is already being considered for NoM.

The SEPEM RDS v3 has been a successful application of GOES/HEPAD data to extend the energy range beyond 300 MeV. For low flux events, comparison with SOHO/ERNE observations highlights the problems of measuring the lowest SEP fluxes with GOES instruments. For low flux events, SOHO/ERNE could be used as one source of re-calibration data in combination with the Wind (1994–present) and ACE (1997–present) missions, from the 3DP and EPAM instruments, respectively. However, there are known contamination issues with these instruments, which should be properly treated before using the data in modelling. Using SOHO/ERNE He data would allow assessing the spectrum at higher energies in events that in GOES observations are masked by background.

The remaining main issues in SAPPHIRE in modelling methodology (besides data issues) are in the handling of anomalous events that skew the flux or fluence distributions somehow and make in particular long mission durations unstable in the model outcome. The issue is twofold, related to very impulsive GLE events (Jan 2005) and very strong ESP events (Mar 1991). The handling of ESP events in a databased way would most likely be easier.