# Open and new requirements - Space science and engineering

29th Geant4 Collaboration Meeting
Aci Castello – Catania

Giovanni Santin

ESA ESTEC

7/10/2024

# Outline

- Physics
  - EM accuracy and validation
  - new Geant4-DNA features in gold
  - Hadronics
  - Neutrons comparisons and validation
- Geometry / visualization
- Primary generator
- Installation / docker

Collection of requirements either via direct communications, or extracted from publications or discussions at space-related venues (conferences, workshops)

Procedure for formal recording & follow up of requirements from space domain just started

Items not properly tracked

# Accuracy / validation of EM in thin layers

**Protons and electrons in thin layers: Simulation for ATHENA of the soft proton flares detected by XMM-Newton**

Accuracy in transport through very thin layers, such as those used in optical filters and coatings for space applications (~10nm) **degrades at low energies (<100 keV)** and lacks dedicated **validation** campaigns. For instance, the precision of the Bethe-Bloch formula, which describes continuous energy loss due to ionization, degrades below 2 MeV. Geant4 interpolates the NIST proton stopping power (Ivanchenko et al. 2017), which below 500 keV is based on fits from experimental data from the late 1970s.

There is an indication of a systematic overestimation of the predicted energy loss through the optical filters compared to observed data. Forthcoming paper on the XMM-Newton proton response matrix (Fioretti et al.), accepted for publication.

EM Standard (SS) reference physics list, without dedicated studies on the impact of different physics models or lists. To test this, we would **require laboratory measurements under the same conditions, which are currently lacking**.

**Source:**
**Simone Lotti @inaf**
**Valentina Fioretti @inaf**
**Paolo Dondero @swhard**

**Direct exposure of materials to outer space environment**

Significant differences in **dose-depth profile** in thin shielding for electrons and protons among MC tools (and even among Geant4-based applications!)

e- 5 keV (range 400nm) → 10 MeV     proton 10 keV (range 200nm) → 100 MeV

Req: Investigate EM models at <100keV, especially in thin layers

Req: Include electron and proton dose-depth profiles in Geant4 validation suite

**Source: Community study led by I.Jun @NASA JPL**

# Accuracy / validation e- and gamma secondary production

**ESA Athena X-ray telescope development**

Variations with Geant4 version and the physics models of **secondary particle (mainly electrons and gamma) emission spectra and angular distributions**, particularly in the low energy range (<100 keV). Significant increase from 10.4 to 11.2 (increase dependent on the geometry model). Challenge: lack of experimental data for validating the parameters across materials, thicknesses, and incident energies.

Req: Include secondary particle emission (<100 keV) in Geant4 validation suite

**Source:**
**Simone Lotti et al @inaf**
**Valentina Fioretti @inaf**
**Paolo Dondero @swhard**

# Electromagnetic physics implementation in GEANT4-DNA

OPEN: Improvement of S/C internal charging associated with electrons below 1 keV. Accurate models for low-energy electron production and propagation in thin layers of gold.

Context: Test-mass charging on board LISA and LISA-like space interferometers for gravitational wave detection. Mismatch of different Monte Carlo simulation tools and experimental data on free-falling test-mass charging in space due to electrons below 1 keV. Material: gold.

https://doi.org/10.1016/j.rinp.2024.107638

Req. 1: Review and improve cross sections and mean free paths of electrons in gold in GEANT4-DNA below 1 keV

Req. 2: Electron quantum diffraction below 100 eV from gold

Req. 3: Hadron ionization below average ionization potential in gold

# Validation of hadronic models

G4LightIonQMD fragmentation model, new, published in Geant4 11.2

https://pubmed.ncbi.nlm.nih.gov/36240757/

https://indico.cern.ch/event/1366947/contributions/5805304/attachments/2801416/4887428/hadronic_highlights_11.2_15Feb2024.pdf

Parameters optimised and validated for Carbon ion therapy

but the model is still new and needs more tests for other use cases

Req: extend G4LightIonQMD validation to more ions, more energies, more (space scenario) materials

Req: include existing G4LightIonQMD validation in Geant4 validation suite

**Source: S.Guatelli @Wollongong**

# Validation of secondary/tertiary production

Production of secondaries in instrument simulations can be noticeably influenced by the choice of hadronic physics models. These secondaries represent a major source of background noise in X-ray space missions, directly or through tertiary production. This issue is considered as critical for the ATHENA design studies.

Ideally, we would propose studying a range of materials, including Kapton, niobium, silicon, aluminum, copper, gold and stainless steel, both individually and in sequence. As for energies, we would suggest proton energies sampled across these ranges:

- 100–200 MeV
- 900–1100 MeV
- 3–5 GeV

Sampling these energies, gathering data on particle types emitted and their spectra and angular distribution, would give us useful insights across various regimes of secondary particle production across the expected GCR proton spectrum.

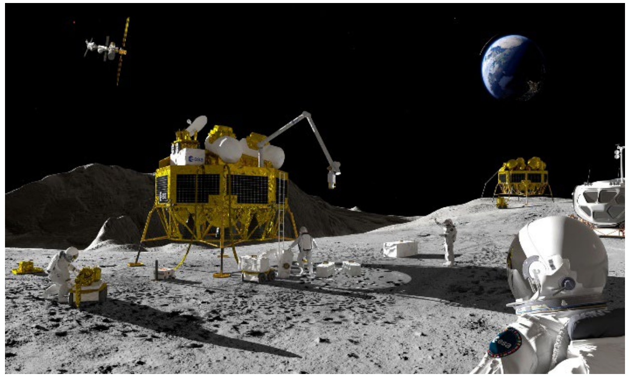
Req: include scenarios relevant for ATHENA background in Geant4 validation suite

**Source:**
**Simone Lotti @inaf**
**Valentina Fioretti @inaf**
**Paolo Dondero @swhard**

# Neutrons

Emerging critical domain

- SEE reliability of electronics
  - Automation, HPC, fusion, avionics, space
- Water equivalent hydrogen (WEH)
  - from spectrum of neutron albedo



**Neutrons from protons**

Feedback from (nuclear) community study: radial distribution of neutrons produced by the impact of protons on different materials. Geant4 shows underproduction of neutrons for certain angles. Results from G4 (v11.2.0) with modified boolean G4ParticleHPManager::PHP_USE_POISSON much closer to (reference) MCNP

Req: Provide user access to G4ParticleHPManager::PHP_USE_POISSON

Req: Include community study scenario in Geant4 validation suite

**Source:** A.Cappe @TRAD
Remi Benacquista @TRAD
Marie-Cecile Ursule @TRAD
Athina Varotsou @TRAD

**Neutron spectrum for soil water detection**

Systematic differences among reference physics lists

Absolute neutron fluxes vary ~30% or more

Req: Include ion-induced neutron albedo in Geant4 validation suite

**Source:** D.Matthiae @DLR
G.Santin @ESA

# Geometry / visualization

**Materials necessary for typical simulations of space scenarios** are missing in the Geant4 material database. Is it possible to extend the G4 internal material database? For example, introducing some standard materials for simulating

- Lunar and the Martian regolith, Martian atmosphere
- Typical Aluminium engineering alloys
- HDPE, Epoxy, CFRP, FR4, …
- Glasses, MCT, …

Req: Add more space materials to the Geant4 material database

**Source: N.Messios @BISA**
**G.Santin @ESA**

In SPENVIS we have been producing the **VRML** outputs e.g. for the visualisation of GRAS simulations. In the G4 Book For Application Developers (Release 11.2, Rev8.0 - Dec 2023) it is mentioned that VRML2FILE created files are supported by most internet browsers. However, I do not believe this is still the case especially since VRML has now been superseded by **X3D** (ISO/IEC 19775-1). Perhaps it will be useful to (also) produce something in the X3D format.

Req: Identify and support modern 3D viewer format with viewers readily available on all platforms

**Source: N.Messios @BISA**

The ROSSINI Reference Radiation Simulation Scenarios was a nice addition to the ESSR. Many thanks for making them publicly available!

**Source: N.Messios @BISA**

# Primary generator - GPS

Automatic implementation of weighted energy bin when using a spectrum as a source

My note: GPS biasAlpha option is maybe already providing the solution ?

Req: Better documentation of GPS option(s) for source biasing

**Source: A.Cappe @TRAD**
**Remi Benacquista @TRAD**
**Marie-Cecile Ursule @TRAD**
**Athina Varotsou @TRAD**

Suggestions about the GPS source definition

- Energy source spectrum is not easy to define (interpolation or not, differential or integral)
  - Related to 2022: Improvement in internal treatment of user spectrum, serious concerns about quality of GPS algorithms
- Source with a “flattened” torus (no thickness) not easy to define
- Old GPS pages from QinetiQ were useful but not copied (?) into the geant4 web page

Req: Improve GPS spectrum definition

Req: Check if any part of original documentation went lost in the transition

**Source: D.Lambert @CEA**

# Docker for installation / distribution

I hope an official release of the g4spaceapps docker container will follow soon.

@ESA, working on a "g4spaceapps" docker container

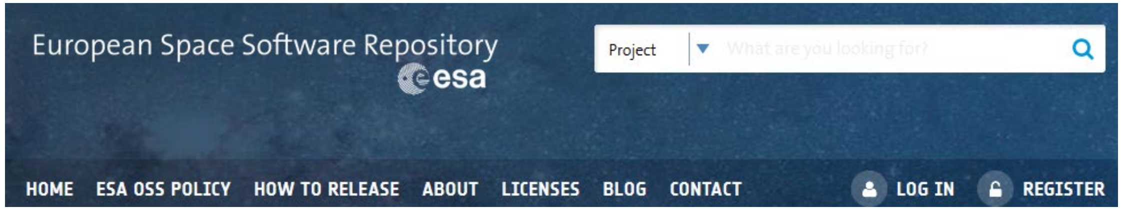
**Source: G.Santin @ESA**
**N.Messios @BISA**

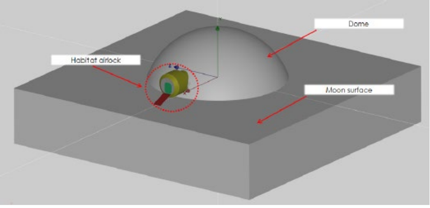
Req: Provide example script in installation manual as official guidance from Geant4 for docker scripts

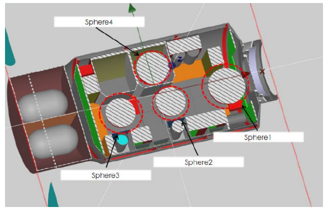
# ESA open community resources

**Geometry**

Reference Radiation Simulation Scenarios: https://essr.esa.int/project/reference-radiation-simulation-scenarios




New Geant4 advanced examples (Geant4 11) from/for the Athena community model of cryostat and optics: "The feedback has been very positive, and we strongly support their continued maintenance and future updates"

**Source: Simone Lotti et al**

**Physics modelling**

Cross Section database (ESA – GSI – NASA)

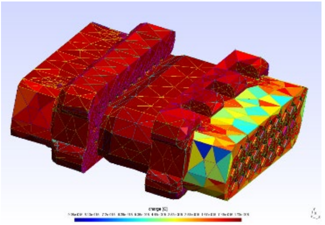

**Geant4-based applications for space radiation analyses**

GRAS (3D) https://essr.esa.int/project/gras-geant4-radiation-analysis-for-space

MULASSIS (1D) https://essr.esa.int/project/mulassis

PLANETOCOSMICS – working on a new release

SPENVIS interfaces to Geant4 GPS, MULASSIS, GRAS, MagnetoCosmics,… https://spenvis.oma.be/



**More info in reference slides below**

# Some relevant user venues

RADSHIELD - Shielding optimization for space – Geant4 heavily used


- https://indico.esa.int/e/radshield2024
- Trapped and Solar - Protons (0.1→1000 MeV) and electrons (0.05→10 MeV)
- GCRs - Heavy Ions 1 MeV/u→10-100 GeV/u – Challenge for hadronic CS models
- Next event ~June 2026

SPACEMON – Radiation instrumentation


- https://indico.esa.int/e/spacemon
- Geant4 used in detector design, ground tests, in-flight response functions
- Next event: ESTEC, 11-12-13 June 2025

Geant4 Space Users' Workshop

- Last edition organised by JPL @Pasadena https://indico.esa.int/event/477/
- Organise at the venue a more official Technical Forum?
- Next event ~2025

# Summary

- EM for electrons and protons
  - Accuracy of transport through (~10nm) thin layers
  - Accuracy of e-, gamma secondaries
  - new Geant4-DNA features in gold
- Heavy ions
  - GCR (10-100GeV/u) sec. variations across physics lists
  - Confidence in cross sections for SEE, sensor noise
  - Need more validation (new light ion model, and overall)
- Neutrons – variations and in general validation
  of production, transport, thermalization
- Usability
  - Geometry – material database extension
  - Visualization – transition from VRML
  - GPS – sampling accuracy, biasing, documentation
  - Docker – example script

- Procedure for recording & follow up of requirements from space domain just started
  - Items not properly tracked – hopefully done within this week

- General high-level summary: users need guidance in their choices, do not know whether they can have confidence in their (physics) results
  - Proposal: including in physics validation suite more space-relevant use cases - and making the results more visible

# Reference slides

Slides with relevant material and requirements from previous years

# 2022
# Reference Radiation Simulation Scenarios

GEANT4 A SIMULATION TOOLKIT

esa

European Space Software Repository (ESSR)

https://essr.esa.int

European Space Software Repository esa

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## REFERENCE RADIATION SIMULATION SCENARIOS

The Reference Radiation Simulation Scenarios includes models compatible with Monte Carlo simulations for radiation transport, including realistic and detailed geometry models of spacecraft modules, and planetary habitats, and guidelines for high energy radiation environment spectra to be used for the simulations.

Its purpose is to provide access to end-users in the space (exploration) domain to realistic modular geometry elements for their radiation simulations, and at the same time to enable meaningful comparisons, among different teams in the community, of simulation results based on common reference input. It also aims at providing an infrastructure for future augmentation of the scenarios dataset with contributions of additional models by the community, developed under other activities.

**Licenses:** European Space Agency Community License – v2.4 Strong Copyleft (Type 1)

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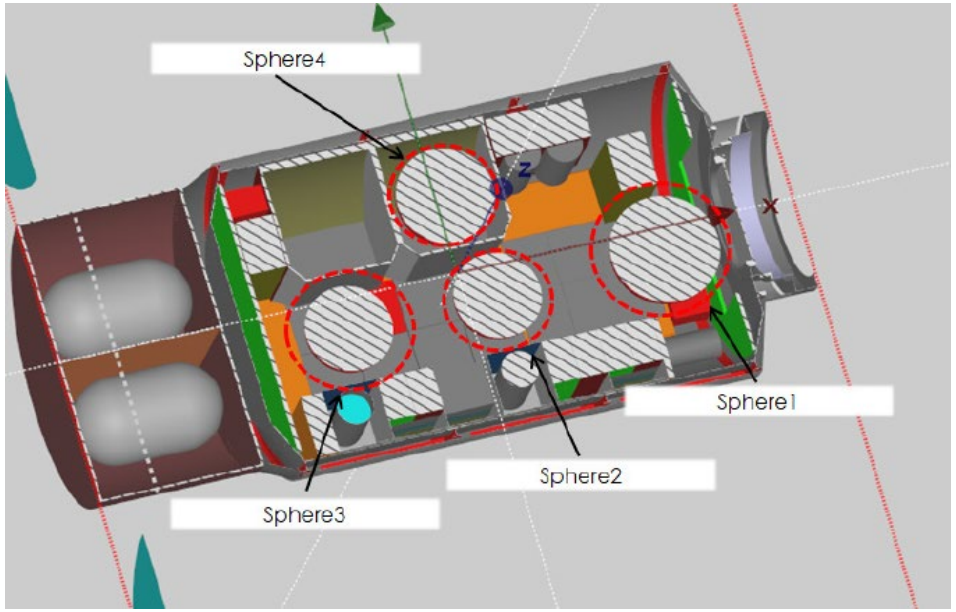
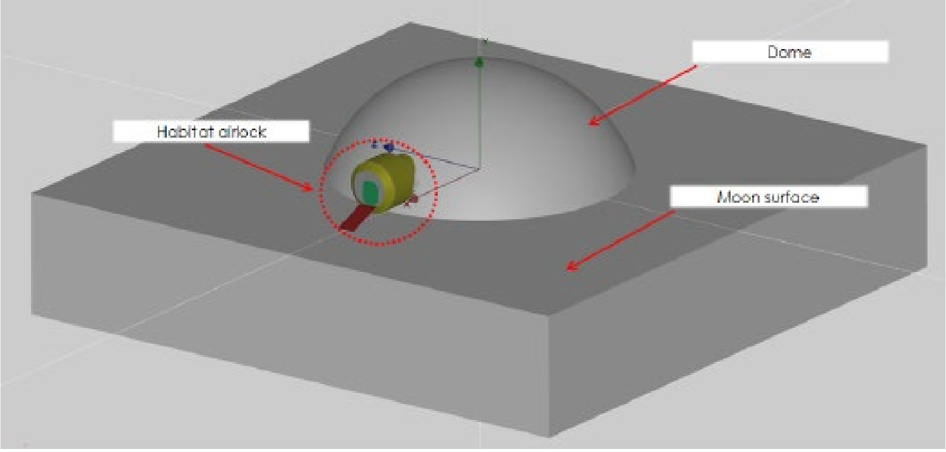
**Updated on:** 08/04/2022
**Created on:** 22/02/2022
**Owner:** TAS-I
**Tags:** simulation Geant4 Radiation Monte Carlo Radiation shielding GDML Radiation environment Exploration



# 2022
# Physics: Protons and Heavy ions (1)

**Open (?) 2015: Cross Sections for High Z - High Energy (HZE) particles**

Context: biological dose in long duration exploration missions to Moon and Mars – dominated by GCRs

ROSSINI 3 project (GCR innovative shielding materials - TAS-I, GSI, UniTo, ESA R&D)

Geant4 physics lists use dramatically different CSs: Fe 1GeV/n Bragg peak curve in Paraffin (reported in 2015 & 2020): **only CS in *INCLXX** reproduce data

**Source: L.Bocchini, M.Giraudo @Thales Alenia Space Italia**

Astronaut radioprotection: **Improve cross sections for hadronic processes (especially fragmentation)**

**Source: S. Guatelli @UoWollongong**

- Req: Review CSs models. Add relevant exp dataset to Geant4 validation suite

Additional information:

New review and useful dataset from ESA **ROSSINI 3 project: Cross Section database (ESA – GSI – NASA)**

- F Luoni et al 2021 New J. Phys. 23 101201 https://iopscience.iop.org/article/10.1088/1367-2630/ac27e1
- Made available at https://www.gsi.de/work/forschung/biophysik/fragmentation

# 2022
# Cross Section database (ESA – GSI – NASA)

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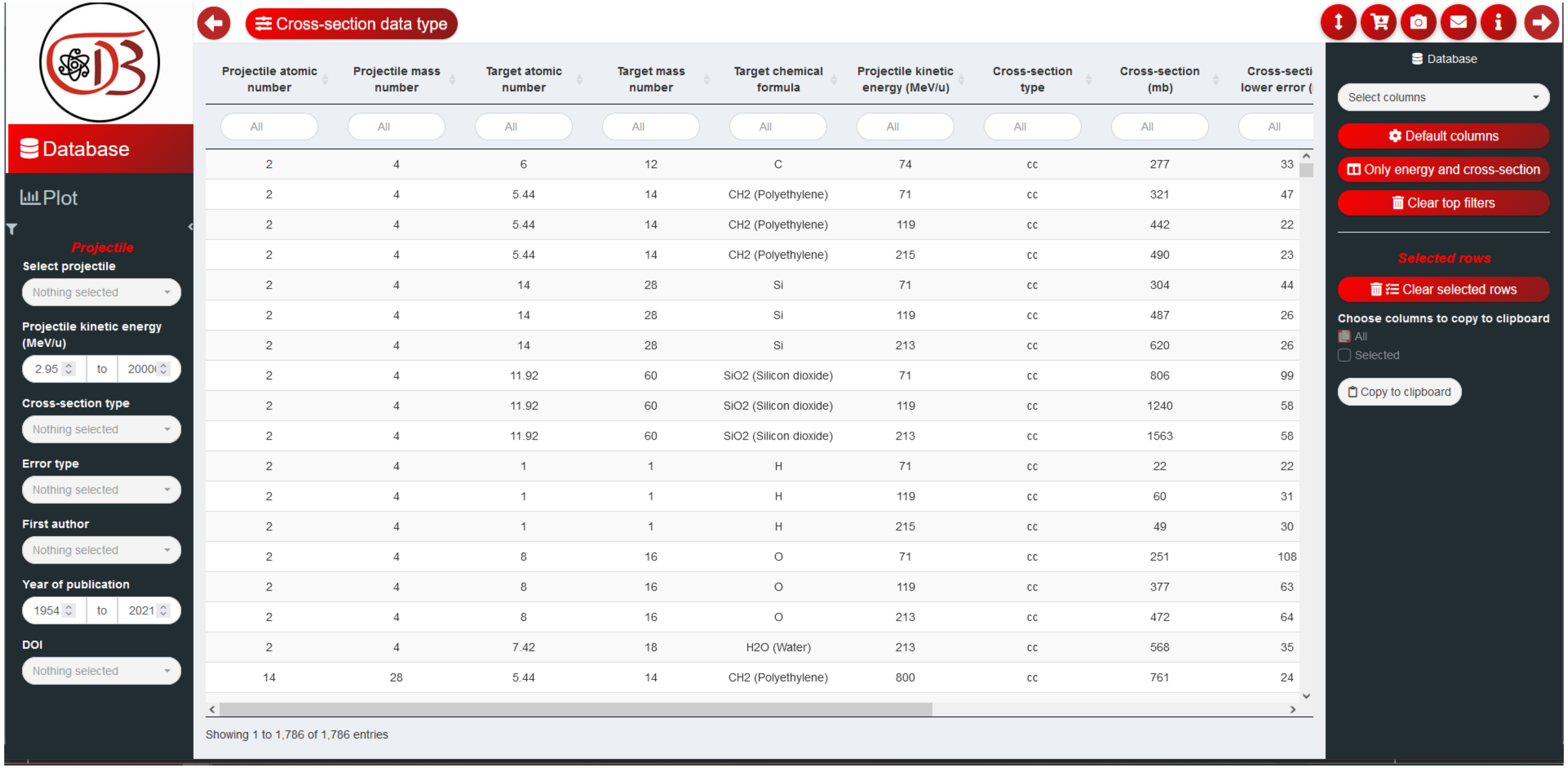


| Projectile atomic number | Projectile mass number | Target atomic number | Target mass number | Target chemical formula | Projectile kinetic energy (MeV/u) | Cross-section type | Cross-section (mb) | Cross-section lower error ( |
|---|---|---|---|---|---|---|---|---|
| All | All | All | All | All | All | All | All | All |
| 2 | 4 | 6 | 12 | C | 74 | cc | 277 | 33 |
| 2 | 4 | 5.44 | 14 | CH2 (Polyethylene) | 71 | cc | 321 | 47 |
| 2 | 4 | 5.44 | 14 | CH2 (Polyethylene) | 119 | cc | 442 | 22 |
| 2 | 4 | 5.44 | 14 | CH2 (Polyethylene) | 215 | cc | 490 | 23 |
| 2 | 4 | 14 | 28 | Si | 71 | cc | 304 | 44 |
| 2 | 4 | 14 | 28 | Si | 119 | cc | 487 | 26 |
| 2 | 4 | 14 | 28 | Si | 213 | cc | 620 | 26 |
| 2 | 4 | 11.92 | 60 | SiO2 (Silicon dioxide) | 71 | cc | 806 | 99 |
| 2 | 4 | 11.92 | 60 | SiO2 (Silicon dioxide) | 119 | cc | 1240 | 58 |
| 2 | 4 | 11.92 | 60 | SiO2 (Silicon dioxide) | 213 | cc | 1563 | 58 |
| 2 | 4 | 1 | 1 | H | 71 | cc | 22 | 22 |
| 2 | 4 | 1 | 1 | H | 119 | cc | 60 | 31 |
| 2 | 4 | 1 | 1 | H | 215 | cc | 49 | 30 |
| 2 | 4 | 8 | 16 | O | 71 | cc | 251 | 108 |
| 2 | 4 | 8 | 16 | O | 119 | cc | 377 | 63 |
| 2 | 4 | 8 | 16 | O | 213 | cc | 472 | 64 |
| 2 | 4 | 7.42 | 18 | H2O (Water) | 213 | cc | 568 | 35 |
| 14 | 28 | 5.44 | 14 | CH2 (Polyethylene) | 800 | cc | 761 | 24 |

# 2022
# Physics: Protons and Heavy ions (2)

**Open (?): Accurate models for low-energy nucl-nucl interactions**

Context: **Single Event Effects** in electronics in space environment (component at <100MeV/nuc very important)

Req: Better model for nuclear fragments from nucl-nucl interactions <50MeV/n regime

**Source: P. Truscott @Kallisto**

**Open (?) 2021:** Complete lack of reasonable **distribution of ion charged states** after thin targets

Context: 10 MeV $O^{4+}$ through ultra thin Al layer. Codes such as LISE++, ETACHA etc. can model this. Not G4

- Req: Model for reasonable distribution of charge in ion final states

**Source: M.Kokkoris @NTU Athens**

**Open (?) 2021: Neutron production**, down to thermal energies from cosmic-ray (protons and HZE particles)

Context: Human exploration missions to Moon and Mars, biological dose and SEE

LRO/CRaTER project (charged-particle sensor aboard Lunar Reconnaissance Orbiter)

- Req: Accurate models for neutrons
- Req: Physics lists: documentation or recommendations for neutron physics and sensor response:

**Source: Mark D. Looper @Aerospace Corporation**

# 2022
# Physics: Protons and Heavy ions (3)

**Open (?) 2020: dE/dx in Si for High Z - High Energy (HZE) particles**

Context: Electronic component tests at CERN SPS with Xe 40GeV/n and Pb 150GeV/n

Energy deposition from sub-um up to 500 um thick Silicon sensitive volumes

- EM, 2020, v10.5.p1: discrepancies in dE/dx in Si: DOI:10.1109/TNS.2019.2958746
- Discussion with Vladimir Ivantchenko: theoretical corrections not easy for ion dE/dx at high energy
- Some work done in recent years (Lindhard–Sørensen) – values moved but still incorrect – still ongoing?

Req: Review and improve the current high-energy ion dE/dx models. Include this case in validation suite

**Source: S.Gerardin,
M.Bagatin @DEI UniPd**

# 2022
# Docker support

**Source: Dávid Lucsányi & CERN R2E**
**Pete Truscott @ Kallisto**
**Neophytos Messios @BISA**
**GS @ ESA**

**Open:** Installation / distribution via docker – starting point for users

Widely used by users but not supported / documented

Req: Provide official Docker support

- Distribute a few standard images – ready for download, users can run examples etc
- Provide scripts for Geant4 containers (including baseline and additional user configurable options)
- Provide guidelines / tips for packaging additional space applications
- Provide instructions for using the G4 libs / running the G4-based apps from a Docker image

Additional information

Recent development at ESA:

- **g4spaceapps** docker container – developed by Pete Truscott for ESA – layered approach
- Now in ESA gitlab repo – standard Geant4 licence conditions – can be input to the collaboration
- Form a small group of interested contributors?

# 2022
# Improvement in source spectra

**Open:** Improvement in internal treatment of user spectrum

- Context: Space applications heavily rely on source energy spectra from external tools
- **Computational accuracy problems in GPS**

Req: Review of GPS algorithms: interpolation, differentiation / integration

**Source: Brian Xiaoyu Zhu @JPL**
**GS@ESA**
**User forum**