Open and new requirements: medical and bio-science

URs in progress: tracked in the Geant4 Requirements Tracker

New URs

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28th Geant4 Collaboration Meeting, 25-29 September, Sapporo, Japan

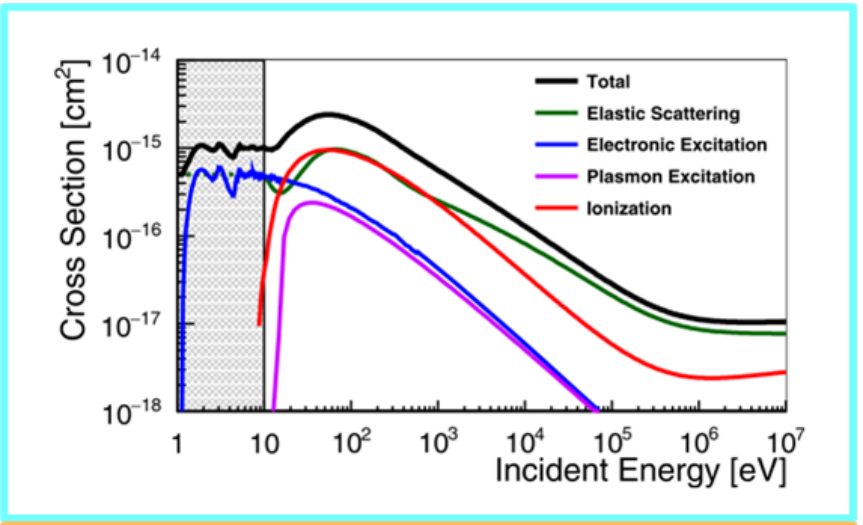
Existing URs (1)

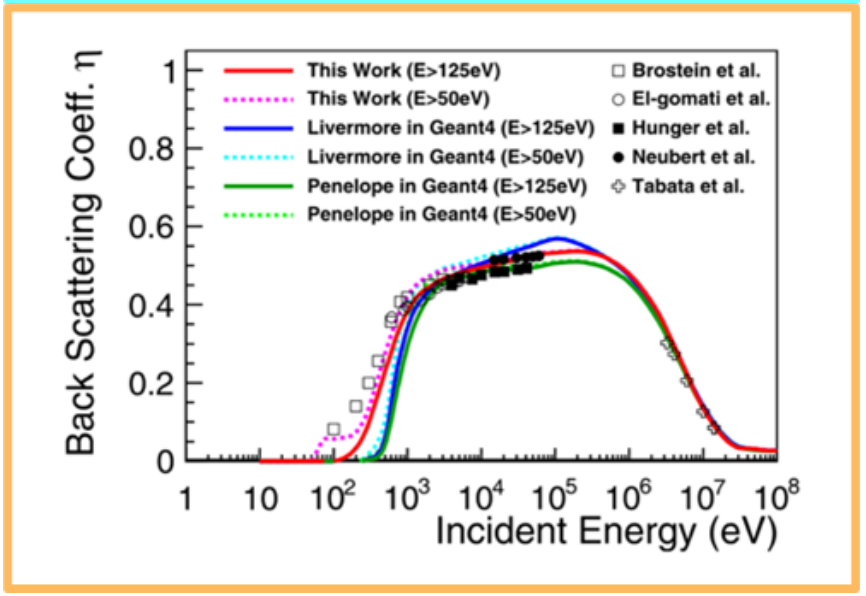
- **UR-54:** Physics models for ions below 1 MeV/u for Boron Proton Capture (Ribon)
  - The aim is to compare the hadronic physics models for the p+B11 —> 3 alpha reaction
  - To start
- **UR-63:** To have an extended example to retrieve directly from the simulation Auger electron energy and associated atomic transition, including in Geant4-DNA processes (Guatelli)
  - To start, no manpower
- **UR-80**. Isotope production from protons using IAEA medical cross-section (Ribon)
  - IAEA has made an extensive work to cover isotope production for medical applications (https://www-nds.iaea.org/medical/)
  - Review and include IAEA medical cross sections into the Geant4 ParticleHP database
  - To start
- **UR-83**: Webpage, with information about Geant4 for medical applications (Guatelli)
  - To start

Existing URs: Geant4-DNA (1)

- **UR-53:** Extend energy and material coverage of G4-DNA beyond DNA and liquid water (S. Incerti)
  - Liquid water, DNA, amino-acids, boron, gas (micro/nanodosimetry), solid state (e.g. high Z materials for nanoparticle aided radiotherapy, microelectronics)
  - Done for gold (Geant4 11.0)
  - Done for protons in water (extension 100 MeV –> 300 MeV) by M. Cortes-Giraldo et al.
  - In progress for electrons: for water (option4 : 10 keV -> 10 MeV) by I. Kyriakou et al, for DNA materials (by S. Zein et al.), for N_2 and O_2 (by C. Villagrasa et al., by C. Mancini, F. Nicolanti et al.)
  - Extensions to MuElec by C. Inguimbert, ONERA, and collaborators
  - Extend ionisation cross sections to heavy ions: Al, Ar, Cl, F, Mg, Na, Ne, P, S (beyond ^{7}Li,^{9}Be,^{11}B,^{12}C, ^{14}N,^{16}O,^{28}Si,^{56}Fe) for space radiation protection. First prototype done by V. Ivanchenko. Further validation needed (V. Ivantchenko, H. Tran, J. Archer)

Gold





Sakata et al (2019) Electron track structure simulations in a gold nanoparticle using Geant4-DNA, Physica Medica, 63: 98-104

Existing URs: Geant4-DNA (2)

- **UR-82**: Geant4-DNA physics processes for positrons (Ivantchenko)
  - Positrons are included in the DNA Physics Lists, using standard condensed history approach. No manpower to start developments on discrete models
- **UR-62:** Model for positronium creation and annihilation (Ivantchenko)
  - To start – no manpower
- **UR-77**: Multiscale combination. Mixing condensed-history and Geant4-DNA, e.g. for radioprotection in space
  - Done but more validation is required (V. Ivantcheko, H. Tran and J. Archer)
  - BioRad3 Multi-scale prototype framework to be made available (Paolo Dondero et al., SWHARD).
- **UR-78:** Provide an example of physics list activating both Geant4-DNA and hadronic physics, including radioactive decay (Ivantchenko)
  - This needs to be demonstrated in an example

Existing URs: Geant4-DNA (3)

- **UR-76**: Provide (external) files to describe geometries of biomolecules (e.g. plasmids, bacterium, cells, etc) (Incerti et al.)
  - On going through BioRad3
    - Release of two alternative chains (first public BETA release of “moleculardna” in 11.1 BETA, “dnadamage1” in 11.1) and more upgrades in 2023
    - See “moleculardna” web site : https://geant4-dna.github.io/molecular-docs/

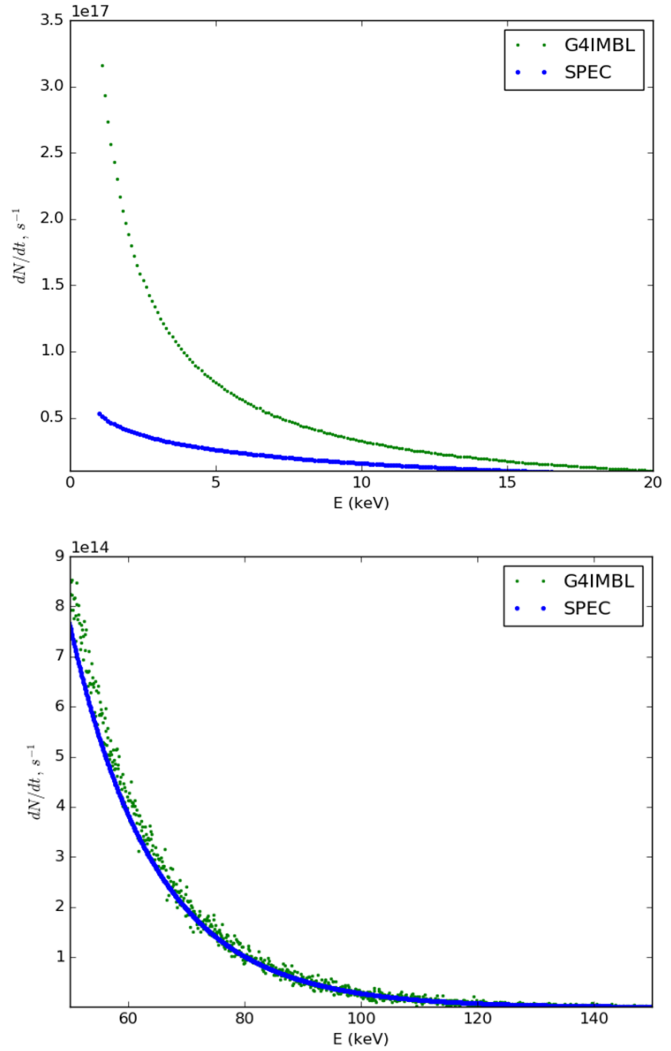
- **UR-79**: Mesoscopic approach development for chemistry / water radiolysis (high dose rates, longer times), including an extended example
  - Under development (high dose rates, longer times) and compared to existing Geant4 (step by step) approaches
  - Activate three Time-Step models (SBS,IRT, IRT-syn) in chem6 example using IU macro.
  - ”scavenger” example for radiolysis simulation in scavengers – released in Geant4 11.0
  - “UHDR” example released in Geant4 11.2 BETA

New URs

- **UR#**: couple the Bearden energy lines with the ANSTO fluorescence data libraries
  - Source: Geant4 User Forum

- **UR#**: revision of G4SynchrotronRadiation process
  - Source: S. Guatelli
  - In progress (S. Guatelli and J. Paino, CMRP, UOW)
  - Comparison of wiggler spectra:
    Geant4 v.s. SPEC
  - SPEC verified against XOP (https://aip.scitation.org/doi/10.1063/1.1147376)
  - <50 keV: Geant4 overestimates flux relative to SPEC
  - G4:SPEC flux ratio 1-20keV = 2.922
  - >50keV: Geant4 and SPEC spectra agree

Comparison of Geant4 and SPEC: Synchrotron radiation



Python wrapping

- **UR#**: contribution to develop the G4 Python wrapping
- Source: David Sarrut
- The current Geant4 python wrapping is not adequate for the needs of GATE.
- A first pybind11-based G4 wrapping has been developed tailored for GATE users. The code is open source and it is here : https://github.com/OpenGATE/opengate/tree/master/core/opengate_core/g4_bindings
- There is strong interest to collaborate to develop further the Geant4 python wrapping for the wider Geant4 community

Not URs,
but very important for bio-medical applications

Validation for radiobiology

On-going verification & validation

- Continue efforts in chemistry under irradiation (LET, doses rates) & radiobiology
- Calculation of G-values, under variety of exp. conditions : T, pH, scavengers, high LET
- Radiobiological damage: beyond strand-breaks towards macroscopic observables (e.g. requiring analytical repair models)
- Addition of related extended and advanced examples for users
- Some of these activities are currently on-going through
  - the ESA BioRad III project (2021-2023): CEA (FR), CHUV (CH), G4AI Ltd. (UK), IN2P3 (FR –coord.), INFN (IT), Ioannina U. (GR), IRSN (FR), Sevilla U. (ES), Swhard (IT)
  - the MAGIC project (2020-2023): CHUV (CH – coord.), LP2i (FR)
  - The FLASHMod project (2021-…): LPC (France), LP2i

Validation for bio-medical applications: the G4-Med suite

Extend the tests of G4-Med to other medical applications

- 19 tests, on geant-val

- New:

- Included Geant4-DNA physics lists where applicable (Microdosimetry and DPK)
- Chemistry / water radiolysis – H. Tran et al.
- EPICS17 data libraries included in the photon attenuation tests

- Later:

- Radioactive decay – L. Desorgher et al
- Nuclear medicine tests – A. Malaroda, S. Guatelli et al, help needed
- Photon energy fluence profile and thick target photon backscatter benchmark - By J. Carrasco Hernandez, B. Faddegon and J. Ramos Mendez, UCSF
- Calculation of the wall correction factors, kwall, for two graphite ionization chambers – P. Arce
- Include benchmark against ICRU Report 90: Stopping Powers of electrons (and positrons), protons, α particles and carbon ions for three key materials: graphite, air, and liquid water – help needed
- Include total inelastic cross section tests of production of C-10 and C-11 important for carbon ion in-vivo PET and Prompt Gamma imaging, E. Simpson, ANU – help needed
- Validate Medical Linac advanced examples against EURADOS Report 2020-05 – C. Caccia

UR for geant-val: Provide documentation on how to include and run tests via geant-val

New QMD model for hadron therapy: G4LiQMD

- See presentation by Y. Sato, Parallel 3A Hadronic 1, Tuesday 26th Sept
- To be released soon

Next steps:

- Validation of fragmentation for proton therapy
  - cross section (thick and thin targets), in-vivo PET, Prompt Gamma, etc. - A. Haga.
- Improvement of computation speed
  - Parameter tuning in QMD model – Y. Sato
  - Application of machine learning model – Y. Sato

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PAPER

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Development of a more accurate Geant4 quantum molecular dynamics model for hadron therapy

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Supplementary material for this article is available online

Abstract

Objective. Although in heavy-ion therapy, the quantum molecular dynamics (QMD) model is one of the most fundamental physics models providing an accurate daughter-ion production yield in the final state, there are still non-negligible differences with the experimental results. The aim of this study is to improve fragment production in water phantoms by developing a more accurate QMD model in Geant4. *Approach*. A QMD model was developed by implementing modern Skyrme interaction parameter sets, as well as by incorporating with an ad hoc α-cluster model in the initial nuclear state. Two adjusting parameters were selected that can significantly affect the fragment productions in the QMD model: the radius to discriminate a cluster to which nucleons belong after the nucleus–nucleus reaction, denoted by R, and the squared standard deviation of the Gaussian packet, denoted by L. Squared Mahalanobis's distance of fragment yields and angular distributions with 1, 2, and the higher atomic number for the produced fragments were employed as objective functions, and multi-objective optimization (MOO), which make it possible to compare quantitatively the simulated production yields with the reference experimental data, was performed. *Main results*. The MOO analysis showed that the QMD model with modern Skyrme parameters coupled with the proposed α-cluster model, denoted as SkM*α, can drastically improve light fragments yields in water. In addition, the proposed model reproduced the kinetic energy distribution of the fragments accurately. The optimized L in SkM*α was confirmed to be realistic by the charge radii analysis in the ground state formation. *Significance*. The proposed framework using MOO was demonstrated to be very useful in judging the superiority of the proposed nuclear model. The optimized QMD model is expected to improve the accuracy of heavy-ion therapy dosimetry.