Open and new requirements: medical and bio science

URs in progress: tracked in the Geant4 Requirements Tracker

URs emerged from last year workshop but not included in Jira yet

New URs

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27th Geant4 Collaboration Meeting, 26th-30th September 2022, Rennes, France

In progress (1)

- **UR-52**: Make EPICS2017 models available in Geant4 (electrons, photons) as an alternative to Livermore (S. Incerti)
  - Li Z et al (2022) Implementation of the EPICS2017 database for photons in Geant4, Physica Medica, 95: 94-115.
  - Now available for photons, since Geant4 11.0
  - It was decided not to update electron models (similar to Livermore)
  - This UR could then be closed
  - **More information in the last 2 slides**

- **UR-63:** To have an extended example to retrieve directly from the simulation Auger electron energy and associated atomic transition (S. Guatelli)
  - To start

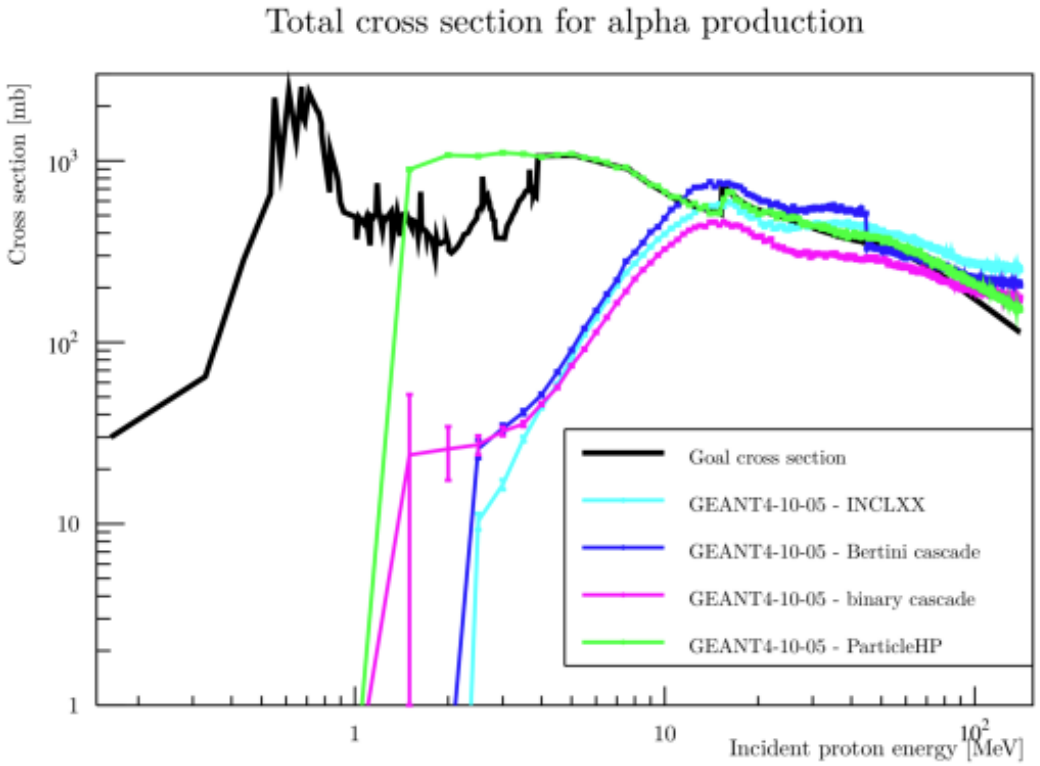
- **UR-62:** Model for positronium creation and annihilation (V. Ivantchenko)
  - In progress

In progress (2)

- **UR-54:** Physics models for ions below 1 MeV/u for Boron Proton Capture
- Source: P. Cirrone
- The aim is to compare the hadronic physics models for the p+B11 —> 3 alpha reaction

In order to do that:

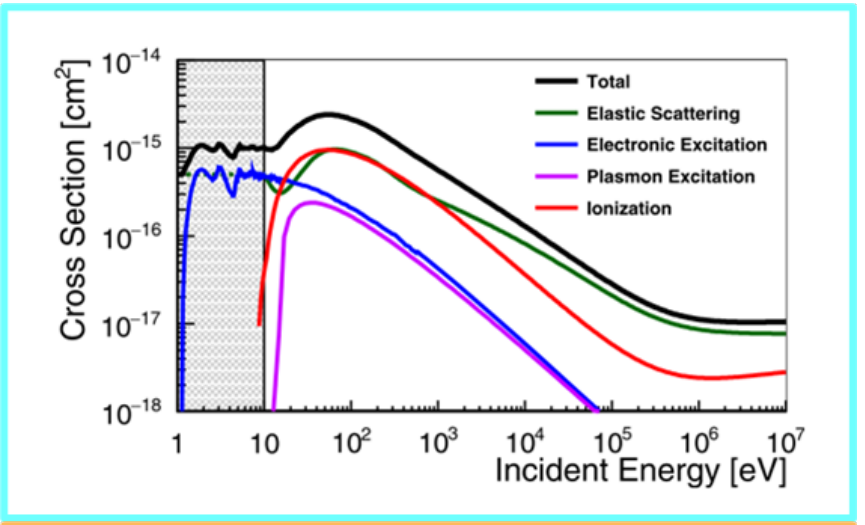
- Extend the hadronic physics models below 1 MeV
- Improve the issue of non conservation of the baryonic number in ParticleHP

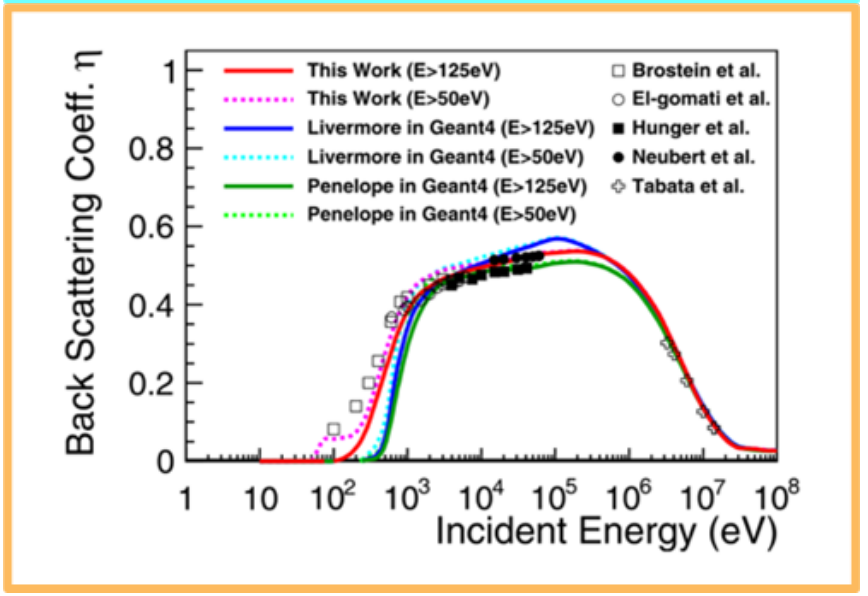


In progress (3)

- **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 N2 (by C. Villagrasa et al.)
  - 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, by D. Bolst, D. Sakata, J. Archer, S. Guatelli

Gold





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

New URs

- Some documented in the talk of G. Petringa “Open and new requirements: medical and bio science 2021” 26th Geant4 Collaboration Meeting 20/09/2021 (But not included in JIRA)

- Some are new

UR: geometries of interest for radiobiology

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

Radiobiological studies for space radiation protection

- UR: Multiscale combination. Mixing condensed-history and Geant4-DNA, e.g. for radioprotection in space :
  - cosmic spectra – space habitats
  - human phantom – « microscopic » & « macroscopic » biological end-points
  - Delivery of BioRad3 expected in 2023

- UR: em + hadronic. Provide an example of physics list activating both Geant4-DNA and hadronic physics, including radioactive decay

- This is on-going

UR: chemistry

- Mesoscopic approach under development (high dose rates, longer times) compared to existing Geant4 (step by step) approaches, including extended example
- 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
- On-going activity

Other URs

- UR: Isotope production from protons
  - 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
- UR – biasing : Add AtRest in Geant4 Biasing framework
  - Source: P. Arce
- UR – geometry: for DNA geometries, include the option to change the copy number of geometries from a G4int to a long in Replica and parameterized volumes, with a lot of geometries (DNA, 6 billion x 2 bases x 4 section geometries),
  - Source: J. Schuemann, & A. McNamara
  - Run out of copy numbers in G4int
- UR - examples: modelling radiation damage in semiconductor devices
  - Source: Geant4 User Forum
  - Develop a Geant4 example, or a macro in an already existing G4 example, to show how to calculate radiation damage (with G4NIELCalculator and G4NuclearStopping)

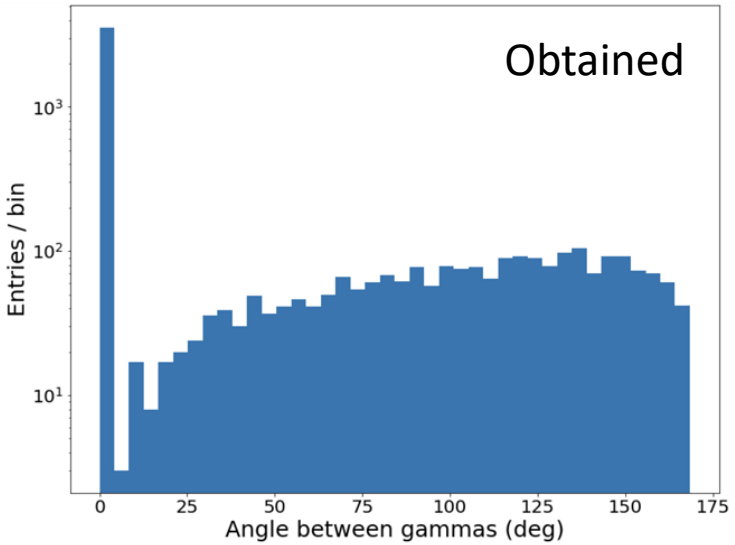
Positrons

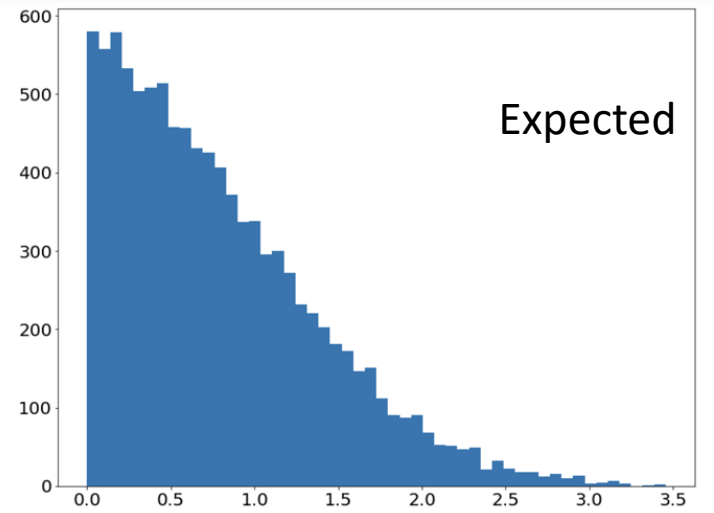
UR: Geant4-DNA physics processes for positrons

- Source: Geant4 user forum
- Model the radiation transport of positrons at low energies, similarly to what done for electrons

UR: Positron annihilation and photon a-collinearity

- Source: Mirjam Schöneck, mirjam.schoeneck@uk-koeln.de, Maxime Toussaint: Maxime.Toussaint@USherbrooke.ca)
- Documented in: https://geant4-forum.web.cern.ch/t/non-collinearity-of-gammas-in-e-e-annihilation/7259/13



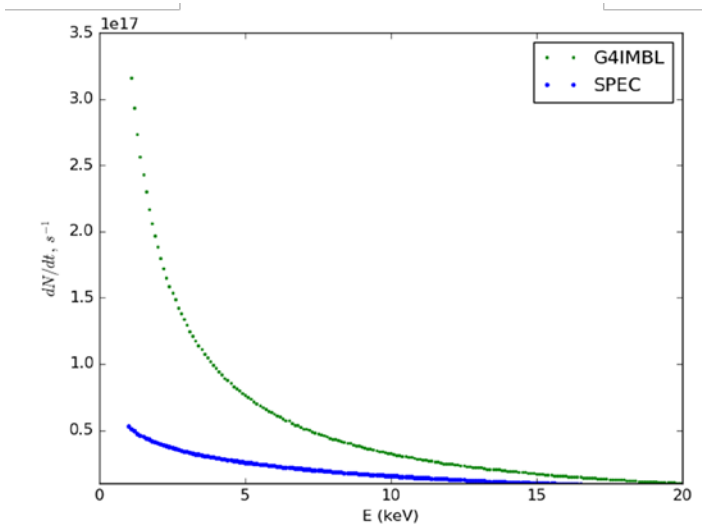


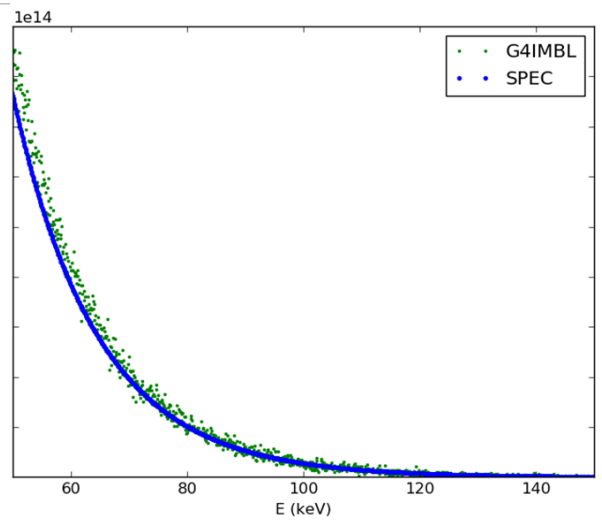
Synchrotron radiation production in a wiggler

UR: revision of G4SynchrotronRadiation process

- Source: S. Guatelli
- 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

Australian Synchrotron





Python wrapping

- UR: G4 Python wrapping
- Source: David Sarrut
- python wrapping of some Geant4 classes and functions for the new GATE version. The current Geant4 version 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

Validation for radiobiology

On-going verification & validation

- Continue efforts in chemistry under irradiation & 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

UR: extend the tests to other medical applications

- 19 tests, on geant-val

- Next in the pineline:

- Include Geant4-DNA physics lists where applicable (e.g. Microdosimetry and DPK)
- X-ray small field dosimetry – S. Guatelli, I. Filipev, G. Biasi, A. Rozenfeld, CMRP, UOW
- Include EPICS17 data libraries in the photon attenuation tests

- Later:

- Radioactive decay – L. Desorgher et al
- Nuclear medicine tests – A. Malaroda, S. Guatelli et al
- 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
- 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
- Validate Medical Linac advanced examples against EURADOS Report 2020-05 – C. Caccia

UR: It would be important to find a way to run all the tests before beta and public releases.

UR: In a longer term vision, it would help to have documentation on how to run the tests via geant-val and eventually, on how to set them up

Other

- UR: documentation. Have a webpage linked to www.geant4.org, with information about Geant4 for medical applications
  - Examples
  - G4 medical physics activity
  - Useful information, e.g. how to activate biasing for bremsstrahlung, etc.
  - Promote events (workshops, conferences, schools)
  - Source: S. Guatelli
  - Status: to start

More information

Implementation of EPICS2017 for Livermore photon models

Z. Li, C. Michelet, S. Incerti, I. Ivanchenko, M. Novak, S. Guatelli

- Database EPICS2017 (Electron Photon Interaction Cross Section library) contains physical data (cross section…) for electron and photon transport calculation, has been implemented for Livermore photon models, available from Geant4 11.0.
- EPICS2017 database is triggered by ***/process/em/LivermoreData epics_2017*** if G4EmLivermorePhysics is used.
- **Models involved**:
  - G4LivermoreGammaConversionModel
  - G4LivermoreGammaConversion5DModel
  - G4LivermoreComptonModel
  - G4LivermorePhotoElectricModel
  - G4LivermoreRayleighModel
- Tabulated cross-sections have been updated, new parameterizations with better precision regarding scattering functions of Compton effect, cross-sections of photoelectric and form factors of Rayleigh scattering have been applied.
- **Publication**: *Z. Li, C. Michelet, S. Incerti, I. Ivanchenko, M. Novak, S. Guatelli, H. Seznec. Implementation of the EPICS2017 database for photons in Geant4, Physica Medica 95 (2022) 94-115.*
- **Technical notes** are available on the *Geant4@IN2P3* website*: http://geant4.in2p3.fr/styled-4/styled-8/*

Work on EPICS2017 electron data

Z. Li, C. Michelet, S. Incerti, I. Ivanchenko, M. Novak

Method:

The following comparisons were performed:

- Subshell ionization cross-section for Z: 1-100 between EPICS2017 and previous version EPICS2014 (=EEDL91)
- Ionization cross-section and stopping power for Z: 1-97 calculated by Livermore, Penelope and MollerBhabha models
- Ionization stopping power between Livermore ionization models and ESTAR data.
  - for elements: H, C, Si, Fe, Cs, Pb, U
  - for materials: air, graphite and water

Conclusion:

There is no need to update Livermore electron ionization model for EPICS2017 electron data.

A technical note summarizing the work is in progress and will be available soon.