Update on Requirements

56th Geant4 Technical Forum March 24th 2022 Virtual Meeting

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Requirements Tracking System Page: https://jira-geant4.kek.jp/secure/Dashboard.jspa?selectPageId=10000

New/analyzed requirements

Requirements from 2021Geant4 Collaboration Meeting (CM)

- Requirement sessions during CM are quite productive
 - > 2021 session ended with O(> 50) requirements expressed !
 - https://indico.cern.ch/event/1052654/sessions/401937/#20210920
- Some first level of filter done, but analysis process is on-going
 - > Is requirement new ? Is it relevant to Geant4 ? Does it need clarification ? Etc.
 - In interaction / iteration with requesters
- Requirement analysis work shared among several volunteers:
 - > HEP : Alberto Ribon
 - Intensity Frontier : Soon Yung Jun
 - > Nuclear Physics : no new requirements !
 - Space Science and Engineering : Makoto Asai
 - Medical and Bio Science : Susanna Guatelli
- Requirements will be added to JIRA as they are validated
- Thank you for your patience !

Validated requirements (HEP)

Source	Requirement	Responsible
CMS	 Extended decay module of Geant4 More accurate branching ratios for baryons and mesons Improved final state sampling Addition of detailed tau, c-, and b- particle decays Native or via interface to generator packages 	Alberto Ribon
ATLAS	 Quasi-stable particle Simulation : Improved robustness of Geant4 when using pre-defined decay chains from Generators. Perhaps implementing some kind of sanity checker for G4Events with predefined decays to spot potential problems. (Unknown particle types, particles with no physics models attached, zero lifetime particles.) 	Alberto Ribon
ATLAS	 Quasi-stable particle Simulation : Establish conventions on consistency of decay models between G4 and Generators where there are overlaps ? Or possibly common work to directly integrate event generators for certain decays and interactions? 	Alberto Ribon
ATLAS	Quasi-stable particle Simulation : Dealing with hadronic interactions of oscillating neutral mesons	Alberto Ribon

Validated requirements (IF)

Source	Requirement	Responsible
DUNE	Propagation of polarized muons and taus in dense media	John Apostolakis & Krzysztof Genser (contact IF)
Mu2e	 pbar annihilation process to be improved including being able to affect the nuclear destruction process at energy below 2GeV 	Davide Mancusi
Muon g-2	Muon g-2 is interested in having a symplectic stepper	John Apostolakis (but need humanpower)

Validated requirements (medical)

Source	Requirement	Responsible
Medical	Provide an example of physics list activating both Geant4-DNA and hadronic physics, including radioactive decay	Sébastien Incerti & Susanna Guatelli
Medical	 Isotope production from protons: IAEA has made an extensive work to cover isotope production for medical applications (https://www-nds.iaea.org/medical/) Put IAEA medical cross section into Geant4 ParticleHP database 	Alberto Ribon
Medical	AtRest in Geant4 Biasing framework add AtRest in Geant4 Biasing framework 	Marc Verderi
Medical	 Modelling Radiation damage in Semiconductor devices https://geant4-forum.web.cern.ch/t/modelling-radiation-damage-in-semiconductor-devices/5751 Include a Geant4 example to show how to calculate radiation damage (with G4NIELCalculator and G4NuclearStopping) 	Susanna Guatelli & Ivana Hrivnacova

Open requirements

4702 : Inclusion of γ polarization effects in the high energy EM models

- Originator:
 - > CMS
 - > 47th Technical Forum (link)
- Scope:
 - > Include Linear Polarization into HE y Models
 - > This has potential usage in the analysis of $H \rightarrow \gamma \ \gamma$
 - Polarization planes of scalar (pseudo-scalar) particle to γ's are parallel (perpendicular)
 - Investigate the effect of polarization in the shower shape of photons
 - May give additional handles to distinguish direct γ's from H decay from BG
- Responsible:
 - Vladimir Ivantchenko
- Status:
 - > In progress, continuing this year.
 - > Open.

5002 : Support for "sub-event" parallelism across G4 threads

- Originator:
 - > ALICE
 - > Page 6 of Requirements from energy frontier
 - > Declined by ALICE last year, but requirement still considered of interest
- Scope:
 - ALICE handles For experiments which handle very big events
 - > These would be processed faster if one event could be split into "sub-events" (= {subset of primary tracks}) -each processed on one thread- with merging back of sub-events into the event at the end
- Responsible:
 - > Makoto Asai
- Status:
 - > This comes along with the tasking model, released with 11.0.
 - > Reproducibility is the main issue
 - > Will be continued this year
 - > Open

5005: Neutron self-shielding effect

- Originator:
 - > LZ (LUX-ZEPLIN), SuperCDMS
 - Page 7 of <u>Requirements from intensity frontier</u>
- Scope:
 - Significant reduction of the neutron flux in material when neutron energy is in the resonance region
 - The capture process can reduce the flux at one position in a crystal creating a kind of shadow in which the downstream atoms see a reduced flux (a ~10% effect)
- Responsible:
 - > Vladimir Ivanchenko
- Status:
 - > Valid requirement but big work
 - Needs theoretician support as well as manpower.
 - > Collection of publications and references on-going.
 - > Not expected to be concluded in the short term.
 - > Open.

5006 : Improve simulation of gamma induced neutron background

- Originator:
 - > LZ (LUX-ZEPLIN), SuperCDMS
 - > Page 7 of <u>Requirements from intensity frontier</u>
- Scope:
 - > Low energy gammas producing neutrons in various materials can generate a significant background
 - > But photo-nuclear process does not model this well below 30 MeV
 - > Point that G4LEND gamma models might resolve the issue
- Responsible:
 - > Vladimir Grichine
- Status:
 - > Improved gamma-nuclear cross sections in G4 11.0.
 - > Next step is the final-state; in the work-plan for this year.
 - > Open.

5007 : Improve electro-nuclear models

- Originator:
 - Markus Diefenthaler (EIC Center, EICUG) for:
 - JLAB 12 GeV Science program
 - Electron-Ion Collider (EIC)
 - > Page 12 of <u>Requirements from nuclear physics experiments</u>
- Scope:
 - > Electro-nuclear models rely on Weizsacker-Williams approximation.
 - > Not sufficient for high-intensity and high precision electron scattering.
 - > The full, off-shell electron scattering vertex must be implemented for nucleons within the nuclear target.
- Responsible:
 - > Vladimir Grichine
- Status:
 - > Will be continued this year.
 - > New collaborator, Maurizio Ungaro (JLab), involved on this.
 - > Open.

5008 : Make EPICS2017 models (electrons, photons) as an alternative to Livermore

- Originator:
 - > General demand
 - > Page 11 of Requirements from Medical and bio science
- Scope:
 - EPICS2017 : Electron and Photon Interaction Cross Sections
 - Mention : these data supersede all earlier versions of the data libraries EADL, EEDL and EPDL
- Responsibles:
 - Sébastien Incerti, Claire Michelet
- Status:
 - > On-going in framework of thesis of Z. Li (CENBG/LP2I Bordeaux+CERN EM group)
 - Thesis will end in 2023
 - > Gamma models have been released, in the plan for this year for electrons
 - > Open.

5009 : Extend energy and material coverage of G4-DNA beyond DNA and liquid water

- Originator:
 - > General demand
 - Page 11 of <u>Requirements from Medical and bio science</u>
- Scope:
 - > Develop track structure models for specific materials (beyond liquid water and DNA)
 - > Extend energy coverage of existing models
 - Need to fill the gap from where DNA model stop (~100-500 keV) up to at least ~100 MeV.
- Responsible:
 - Sébastien Incerti
- Status:
 - > Gold G4-DNA model has been included in 11.0 beta release.
 - > Will be continued this year (with, eg, DNA bases + sugar/phosphate).
 - > Open.

5010 : Physics models for ions below 1 MeV/u for Boron Neutron Capture

- Originator:
 - > General demand
 - > Page 12 of Requirements from Medical and bio science
- Scope:
 - > Allows usage of Geant4 in BNC therapy field
- Responsible:
 - > Sébastien Incerti & Jose Ramos-Mendez (University of California, San Francisco)
- Status:
 - Work taken care by Naoki Domínguez (Ph.D. student at BUAP, México), and José Ramos (UCSF)
 - > In development since 2021, will be continued this year.
 - > Open.

5201 : To extend "force collision" biasing to charged particles

- Originator:
 - > NA62
- Scope:
 - > A "force collision" biasing scheme exists in Geant4, but is adapted to neutral particles.
 - NA62 uses a K+ beam
 - > A biasing with forced collisions for charged particles would allow for generating samples of useful statistics within a reasonable time to study the rare inelastic interactions in thin material in more detail.
 - > Space domain also expresses its interest for this (requirement session CM 2021)
- Responsible:
 - Marc Verderi
- Status:
 - > Will be continued this year.
 - > Open.

5202 : Precision versus speed optimized EM physics simulation configuration for ATLAS

- Originator:
 - > ATLAS, from 2020 LPCC workshop
- Scope:
 - > The most precise Geant4 (_EMZ) EM physics option provides more accurate simulation results in some cases (compared to the standard EM option). However, this precision gain comes at the expense of a significant increase of the simulation time.
 - > The goal is to find the EM physics configuration that provides the optimum in terms of computing time and simulation accuracy.
- Responsible:
 - > Mihaly Novak
- Status:
 - > Effort started in 2021, the related studies and optimizations are ongoing together with our ATLAS colleagues.
 - > On-going, complex task. Will continue in 2022
 - > Open.

5203 : Improve the inelastic cross sections of \overline{d} and anti_He3 at low energies (< 1-2 GeV/c).

- Originator:
 - > ALICE, from 2020 LPCC workshop
- Scope:
 - > Inelastic cross-section of anti-deuteron and anti_He3 is too low at low energies
 - > Likely, the same is needed for anti_triton and anti_alpha cross sections.
- Responsible:
 - Vladimir Uzhinsky
- Status:
 - > Started in 2021, will continue in 2022.
 - > Impact of war ?
 - > Open.

5301: Model for positronium (aka Ps) creation and annihilation

- Originator:
 - David Sarrut and Lydia Maigne, on behalf of GATE community
 - From CM2020 requirements session
- Scope:
 - > The e⁺ annihilation proceeds in tissue via Ps creation in > 40% cases
 - > Ortho-positronium (o-Ps; triplet spin state : s=1; m=-1,0,1) formed with 25% probability (in water)
 - Decay via 2γ (pickoff) or 3 γ (0.5% in tissue, 100% in vacuum)
 - $\langle \tau \rangle$ o-Ps maybe correlated with metabolic disorders ($\langle \tau \rangle$ depends on the size of the free volumes between atoms; varies from 142 ns in vacuum, down to below O(few10 ps) in matter).
 - > Feasibility study in Phys. Med. Biol. 64 (2019) 055017 to measure $\langle \tau \rangle$ using o-Ps $\rightarrow \gamma \gamma \gamma$ decay.
- Responsible:
 - Vladimir Ivanchenko
- Status:
 - > Some implementation already in 10.7
 - 3-γ annihilation is available in G4EmStandardPhysicsWVI Physics List
 - > One person now working on the topic
 - > Open

5302 : Extended example to directly retrieve Auger e- E & associated atomic transition

• Originator:

- Alfonso Mantero
- > From CM2020 requirements session
- Scope:
 - > Have better/complete "MC truth" information for these emissions
- Responsible:
 - > Susanna Guatelli
- Status:
 - > In the work plan for this year to add a model sub-type
 - which will make it easy to identify Auger electrons.
 - Seeking for a student to work on the topic
 - > Open

5303 : GIDI - LEND Models : install new GIDI when ready & validate with updated LEND

- Originator:
 - From CM2020 requirements session
- Scope:
 - Future of high precision neutrons looks like it will be GND (Generalized Nuclear Data)
 - New & simpler data format (will replace ENDF) & includes low- to medium-energy nuclear data
 - however, not as complete as ENDF
 - > Current LEND models in Geant4 are based on this
 - GIDI (General Interaction Data Interface) = interface between GND data and LEND physics models
 - Written in C
 - Many bugs uncovered by users and LEND validation effort
 - Livermore is writing a new, redesigned version in C++
 - > Makes this available when ready
- Responsible:
 - Alberto Ribon
- Status:
 - > Was in the plan of work for 2021, but it is often postponed
 - > Livermore got some grant to work on this year
 - > Open

Requirements pending because of "Lack of resources"

Valid requirements, but no resources to address them

- 5305, "Fix overproduction of n and p near endpoints of reactions at 4.5 GeV"
- 5304, "Beta-delayed Neutrons : develop understanding of highly excited level densities in nucleus and model neutron decay from this region"
- 5005, "Neutron self-shielding effect"
- 4005, "Neutron production in muon showers at the %-level"
- 4001, "Anti-proton production from proton beam (Mu2e request)"
- Ontribution/resources welcome to address these requirements !