Simulation Work Plan for 2025

Alberto Ribon
CERN EP-SFT
On behalf of the Simulation team

CERN EP-SFT group meeting, 22 January 2025

Outline

- Highlights of the Simulation achievements in 2024
  - Part of these have been included in the latest Geant4 release, 11.3 (December 2024)

- **Program of Work for 2025**
  - **Focus on HEP domain and EP-SFT team**
    - The full version will be presented to the users in a dedicated Geant4 Technical Forum (in March/April)

Notes

- *Fast Simulation will be covered in ML4EP by Lorenzo Moneta*
- *A large fraction of the work goes to support, and regular testing & validation, which do not appear in the work program!*
- *Names are present only in the achievements*

Project Purpose

- Provide support for the Geant4 **detector simulations** of the CERN experiments and projects
  - According to the Lab's priorities : **LHC experiments**, fixed-target experiments, future colliders, *etc.*
- Contribute to the development and maintenance of the **Geant4 toolkit**
  - Large, **international** and **multi-science** effort

Project Objectives

- Objectives and priorities driven by **user needs**
  - Often via explicit requirements, sometimes anticipated by us
- We strive for **better Geant4 detector simulations**, in all aspects:
  - More accurate physics models
    - Always useful, even when not used in production, for clarifying open physics issues, as well as for tuning/training fast simulation
    - With an extended physics validation program
  - Faster, more robust/reliable, smaller memory footprint
  - Capable of more things and covering more use-cases
  - Easier to use

1st Part

Highlights of Achievements in 2024 (part of these are included in G4 11.3)

Geometry

- VecGeom bounded-surface based modeller *(S. Diederichs, A. Gheata, J. Gonzalez)*
  - Portable, with CUDA/GPU first target
  - Prototype grew to working model for complex, experiment-level geometries
  - Multiple optimisation techniques adapted; now performance is competitive with solid model (for both simple and complex set-ups)
  - Identified path for further optimisations
- Parallelisation of voxel creation during geometry initialisation *(J. Apostolakis)*
  - Parallelised over logical volumes, using threads/tasks
- Revision of *G4GenericTrap* *(E. Tcherniaev)*
  - Main Geant4 solid used to replace the ATLAS custom solid for the EMEC
- New ‘builder’ method to initialise field classes *(I. Hrivnacova)*
  - Includes new UI commands to change propagation parameters
    - Originally developed in ALICE

Electromagnetic Physics

- Revised initialisation of EM tables and data structures *(V. Ivanchenko)*
  - To make them thread safe, as a necessary condition towards the parallelisation of the initialisation of physics, expected for 2025 (G4 11.4)
- EM physics for transporting exotic charged particles *(V. Ivanchenko, A. Ribon)*
  - As required by ATLAS and LHCb, ionisation and multiple scattering (as well transportation in magnetic field and decay) are included for charged particles with well defined PDG code but unknown to Geant4
- Positron annihilation into 3 gammas, and positronium production and decay *(J. Allison, D. Bernard, I. Semeniouk – H.T. Hong, V. Ivanchenko)*
  - In-flight positron annihilation is relevant for HEP: it may affect EM shower shapes at the per-mille level
  - Creation of positronium at-rest is relevant for medical applications (PET)
- Extension of models and examples for channeling *(A. Sytov)*

G4HepEm

Specialised EM physics library for electron, gamma and positron for HEP (CPU & GPUs)

- Completed the needed extensions *(M. Novak, J. Hahnfeld)*
  - To provide the full functionality of native Geant4 electromagnetic physics
    - Configuration per detector region (*e.g.* multiple scattering for CMS)
    - Gamma / electron / positron – nuclear interactions
  - To gain extra computing performances
    - Data re-structuring (*e.g.* of the macroscopic cross sections)
    - “General Process”-like handling of macroscopic cross sections
    - Woodcock tracking for gamma particles
  - To maintain the GPU support of the library for AdePT

Very promising speed-up observed in initial ATLAS tests: stay tuned!

Hadronic Physics

- Refined hadronic datasets and low-energy hadronic models for detailed investigations of hadronic observables
  - New hadronic datasets *(L. Desorgher)*
    - Updated with latest ENSDF (Evaluated Nuclear Structure Data File) data from March 2024
    - More consistent treatment of nuclides with incomplete information, and with fewer unphysical nuclear states => thanks to these datasets, closed already a number of open bugs
  - Improved simulation of low-energy neutrons *(M. Zmeskal, L. Thulliez)*
    - Included the possibility (off by default) to treat the Unresolved Resonance Region (URR) by Particle Tables (PT) for low-energy (< 20 MeV) neutrons, relevant for more precise simulations of nuclear reactor criticality and shielding applications
    - Making Geant4 another step closer to MCNP and TRIPOLI − reference codes for neutronics
  - New alternative nuclear de-excitation model (NuDEX) *(E. Mendoza, D. Cano)*
    - Optional, more sophisticated model, useful for precise simulations of nuclear reactions in particular concerning the emissions of gammas and internal conversion electrons

Fluka-Cern and Geant4 integration

Since G4 11.2 (2023), interface to Fortran Fluka-Cern available for Geant4 applications to get inelastic cross sections and final states

- Understood some disagreements between Geant4 and Fluka-Cern
  - Due to the different **quasi-elastic** treatment: considered as *inelastic* (in Geant4) vs. *elastic* (in Fluka)
  - Fixed bug in the interface, related to the rotation of final-state particles
- Evaluating possible extensions (elastic, ion-ion, gamma/lepton-nuclear, *etc.*)
- Areas of common interest − where resources could be shared
  - Physics validation
  - Hadronic datasets
  - Low-energy neutrons
  - Very high-energy (above a few TeV in Lab frame) hadronic models
- Progress towards Fluka-Cern 5 (C++, compatible with Geant4)
  - Ready new C++ point-wise low-energy neutron treatment
  - On-going migration of the nuclear de-excitation models

geant-val.cern.ch

- Key validation tool for Geant4
  - *geant-val* is essential for validating Geant4 simulations across multiple areas, including electromagnetic and hadronic physics
- Sustained development efforts *(D. Konstantinov)*
  - Continuous work is underway to maintain, improve, and run *geant-val*
- Recent test integrations
  - CMS HGCal calorimeter test-beam *(L. Pezzotti)*
    - This test expands *geant-val*'s reach in calorimeter validation, as well as supports GPU R&D initiatives AdePT and Celeritas
  - Low-energy neutron benchmarks *(L. Thulliez, M. Zmeskal, D. Konstantinov)*
    - New tests are being integrated, primarily through comparisons with the reference codes MCNP and TRIPOLI
    - These demonstrate the value of non-experimental tests

Kernel

- First prototype of task-based sub-event level parallelism *(M. Asai)*
  - Event split in sub-events, with automatic merging of the hits at the end of the event
    - In “Phase I” (*i.e.* already included in G4 11.3): all tasks have the same physics processes and see the same detector geometry
      - Useful for large events, *e.g.* heavy-ion collisions
      - Example in *examples/extended/runAndEvent/RE03*
    - In “Phase II” (*i.e.* after G4 11.3): each task has only the necessary physics processes and see the limited detector geometry which are needed for that particular task
      - Useful for heterogeneous simulation

Note: the threading model of Geant4 has been stable since its introduction with G4 10.0 (2013), from sequential to multi-threading (always keeping backward-compatibility with pure sequential mode) and with the addition of tasking in G4 11.0 (2021), as an alternative parallelism approach.
The introduction of sub-event parallelism is not going to change the threading model, and will be optional.

AdePT (**A**ccelerator **d**emonstrator of **e**lectromagnetic **P**article **T**ransport)

- Progress on the surface model *(S. Diederichs, A. Gheata, J. Gonzalez Caminero)*
  - **All solids relevant for LHC are supported**
    - CMS (2018, 2026), CMS HGCal test-beam, LHCb ECal & HCal, LHCb upgrade, ATLAS EMEC, *etc*.
  - Treatment of geometry overlaps (which are more problematic for surface model)
  - Performance of the surface model competitive with the solid model
    - On-going optimization of relocation, safety calculations and investigation of mixed precision
- Various developments *(S. Diederichs, A. Gheata, J. Gonzalez, S. Hagebock, W. Pokorski)*
  - Common interface between AdePT and Celeritas for integration in Geant4 applications and frameworks
  - Refactoring of AdePT into a library
  - New method of integration on Geant4 (based on specialised tracking manager), and new scoring
  - Asynchronous kernel scheduling
- Integration with experiments *(S. Diederichs, A. Gheata, J. Gonzalez, W. Pokorski)*
  - Hackathon dedicated to the integration of AdePT & Celeritas in the ATLAS software framework
  - On-going integration of AdePT in LHCb Gaussino (simulation software framework)
- Geant4 delta-assessment of AdePT & Celeritas postponed to March 2025
  - Check-point of these projects, likely the last one by Geant4

2nd Part

Work Plan for 2025

Geometry

- Main goal / effort
  - Finalise the first version of the VecGeom surface-based modeller for overlap-free setups
    - Targets: AdePT, portable GPU support
  - Further improve stability and performance
- Intermediate effort goals
  - Extend and improve parallel geometry initialisation (creates voxels)
  - Parallelise overlap checking (first implementation)
  - Investigate re-implementation of Navigation History (for memory and speed)
  - Improve implementation of QSS integration method *(tbc - University of Buenos Aires team)*
- Ongoing effort, fixes, maintenance, refinement
  - Improve robustness, performance of selected Geant4 solids (for LHC production use)
  - Aid to improve description of complex experiment setups (based on need, opportunity, resources)
  - Improve default values of parameters for field propagation and adopt these defaults in new ‘builder’/UI way

Electromagnetic Physics (1/2)

- Optimisation of CMS HGCal simulation
- General infrastructure
  - Parallel initialisation of physics
    - For limited number of particles: γ, e-, e+, μ-, μ+, and others
  - Possibility to switch off energy-loss fluctuation per-region
- Standard, muons, and low-energy
  - Implement electron bremsstrahlung on atomic electrons
  - Extend angular generators for EM models
  - For muons, try to use new 5D e+e- pair production generators
    - Compare them with the default model
  - EPICS-2017 cross section for the Compton as an alternative
- X-rays and optical
  - Refine design of X-ray production processes − Cerenkov and Scintillation
    - With new examples
  - Redesign optical surface handling

Electromagnetic Physics (2/2)

- G4HepEm
  - Completing the integration into the experimental frameworks (ATLAS, CMS, *etc.*)
    - Including the physics validation and the evaluation of the performance gain
  - Publishing a paper on G4HepEm, including the results
  - Keep supporting AdePT
    - To use of G4HepEm on GPUs

Hadronic Physics (1/2)

- Review of Birks' treatment in hadronic calorimeters to take into account the interplay between string (FTF) and intra-nuclear cascade (BERT) models
  - To tackle an issue (lower energy response at low energies) reported by ATLAS TileCal test-beam
- Validation and refinement of strange and charm particle production of string models (FTF and QGS) in hadron-nucleus and nucleus-nucleus interactions
  - To improve the description of thin-target data
  - Extend the physics validation tests
- Exploring different approaches for nuclear de-excitation
  - Ordering and threshold between PreCompound and MultiFragmentation
  - Can impact hadronic showers
- Continue the development of the charge exchange model
  - Critical process for NA64

Hadronic Physics (2/2)

- Refinements of the latest hadronic datasets (released in G4 11.3)
  - To have a more consistent treatment of nuclear fragments
  - Relevant mostly for nuclear and medical physics
- ParticleHP (*i.e.* low-energy − below 20 MeV kinetic energy − neutrons)
  - Introduce cross sections at fixed temperature (to avoid on-the-fly Doppler broadening from 0 K cross sections, which is computationally expensive)
  - Continue the alternative software implementation of the ParticleHP package

- Utilise regularly the validation and testing suite to monitor development
- Maintenance and update of the infrastructure
- Keep extending its coverage
  - Adding/updating/refining calorimeter test-beam set-ups
  - Completing the low-energy neutron benchmarks, recently introduced
  - Importing experiment-specific Geant4 validation tests
    - Long-term effort aimed to accelerate the adoption of new Geant4 versions for large production
- Review of the code for all tests, making them more consistent
  - Long-term work

Kernel

- Consolidation of the sub-event parallelism *(M. Asai)*
  - Check rare race conditions, unexpected performance bottleneck, *etc.*
  - Start developing the infrastructure needed for the “Phase II”
    - Each task can have different physics and see different detector geometry
    - Completion of “Phase II” expected after 11.4

AdePT

- Performance
  - Finalise the asynchronous kernel scheduling
  - Improve and evaluate the split-kernel approach
  - Accelerate the Runge-Kutta magnetic field integrator
- Adding features
  - Add missing information as required by experiments (MC truth, vertex information, *etc.*)
  - Add handling of gamma/electron/positron-nuclear reactions
  - Add an extended continuous integration
- Integration into experiments
  - Validate physics in Gaussino and Athena (and potentially CMSSW in the future)
  - Achieve comparability against full production simulations
- Benchmarks and preparation for the project assessment on March 26th- 27th
- If sufficient level of maturity is reached, write proper publication

Thanks for your attention!

Team (as of today)

- Staffs
  - John Apostolakis, Gabriele Cosmo, Andrea Dell'Acqua, Andrei Gheata, Mihaly Novak, Witek Pokorski, Alberto Ribon, Anna Zaborowska
- Fellows
  - Severin Diederichs, Juan Gonzalez Caminero, Peter McKeown, Piyush Raikwar
- Associates and visitors
  - Alexandre Bagulya, Aida Galoyan, Vladimir Grichine, Vladimir Ivanchenko, Dmitri Konstantinov, Lorenzo Pezzotti, Evgueni Tcherniaev, Vladimir Uzhinsky