A perspective on detector simulations as done by (smaller) HEP experiments (and related challenges)

Krzysztof Genser/Fermilab

Software and Computing for Small HEP Experiments

Snowmass21 Computational Frontier Workshop

November 16, 2021

Outline/Acknowledgments

- Introduction/Geant4 and other packages used
- Geant4 development cycle & Physics Lists
- Observations and comments
- Selected Geant4 open requirements
- Selected R&D activities
- Varying Geant4 model parameters
- Selected highlights of Geant4 v11
- Places where to find/share/discuss information about detector simulations
- Summary and comments

This talk is based in part on the information and input collected for the "requirements" and other talks (see acknowledgments in them) given at several recent Geant4 collaboration meetings, as well as Geant4 documentation and training materials, available from https://geant4.web.cern.ch

Comments/opinions are mine

I have been involved in Geant4 integration/deployment, support and development for more than last ten years

Introduction

- While HEP experiments use variety of tools to perform detector simulations, Geant4 is a tool used by all of them for at least some aspects of those simulations
  - Simulations are used both at the design and analysis stages
- Geant4 may be augmented by other physics packages, such as NEST, G4CMP, Opticks or geometry related packages e.g., VecGeom, CADMesh, with GDML usually used to exchange geometry/material information among software components (with DD4hep starting to used)
- Other packages, such as FLUKA, MARS, MCNP, are used as well (e.g., to crosscheck Geant4 results, or to make specialized calculations)
- Many experiments extend or replace Geant4 models with private/specialized code

Geant4 usage by neutrino, rare process & precision measurements and cosmic frontier experiments

- The versions of Geant4 currently in use or being commissioned for use (sometimes with patches developed by experiments) (with the date of the main and patch release)
  - 10.7.p02 (2020/12/04, 2021/06/11)
  - 10.6.p03 (2019/12/06, 2020/11/06)
  - 10.6.p01 (2019/12/06, 2020/02/14)
  - 10.5.p01 (2018/12/07, 2019/04/17)
  - 10.4.p02 (2017/12/08, 2018/05/25)
  - 10.3.p03 (2016/12/09, 2017/10/20)
  - 10.3.p02 (2016/12/09, 2017/07/27)
  - 10.1.p03 (2014/12/05, 2016/02/05)
  - Most experiments use Geant4 in the sequential mode, a small number of experiments runs in the MT mode (saves memory, as geometry and x-sections are shared among threads)
- Physics list used by the experiments
  - FTFP_BERT, QGSP_BERT, QGSP_BERT_HP, QGSP_BERT_EMZ, QGSP_BIC_HP_LIV, Shielding(M),
  - plus, custom lists based on the above that add optical processes, LEND and augment Geant4 with additional packages, e.g., NEST, G4CMP, Opticks

Geant4 development cycle

- Geant4 has been released on a yearly basis for many years now
  - With the yearly release in December, beta/preview release in June
  - A few patch releases occur per year for (predominantly most recent) previous releases
    - Patch releases are meant to correct the code, not to introduce new features
- Geant4 API is kept backward compatible for the minor versions (as in Major.Minor)
  - API can be expanded, but not changed for minor releases
  - API can change for major releases
    - The changes are usually small and mostly driven by code improvements and optimizations
- While the API is kept stable, *the internal code evolves significantly*, even during the years when only minor releases occur
- Newer versions are more accurate, more efficient and offer more flexibility (e.g., new/better models, faster field steppers, better pRNGs, better configurability options/ability to vary parameters; with the code being incrementally faster and using hardware more efficiently)

Geant4 Physics Lists

- Physics List specifies particles to be used and processes assigned to each individual particle
- Prepackaged, so-called reference physics lists are available, including a group of production level physics lists which are well documented, maintained, validated and changed more conservatively; They, among others, include
  - FTFP_BERT - the recommended list for most HEP experiments
  - QGSP_BERT - the previously recommended list
  - QGSP_BIC - typically used in medical applications together with more accurate electromagnetic physics options
  - Shielding - often used in shielding applications (it uses more accurate low energy neutron transport and enables radioactive decays among other additions)

Geant4 Physics Lists (cont'd)

- Most physics list names are derived from the names of the hadronic inelastic model used, going from high to low energies, optionally followed by the name of a higher precision neutron transport package and electromagnetic option name;   below are some names appearing in the lists used by the experiments mentioned earlier
  - High energy models: QGS - Quark Gluon String (above ~12GeV), FTF - Fritiof String, (above ~3GeV)
  - Intermediate energy models, below ~10 GeV: BERT - Bertini-like Intranuclear Cascade, BIC - Binary (also Ion) Cascade
  - P - Precompund/De-excitation model used to de-excite the remnant nucleus
  - Low energy neutron/particle transport: HP, LEND
  - Electromagnetic physics options, e.g., EMZ - uses the most accurate EM models (as opposed to "default" EM models used in other lists), LIV - uses Livermore models for some EM processes

- Note that while not explicitly spelled out in some lists, Bertini and FTF models are used in all lists mentioned above (at least for some of the particles); Other models exist, e.g., INCL (another Intranuclear Cascade model used instead of the Bertini model in some physics lists)

Interfacing with Event Generators

- Primary events are often simulated with external event generators interfaced with Geant4
- The generators can also be interfaced with Geant4 to assure model consistency (e.g., GENIE - Geant4 Bertini intra nuclear cascade) or for enabling certain (e.g., charm, tau) decays, or consistency thereof (GEANT4 - PYTHIA8)
  - An example demonstrating the latter to be available in the upcoming Geant4 v11 release

Observations/comments regarding Geant4 use

- There are many Geant4 versions in use
  - This poses a support challenge
- Some experiments use quite old versions of Geant4
  - It makes it harder to address new Geant4 related needs of such experiments
  - While there are many constraints on experiments upgrading versions of Geant4, at some point benefits of using newer version start to prevail
    - An upgrade at least every few years should be an integral element of the simulation plans
- Some experiments hardcode their own solutions, copying fragments of the Geant4 code and not using the official API
  - It is one of the reasons why it is difficult for such experiments to upgrade to newer versions of Geant4 since Geant4 internals evolve
  - A better alternative is to work with the Geant4 Collaboration to develop new code as a part of the Geant4 toolkit
    - A successful collaboration/co-development model is when a person is a member of an experiment and the Geant4 Collaboration, e.g., working on a Geant4 aspect used/needed(and tested while being developed) by the specific experiment
      - Experiments employing such a model tend to use newer versions of Geant4 and benefit more from the ongoing improvements
    - A currently being introduced *Geant4 contributor status* should lower the threshold for such a collaboration
- It is beneficial to have experiment's Geant4 related code being implemented by (or under the guidance of) a person very knowledgeable about Geant4 and aware of its internals and evolution plans
  - One needs to take into account the fact that learning Geant4 takes a long time, and that one needs to keep that knowledge up-to-date as Geant4 evolves

Some related, open Geant4 requirements https://jira-geant4.kek.jp/projects/UR

- UR-28 Anti-proton production from proton beam
  - Correct the discrepancy in anti-proton production for proton beam at about 10 GeV on various targets
    - Currently no manpower to implement it, but important
- UR-49 Neutron self-shielding effect
  - Neutron flux through a material can be significantly modified when the 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 different background flux (a ~10% effect)
  - Accepted as a valid requirement, currently no manpower to implement it
- UR-50 Improve simulation of gamma induced neutron background
  - Low energy gammas producing neutrons in various materials can be a significant background
    - Photo-nuclear process does not model this well below 30 MeV
      - An improved process using the G4LEND gamma models is required
  - Accepted as a valid requirement
    - In ShieldingLEND physics list since 10.4/10.5
      - Below 20 MeV
    - Careful verification of code aspects in various areas needed

- While many requirements have been fulfilled or became part of the working group work plans, there are some which (are very old and) have no or little manpower assigned to them

More on physics requirements

- As new experiments are designed and come online, more accurate (and often new) models are required
  - There is a constant need to improve old models and introduce new ones, handling new processes
  - Some recent requests (not in the requirements system yet):
    - Ability to perform fast (and accurate) simulations of optical photon processes (i.e., have Opticks integrated with Geant4)
    - A(n external) decayer handling taus (including the polarization aspect)
    - Charm production and decays (in order to model the tau neutrino component of the beam)
    - Propagation of polarized muons and taus in dense media
    - Ability to adjust parameters of pion inelastic process and obtain more information about its intermediate states
    - Improved pbar annihilation process, including being able to affect the nuclear destruction process at energy below 2GeV;
    - Address an observed excess ratio of pi-/pi+ in p W reaction, when using Bertini cascade
    - A symplectic stepper

R&D efforts to develop code to run on GPU/HPC(I)

- To address the need to speed up simulations and utilize new computing hardware hardware, R&D efforts are undertaken to accelerate Geant4 execution by targeting the most compute intensive parts: i.e., EM processes and optical photons

- G4HepEm - R&D project to make e–/e+/gamma transport faster by restructuring, specializing and separating underlying libraries, targeting optimization of execution on CPU as well as on GPU
  - https://github.com/mnovak42/g4hepem, https://indico.cern.ch/event/1052654/contributions/4524767

- AdePT (Accelerated demonstrator for electromagnetic Particle Transport) - R&D project to transport e–/e+/gammas on GPUs
  - Makes use of G4HepEM and VecGeom which is also being redesigned to improve its GPU performance
  - https://github.com/apt-sim/AdePT, https://indico.cern.ch/event/1052654/contributions/4525306

- AdePT is being integrated with Geant4 to offload processing of e–/e+/gamma to GPUs
  - https://indico.cern.ch/event/1052654/contributions/4525308

R&D efforts to develop code to run on GPU/HPC(II)

- Celeritas
  - HPC/GPU-targeted re-implementation of a subset of Geant4 physics leveraging both HEP physics community and HPC/GPU particle transport domain knowledge
  - Short-term goal: offloading EM tracks from Geant4 to GPU through a bridge library
  - Long-term goal: direct access library for higher performance integration into LHC/HEP workflows

  - For more info see: https://github.com/celeritas-project and talks
    - https://indico.cern.ch/event/948465/contributions/4324114
    - https://indico.cern.ch/event/1019940/#4-celeritas-status-plan

R&D efforts to develop code to run on GPU/HPC(III)

- Opticks integration with (most recent version of) Geant4
  - Opticks is a GPU Accelerated Optical Photon Simulation using NVIDIA OptiX GPU ray tracing library
    - Fast simulation, eliminating the use of pre-generated photon lookup tables
    - https://bitbucket.org/simoncblyth/opticks
    - https://doi.org/10.1051/epjconf/20192140202
  - A Geant4 advanced example (called CaTS) is to be released as a part of Geant4 v11, allowing to use either Geant4 or Optics to simulate optical photons
    - Integrating Opticks (v0.1.6) with Geant4 (v10.7.p02) for concurrent processing of optical photons on the GPU while performing the rest of the simulation on the CPU
    - Small changes to Geant4 v10.7 API were introduced as needed
      - Another small set of changes was made to Opticks/CaTS to make it work with the upcoming Geant4 v11 (to accommodate API evolution)
    - See, e.g., https://indico.cern.ch/event/1052654/contributions/4525304
    - To be followed by more changes to Opticks (model/material properties) to accommodate Geant4 improvements and by implementation of additional process (e.g., WLS)
      - And then by integration with LArSoft

Study varying Geant4 model parameters

- An effort to improve Geant4 physics models' agreement with data and to provide ways to estimate simulation systematic uncertainties by varying model parameters is ongoing
  - One of the conclusions of an early study of the impact of varying of (some) parameters of hadronic models (Bertini, PreCompound, FTF)
    - ”varying parameters produces substantially better agreement with some datasets, but that more degrees of freedom are required for full agreement”
      - See: GEANT4 Parameter Tuning Using Professor, V. Elvira, at al., JINST 15 (2020) 02, P02025
  - Note that the Bertini model is currently not being actively developed due to the lack of manpower

Selected highlights of the upcoming Geant4 v11 scheduled for December 10th

- Tasking
  - A more flexible approach to multithreading, enabling sub event parallelism and a way to enable hybrid computing
- G4HepEm
- Updated VecGeom, including navigation features and more geometrical shapes
- C++17 will be the minimum standard required
- Examples showing Opticks & Pythia8 integration
  - (Another example of the latter also is available in LArSoft)

- BTW: v10.7.p03 is to be released this week
- The complete details of both releases are to be presented at the to be announced Geant4 Technical Forum (see next page)

Fora to learn about and discuss simulation tools, share experiences and voice requirements

- HSF Detector Simulation Working Group
  - Presentations and discussions related to Detector Simulations
  - https://hepsoftwarefoundation.org/workinggroups/detsim.html

- Geant4 (main link: https://geant4.web.cern.ch)
  - Geant4 Technical Forum
    - A place where new releases are described, work plans and user requirements/experiences presented
    - https://geant4.web.cern.ch/collaboration/technical_forum
  - Geant4 User Forum https://geant4-forum.web.cern.ch
  - Geant4 Bug Report System https://bugzilla-geant4.kek.jp
  - Geant4 documentation (follow the main link above)

- Snowmass 21 Detector and Beam Simulations subdomain of the Computational Frontier
  - Subscribe to SNOWMASS-COMPF02-DETBEAMLNSIM
  - Some topics related to this talk are also mentioned in this CompF2 LOI
    - https://www.snowmass21.org/docs/files/summaries/CompF/SNOWMASS21-CompF2_CompF1_Pascuzzi-119.pdf

Summary and additional comments

- Geant4 has been successfully used to design HEP experiments and analyze their data for many years now
  - To assure the high quality of the current and future experimental results, *continuous* development of Geant4 models and code is needed
    - This implies the need for continuous, *long-term support*, recruitment, training and retention of both Geant4 developers and Geant4 users writing related code for experiments;
      - See similar remarks e.g., in [Challenges in Monte Carlo Event Generator Software for High-Luminosity LHC]
- Some requirements, in particular those related to more rare physics processes, even though deemed important, do not currently have people assigned to work on them. More requirements are in the pipeline
- Some heavily relied on models, and detailed models of some more rare processes, are currently not (or not actively) being developed
- As computing architectures evolve, so must the code which runs on them
  - Efforts to write the corresponding code are underway
- Efforts to enable estimation of systematic uncertainties and adjusting Geant4 parameters are undertaken
- Both Geant4 and packages used together with it must be continuously co-developed in response to new requirements and new (hardware and software) environments
  - This again requires long term and continuous support of people developing such packages
- Tightening the collaboration among HEP experiments and Geant4 Collaboration is always welcome, appreciated and, in the past, has led to many Geant4 enhancements benefiting then current and subsequent experiments
  - This also applies to the groups developing packages used together with Geant4
  - The currently being introduced *Geant4 contributor status* should make it easier to collaborate
  - It may also help in experiments using newer versions of Geant4 and benefiting from ongoing improvements

- See the previous page for selected places to obtain or exchange detector simulation related information including the upcoming Geant4 v11 release

Additional Slides

NEST - Noble Element Simulation Technique

a symphony of scintillation

- Adapted from https://nest.physics.ucdavis.edu
  – See references therein
  – Also see: https://indico.cern.ch/event/1009384/#2-nest-noble-element-simulatio
- Comprehensive, accurate, and precise simulation of the excitation, ionization, and corresponding scintillation and electroluminescence processes in liquid noble elements, verified against a long list of past experimental results
  – Providing robust calculation of the scintillation and ionization yields using empirical models which take into account the energy and field dependence, as well as the intrinsic fluctuations and recombination physics.

G4CMP - Condensed Matter Physics for Geant4

- Slide based on: https://indico.cern.ch/event/1016632/#2-simulating-solid-state-micro, also see: https://github.com/kelseymh/G4CMP

- Transport of eV-scale (conduction band) electrons and holes in crystals
  - Anisotropic transport of electrons
  - Scattering, phonon emission (NTL), trapping
- Transport of meV-scale (acoustic) phonons in deeply cryogenic crystals
  - Mode-specific relationship between wavevector and group velocity
  - Impurity scattering (mode mixing), anharmonic decays
- Production of electron/hole pairs and phonons from energy deposits
- Utility classes to support detector response
  - Finite-element mesh electric fields (2D and 3D)
  - Phonon absorption, detection in superconducting films