Detector Simulation

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Outline/Acknowledgments

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This talk is based in on the following white paper:

“Detector and Beamline Simulation for Next-Generation High Energy Physics Experiments”
https://arxiv.org/abs/2203.07614

See the details, list of co-authors, references and acknowledgements therein

Thank you to all who contributed to the paper

Apologies for omitting some items due to the time limit imposed on this talk

Introduction/Simulation needs and their drivers

- Detector simulations are necessary in the design of new detectors and HEP facilities, in the development of reconstruction algorithms and validation and interpretation of experimental results

- Physics-Related Needs
  - Are driven by complexity of detectors, increasing size of datasets, higher precision measurements and attempts to measure rarer processes
    - Result in the demand for more accurate simulations and larger numbers of simulated events, additional and more complete physics models
      - including those used to model beam interactions with thick targets to describe secondary beam production
- Some experiments need significant speed-ups of detector simulation and drive the development of e.g., parameterized or machine-learned models

Simulation needs and their drivers (cont'd)

- Computing Hardware Evolution
  - Imposes new constraints on the way the simulations can and need to be performed, forcing the simulation software, algorithms, and techniques to also evolve in order to allow for the efficient use of the available computing infrastructure where CPUs are accompanied by more and more GPUs, FPGAs, and other hardware accelerators

Current simulation tools and the central role played by Geant4

- While HEP experiments use variety of tools to perform detector simulations, Geant4 is a toolkit used by most, if not all of them and has become a de-facto standard for many aspects of the HEP detector simulations
- Geant4 may be augmented by other physics packages, such as G4CMP, NEST, Opticks or geometry related packages— (e.g., VecGeom, CADMesh, GDML, DD4hep)
- Other packages, such as FLUKA, MARS, and MCNP, are also used e.g., to crosscheck Geant4 results or to make specialized calculations

Current simulation tools and the central role played by Geant4 (cont'd)

- While Geant4 fulfills most of the current needs, and is supported by a worldwide collaboration, it is being pushed to its limits by new experiments and changing computing hardware
  - To address missing Geant4 features, many experiments extend or replace Geant4 models with specialized code
    - Most such developments are needed for experiments outside of the Energy Frontier for which Geant4 had predominantly been developed initially

Extending Geant4 by interfacing other packages with it

The packages used to enhance Geant4 capabilities include:

- G4CMP – a Condensed Matter Physics for Geant4 package, which, among other features, models the production of electron-hole pairs and phonons from energy deposits and the subsequent transport and interactions of the produced objects
- NEST – the Noble Element Simulation Technique package, that simulates excitation, ionization, and corresponding scintillation and electroluminescence in liquid noble elements
- Opticks – a GPU Accelerated Optical Photon Simulation using NVIDIA OptiX (GPU ray tracing library)
- PYTHIA 8 – a general purpose Monte Carlo event generator, that can also be interfaced with Geant4 to perform particle decays or to replace certain Geant4 decay tables to assure consistency when the two packages are used together

Most of such packages can be used standalone or as an extension of Geant4

This is in addition to event generator packages that are used to define primary particles for a given event

Other slightly different packages include, e.g.,

Geant4Reweight – a framework for evaluating and propagating uncertainties of Geant4 hadronic interactions

Some specific detector simulation needs - modeling of hadronic interactions

- New experiments, either reaching out to higher energies or searching for very rare processes, require improvements in the range, precision, and flexibility of the current models, as well as implementation of the new ones

- Experiments in which the beam energies require modeling of hadronic interactions below 10 GeV, rely predominantly on Geant4 models such as Bertini-like intranuclear cascade, Fritiof (FTF) string, Geant4 precompound, evaporation and breakup to simulate the relevant interactions
  - In a dedicated study it has been shown that e.g., the Bertini model needs more degrees of freedom and more work to describe the existing data
    - Unfortunately, despite being widely used, the model has not been actively developed over the last few years due to the lack of personpower

- All the above needs could be better addressed if additional personpower were available

Some specific detector simulation needs - performing dedicated measurements

- Physics model parameter studies and related model developments require experimental data that can be used to validate the models
  - One of recent examples of such data is a set of measurements of the negative pion total hadronic cross section on Argon performed by LArIAT (arXiv 2108.00040)
  - (ProtoDUNE plans to publish results on the hadron-Argon cross sections for positive pions, protons, and positive kaons)
  - Such measurements can be used to improve the modeling of hadron-Argon interactions
    - They help to reduce the simulation systematic uncertainties for the current and future neutrino experiments using LArTPCs, in particular the short- and long-baseline neutrino experiments at Fermilab
- Performing such measurements should be considered an integral part of the design process of new experiments, in order to be able to accurately simulate them and interpret their results

Specific R&D efforts addressing the needs

- Some US R&D activities:
  - Celeritas: a new GPU-optimized (targeting ATLAS and CMS) detector simulation code, including "Acceleritas", a direct Geant4 interface for offloading EM tracks to GPU
    - See the white paper https://arxiv.org/abs/2203.09467 and poster in the poster session https://indico.fnal.gov/event/22303/contributions/243736/
  - Simulating Optical Photons in HEP experiments on GPUs - an effort integrating current versions of Geant4 and Opticks into a hybrid CPU/GPU application (CaTS Geant4 extended example)
  - G4VMP - an activity to optimize Geant4 parameters and to enable estimating related systematic uncertainties
  - Proposal to investigate the interconnection of HPC systems for event simulation and task scheduling
- Two related European HEP efforts:
  - G4HepEm – an R&D project to make Geant4 electron/positron/gamma transport faster, targeting optimization of execution on CPU as well as on GPU
  - AdePT (Accelerated demonstrator for electromagnetic Particle Transport) – an R&D project to transport electron, positrons and gammas on GPUs; it makes use of G4HepEm and VecGeom, with the latter also being redesigned to improve its GPU performance; AdePT is being integrated with Geant4 to offload processing of electrons/positrons/gammas to GPUs
  - A very active communication occurs among Celeritas and Geant4/AdePT(G4HepEm) teams

Machine learning and fast simulations

- Machine learning (ML) is one of the most promising alternatives to traditional parameterization-based method
  - It can naturally be accelerated on coprocessors such as GPUs or FPGAs, utilizing the new computing hardware
  - However, it still requires computationally expensive training and validation, that needs to rely on some well-established simulation software like Geant4
  - Therefore, ML does not eliminate the need to improve the speed and fidelity of the existing detector simulation software and to make it run efficiently on modern computing hardware
- Please see e.g., this white paper https://arxiv.org/abs/2203.08806) the session on AI/ML Modern Machine Learning for HEP for information on using ML for detector simulation

Need for experts and their training - the “Human Challenge”

- Detector simulation tools require people to improve physics models, maintenance, modernizing code, and to adapt them to evolving computing environments, as well as for long-term support
- These efforts are not viable without comprehensive and intensive training of both application developers and end users
- Due to the long lifetimes of current and future HEP experiments, it is crucial to continuously recruit, train, and retain multidisciplinary teams of experts, and to create attractive career paths for people developing and maintaining the software.
- Continuous funding is required for High-Energy, Nuclear and Condensed Matter physicists as well as software developers working on simulation tools throughout the (long) life cycles of HEP software toolkits
- An example of the size of the size of the effort required: Geant4 is maintained by an almost 30-year-old collaboration of well more than 100 members (and more than 30 FTEs) distributed worldwide, serving a very diverse set of user domains

Summary (1/2)

- Detector simulations play a central role in the design of new detectors and facilities, in the development of reconstruction algorithms, as well as in the validation and interpretation of experimental results.
  - Geant4 and the packages used with it are the main simulations tools in use; Geant4 is also used as a de-facto standard when developing other simulation tools (e.g., ML-based)
- The main detector simulation needs are
  - The ability to adequately simulate all important physics processes, the speed and accuracy, and the ability to run and efficiently use the current and future computing hardware
- Dedicated measurements enabling validation of the physics models are needed to complement the software efforts

Summary (2/2)

- Several technical efforts are undertaken to address some of the needs
- The importance of detector simulation and the evolving requirements and changing computing hardware motivates the need to continuously develop and maintain the simulation software and Geant4 in particular
- Challenges facing the simulation community include concerning discontinuities and dormancy of some of the physics developments
- The magnitude of the human efforts needed to develop and support the main software simulation tools (necessary to successfully carry out the simulation tasks for the current and future US HEP experiments) is quite large and the efforts require adequate and uninterrupted funding