WG Charge and Scope

CWP WG: Simulation

Charge and scope:

Identify challenges and opportunities for full and fast simulation applications of HEP experiments, including modeling of detectors and beamlines, and establish a plan to address them. The components of a HEP simulation application are: MC truth, geometry, particle propagation in materials and fields, physics modeling, pileup and other backgrounds, digitization, analysis and monitoring tools. Anticipate the needs and plan for the associated software and physics support and training.

(Outside of scope elements: generators, event visualization, accelerator facilities other than experimental beamlines, space or medical applications)

Key challenges and opportunities

- Continuous maintenance, support and improvement of the Geant4 simulation toolkit with minimal API changes visible to the experiments at least until production versions of potentially alternative engines, such as GeantV, become available, integrated, and validated by experiments.
- Redesigning, developing, commissioning detector simulation toolkits to be more efficient when executed on emerging computing architectures (e.g SIMD vectorization, NUMA hierarchies, MIC/GPU offloading, tensor processing units, etc);
- exploring different fast simulation options, including common frameworks for fast tuning and validation, i.e. using machine learning (ML) techniques;
- porting and optimizing simulation applications, or developing new ones to allow exploitation of High Performance Computing facilities (HPC);

Key challenges and opportunities

- developing, improving, optimizing geometry tools (e.g. DD4HEP, USolids, VecGeom) which can be shared among experiments and software tools (Geant4, GeantV, ROOT) to make the modeling of complex detectors computationally more efficient, modular, transparent;

- enhancing the accuracy of the physics models for interaction of particles with matter embedded in detector simulation toolkits, in particular for the support of future physics programs;

- developing techniques for background modeling, including contributions of multiple hard interactions overlapping the event of interest in collider experiments (pile-up);

- revisiting digitization algorithms to improve performance by means of vectorization and sub-system parallelization techniques, and exploring opportunities for code sharing among experiments, i.e. LArSoft;

- recruiting, retaining, training human resources in all areas of expertise pertaining to the simulation domain, including software and physics.

Big ideas: Physics Modelling

LHC, IF experiments, and future programs need improvements to physics models in particle transport codes. Ongoing and future efforts to re-implement code to give better physics and computing performance. (Modular packages available for Geant4 and GeantV.)

- EM physics largest consumer of computing resources. Examples of processes being revisited or added: multiple-scattering, Bremsstrahlung , Landau-Pomeranchuk-Migdal effect.

- Hadronic physics: intermediate energies (Bertini, Binary, further development of the INCL++ model), evolution to a theory-based model (QGSP) seen as crucial for extrapolation to high energies, important for programs such as FCC, neutron interactions important for modeling of shower shapes.

- Neutrino experiments: ν-nucleus interactions in GENIE, G4 takes over for nuclear de-excitation and hadronisation – GENIE-G4 interfaces underway, validation/improvement of neutrino interactions in liquid argon. G4 predictions with systematic uncertainties from model parameters.

Big ideas: Fast Simulation

Fast simulation means different things for different experiments. There is consensus that future experiments will extend its use to adjust to the computing resources available.

- Parametrized simulation, separate from Geant4-based simulation, may share components such as geometry, fields. (Example: CMS.)
- Flexible integrated simulation framework that combines different techniques to provide optimal accuracy and speed. Mixture of G4 showers, GFLASH or other parametrizations, frozen showers depending on particle, energy range, detector region. (Example: ATLAS.)
- Framework that integrates Full and Fast Simulation to facilitate the tuning and validation of fast simulation with respect to full simulation. (Example: R&D in the context of GeantV.)
- Machine Learning techniques fast and accurate modeling of particle shower.

Big ideas: Software Performance

Exploit benefits of new software paradigms and computing architectures.

- Implement particle-level parallelization (track-level in Geant4 jargon) in particle transport engine.
- Use programming techniques such as instruction pipelining, SIMD explicit vectorization, data locality.
- Offload tasks to different computing architectures in a hybrid computing model, e.g. EM physics running on GPUs.
- Adapt and optimize simulation code to run in HPC facilities.

Basketization for track-level parallelization (GeantV), use of above-mentioned techniques to develop modular packages for use in Geant4 (scalar mode) and GeantV (vector mode). Examples are the VecGeom geometry package (delivered), EM physics package.

Big ideas: Other topics

- MC truth: challenge is to save MC truth information without memory and CPU overheads.
- Geometry : common shapes library (USolids), VecGeom (vectorized geometry and navigation), DD4HEP (full detector description).
- Readout modelling: expensive for TPC detectors (ALICE, DUNE), exploit SIMD vectorization and parallelism to speedup code - pending. The neutrino experiments' LArSoft framework allows sharing of digitization code among experiments. Digitization + pileup is computationally expensive.
- Pileup: I/O intensive, overlay of real zero-bias events brings trigger and ideal-to-real geometry association challenges – pending.
- Pseudorandom Number Generators, e.g. MIXMAX : ensure reproducibility in fine-grained parallel environment, while achieving high speed and quality of sequences – ongoing.

Practical Consideration for Progress in the WG Area

How will the proposed activities empower HEP physicists to get the most physics out of the experiments during the 2025-2035 era? What new physics capabilities might these bring?

Higher event throughput of simulated events with more accurate physics means better physics results, with smaller systematic uncertainties and higher BSM reach, within the available computing resources.

What are the proposed R&D activities over the next 5 years toward these applications?

R&D activities described before are underway in the context of Geant4, GeantV, and experimental programs.

Practical Consideration for Progress in the WG Area

How will the software be deployed by the experiments and sustained for the duration of the experimental programs?

In the case of the detector simulation tool kits, the G4 Collaboration has already established a mechanism of communication, interaction, collaboration with the experiments: technical forum, direct contribution to experiments, contact person responsibilities, support, etc. Nevertheless, improving communication and collaboration between experiments and toolkit developers is essential in order to understand needs and issues, and to prepare simulation to match future needs.

What is the likely impact that the techniques and applications will have on overcoming the challenges of experimental programs in the next 10 years?

The goal is to deliver simulation tools and event samples that meet or exceed expectations in what relates features and physics, within the available computing resources.

Practical Consideration for Progress in the WG Area

Are there risks associated with going in the direction of each of the proposed ideas/R&D? What are the associated costs and is the development and implementation realistic in this regard?

The R&D program is already delivering and exceeding expectations. Examples are VecGeom, and improved and new physics models. More prototyping is needed to demonstrate the benefits of track-level parallelization in particle transport. Large physics program of work to incorporate, improve, fixe physics models is not straightforward. Milestones are realistic with modular packages already delivered or underway, and the more revolutionary elements expected to be available within the timescale of the HL-LHC physics program.

Consolidation of existing person-power, and continuous support and funding from experiments and agencies are essential to ensure the success of the R&D programs and a timely delivery.

Commonality and Leveraging S&C beyond HEP domain

What are the opportunities for common tools across experiments in this WG area? What are the challenges and barriers to commonality?

Examples: Geant toolkit (used by most experiments), geometry packages (shape libraries, tools for detector implementation), math libraries (e.g. PRNG), databases and web interfaces to store validation data and data-to-MC comparison plots (DoSSIER used in Geant4, GeantV, potentially in GENIE), visualization packages.

Similar readout chips in future ATLAS, CMS trackers offer the possibility to share readout modeling code.

In what ways can this WG area leverage software and computing techniques and technologies outside of the traditional HEP domain (e.g. from industry and CS)?

Not studied in depth. Some examples are collaboration with Intel for optimization of machines for use in simulation, neutral network and Machine Learning software, differential equation solvers, math libraries (random number generators – MIXMAX), visualization tools.

High Performance Computing facilities, cloud computing services from industry will be used in addition of in-house (HEP) computing resources.

Cross-cutting Elements

What are the elements of your ideas and R&D that cut across other WGs? Which ones? Can synergistic activities be identified which would positively impact not only the area of this WG but also other WGs?

- Generators – interfaces a la HEPMC, tools for physics validation, regression testing, etc.
- Frameworks – multithreading, event model, consistent with simulation tool's engine.
- Reconstruction and analysis – Machine Learning techniques to be used in fast simulation.
- Visualization - visualization WG suggests to develop common tools for experiments for which we need common data exchange software for geometry and event data: a layer for common data plus experiment specific layers.

CWP Chapter Status and Plans

What is the status of the CWP Chapter? Are the key ideas and R&D in place?

- Large participation from most experiments and projects associated with detector simulation.
- The note contains more than 50 pages of detailed descriptions of the ongoing and planned activities.
- The key ideas are in place and so are most of the on-going R&D activities. There is no “CWP simulation plan or roadmap” although detailed plans exist within the experiments and projects and a large degree of collaboration among them already exists.
- Within the CWP initiative, a collaboration was established between ATLAS and CMS for an as-much-as-possible apples-to-apples comparison of the computing performance of the Geant4 module of their simulation applications.

CWP Chapter Status and Plans

How do you plan to complete your chapter?

We have a stand-alone Simulation White Paper (>50 pages) that needs some (significant) editing to read well. We suggest that every WG produces an executive summary (ES) 2-3 pages long, which describes the challenges and the elements of a plan for their domain.

The final CWP would be composed by merging the ES's from each WG, with the addition of introductions and other sections to link the chapters. We suggest that an ES template is provided to the WG's.

What do you expect to accomplish by the end of this workshop?

Executive Summary for the Simulation CWP. A final version of the simulation white paper will come at a later time. Need to incorporate comments, missing elements, input from LPPC-Simulation workshop.

Auxillary Material

Simulation WG: Primary Activities

Strong participation from projects (Geant4, GeantV) and experiments (ALICE, ATLAS, CMS, LHCb, muon and neutrino experiments), 44 subscribers to google group

Four meetings with large participation to discuss four topics:

- computing performance (https://indico.cern.ch/event/615703/);
- fast simulation (https://indico.cern.ch/event/623453/);
- geometry and readout modeling-digi/pileup (https://indico.cern.ch/event/627793/);
- Physics modeling (https://indico.cern.ch/event/635947/)

Simulation WG: Main Contributors

Conveners: D. Elvira, J. Harvey

Main contributors to the working group:

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Simulation white paper google document:
https://docs.google.com/document/d/1Qm8btmDti1dcu5G2FMez3J6FLyzv0k6fag0clD25JSo/edit?ts=58e343c1#heading=h.6w9orc8rysri