

# Full Simulation Group Report

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on behalf of the ATLAS Simulation Group

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Celeritas/Adept Hackathon

Geant4 Nightly Builds

Physics Stability

Improve I/O Robustness

Energy Loss Fluctuation

- **Description:** Integrate and test AdePT and Celeritas in Athena to achieve increase in events/seconds/Watt (14–18 Oct 2024)
- **Attendance:** 6-7 people from AdePT/Celeritas teams and 6-7 people from ATLAS
- **Completed Tasks:**
  - ▶ CPU-only build of Celeritas and G4HepEM in AthenaExternals
  - ▶ CUDA-enabled build of VecGeom, AdePT, Celeritas, G4HepEM in AthenaExternals
  - ▶ CPU/GPU-enabled builds linked into Athena
  - ▶ AdePT/Celeritas developers able to build on Perlmutter HPC/SFT GPU systems
  - ▶ Use of Celeritas Geant4 user actions to offload in Simulation
  - ▶ Use of AdePT G4VTrackingManager implementation to provide offload as a new ATLAS physics list (GPU-only)

Contact: Ben Morgan

## ■ Ongoing Tasks:

- ▶ Separate branches for CPU/GPU builds need unifying, so GPU enabled when CUDA available (disabled otherwise) following ATLAS practice in other areas
- ▶ Use LTO in VecGeom results in  $\gg 20$  min link times (limit not found)  $\rightarrow$  not triaged further
- ▶ Offload using Celeritas G4VTrackingManager ala AdePT (requires some technical work in Celeritas on initialization/event boundaries)
- ▶ Celeritas offload could only run in CPU mode (GPU runs had stuck tracks in TileCal glue layer(s) and other runtime issues with CUDA architectures)
- ▶ AdePT offload could only run in GPU mode
- ▶ Geant4 physics optimizations are critically important for comparison  $\rightarrow$  still need well defined setups to ensure we do like-for-like comparisons of scoring outputs

## ■ Results:

- ▶ Celeritas results compared against Athena with some physics optimizations disabled, AdePT results against fully optimized Athena physics
- ▶ Celeritas results are pure CPU, AdePT are Athena CPU + AdePT GPU

# Faster Adoption of Geant4

- **Description:** Automatic calibration and validation of new Geant4 version
- **Motivation:**
  - ▶ Use Athena CI to run regular builds against given Geant4 version(s), as is done for Gaudi and ACTS
  - ▶ Run regular high level validations of these builds as early warning of discrepancies to help understanding before committing to a full validation
  - ▶ Nightly build with the newest Geant4 versions using preInclude directives to specify the Geant4 version
  - ▶ Automated calibration (sampling fractions and rederiving noise) and SPOT
- **Next Steps:**
  - ▶ Make a tag of atlasexternals including necessary changes to build the version of Geant4 for testing
  - ▶ Set up the Jenkins job that builds the nightly to use dedicated version of atlasexternals instead of default selection

Contact: Mustafa Schmidt, Attila Krasznahorkay



# Physics Stability

- **Description:** Guarantee physics stability through Geant4 versions

- **Motivation:**

- ▶ In ATLAS changes in physics modeling within the Monte Carlo (MC) simulations require updated recommendations for physics objects
- ▶ Resource-intensive process (mainly in terms of person-power but also computing power and typically undertaken only once or twice per LHC run)
- ▶ Improvements in physics modeling can only be incorporated into production releases when new physics object recommendations are scheduled
- ▶ Technical optimizations that enhance performance can be added to production releases between data-taking years in an LHC run, provided they do not affect the physics modeling
- ▶ These requirements slow down adoption of new Geant4 versions (if physics is changed)

- **Requirement:**

- ▶ Experiments should be able to request that a "tag" of a particular physics list they have validated be retained in future Geant4 versions with frozen physics output until it is no longer required
- ▶ This would reduce the need to support old Geant4 versions for many years and allow experiments to test the latest versions at large scales more rapidly

Contact: Marilena Bandieramonte, Jana Schaarschmidt, Walter Hopkins



■ **Description:** Improve Robustness of G4 Data I/O

■ **Motivation:**

- ▶ Recently the CI for Athena was hit by some EOS infrastructure issues resulting in unavailability of Geant4 data files or corrupted version of some Geant4 data
- ▶ Debugging this was made more complicated by the fact that the Geant4 code does not seem to have a robust and consistent way of dealing with cases where data files are not properly accessed (either not available or corrupted so that only part of the file is readable)

■ **Requirement:**

- ▶ Add additional and consistent checks when reading in G4 data files
- ▶ Harmonize the handling of data files?
- ▶ Consider providing the Geant4 data files in a versioned database in the future?

**Contact:** John Chapman, Marilena Bandieramonte, Jana Schaarschmidt



# Energy Loss Fluctuation

■ **Description:** Switch-off energy loss fluctuation in Geant4

■ **Motivation:**

- ▶ In Geant4 energy loss process calculates continuous and discrete losses per step
  - Both are stochastic processes (mean value of continuous loss can be calculated from restricted stopping power)
  - Statistical fluctuation around this mean from Urban/PAI models in Geant4
- ▶ Sampling these models adds (small) compute time per step, but fluctuation can often be ignored if number of steps is large in important volumes
- ▶ Statistical variation in energy loss over steps dominates per-step fluctuation
- ▶ Switching this process OFF → ATLAS observed Changes on Egamma energy scale larger than calibration systematic and a higher catastrophic energy loss with a 1% mismatch for muons with  $p_T > 500$  GeV

■ **Requirements:** Add possibility to enable the switch-off option depending on particle types / detector regions

Contact: Meryem Nouri, Marilena Bandieramonte



**Thank you very much for your  
attention!**