Report of usage of Geant4 within ATLAS

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On behalf of the ATLAS collaboration



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REMINDER OF PREVIOUS SUMMARY

- Previous update was shown on in the January 20, 2022 Geant4 Technical Forum
- Implemented improvements (resulting in 50%) increase in event throughput)
 - Usage of Gamma General Process and VecGeom
 - Magnetic field tailored switch off and vectorized sin/cos calculations in the EMEC.
 - Russian Roulette and EM range cuts.
 - Simplified Geometries.

- Ongoing R& D and new ideas:
 - Big static library and thread local storage.
 - TRT Geometry optimization.
 - GPU friendly EMEC.
 - Woodcock tracking.
 - Quantized state system stepper.
 - G4HepEM library integration.
 - EM Physics tuning.

 - ML Correction for Aggressive Range Cuts. New particle filter and voxel density tuning.

WILL ONLY HIGHLIGHT NEW DEVELOPMENTS IN THIS TALK.

OVERVIEW

ATLAS SIMULATION TOWARDS RUN 3

VECGEOM PERFORMANCE

BUGS IN RADIATION MODELLING

LAR SPECIAL SHAPE (EMEC) CODE

WOODCOCK TRACKING

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STATUS OF ATLAS SIMULATION TOWARDS RUN 3

- ATLAS used Geant4 10.1 during Run 2 for the majority of its background Monte Carlo.
- Plan for Run 3:
 - Use Geant4 10.6.3.3 with Birk's law tune and additional optimizations.
 - Include release with VecGeom.
- Geant4 10.6 is already being used for HL-LHC studies.
- Big library effort will hopefully converge soon.
- Birk's law tuning finalized
 - Geant4 strongly suggested ATLAS' Birk's law tuning be revisited for Geant4 10.6 due to change in hadronic models.
 - Tunes were checked with e/p (LAr) and Tile test beam.
 - Final tune is 20% higher for LAr and 54% higher for Tile when compared to the Birk's law parameterization used in Geant4 10.1.

VECGEOM: REMINDER GEOMETRIES IN ATLAS



- Fastest Run 3 simulation configuration uses slices (instead of cones) for EMEC.
- Previously the EMEC was described by a custom solid using G4Polycone.
- Now there are 3 implementations of the custom solid.
 - Wheel: default with G4Polycone.
 - Cone: outer wheel divided into two conical section using G4ShiftedCone.
 - Slices (fastest): new LArWheelSliceSolid → each wheel is divided into thick slices in Z. • Provides 5-6% speed up without
- - VecGeom.

VECGEOM PERFORMANCE WITH NEW GEOMETRIES

- When enabling VecGeom, EMEC configuration with slices is no longer the fastest.
 - Wheel configuration is faster when using VecGeom.
 - VecGeom is optimized for PolyCone so no gain from using slices.
- Profiling studies, including differences in CPU cycles, are still ongoing.
- Not yet clear what the reason for these differences are.



VECGEOM AND DIFFERENT ARCHITECTURES



	BNL Cluster, 1000 Jobs 100 tt-bar events/job	Walltime,s	sigma	Uncertanty	Speedup Throughput	Speedup CPU time
	Athena 22.0.47 (baseline)	28.0k	2.28k	~0.25%	-	
	Athena 22.0.47+Run3Opt	21.0k	1.7k	~0.26%	33%	-25%
	Athena 22.0.47+VecGeom	25.8k	2.27k	~0.28%	8,52%	-7,85%
	Athena 22.0.47+VecGeom+Run3Opt	18.1k	2.64k	~0.46%	54,69%	-35,35%
	Athena 22.0.47+VecGeom+Run3Opt (EMEC Wheel)	20.6k	1.37k	~0.21%	35.9%	-26.42%
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Color to architecture mapping is different for each plot.

DIFFERENT PERFORMANCE ON DIFFERENT ARCHITECTURES (INTEL AND AMD EPYC MACHINE)



on(B) CPU E5-2690 v4 @ 2 60GHz 35840 KB+AVX2 eon(R) Gold 6150 CPU @ 2.70GHz 25344 KB+AVX2 eon(R) Gold 5120 CPU @ 2.20GHz 19712 KB+AVX2

RADIATION MODELLING

- Geant4 10.6 showed more total ionizing dose (TID) and neutron fluence compared to Geant4 10.1.
- TID difference was due to buggy treatment of final states (FS) in neutron capture for HP physics lists.
 - This is specifically for all _HP physics lists (e.g., Shielding) because only these use the ParticleHP (10.6 and newer) (or NeutronHP in 10.1) classes. FTFP_BERT_ATL lists do not have these problems.
 - Geant4 10.1 also had problematic treatment of FS but FS data was barely used in 10.1.
 - More details in Geant4 bug report: https://bugzilla-geant4.kek.jp/show_bug.cgi?id=2468
 - Treatment of FS partially caused by new caching (needed for multi-threading).
 - Might be good for G4 experts to look into the caching code for ParticleHP in case something suspicious is happening there.
 - Patch provided which solves the TID issue \rightarrow already added to the official Geant4 patches.
- Increase in neutron flux still not understood.
 - Change to transition between FTF and BERT had no impact.
 - Alberto Ribon provided G4 10.1-like BERT and FTF code to partially revert to old setup. Tests ongoing.

RADIATION MODELLING: NEUTRON FLUX CHECKS STATUS

- Compare radiation fields of FLUKA and Geant4 for 10 GeV n, p, π^{\pm} on Cu.
- Use FTF and BERT from Geant4 10.1 with Geant4 10.6: lowers the neutron flux by $\mathcal{O}(10\%)$ (about 1/3) of the total effect is from BERT)
 - 10% reduction of backscattered neutrons into the inner detector (compared to 10.1) does NOT change when reverting to the old BERT.

1st row: 10.6 vs 10.1

2nd row: 10.6 vs 10.6 with old BERT



LAR SPECIAL SHAPE (EMEC) CODE

- The code that describes the EMEC custom solid was extracted from Athena in order to make it available in a stand-alone way within FullSimLight.
- It was also duplicated in the LArPlugin code under the GeoModelATLAS repository as part of the **Detector Description.**

Previous situation



LAR SPECIAL SHAPE (EMEC) CODE

- EMEC custom solid code (with all variation: wheel, and cones) has been refactored in Athena in order to make it portable.
- A copy of this code is available in the stand-alone repository: https://gitlab.cern.ch/SolidExtensions/LArCustomSolidExtension
- The stand-alone code can be synchronized with Athena using a script.



master · LArCustomSolidExtension / + · History Find file Web IDE & Clone ·							
Update README.md 6a14a4cd 🚯							
Name	Last commit	Last update					
LArCustomShapeExtensionSolid	Import files from the version in GeoModelA	21 hours ago					
🗅 import	Import files from the version in GeoModelA	21 hours ago					
CMakeLists.txt	Import files from the version in GeoModelA	21 hours ago					
M README.md	Update README.md	4 hours ago					
Σ autonomous-lar.sh	Update autonomous-lar.sh	4 hours ago					
README.md							
LArCustomSolid Exten	ArCustomSolid Extension						
This repository contains the LArCustomSolid Extension that describe the ATLAS LAR EMEC custom shape. The LAR EMEC custom shape extension is build starting from a copy of the corresponding code in the Athena repository.							
How to build the LArCustom Solid Extension							

FULLSIMLIGHT UPDATES

- LArCustomSolidExtension
 - LAr special shape code has been removed.
 - LArCustomSolid extension repository has been added to GeoModel as a submodule.
 - To run FullSimLight with the full ATLAS detector geometry, the LArCustomSolid extension has to be build and made available:
 - Requires specifying build flag when building GeoModel:

DGEOMODEL_BUILD_LARCUSTOMSOLIDEXTENSION=TRUE

- The extension is searched for in standard locations and if not found, the environment variable G4EXTENSION SOLID DIR is checked.
- FullSimLight is now compatible with Geant4 11.





WOODCOCK TRACKING

- EMEC is highly granular: steps are mostly limited by geometric boundaries.
 - One contributor of the EMEC's large CPU consumption.
- Woodcock tracking performs tracking in densest material to reduce number of steps in granular detectors.
 - Without loss of accuracy.
- Woodcock tracking has been implemented (by M. Novak) now within FullSimLight with full ATLAS geometry.
- Initial results show 10-15% improvement in running time with Woodcock tracking with FullSimLight (based on ttbar events).
 - Work on implementation in Athena has started.
 - Need to consider how the ATLAS implementation of Geant4 uses step information (Woodcock tracking removes some information).
 - For example, Athena uses Pre and PostStepPoint to calculate Birk's law corrections.



CONCLUSION

- ATLAS plans to move from Geant4 10.1 to Geant4 10.6.3.3 with Birk's law tune and additional opimizatons for Run 3.
 - Includes the ability to use of VecGeom and various speed ups (e.g. big library).
 - Final Birk's law tunes: increase of 20% for LAr and 54% for Tile when compared to Geant4 10.1.
- Using VecGeom seems cause stronger dependence on processor architecture and different optimal EMEC special shape.
- Bugs in radiation modelling found and partially fixed (total irradiated dose).
- New framework in FullSimLight and GeoModel to avoid duplication of LAr Special Shape code.
- Work on implementing Woodcock tracking within Athena has started.