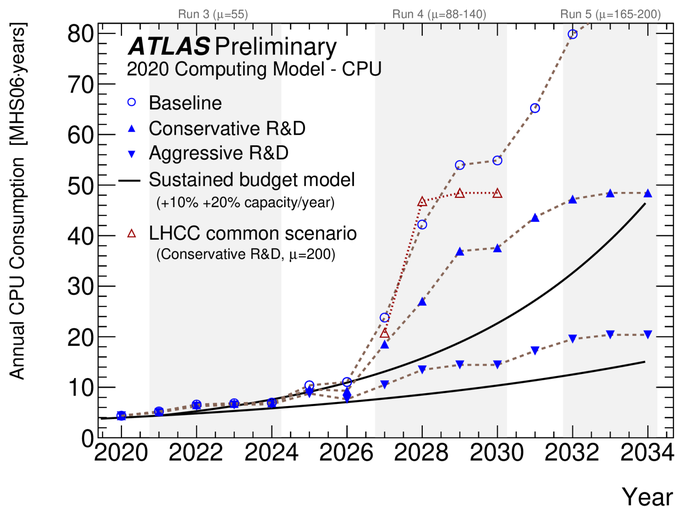
Celeritas: HEP detector simulation on GPUs

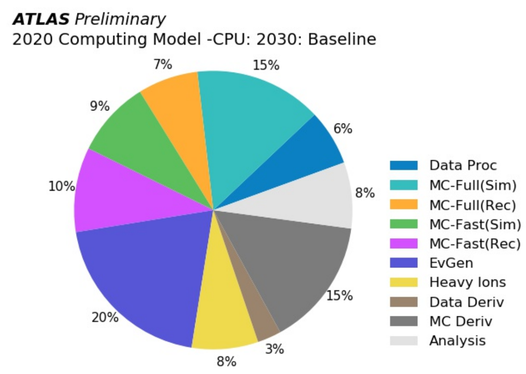
S. C. Tognini, S. R. Johnson and T. M. Evans — **Oak Ridge National Laboratory**
P. K. Romano and A. L. Lund — **Argonne National Laboratory**
P. Canal, G. Lima and S. Y. Jun — **Fermi National Accelerator Laboratory**
V. R. Pascuzzi — **Brookhaven National Laboratory**

arXiv white paper

MOTIVATION

- **Unprecedented computing demand on both HL-LHC and DUNE**



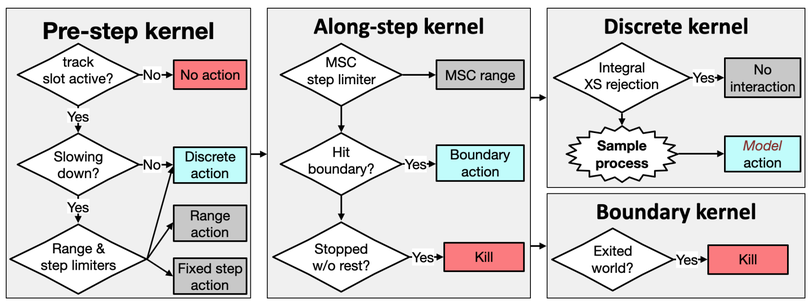


ATLAS HL-LHC Computing Conceptual Design Report. CERN-LHCC-2020-015/LHCC-G-178 (2020)

- Detector simulation can take up a large fraction of the total CPU time

CODE ARCHITECTURE & PHYSICS

- Data-oriented programming
- Composition-based classes
- Extensive unit-testing

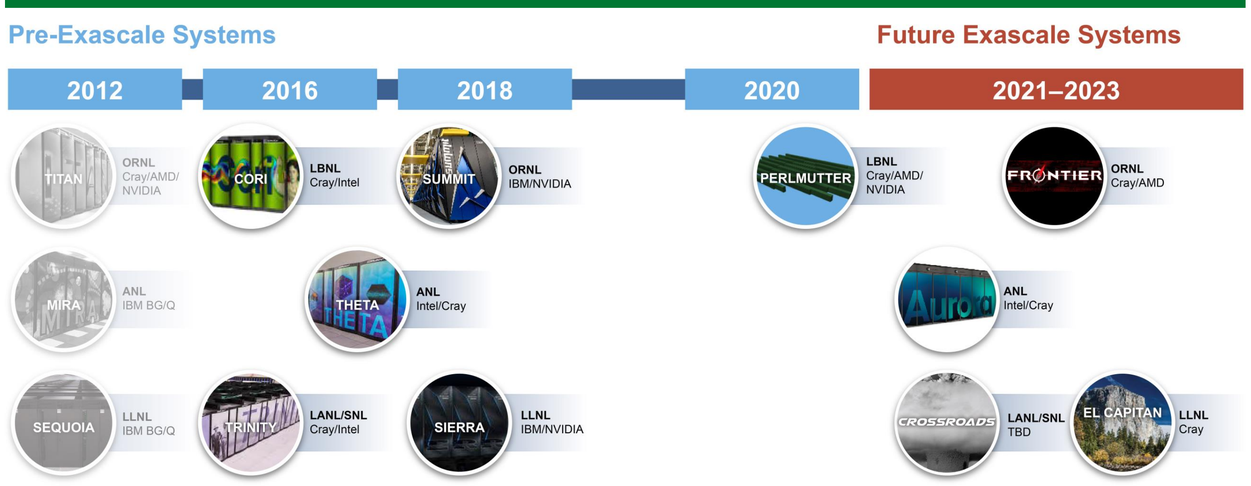


- Geometries:
  - **ORANGE** (Oak Ridge Advanced Nested Geometry Engine)
  - **VecGeom**
- Multi-architecture:
  - **NVIDIA** & **AMD** currently

Particle	Process	Model(s)
γ	photon conversion	Bethe–Heitler
	Compton scattering	Klein–Nishina
	photoelectric effect	Livermore
	Rayleigh scattering	Livermore
$e^{\pm}$	ionization	Møller–Bhabha
	bremsstrahlung	Seltzer–Berger, relativistic
	pair annihilation	EPlusGG
	multiple scattering	Urban, WentzelVI

- Comprehensive EM physics
- **Tag release v0.1 imminent**

EXASCALE COMPUTING SYSTEMS & PROJECT



D. B. Kothe, *et al*. **The US DOE Exascale Computing Project (ECP) Perspective for the HEP Community** A Coordinated Ecosystem for HL-LHC Computing R&D. Washington D.C. (2019)

- 24 open science applications have been ported and deployed on LCFs—most resulted in complete rewrites
- *ExaSMR: Coupled Monte Carlo Neutronics and Fluid Flow Simulation of Small Modular Reactors*
  - **Summit: 1 GPU ≡ 160 CPU cores**†

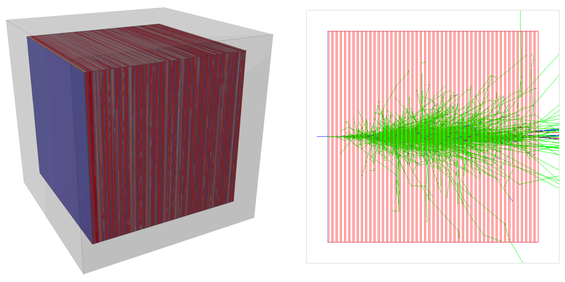
†S. P. Hamilton, *et al.* **Continuous-energy Monte Carlo neutron transport on GPUs in the Shift code** Annals of Nuclear Energy, vol. **128**, pp. 236–247 (2019)

PRELIMINARY PERFORMANCE RESULTS

Summit

CPU IBM Power9 22C @ 3.07 GHz
GPU NVIDIA Tesla V100 @ 1.53 GHz
(80 SM, 64 cores each, 16 GB mem.)

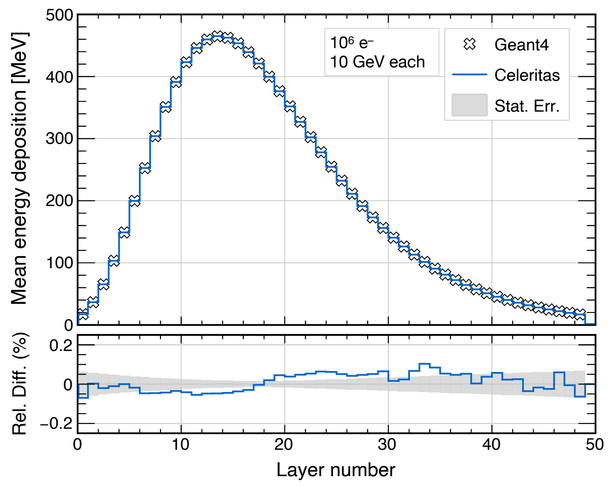
- Geometry: 50 layers of LAr + Pb



- **CPU**: 7 cores multithread
- **GPU**: 1 core per GPU

Celeritas per-node performance
- **~40× faster on GPU**
- **1 GPU ≡ ~280 CPU cores**

New preliminary results; **NOT** published yet



Input

Application	Arch.	Events
Geant4 (v10.7.1)	CPU	10^4
Celeritas	CPU	10^3
	GPU	10^5

Wall time per primary

Application	Geo.	Arch.	Mean (ms)
Geant4 (10.7.1)	Geant4	CPU	2.9 ± 0.1
Celeritas	ORANGE*	CPU	2.09 ± 0.02
		GPU	0.046 ± 0.001
	VecGeom	CPU	1.95 ± 0.04
		GPU	0.0627 ± 0.0004

*Oak Ridge Advanced Nested Geometry Engine

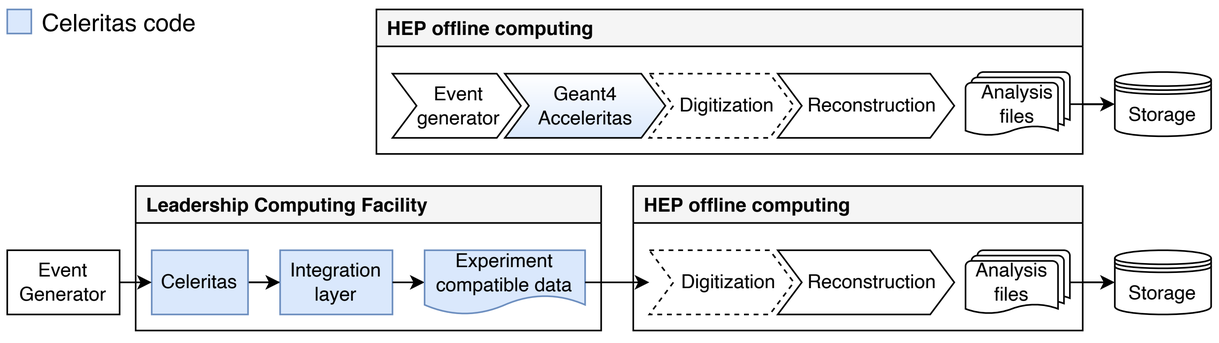
IMPACT

- *Celeritas* is designed to take full advantage of DOE LCFs
- ORNL alone is home of both Summit and Frontier
- If *Celeritas* reaches a CPU to GPU factor of 160 (such as ExaSMR)
  - **Summit: 27,648 GPUs → 4,423,680 CPU cores**
  - The Worldwide LHC Computing Grid (WLCG) had ~500,000 CPU cores in 2017††
  - **Summit can reach an equivalent computing power of 8 WLCG**

†† **A Roadmap for HEP Software and Computing R&D for the 2020s.** Comput. Softw. Big Sci. **3**, 7 (2019)

EXPERIMENT INTEGRATION

- Working with experiments to provide a proof-of-principle workflow
- *Acceleritas*: Geant4-*Celeritas* hybrid that offloads EM physics to GPU



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