OAK RIDGE National Laboratory

Celeritas for platform portable HEP comparison

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Scalable Engineering Applications

CELERITAS

Celeritas core team:

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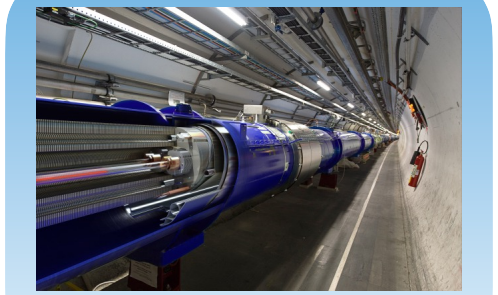
U.S. DEPARTMENT OF ENERGY

HEPiX meeting
6 March, 2024

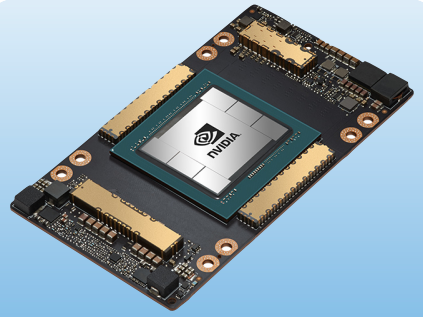
Celeritas project goal

- **Accelerate scientific discovery** by improving detector simulation throughput and energy efficiency for LHC production simulation
  - Long term goal: as much work as possible on GPU
  - Initial funding: focus on EM physics (but keep door open for more!)
- Multidisciplinary approach
  - **Research and develop** novel algorithms for GPU-based Monte Carlo simulation in High Energy Physics
  - **Implement** production-quality code for GPU simulation
  - **Integrate** collaboratively into experiment frameworks



LHC beamline ©CERN

CELERITAS



Nvidia A100 GPU @Nvidia

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Background

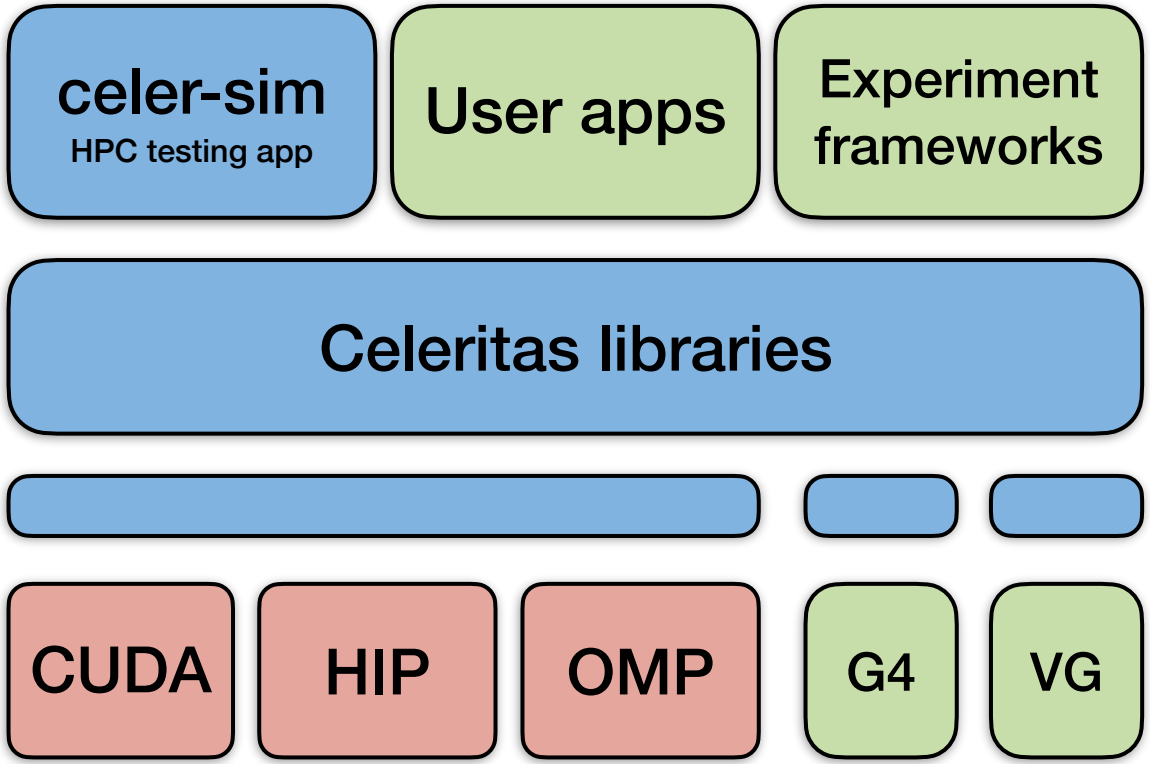
Methods

Results

Conclusions

Software stack

- Every dependency is optional
  - Needed for testing on oddball HPC systems
  - Minimum useful simulation requires Geant4 or ROOT for physics data input
  - HEP detector geometry requires VecGeom
- In-house data model supports platform performance portability
  - Most code is just C++ (<1% is CUDA/HIP)
  - Data management layer abstracts memory location and transfer
  - “Launcher” helper abstracts code execution
  - Plan this year to add Intel via DPC++

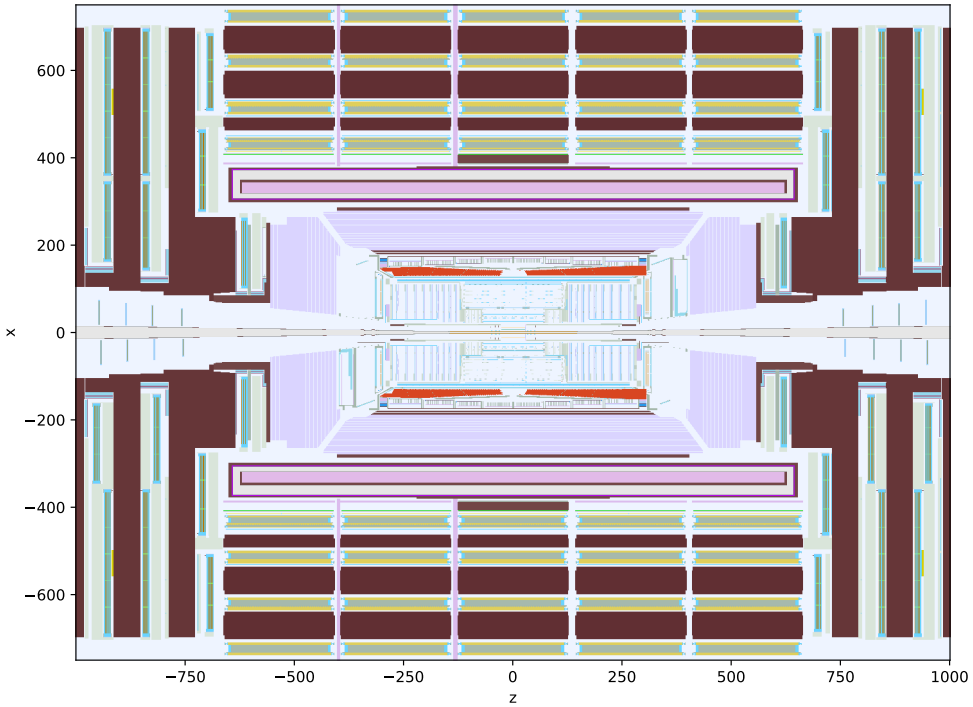


Optional dependencies:
- nlohmann/json
- HepMC3
- googletest

Documentation:
- Doxygen
- Sphinx
- Breathe

High-level capabilities targeting LHC simulation

- Equivalent to `G4EmStandardPhysics`
  …using Urban MSC for high-E MSC; only γ, $e^{\pm}$
- Full-featured Geant4 detector geometries using VecGeom 1.x
- Runtime selectable processes, physics options, field definition
- Execution on CUDA (Nvidia), HIP* (AMD), ***and CPU*** devices

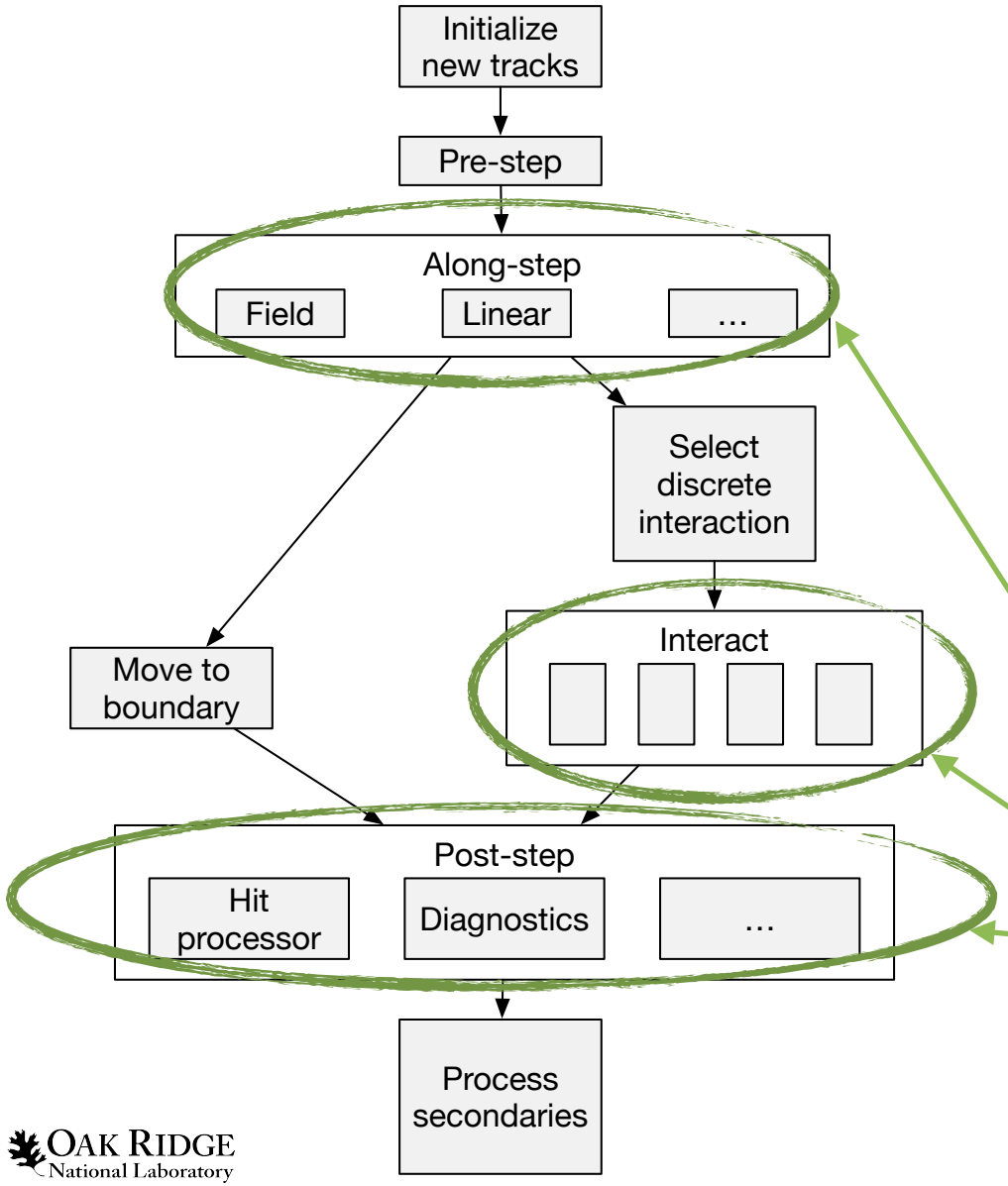


GPU-traced rasterization of CMS 2018

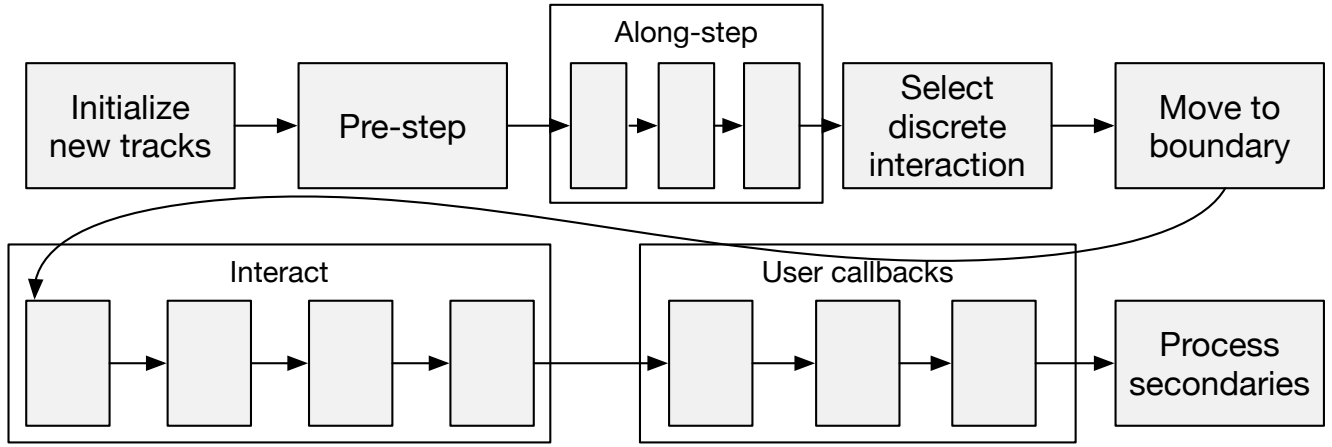
**VecGeom currently requires CUDA: ORANGE navigation required for AMD*

Source: Johnson, S.R. Geant4 Meeting 2023

Stepping loop on a GPU



Process large batches of tracks through all kernels (10^3–10^6)



Topological sort: a loop over kernels

Using many small kernels improves extensibility

Source: Johnson, S.R. Geant4 R&D Summary 2023

Celeritas/Geant4 integration

- **Imports** EM physics selection, cross sections, parameters
- **Converts** geometry to VecGeom model without I/O
- **Offloads** EM tracks from Geant4
  *(Via `G4UserTrackingAction`, `G4VFastSimulationModel`, or **`G4VTrackingManager`**)*
- **Scores** hits to user "sensitive detectors"
  (Copies from GPU to CPU; reconstructs `G4Hit`, `G4Step`, `G4Track`; calls `Hit`)
- **Builds** against Geant4 10.5–11.2 with no patches required

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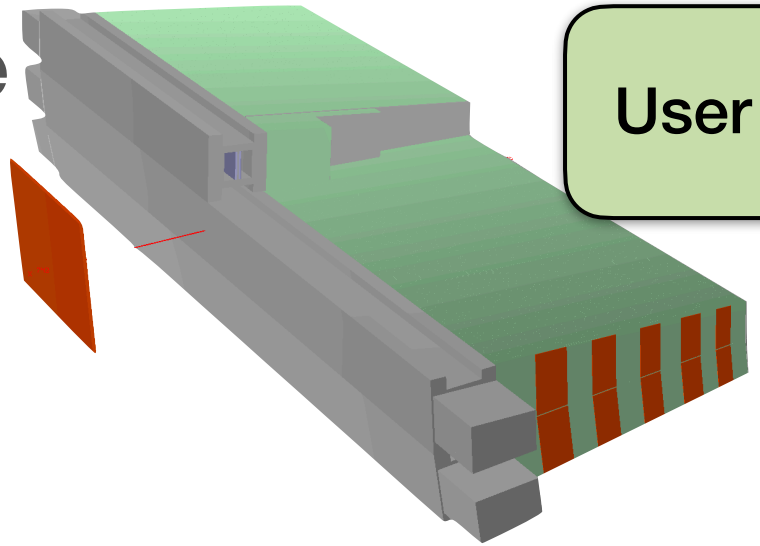
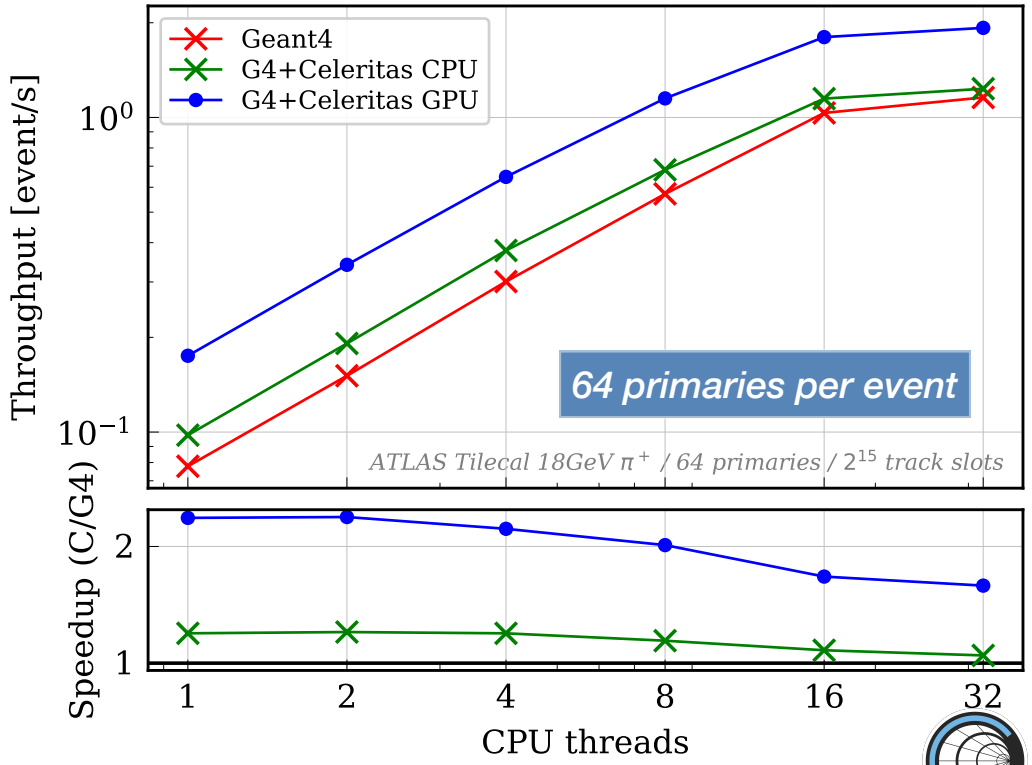
ATLAS Tile Calorimeter performance



- Example of combined GPU/CPU comparison
- 1/4 of a Perlmutter (NERSC) GPU node
  16 cores of AMD EPYC, 1 Nvidia A100
- GPU speedup: **1.7×** at full occupancy
  Using all CPU cores with a single GPU
- CPU-only speedup: **1.1–1.3×**
- Theoretical maximum speedup: **2.2–2.5×**
  Instantly killing e-, e+, γ when born
- **One GPU is effective with many-CPU Geant4**

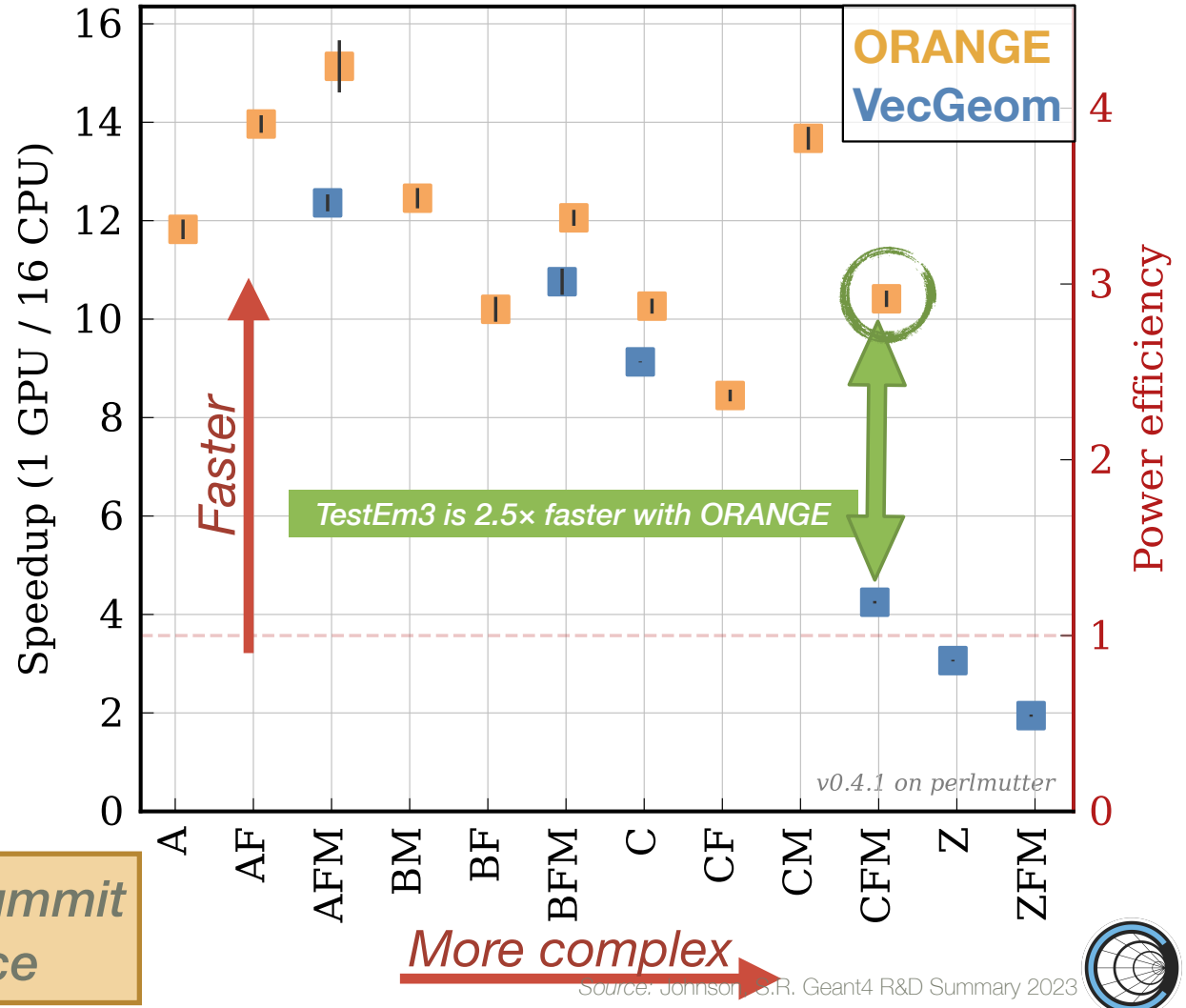


Standalone EM performance

Modifier		Problem definition	
		A	“infinite” medium
		B	simple-cms
F	+field	C	idealized calorimeter
M	+msc	Z	cms2018

celer-sim
Performance testing app

- 1300 × 10 GeV e^-, 16 events
- ¼ Perlmutter node (NERSC)
  1 × Nvidia A100 GPU, ¼ × 64-core AMD EPYC 7763
- Celeritas GPU vs CPU
  CUDA (1 CPU thread) vs OpenMP (16 CPU threads)
- Key metrics favor GPU
  - *Capacity:* **50–94% loss** if GPUs are ignored
  - *Efficiency:* up to **4×** performance per watt



Previous versions of this slide used Summit which has slower CPU performance

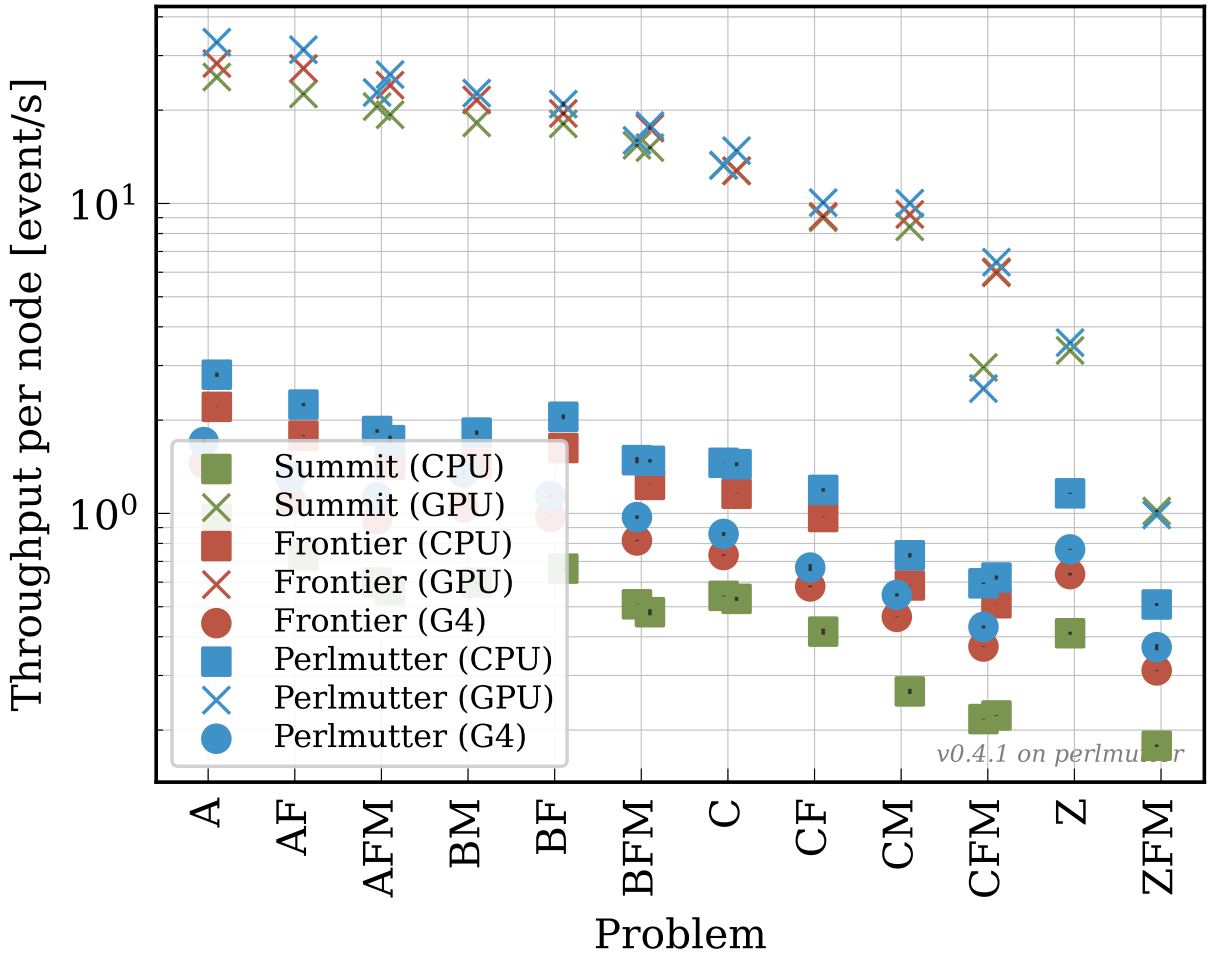
Source: Johnson S.R. Geant4 R&D Summary 2023

Figure of merit: throughput

- **Cross-platform comparison**
- GPUs *cannot* be ignored if present
- AI/ML "revolution" guarantees more coprocessors at all scales

Per-node stats for DOE supercomputers

Machine	Arch	Card	TDP (W)	Cores*	Cards
Summit	CPU	IBM Power9	190	‡22	2
	GPU	Nvidia V100	250	80	6
Perlmutter	CPU	AMD EPYC 7763	280	64	1
	GPU	Nvidia A100	250	108	4
Frontier	CPU	AMD EPYC 7453	225	‡64	1
	GPU	AMD MI250x	500	220	†4



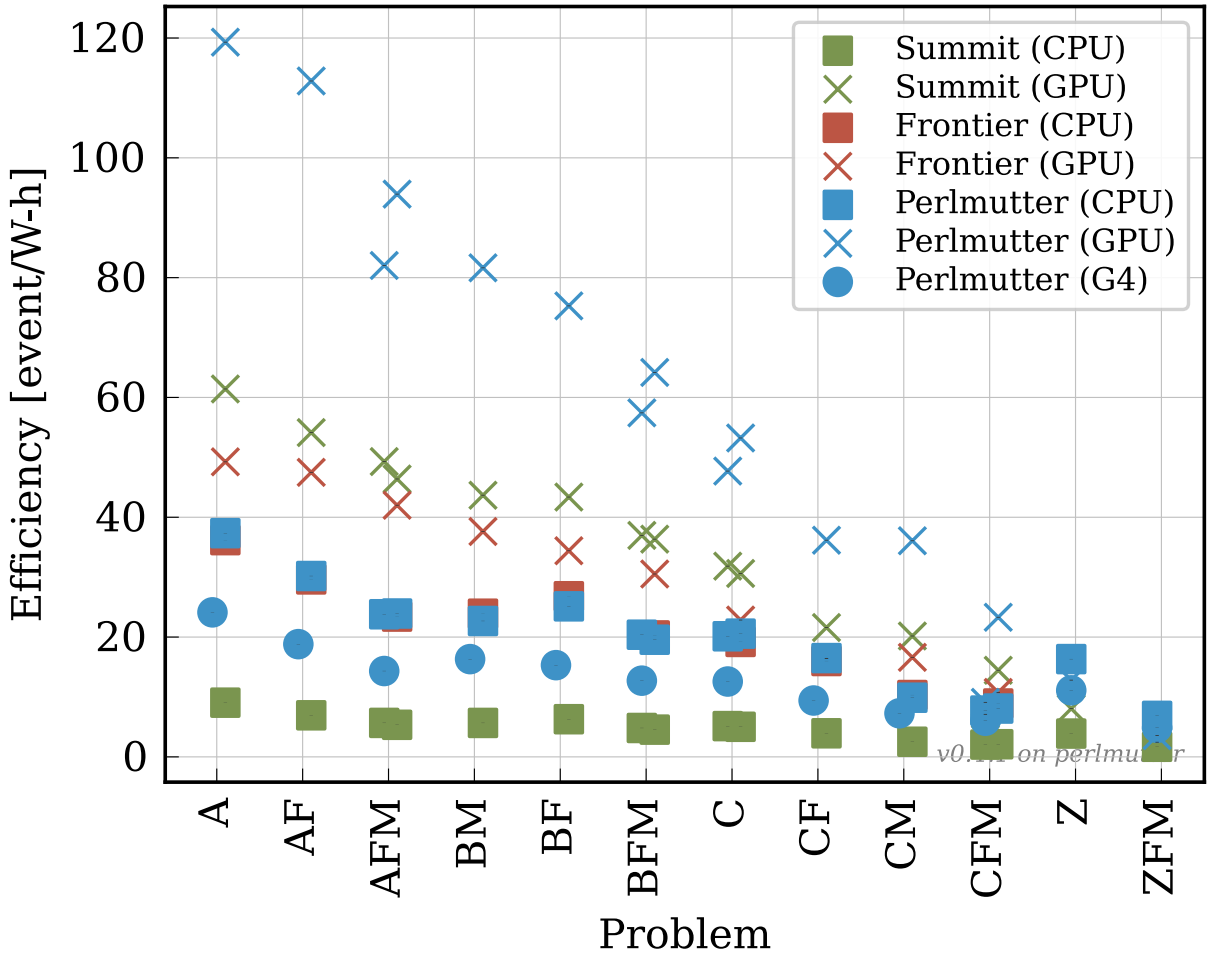
EM only, no SDs

*or SMs;
†Each card has 2 GPUs
‡One core reserved per GPU

Source: Johnson, S.R. Geant4 R&D Summary 2023

Figure of merit: efficiency

- **Estimated** using reported Thermal Design Power (TDP) and Celeritas throughput
  - Likely *conservative* based on nvidia-smi readings, since we use only a fraction of GPU hardware
  - **Really excited to work with your group on potential real-life power draw!**
- GPU consistently shows higher energy efficiency 🌱
- A100:EPYC price is ~4× 💸



EM only, no SDs

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Resources and installation

- Detailed installation, usage, development documentation
  - User documentation: celeritas-project.github.io/celeritas/user/
  - Doxygen: celeritas-project.github.io/celeritas/dev/
  - Github: github.com/celeritas-project/celeritas
  - Slack workspace, or AdePT/Celeritas Mattermost
- Installation
  - Automatic CMake-based detection of available options
  - Full spack environment definition and installable package
  - Docker image with dependencies (used for CI)
  - Rigorous CI matrix gives us confidence in build/test on new platforms

Continuing work

- Concluding efforts funded by SciDAC V
  - EM physics validation
  - Integration with experiment frameworks
- Now officially funded by HEP-CCE (US DOE program)

  High Energy Physics - Center for Computational Excellence
  - Optical physics for LZ, LEGEND, JUNO, etc.
  - GPU-optimized, platform portable computational geometry for HEP
  - Implementation and testing on **Intel GPUs**
  - **Platform portability and energy efficiency are central to this program**

Next steps

- Identify multiple testing hardware
- Configure software stack
- Determine test problems, targeted run time
- Perform cross-hardware efficiency comparisons?
- Incorporate into HEPScore benchmarking?

Acknowledgments

Celeritas v0.4 code contributors:

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- Philippe Canal (@pcanal)
- Julien Esseiva (@esseivaju)
- Tom Evans (@tmdelellis)
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- Amanda Lund (@amandalund)
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https://github.com/celeritas-project/celeritas