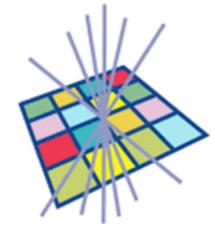
Power efficiency gains from **GPU optimised workloads Geant4 based detector simulations** with Celeritas

Albert (Bruno) Borbely, David Britton, Emanuele Simili, Gordon Stewart, Samuel Skipsey





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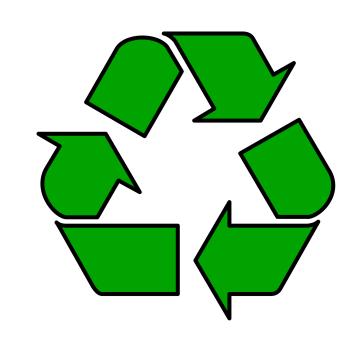


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Processors CO2 life cycle Embodied + Energy Fraction (EF) CO2



- Embodied CO2 due to manufacturing + shipping, fixed value for each component (may have a geographical component due to shipping)
- Energy fraction is the CO2 emitted by the local energy GRID and depends upon the length of its lifetime (KWh)







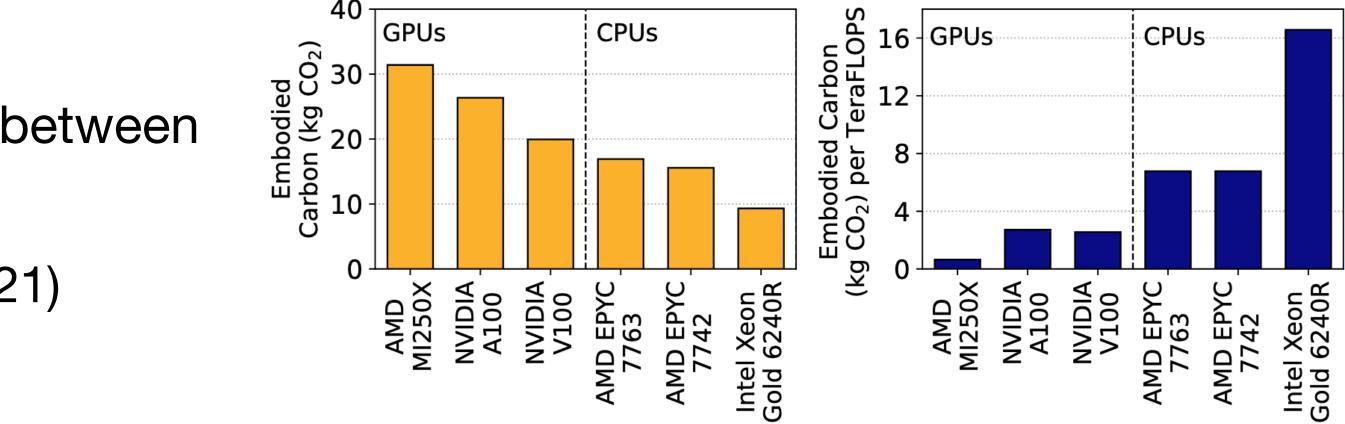




Embodied Carbon in Processor Components

- Embodied carbon in typical CPU / GPU normalised by double floating point precision (64FP)
- AMD CPUs have similar kg CO2 / TFLOPS between generations
 - AMD EPYC 64 core 7742 (2019), 7763 (2021)
 - Intel CPUs are uncompetitive
- Overall GPUs perform better when performance in normalised
 - Nvidia GPUs perform ~ 2x than AMD CPU
 - AMD GPUs perform ~ 6x than AMD CPU
 - Raw double floating point precision (64FP) isn't the full story, Nvidia focusing on 32, 16, 8 in recent years for ML





https://arxiv.org/pdf/2306.13177

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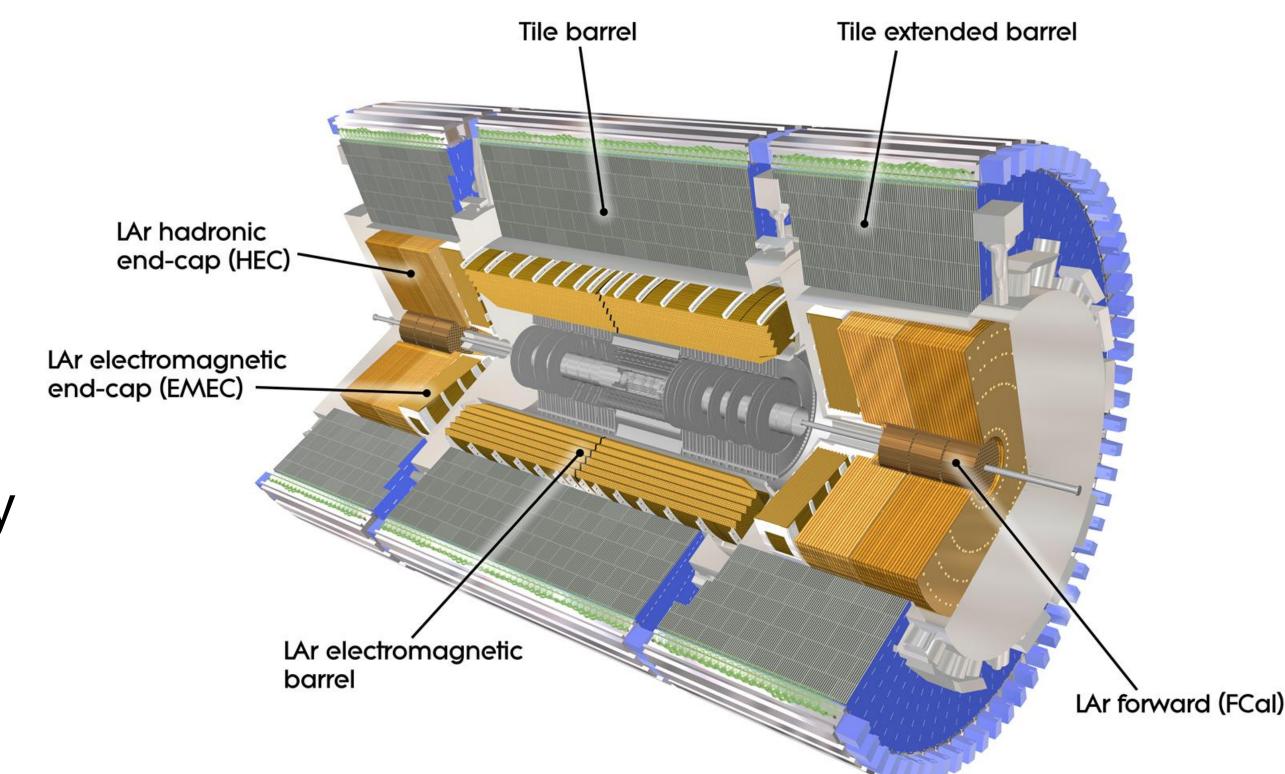






- The Celeritas project is aimed at developing GPU-based Monte Carlo simulations in HEP
- Currently focused on EM physics e.g. the ATLAS Tile calorimeter
- Detector simulation is particularly costly in terms of CPU
 - ATLAS spends ~ 40% of its CPU
 - 20% spent on Geant-4 based full detector simulation















GPU benchmarking: step 1 **CPU vs GPU comparison**

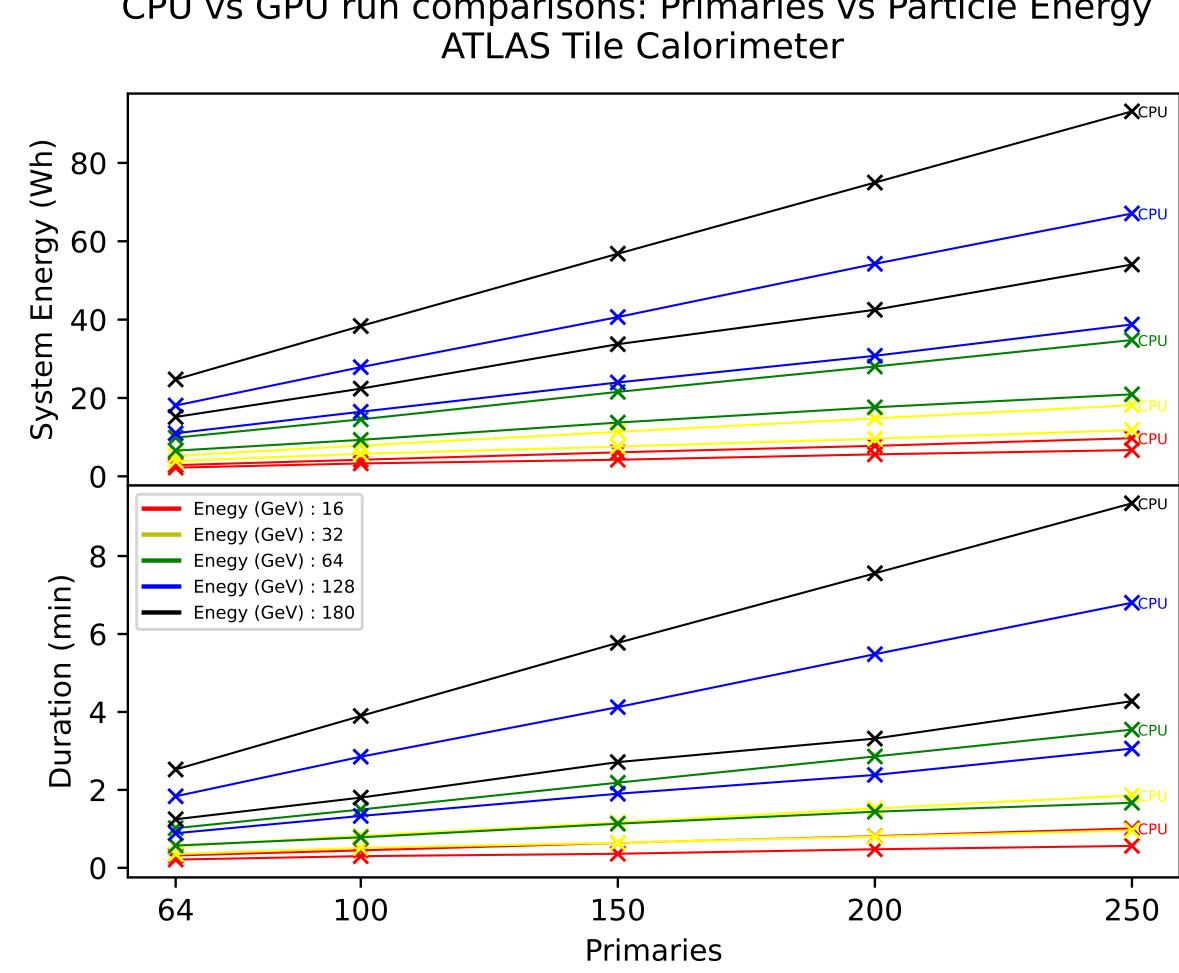
- Using the ATLAS Tile Calorimeter as a test geometry
- Using Celeritas in GPU and CPU mode
- 2 run parameters were varied:
 - Number of primaries
 - Initial particle energy
- The higher the parameters
 - -> more intensive job
 - -> more work offloaded to GPU
 - -> greater reduction in duration/energy
- @ lowest (N64 & E16 GeV) ~ 22% & 33% decrease in job energy & duration respectively with GPU
- @ highest (N250 & E180 GeV) ~ 42% & 54% decrease in job energy & duration respectively with GPU
- Plenty of gains to be had

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CPU vs GPU run comparisons: Primaries vs Particle Energy **ATLAS Tile Calorimeter**



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GPU benchmarking: step 2

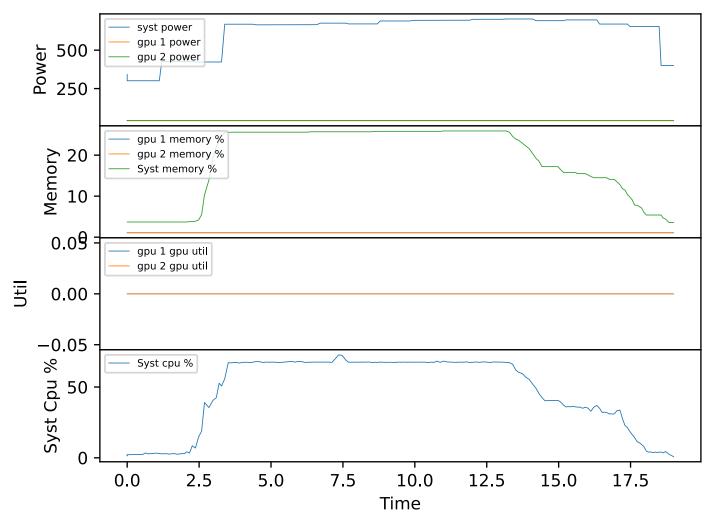
Details

- CPU threads set to 32
- System Power gathered with IPMI
- GPU Power gathered with NVML
- CPU only Energy ~ Syst. energy idle GPU energy
 - Verified with unplugged GPUs
- System: GPU 2xa100 (80GB), CPU 2x AMD EPYC 7443 x48 cores (2021), **RAM 251 GB**
- To keep things consistent 2 cpu jobs were launched in parallel as well as 2 gpu jobs (one targeting each card), so values shown are for two jobs in parallel in both cases
- GPU variant doesn't always maximise GPU utilisation -> need to think about CPU/GPU -> to maximise GPU utilisation
- All jobs being launched in docker containers, to deal with dependancies, environment and installation. Also makes GPU management easier.

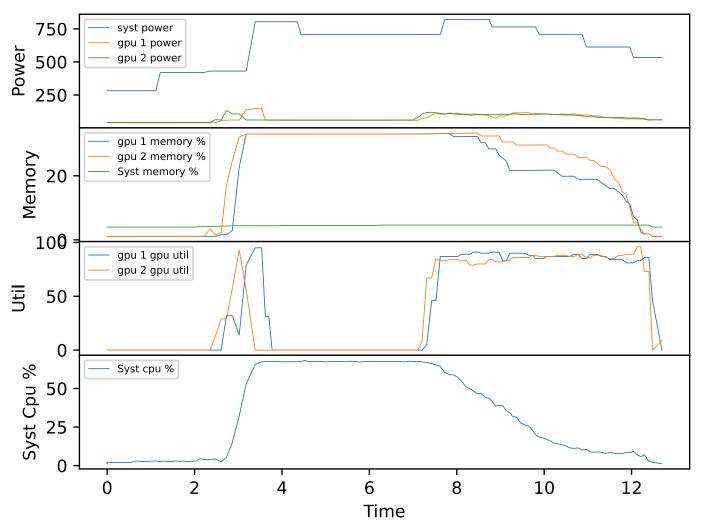




(Wh) syst: energy 3.28; gpu 1: energy 0.21; gpu 2: energy 0.22; Duration: 19.0 s



(Wh) syst: energy 2.21; gpu 1: energy 0.26; gpu 2: energy 0.26; Duration: 12.69 s



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GPU benchmarking: step 3 **Node considerations**

- Compute node now consists of GPU + CPU
- Nvidia a100 GPU 1.55x AMD EPYC 7763 CPU embodied carbon (EC)
- A compute node with: x2 AMD CPU, x2 Nvidia GPU ~ 5x EC
- Its normalised EC (kg CO2/ 64FP) is 70% (5) for the GPU version vs (7) for the CPU version
 - More compute in 1 node will leads to less EC / TFLOPS
 - Life cycle CO2 will also heavily depend on GPU utilisation
 - CPU is idle when offloading to the GPU
 - The above number assumes full CPU and GPU utilisation throughout lifecycle not necessarily realistic, still learning on how to utilise GPUs fully

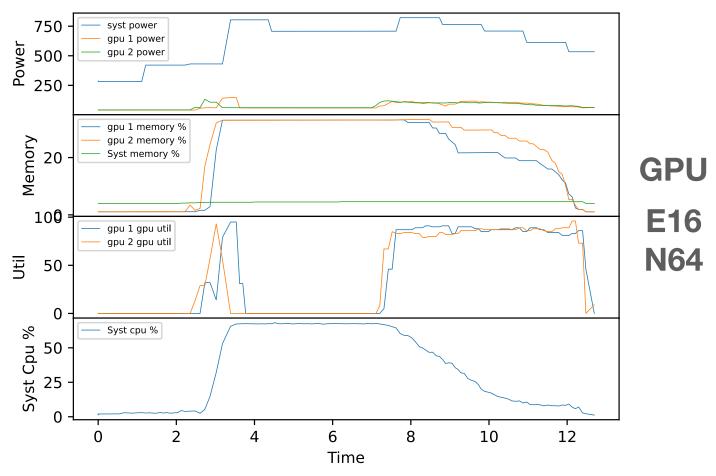


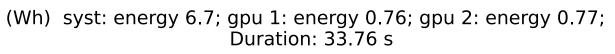


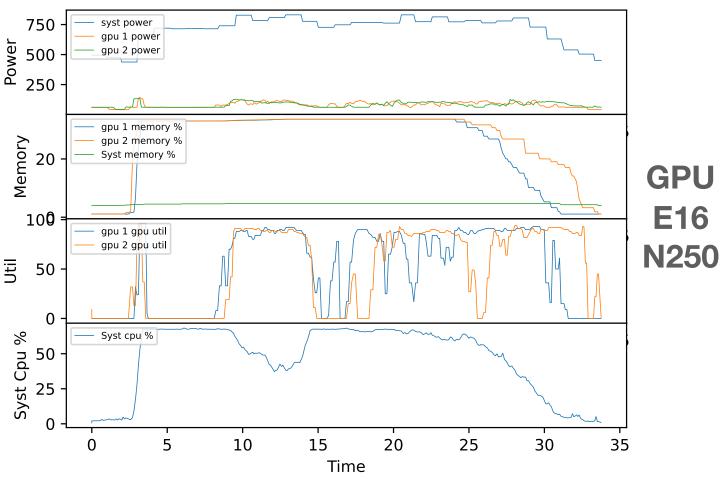




(Wh) syst: energy 2.21; gpu 1: energy 0.26; gpu 2: energy 0.26; Duration: 12.69 s







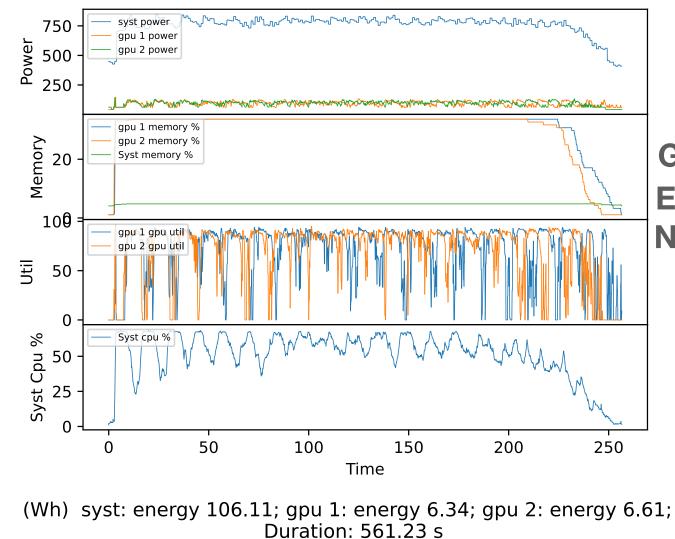
GPU benchmarking: step4 Job considerations

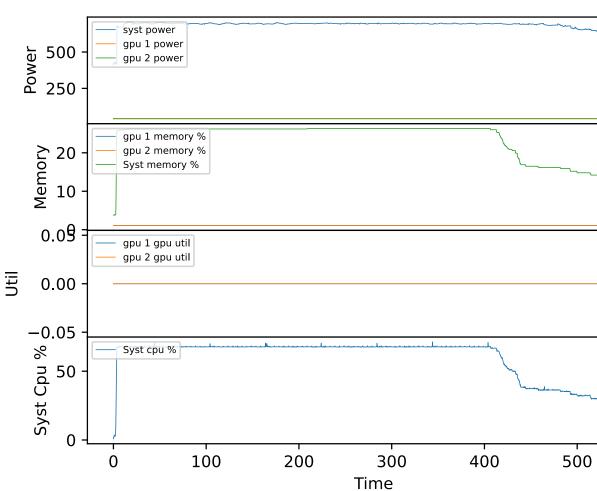
- used
- CPU variants effectively use a constant fraction of CPU resources (32 threads per job)
 - GPU variant is constantly offloading parts of the job to the GPU
 - -> This causes fluctuations in GPU utilisation (see left/top-right plots)
 - Need to think about how to maximise GPU utilisation, often most expensive part should not be sitting idle
 - Current setup allows a job to hog 1 GPU \bullet
 - -> Potential solution to allow multiple job slots to share a GPU resource

Job "work" heavily depends on parameters

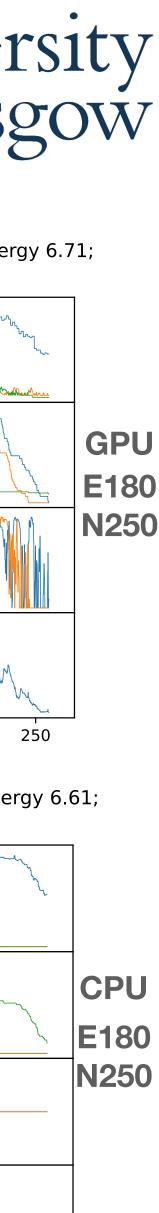


(Wh) syst: energy 54.06; gpu 1: energy 6.61; gpu 2: energy 6.71; Duration: 256.59 s





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GPU benchmarking: step 5 **Putting things together**

- Node + Job consideration
- The CPU + GPU version of a node has ~ 2.5x the EC of the corresponding CPU node
- With a normalised EC of 0.7x corresponding CPU node in terms of double floating point precision -> assumes 100% utilisation of both CPU and GPU resources
- With the best possible job run conditions the Celeritas benchmark achieved a 42% decrease in real world energy use -> does not fully utilise CPU or GPU -> utilisation fraction dependent on run parameters -> the more work offloaded to the GPU the greater the energy savings
- · Break even point will depend on where node is geographically located
 - -> lots of dirty power -> EC is a negligible fraction, CO2 due to energy mix will dominate -> frequent component upgrade cycle
- Component utilisation rates also play a factor:
 - If a resource is under utilised then a negative factor appears in-terms of idle energy
 - This is not really an issue with CPU only as the job can maximise the CPUs capabilities
 - But with CPU + GPU architectures one of the resources is by definition waiting for the other



• -> lots of clean power -> EC is a dominant fraction -> longer running time required to break even -> infrequent component upgrade cycle

• Overall good progress is shown in achieving energy savings in calorimeter simulation using FullSim Geant-4 when high calorimeter fidelity is required

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