First experiences at the exascale with Parthenon – a performance portable block-structured adaptive mesh refinement framework

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in collaboration with the Parthenon community (J. Dolence, F. Glines, J. Miller, P. Mullen, B. Prather, B. Ryan, L. Roberts, J. Stone, and more) and J. Holmen (OLCF)

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Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

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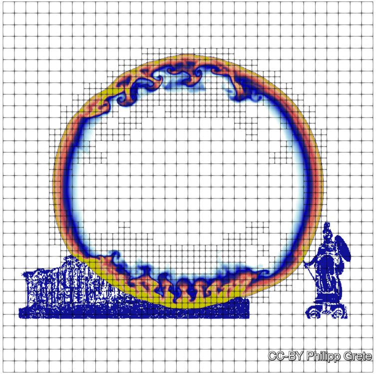
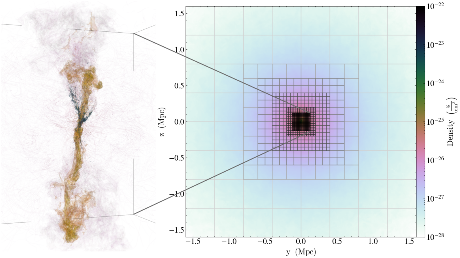
(Adaptive) Mesh Refinement (AMR)

- Decompose domain into blocks
- Blocks
  - are logically independent
  - have fixed size
  - communicate with their neighbor through ghost cells/buffer zones
- "Refine" (split block into more blocks) to
  - increase spatial resolution in region(s) of interest
  - save computational resources
- Block size is important
  - ratio of active to passive zones
  - number of neighbors
  - thickness of transition regions



Parthenon – Performance portable AMR framework

- Open collaboration (10+ active developers)
- AMR framework heavily expanded from Athena++
- Intermediate abstraction layer hiding Kokkos
- Key performance design decisions
  - device first/resident
  - block packing
  - device-to-device communication via one-sided, async. MPI
- Advanced features (e.g., abstract data containers, package system, task-based parallelism, sparse variables)
- Multiple downstream codes
  - AthenaPK (MHD), Phoebus (GRMHD), KHARMA (GRMHD), parthenon-hydro (miniapp)

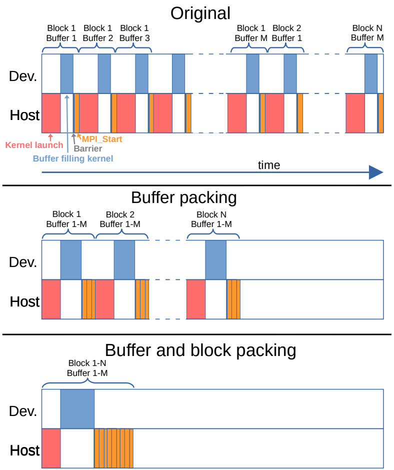


Packing #1: Kernel fusing $\leftrightarrow$ block packing

[Grete+ IJHPCA 2023 – Parthenon collaboration]

- Launch overhead
  - $\approx 5\mu$s launch, inherently serial (launching in parallel does not help)
  - possibly $> 100,000$ buffers per device
- Small blocks $\Rightarrow$ little work
  - $16^3 = 4$k cells $\leftrightarrow$ >1k cores/device
  - even Riemann solve is $< 5\mu$s

$\Rightarrow$ Combine work into fewer kernels



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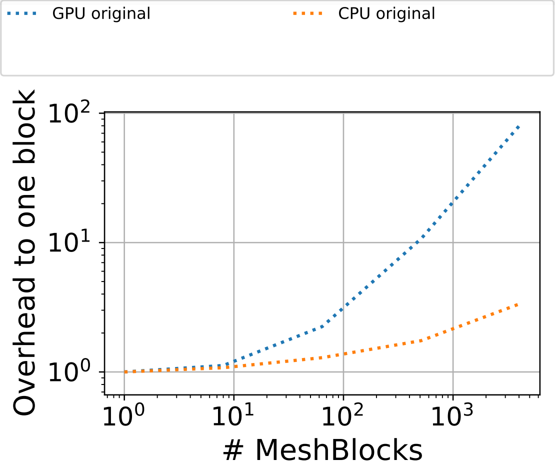

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- CPU 128^3 mesh with blocks 128^3 to 8^3

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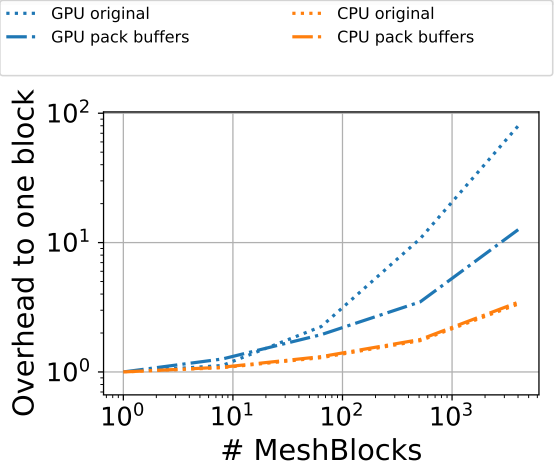

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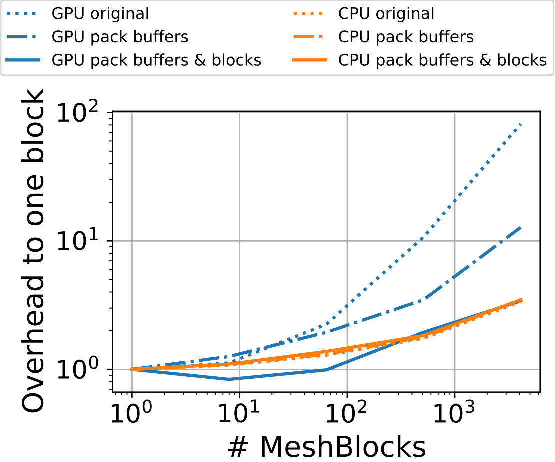

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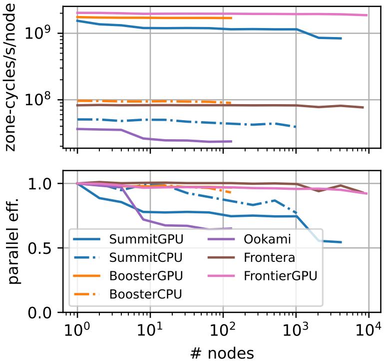
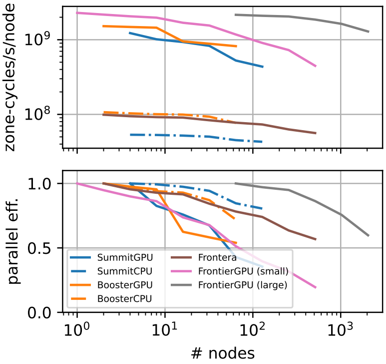
Scaling on TOP500 #1 Frontier

[Grete+ IJHPCA 2023 – Parthenon collaboration]



Uniform mesh (weak)



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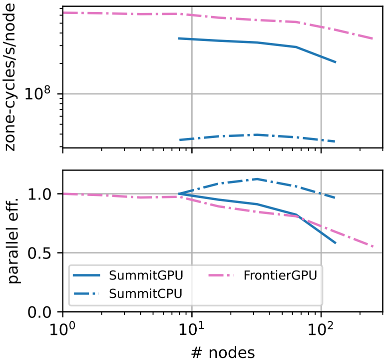


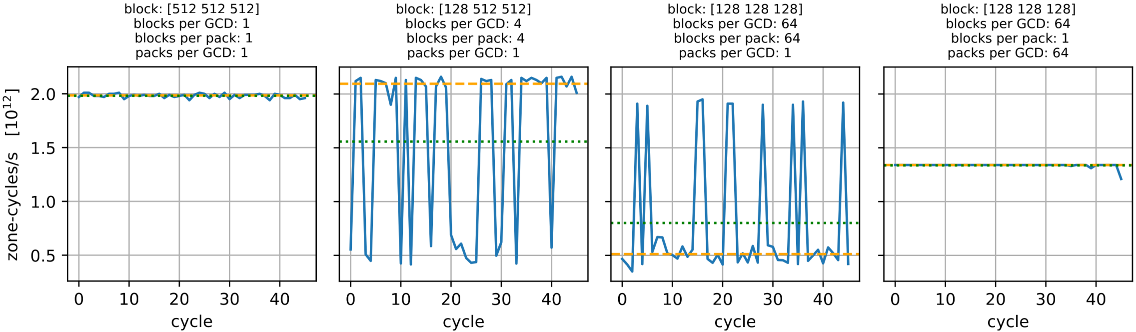
Multilevel mesh (strong)
(24k 32^3 blocks)

$\Rightarrow$ 92% weak scaling efficiency on 73,728 GPUs and

$\Rightarrow$ $\gtrsim$ 50% strong scaling efficiency for 100x increase in resources

Packing #2: Messages in a bottle(neck)

[Holmen, Grete & Melesse Vergara CUG23]



- 1024 nodes
- 16384x8192^2 mesh
- Vary block sizes and pack sizes

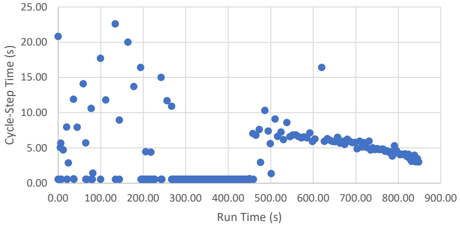
$\Rightarrow$ Messaging matters

$\Rightarrow$ Room for more optimizations

IO #1: 1x9000 vs 9000x1 – What could possibly go wrong?

[Holmen, Grete & Melesse Vergara CUG23]

- `parthenon-hydro` part of OLCF test harness (used for system testing)
- "All nodes" versus "every node" tests
- Goal: Isolate "bad" nodes
- Observed strong variability



performance over time of a random node in "every node" test case

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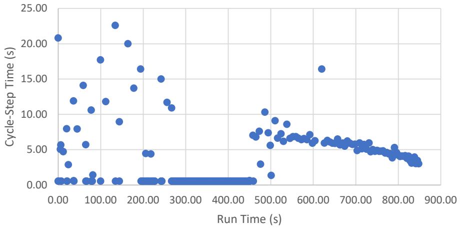
⇒ `stat` on parallel file systems does **not** scale

- Potentially relevant to parameter sweeps



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IO #2: Writing (a) “large” file(s)

- Parallel HDF5 (with MPI IO)
- Single file per output
- No issues on Alpine (GPFS)
  - writing 6TB files in $<15\,\mathrm{s}$
  - using collective buffering (one rank per node with 16MB buffer size)

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- On Orion (Lustre) for INCITE runs (2.7TB)
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⇒ Monitoring script for silent failures

- Single file per output does not scale (for us on Lustre)

⇒ HDF5 subfiling (I did not get it working)

⇒ OpenPMD/ADIOS2 (tests successfully wrote 4.5TB file in <1 s)

- * use “capacity” tier not “performance”

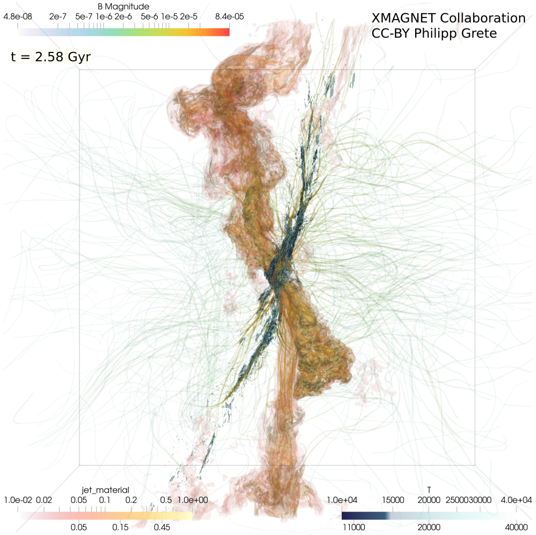
Large scale visualization

Paraview on Andes

- Establishing connection takes a long time (⇒ increase timeout)
- Preselect data (⇒ reduce memory footprint)
- Be patient!

Next: In-situ with Ascent

- Still fighting performance degradation



Conclusions – Take home message(s)

[Grete+ IJHPCA 2023 – Parthenon collaboration]

- Fuse kernels
- Remain flexible wrt. communication
- Do not write to a single large file
- Introduce safety checks (e.g., for timeouts)
- BENCHMARK!

We are an open, welcoming community. Meet us at/on

- `https://github.com/parthenon-hpc-lab`
- Matrix chat: `#parthenon-general:matrix.org`