Parthenon – a performance portable block-structured adaptive mesh refinement framework

Philipp Grete
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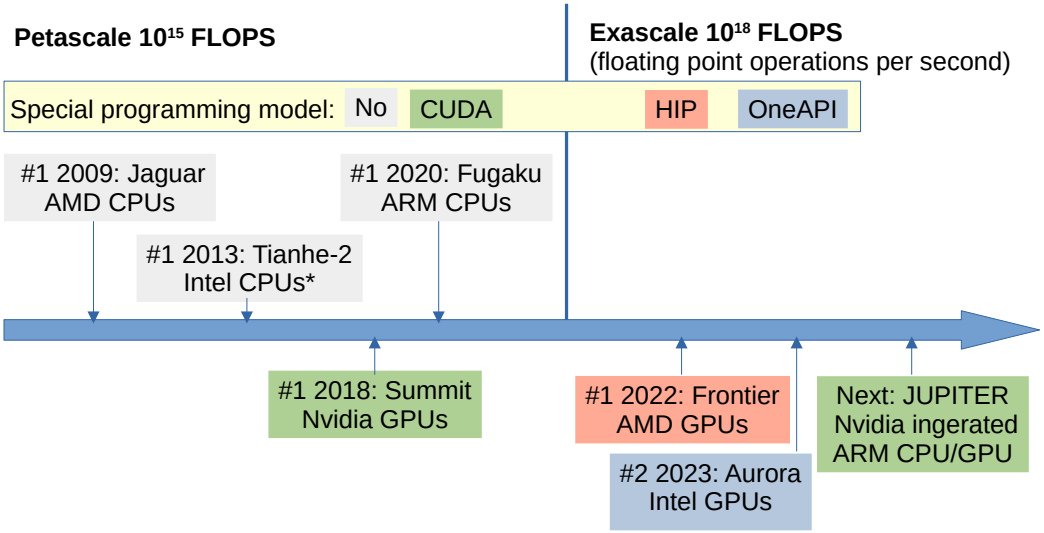
in collaboration with F. Glines, B. O'Shea, J. Holmen, and the Parthenon community (A. Dempsey, J. Dolence, J. Miller, P. Mullen, C. Prather, A. Reyes, L. Roberts, and more)

Kokkos Tea-Time

Funded by
DFG Deutsche Forschungsgemeinschaft
German Research Foundation

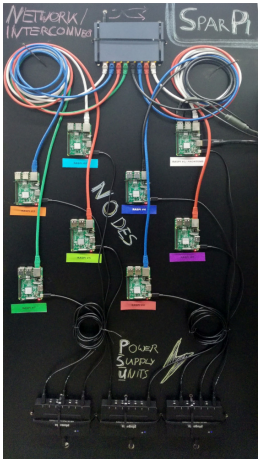
A changing HPC landscape – architecture & programming models



A changing HPC landscape – key challenges

- Computational
  - Multicore ⇒ manycore
  - Diverse hardware **and** programming models
  - Traditional scale-up/out not applicable
- Scientific: Porting code is not sustainable
- Societal: HPC uses large amounts of resources

⇒ Need: effective and efficient use of capabilities



SparPi supercomputer model

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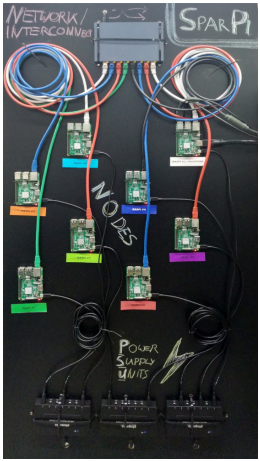
Performance portability... *broadly refers to portable (single) source code that makes efficient use of the hardware architecture whatever it may be*

[performanceportability.org]



SparPi supercomputer model

From CPU to any GPU

[Grete, Glines, & O'Shea TPDS 2021]
[Grete+ IJHPCA 2022]

Standard C++ CPU code

- Example 3D loop:

```
for( int k = ks; k < ke; k++){
 for( int j = js; j < je; j++){
  #pragma omp simd
  for( int i = is; i < ie; i++){
   /* Loop Body */
   u(k,j,i) = ...
}}}
```

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```

Kokkos abstraction (exposes full control)

```
parallel_for(team_policy(nk, AUTO),
 KOKKOS_LAMBDA(member_type team) {
  const int k = team.league_rank()+ks;
  parallel_for(
   TeamThreadRange<>(team,js,je,
    [&] (const int j) {
     parallel_for(
      ThreadVectorRange<>(team,is,ie,
       [=] (const int i) {
        /* Loop Body */
        u(k,j,i) = ...
});});});});
```

From CPU to any GPU

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   u(k,j,i) = ...
}}}
```

Our (and other) codes

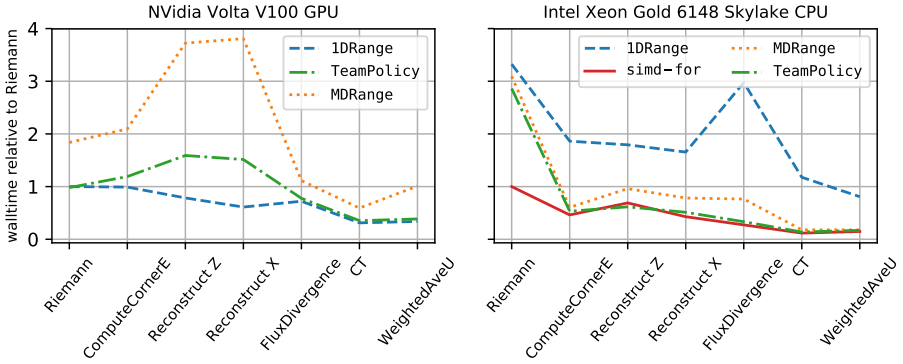
```
par_for("name",ks,ke,js,je,is,ie,
 KOKKOS_LAMBDA (int k,int j,int i) {
  /* Loop Body */
  u(k,j,i) = ...
});
```

- Introduced intermediate abstraction layer
- Runs on any GPU (and CPU)
- Simple things stay simple
- No expert knowledge required

⇒ proof-of-concept code `K-Athena` with 76% parallel efficiency on all of Summit

Intermediate abstraction layer and execution policies

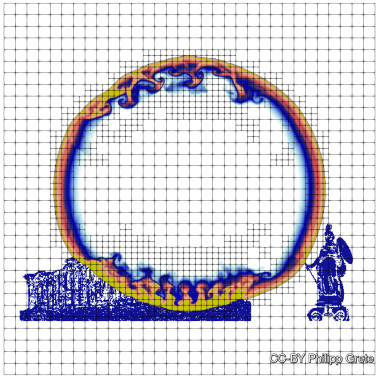
[Grete, Glines, & O'Shea TPDS 2021]



- Execution policies have significant impact on performance
- No "one size fits all" solution yet
- In some codes: manual pointers extraction to aid compiler vectorization

(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



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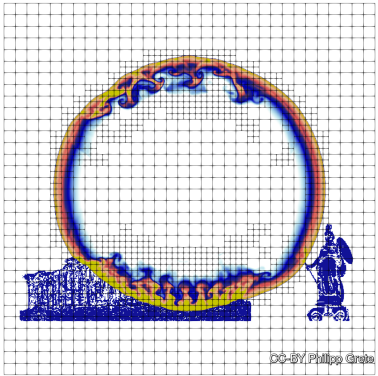
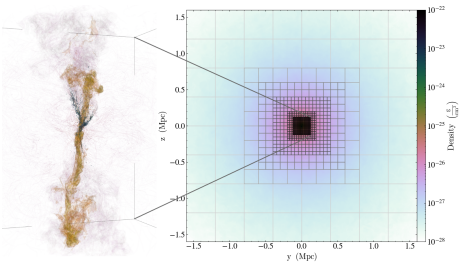
- "Refine" (split block into more blocks) to
  - increase spatial resolution in region(s) of interest
  - save computational resources
- Block size is important
  - ratio of active to passive zones
  - number of neighbors
  - thickness of transition regions



Parthenon – Performance portable AMR framework

- Goal: Hide complexity of device-accelerated AMR
- Open collaboration (20+ contributors)
  github.com/parthenon-hpc-lab
- Key performance design decisions
  - device first/resident
  - block packing/kernel fusing
  - device-to-device communication via async. MPI



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- Key performance design decisions
  - device first/resident
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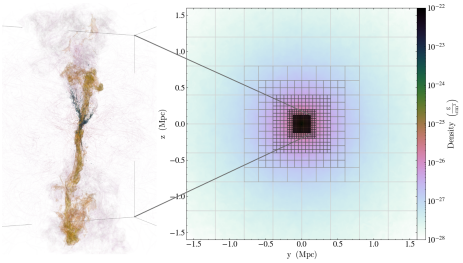
  - device-to-device communication via async. MPI
- Advanced features (e.g., abstract data containers, package system, task-based parallelism, sparse variables, particles, integrated solvers)
- Multiple downstream codes

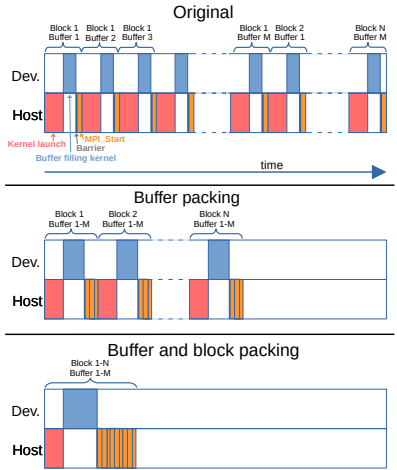


Packing: Kernel fusing ↔ block packing

[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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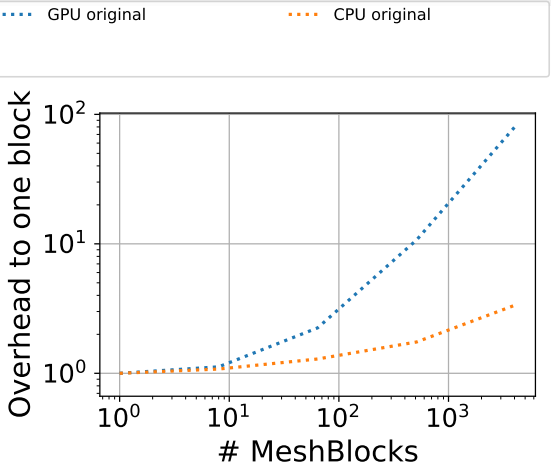

- GPU 256^3 mesh with blocks 256^3 to 16^3
- CPU 128^3 mesh with blocks 128^3 to 8^3

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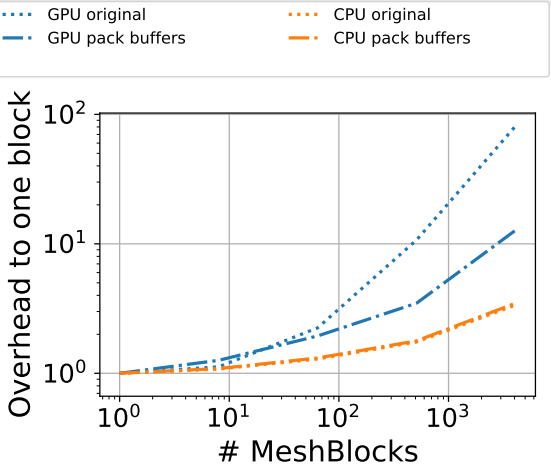

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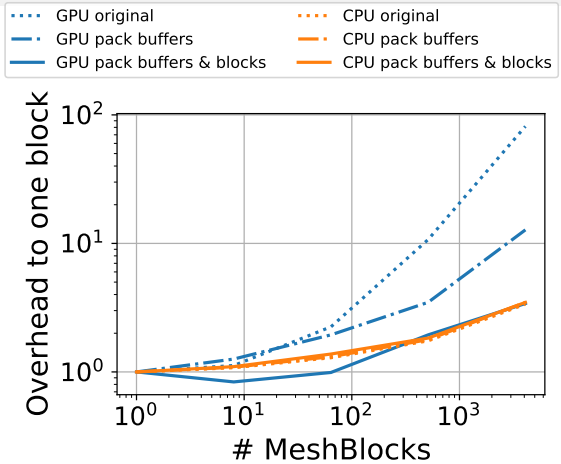

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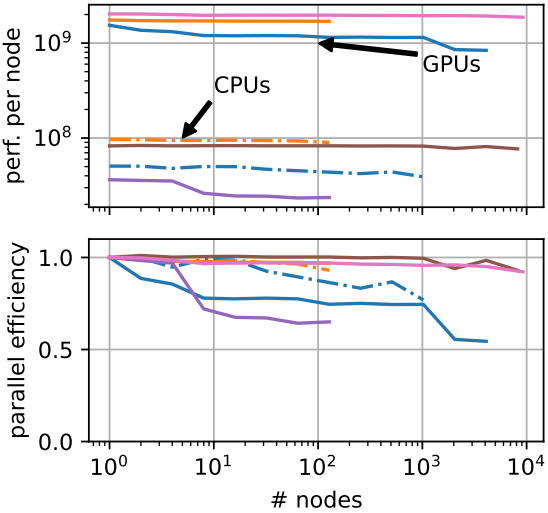
Parthenon – a performance portable AMR *framework*

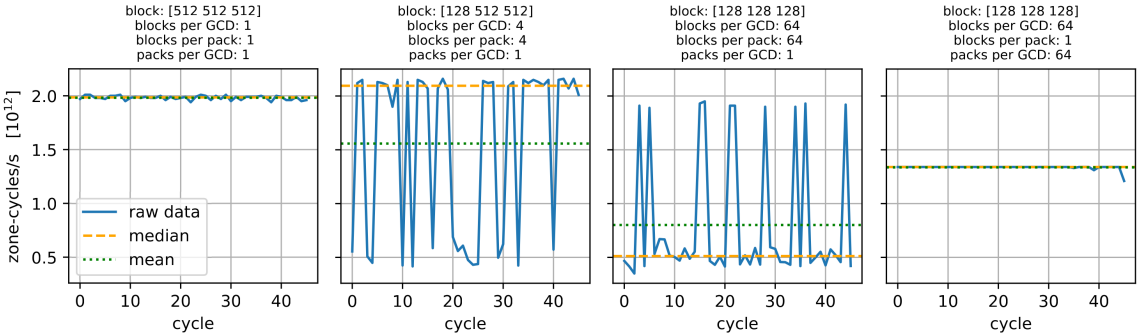
[Grete+ IJHPCA 2022]

- Performance across architectures:
  - CPU: x86, ARM, Power9
  - GPU: CUDA, HIP
- #1 TOP500: Frontier (9472 nodes)
  - 92% weak scaling efficiency on 73,728 GPUs (eff. 500 million cores)
- Performance portable GPU-acceleated AMR works in practice*!



Packing #2: Messages in a bottle(neck)

[Holmen, Grete & Melesse Vergara CUG23]



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

$\Rightarrow$ Messaging matters

$\Rightarrow$ Support for coalesced messages with index splitting ($\rightarrow$ incr. occupancy)

Advanced features: packing of (sparse) variables on blocks

- `View` + `Metadata` = `Variable`
- Multiple `Variable` = `MeshBlockData`
- `MeshBlockData` across multiple blocks = `MeshData`
- Arb. selection of variable and blocks = `Pack` (read: `View` of `View` (of `View`)

```
struct my_var_t : public variable_names::base_t<false> {
  template <class... Ts>
  KOKKOS_INLINE_FUNCTION varname(Ts &&...args)
      : variable_names::base_t<false>(std::forward<Ts>(args)...) {}
  static std::string name() { return "my_var"; }
}
...

pkg->AddField<my_var_t>(Metadata(...));
pkg->AddSparsePool<my_sparse_var_t>(Metadata(...), sparse_idxs);
...
```

Define a variable name type that uniquely identifies your field. Needs to inherit from `variable_names::base_t` and provide `name()` which returns a unique string.

Add fields and sparse fields to your package using the type

[Credit: L. Roberts LA-UR 25-25420]

Advanced features: packing of (sparse) variables on blocks cont.

```
/*static*/ auto desc = MakePackDescriptor<my_var_t, my_other_var_t>(md);
...

auto pack = desc.GetPack(md);
...

par_for(PARTHENON_AUTO_LABEL, 0, pack.GetNBlocks() - 1, kb.s, kb.e, jb.s, jb.e, ib.s, ib.e,
    KOKKOS_LAMBDA(const int b, const int k, const int j, const int i) {
      pack(b, TE::F1, my_var_t(), k, j, i) = ...;
      for (int l = pack.GetLowerBound(b, my_sparse_var_t());
           l <= pack.GetUpperBound(b, my_sparse_var_t()); ++l) {
        pack(b, my_sparse_var_t(l), k, j, i) = ...; // Default assumption is TE::CC
      }
    });
```

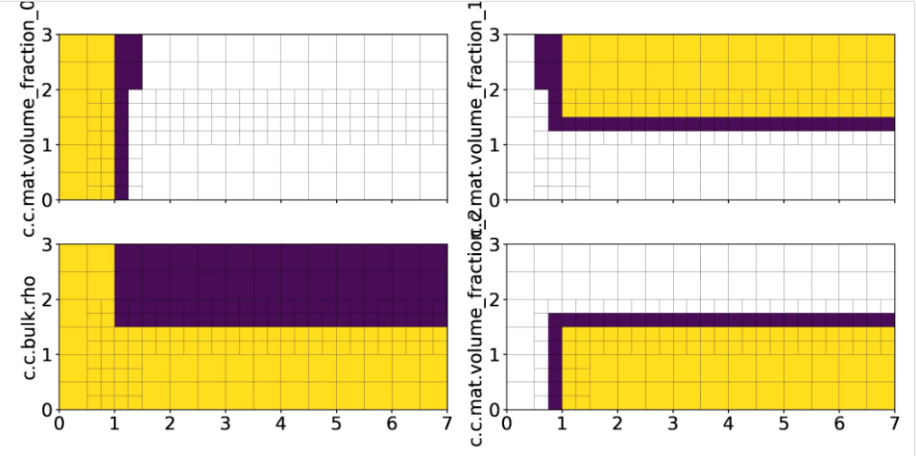
A `PackDescriptor` defines a list of fields to be packed. Also can take `PDOpt` options and `Metadata` flags to further define selection of fields.

Actually get the pack from a `MeshData` object

Access the pack in a kernel

[Credit: L. Roberts LA-UR 25-25420]

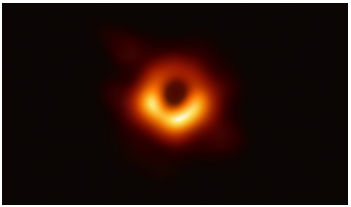
Sparse variables in action (white blocks are not allocated)



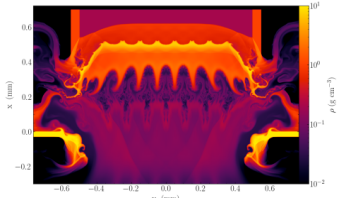
[Credit: J. Dolence LA-UR-26-22714]

Parthenon-enabled applications and ecosystem

- `AthenaPK` (astrophysical) MHD and turbulence
- `Phoebus` GRRMHD (e.g., neutron star mergers)
- `KHARMA` GRMHD (used within EHT collaboration)
- `RIOT` multi-material physics
- `Artemis` multi-fluid, radiation hydro
- `Flash` fusion power
- `parthenon-hydro`: just 1000 lines of code including test infrastructure ($\Rightarrow$ tutorials/teaching)



[EHT collaboration]



[RIOT LA-UR-26-22714]

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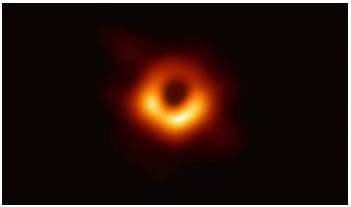
- `Singularity-eos` microphysics
- `Jaybenne` Monte Carlo radiation transport
- ...



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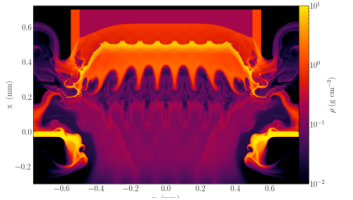

[RIOT LA-UR-26-22714]

Pushing limits with AthenaPK through Parthenon

- Own downstream code: AthenaPK targeting processes/systems involving astrophysical plasmas
  - Supernova remnants
  - Cloud/galaxies in wind (example right)
  - Jets from active galaxies
  - Magnetized turbulence
    GCS Exascale Pioneer Application on JUPITER

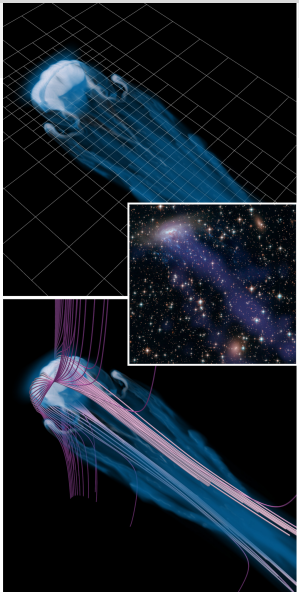

Image credit (inset): NASA/HST

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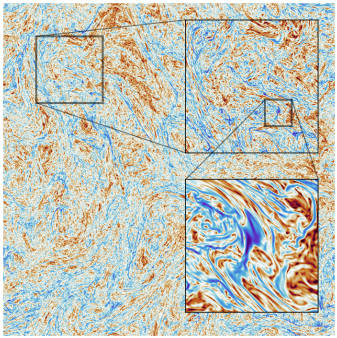
    GCS Exascale Pioneer Application on JUPITER
- Successfully (more or less)
  - running 4 trillion cells MHD turbulence simulation
  - writing/restarting from 289TB checkpoint
  - running with 26 cell wide ghost layer
  - running with particles 57 fields



MHD turbulence on JUPITER

Conclusions and outlook

- Performance portable AMR works in practice*
  (*but needs non-trivial pooling of resources)
- Enabled by `Kokkos`
- Large, collaborative effort!
- Current challenges
  - High register pressure kernels
  - Memory pools
  - Efficient vectorization
- We are an open, welcoming community. Meet us at/on
  - `https://github.com/parthenon-hpc-lab`
  - Matrix chat: `#parthenon-general:matrix.org`