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

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Abstract
On the path to exascale the landscape of computer device architectures and corresponding programming models has become much more diverse. While various low-level performance portable programming models are available, support at the application level lacks behind. To address this issue, we present the performance portable block-structured adaptive mesh refinement (AMR) framework PARTHENON, derived from the well-tested and widely used ATHENA++ astrophysical magnetohydrodynamics code, but generalized to serve as the foundation for a variety of downstream multi-physics codes. PARTHENON adopts the KOKKOS programming model, and provides various levels of abstractions from multidimensional variables, to packages defining and separating components, to launching of parallel compute kernels. PARTHENON allocates all data in device memory to reduce data movement, supports the logical packing of variables and mesh blocks to reduce kernel launch overhead, and employs one-sided, asynchronous MPI calls to reduce communication overhead in multi-node simulations. Using a hydrodynamics miniapp, we demonstrate weak and strong scaling on various architectures including AMD and NVIDIA GPUs, Intel and AMD x86 CPUs, IBM Power9 CPUs, as well as Fujitsu A64FX CPUs. At the largest scale on Frontier (the first TOP500 exascale machine), the miniapp reaches a total of $1.7 \times 10^{13}$ zone-cycles/s on 9216 nodes ($73,728$ logical GPUs) at $\approx 92\%$ weak scaling parallel efficiency (starting from a single node). In combination with being an open, collaborative project, this makes PARTHENON an ideal framework to target exascale simulations in which the downstream developers can focus on their specific application rather than on the complexity of handling massively-parallel, device-accelerated AMR.

Keywords
Adaptive mesh refinement, performance portability, high-performance computing, parallel computing

1. Introduction
Many open problems in physics involve vastly varying length- and time-scales. Some examples, drawn from astrophysics, include the deposition and redistribution of energy from active galactic nuclei (Bourne and Sijacki 2021; Glines et al., 2020; Meece et al., 2017; Prasad et al., 2020) relativistic accretion flows around compact objects (Miller et al., 2019b, 2020; Ryan et al., 2018; Ressler et al., 2020), the in-spiral and merger of neutron stars and black holes Alcubierre (2008); Miller and Schnetter (2016), and, more generally, turbulence simulations (Federrath et al., 2021; Grete et al., 2021b).

From a computational point of view, simulating these problems involves solving (various types of) partial
differential equation—often on a structured grid using finite volume or finite difference methods. However, given the physical scale separation these problems typically cannot be globally represented in simulations—even on the next generation, exascale supercomputers. One option to make these kinds of simulations feasible is the use of (adaptive) mesh refinement (AMR), that is, a mesh that increases the spatial resolution in regions of interest. AMR frameworks using varying refinement approaches have successfully been used for many years. These include refinement based on individual cells, for example in RAMSES (Teyssier, 2002) or xRAGE (Gittings et al., 2008), based on separate patches (of arbitrary shape and size), for example, by Berger and Colella (1989) implemented in ENZO (Brummel-Smith et al., 2019) and PLUTO (Mignone et al., 2011), or based on blocks of fixed size, for example, as in PARAMESH (MacNeice et al., 2000). With respect to parallelization all these “legacy” frameworks are primarily concerned with handling the mesh (and its refinement) across multiple nodes in parallel, see, for example, Dubey et al. (2014) for a comparative review. Given that they were developed prior to the broad availability of accelerators/GPUs, the additional levels of parallelism and memory hierarchy provided by these devices are typically not leveraged. This prevents an efficient use of those frameworks on many next generation, exascale supercomputers.

From a technical point of view, achieving sustained application-level exascale performance will require maximizing concurrency throughout the application while simultaneously minimizing the impact of data movement within the system. Both issues will be significantly more challenging at exascale than they are on today’s petascale systems: Amdahl’s law will require ever more levels of parallelism to be exploited in applications to remove or hide even small sequential bottlenecks. At the same time, technological trends will continue to increase the expense of data movement relative to compute for most applications as well as introduce more dynamic performance characteristics due to power capping and highly tapered network topologies. An additional challenge is that applications will need to achieve this level of performance on two or more radically different system architectures, as typified by the current Summit (IBM/Nvidia) and Frontier (AMD), and future El Capitan (AMD) and Aurora (Intel) systems. These requirements are pushing applications to consider new programming approaches such as additional hardware abstraction layers, and/or compositions of task-based and data parallelism.

In general, the combination of accelerated nodes (with large amounts of device memory and different architectures) and the complexity of AMR introduces new computational challenges. For example, handling many (even up to thousand of) blocks per device with even more compute kernels—especially when small block sizes are involved—can result in significant overheads both with respect to managing the mesh hierarchy as well as with respect to the cumulated kernel launch latency.

To address these challenges, we introduce the performance portable block-structured adaptive mesh refinement framework PARTHENON. It is built on the basis of ATHENA++ (Stone et al., 2020) and K-ATHENA (Grete et al., 2021a) and hides the complexity of AMR and device computing in downstream codes by providing high-level abstractions. These high-level abstractions not only pertain to the handling of the mesh and its data but also address computational complexity, such as parallel execution. To exploit on-node data parallelism, PARTHENON internally uses the performance portability programming model KOKKOS (Carter Edwards et al., 2014; Trott et al., 2021). This way PARTHENON inherits the KOKKOS capability to target various device architectures using a single source code and programming model. To further increase data parallelism, PARTHENON also supports various levels of logical packing of data structures such as variables or entire blocks, which are always allocated in device memory to minimize data transfer. To exploit inter-node parallelism, PARTHENON internally uses asynchronous, one-sided (GPU-aware) MPI calls using buffers located in device memory.

Naturally, the PARTHENON collaboration is not the only collaboration who has identified the various numerical and computational issues of “next generation” AMR frameworks. For example, AMREX (Zhang et al., 2021) shares many design decisions with PARTHENON including data containers and abstraction for parallel regions. Key differences to PARTHENON are the more flexible mesh structure in AMREX (at the cost of increased complexity) and a self-contained performance portability layer rather than relying on an external library such as KOKKOS. Another example is UINTAH (Holmen et al., 2017), which, as a legacy asynchronous many-task runtime system for block-structured AMR, also adopted KOKKOS internally as performance portability layer below an intermediate abstraction layer. While PARTHENON also offers a flexible, asynchronous tasking system, it is operating at the block level whereas UINTAH tasks can be more fine-grained following a directed acyclic graph. However, to our knowledge the impact performance of the interplay of fine-grained tasks with (many) kernel launches and large number of blocks per device is still an open question. This similarly applies to other asynchronous many-task runtime systems such as CHARM++ who also start to incorporate GPU support (Choi et al., 2022). One framework using AMR built on top of CHARM++ is QUINOA (Bakosi et al., 2021) that just started to use GPUs. Finally, GAMER-2 is astrophysical, multi-physics code with support for GPU-accelerated AMR (Zhang et al., 2018). It differs from PARTHENON by being a fully integrated code (physics and mesh) rather than an AMR framework and supporting only CUDA (i.e., Nvidia GPUs).
Moreover, in GAMER-2 all data structures are allocated in host memory so that data required in compute kernels is constantly transferred back and forth between host and device memory.

In the following, we first provide a brief background on block-structured AMR and Kokkos in Section 2 before introducing the key design aspects and features of PARTHENON in Section 3. In Section 4, we provide an overview of various downstream applications that are built on top of PARTHENON including the PARTHENON-HYDRO miniapp. The latter is used in Section 5 to present different performance characteristics of PARTHENON pertaining to the packing of variables and blocks as well as to weak and strong scaling. In Section 6, we describe the software engineering approach taken by the collaboration. Finally, we discuss current limitations and future enhancements in Section 7 before we conclude in Section 8.

2. Background

2.1. Block-structured AMR

Only a brief summary of the block-structured AMR algorithm adopted by PARTHENON is given in what follows, a complete description is given in Stone et al. (2020). Individual cells that span the computational domain are grouped into a regular array of subvolumes termed MeshBlocks. Data associated with the cells on a given MeshBlock are stored as N-dimensional arrays. PARTHENON provides infrastructure for AMR with both cell- and face-centered data. The size of these arrays must be the same on all MeshBlocks, and moreover the overall domain must contain an integer number of MeshBlocks in each dimension. However, the number and size of individual MeshBlocks tiling the computational domain is arbitrary.

The MeshBlocks themselves are arranged into a binary-tree (in 1D), a quad-tree (in 2D), or an oct-tree (in 3D). Use of a tree greatly simplifies finding neighbors (necessary for communicating boundary conditions) and allows distribution of MeshBlocks across multiple processors using Z-ordering, which helps improve load balancing.

For AMR calculations, any number of MeshBlocks can be subdivided into $2^N$ finer MeshBlocks (prolongation), or contiguous blocks of $2^N$ MeshBlocks can be joined into one coarser MeshBlock (restriction), as needed. Figure 1 diagrams how MeshBlocks on a refined grid are stored in the tree. The tree structure ensures that the neighbors of a MeshBlock can easily be found, even if they are at different levels of the grid hierarchy. One great advantage of

![Figure 1](https://example.com/image1.png)

**Figure 1.** Labeling of MeshBlocks (top) and their organization into a quadtree (bottom) for an example simulation with mesh refinement in two dimensions. Reproduced by permission of the AAS from Stone et al. (2020).
this tree structure-based AMR is that any given spatial
location in the domain is covered by one, and only one,
MeshBlock. As a result, only neighbor relationships exist
but no spatial parent–child ones. Thus, except when new
MeshBlocks are created or destroyed, prolongation and
restriction is required only when data is communicated at
MeshBlock boundaries. However, this approach requires
that the entire tree is rebuilt every time (de)refinement is
triggered and MeshBlocks are being destroyed/constructed in place.

2.2. Kokkos

Kokkos is an open source, performance portable pro-
gramming model for many core devices implemented as a
C++ template based library (Carter Edwards et al., 2014;
Trott et al., 2021). As such it provides abstractions to le-
verage hardware features, for example, threading or multi-
level memory hierarchies, through various backends. This
allows device-specific optimization at compile time for
devices from various vendors, for example, using the
CUDA backend for NVIDIA GPUs, the HIP backend for
AMD GPUs, or the OpenMP backend for multi-threading
on CPUs.

Some of the fundamental abstractions provided by
Kokkos include:

- **Execution Spaces** define where (on which device/
through which backend) a computational kernel (in
practice a function object) is executed.
- **Execution Patterns** define how individual work items
within a kernel are related. Examples include
Kokkos::parallel_for for independent work
items that can be handled independently in parallel or
Kokkos::parallel_reduce to execute a par-
allel reduction over all work items.
- **Execution Policies** allow control over how a parallel
region is executed. They can be simple, such as a
RangePolicy that correspond to a single one-
dimensional index for each work item, as well as
nested loops, or they can be complex descriptions
through hierarchical parallelism to control the
(grouping of threads and individual threads.
- **Memory Spaces** define where data is stored, for ex-
ample, on the host or in device memory, or even in
cache-type memory (where supported by hardware).
- **Memory Layout** allows to specify how data is stored,
that is, how multidimensional indices are mapped to
memory locations.
- **Views** are the primary data structure provided by
Kokkos. They correspond to multidimensional arrays
and are parameterized, for example, by a Memory
Spaces and a Memory Layout.

3. Design

3.1. Primary design goals

Many algorithms employed in targeted application domains
have comparatively low arithmetic intensity, for example,
O(1) floating point operations per byte of data moved for
stencil based calculation. At the same time, the peak
compute power of devices has been increasing faster than
the peak memory bandwidth in recent years and is even
worse for the bandwidth between host memory and device
(e.g., GPU) memory. This results in an ever increasing
bottleneck when lots of data needs to be moved. To cir-
cumvent this, PartHENON follows a device first or device
resident approach in which all work data is allocated in
device memory only. In other words, data movement be-
tween host and devices is reduced to a minimum as the work
data used in (expensive) computational kernels is already
close to the execution space.

Another goal is to hide complexity from a downstream
application point of view. Similar to Kokkos, which ab-
stracts the complexity of on-node parallel programming,
PartHENON generally provides additional abstractions to
hide the complexity of multi node, parallel, block-structured
adaptive mesh refinement. This includes simplified loop
abstractions (i.e., setting many default values in the Kokkos
layer) as well as higher level abstractions such as control
over the packing of individual blocks, communication
between nodes via MPI, a tasking infrastructure, or IO, as
detailed in the following sections. At the simplest level, a
downstream application only needs to provide compute
kernels in plain C++ (i.e., no vendor specific backend) that
are concerned with data of a single block and everything
else is handled by PartHENON.

Importantly, the underlying access patterns provided by
these abstractions need to change depending on hardware
and must often be tuned for a given problem. To accomodate
this constraint, we expose in our abstraction layers tuning
parameters, allowing us to tune to individual hardware
configurations.

Finally, PartHENON is designed with extensibility in mind
offering many “plug-and-play” interfaces. This allows for
a straightforward addition of many capabilities in down-
stream codes without requiring changes in PartHENON itself.
At the same time, this also allows different downstream
applications to easily share code as all downstream features
are implemented using those interfaces by construction.

3.2. Intermediate abstraction layer

A given set of hardware may require different loop patterns
and nested parallelism for optimal performance. For ex-
ample, an Intel machine parallelized only with MPI may be
most performant with a standard C++ for loop, enabled with
vectorization pramgas. However, this will obviously not be the case on a GPU. Following the work in Grete et al. (2021a), we introduce a set of loop abstractions, which we call parthenon::par_for and parthenon::par_reduce. At their simplest, these are thin wrappers around kokkos parallel dispatch. However, they have a unified interface suited to parthenon loops over mesh-blocks, regardless of the parallelism pattern used “under the hood.” This enables us to swap out kokkos loops for basic for loops and calls to the C++ standard library. An example two-dimensional using the basic abstraction might look like

```
Listing 1: Example of a two dimensional for loop with the j index going from 0 to je and i index from 0 to ie using the basic abstraction provided by PARTHENON. The loop_pattern_tag controls the Kokkos execution policy and exec_space the Kokkos execution space.
parthenon::par_for(parthenon::loop_pattern_tag, "kernel_name", exec_space, 0, je, 0, ie, Kokkos::LAMBDAG(k,j,i) { 
    u(j,i) = ... 
});
```

For ease of use, PARTHENON sets several default options, such as the parallel pattern, at compile time depending on the target architecture. These are used when the par_for associated with a MeshBlock are used as illustrated in the following listing.

```
Listing 2: Same as in Listing 1 but using the higher level abstraction associated with a MeshBlock.
block->par_for("kernel_name", 0, je, 0, ie, Kokkos::LAMBDAG(k,j,i) { 
    u(j,i) = ... 
});
```

We also introduce an arbitrary rank array abstraction, built on Kokkos::View, which we call ParArrayND. To support kokkos layout machinery, we use a six-dimensional Kokkos::View as the underlying data structure, and provide a suite of methods for accessing the elements of the array, casting it into a Kokkos::View, and getting lower-dimensional slices. This allows us to treat scalar, vector, and tensor variables all in the same way. For example, a three-dimensional array can be allocated as shown in Listing 3.

```
Listing 3: Initializing a three-dimensional ParArrayND.
ParArrayND<double> arr_3d("Array_name", n3, n2, n1);
```

The shape is set by n3, through n1. Our convention is that the slowest-moving index is first in the constructor arguments and higher rank. However, this depends on the underlying kokkos memory layout setting. (We currently assume LayoutLeft.) Our ParArrayND abstraction supports access operators, where missing indexes are assumed zero, slice operators, and access to the underlying Kokkos::View, as shown in Listing 4.

```
Listing 4: Various operations with ParArrayND.
// Parentheses operator for
// accessing and setting elements
arr_3d(k,j,i) = value;
// Missing indices are assumed zero
assert (arr_3d(j,k) == arr_3d(0,j,i));
// For lower-rank arrays,
// extra indices are ignored
assert (arr_3d(1,k,j,i) == arr_3d(k,j,i));
// Returns an array with the second
// dimension bounded by lower and upper
auto sliced = arr_3d.Slice0<2>(lower, upper);
// Returns a three-dimensional
// Kokkos View
auto view_3d = arr_3d.Get<3>();
```

Both host and device ParArrayND objects are supported, but they default to living in device memory.

### 3.3. Packages

PARTHENON is designed to couple multiple disparate components together. To capture this, we introduce packages. Each package is an independent functionality built on top of PARTHENON, with its own registered variables, physics routines, and tasks. Importantly, packages can share variables. In other words, package “A” may register a variable and package “B” may use it. PARTHENON supports dependency tracking between variables registered by packages. A package may register a variable as

- Private
- Provides
- Requires
- Overridable

A Private variable is private to a given package, and lives in the package’s namespace. Other packages should not access it. A Provides variable is provided by a package, with the intent that other packages may use it. However, the providing package is expected “own” the variable. If two packages try to provide the same variable, an error is raised. If a package registers a Requires variable, it is stating that it needs this variable to exist, but does not create or manage it itself. If no package provides a required variable, an error is raised. If a package registers an Overridable variable, it is stating that it can provide this variable, but will defer to another package, if it provides it.
Packages register their variables, as well as global constants within their namespace (called params) in a function we call Initialize. An example Initialize function is shown in Listing 5. All initializations are registered by the parthenon manager object at startup. To tell the code what packages to load, a ProcessPackages function must be provided.

An example function is shown in Listing 6.

Note that although packages create their own variables and provide tasks, these tasks are not automatically called. The tasks must be woven together “by hand” by an expert in the driver code. This will be explained in Section 3.10.

### 3.4. Variables

Variables in parthenon consist of metadata and data. The data is stored on a per-block basis in a multidimensional Kokkos::View. It can live at cell centers, faces, edges, corners, or not be associated with a mesh entity at all. Although in the initial parthenon release, only cell-centered and non-mesh-tied variables are fully implemented. Support for the other types of variables will be added in a later release.

All variables in parthenon must be named. The name is used in simulation output, error messages, and to obtain a handle to the variable data from containers (see Section 3.6). This greatly enhances the readability and self-documentation of the code. The name of a variable is stored in its metadata along with other important information. The metadata also contains the shape of the variable, that is, if it is a scalar, vector, or tensor, along with the number of components in each dimension in the case of vectors and tensors. Finally, the metadata contains a collection of flags that indicate, for example, if the variable is independent or derived, whether it is private, provided, required, or overridable (see previous section), if it is advected, if it needs ghost cells filled, or if it has fluxes.

The metadata information allows the parthenon infrastructure to perform certain tasks on variables without needing to understand their physical meaning. For example, parthenon can write a restart file that includes only the independent variables, since they are all flagged as such. When using reflective boundary conditions, parthenon can reflect the X-component of vector variables in the X-direction, Y-components in the Y-direction, and so on. Furthermore, the metadata flags are also useful for user provided physics packages. For example, the hydro package can advect all variables from all packages flagged as advected, without needing to know what those variables are. By setting the FillGhost and WithFluxes metadata flags, the user can control which variables will have their ghost cells filled by parthenon and which variables will have fluxes buffers allocated.

Typically, variables are allocated on every block in the entire domain. But for some applications, there may be variables that are only relevant in parts of the domain, thus creating opportunities to save both memory and computing resources. For such cases, parthenon provides sparse variables. Sparse variables behave just like ordinary (or dense) variables, with two exceptions: (i) Instead of just a name, sparse variables have a base name and a sparse ID and (ii) sparse variables are only allocated on some blocks.

Sparse variables are added through pools. A sparse pool consists of a base name, a set of sparse IDs, and shared metadata. For each sparse ID in the pool (e.g., 1, 4, 10, and 11), a sparse variable is created whose name is “basename\_X”, where “basename” is the pool’s basename and “X” is the sparse ID. The sparse variables have the same metadata as the pool’s shared metadata, except for the shape and Vector/Tensor flags, which can be set individually per sparse ID. Furthermore, the sparse variables are not allocated on any blocks until the user manually allocates them on specific blocks or they are advected into a block where they were not previously allocated. They can also be deallocated by the parthenon infrastructure if they
completely leave a block. The main use case for sparse variables are multi-material simulations where a particular sparse ID corresponds to a particular material. Currently, only cell-centered variables are supported as sparse variables.

### 3.5. Particles

In addition to the structured multidimensional variables (either tied to mesh entities or not) described above, PARThENON also supports particle data structures, called Swarms. Like variables, swarms combine metadata and data, and are stored on a per-block basis. Swarms hold particle data in a Struct of Arrays pattern; as such, particles that will be iterated over together by the same physics should belong to the same swarm.

Swarms support a subset of Metadata flags used by variables; Provides or Requires are used by individual packages to share particle data, and None is generically set because particles are not grid-based quantities. A swarm is composed of a set of ParticleVariables, which store data in 1D ParArrayNDs. Each particle variable contains its own metadata; in particular, this metadata is used to specify the datatype of the particle variable, either real or integer. Swarms are always created with \( x, y, \) and \( z \) real-valued particle variables; additional variables are enrolled by the package creating the swarm. This approach of user-specified data with memory locality provided by the library has been successfully applied in other particle frameworks (Mniszewski, 2021; Zhang et al., 2021).

In general, the particle population will grow and shrink in size over time, particularly on the scale of a meshblock. This can occur both through physics algorithms that create or destroy particles and communication of particles across meshblocks. Swarms manage their memory dynamically; users request the creation of a certain number of particles. Existing empty elements in the particle list are filled in first, and then if necessary the swarm will internally resize its ParticleVariables to accommodate the remaining particles. This resizing procedure proceeds exponentially to limit the number of memory reallocations required; the size of the memory pool grows by factors of 2. Swarms include a Defrag method that deep copies individual particles’ entries to ensure contiguous memory in each particle variable on demand.

Particle communication is handled by non-blocking send and receive calls as in grid-based data communication. During package functions that update particle positions, particles must be checked for whether they have left the meshblock they are currently on. This will be recorded by the swarm, and during the subsequent send and receive calls the off-block particles will be copied to either send buffers for subsequent MPI communication or copied directly onto the receive buffers of blocks on the same MPI rank. The sent particles are deleted from the sending meshblock’s swarm. Receiving meshblocks then copy the particles from the receiving buffers into their own swarm’s particle variables. Only communication to neighboring meshblocks is supported.

Particle communication between the same meshblocks can be required multiple times per timestep, particularly for algorithms where particles can traverse many meshblocks per timestep. This can be implemented by a separate blocking TaskRegion that is repeatedly called until a global stop criterion is met, as in the provided examples, or through the iterative task list machinery.

Boundary conditions on particles are applied to all particles marked as being off their meshblock by the internal swarm send and receive tasks. Boundary conditions are implemented through separate polymorphic boundary condition classes for each of the six boundary faces. PARThENON provides periodic and outflow boundary conditions; additional boundary conditions can be implemented by driver applications.

Particles are not sorted by grid zone below the scale of an individual meshblock. Particle-mesh interactions are handled via KOKKOS by the downstream application.

### 3.6. Data containers/packing

As discussed above, each package may register its own set of variables. However, it is often useful to loop over all variables, either sparse or dense, with some set of properties such as the need to perform ghost halo exchange. Because launching code on an accelerator comes with some (often significant) latency, it is also often far more performant to bundle work across mesh blocks into a single device kernel launch.

To enable this, we implement VariablePacks and MeshBlockPacks. VariablePacks are objects that collect all desired variables within a single index space. In the process, indices of higher rank variables (e.g., tensors) are flattened so that all variables (and their components) can be accessed by a single running index, typically \( v \) in addition to the spatial \( k, j, \) and \( i \) indices. The underlying data structure is a View of Views allowing efficient access to the existing data on devices. Variables for VariablePacks can be selected via metadata tags registered by a given package, or by name. MeshBlockPacks do the same, but also gather variables from some number of meshblocks on a given MPI rank. This results in an additional, fifth flattened index, typically notated by \( b \). The optimal number of meshblocks to gather is hardware and problem dependent, and so may be set at runtime, see Section 5.2 for some example results. To expose these packing mechanisms, as well as relevant metadata used in a given physics kernel, we implement the MeshBlockData and MeshData data structures. These objects have
methods to generate pack objects and also automatically cache the relevant packs from cycle to cycle. The MeshBlockData and MeshData objects also expose accessors for variables, grid shape information, and parameters set by individual packages. Overall, this allows efficient access to all data of an arbitrary number of variables on an arbitrary number of blocks through tight, 5-dimensional loops.

3.7. Boundary communication

Two important strategies to achieve a high parallel efficiency across multiple ranks are implemented in PARTHENON.

First (and more general), all communication buffers can be exchanged asynchronously by using one-sided, asynchronous MPI calls. Moreover, each Variable uses its own MPI handle so that individual Variables can also be communicated independently. This also applies to flux correction for multilevel meshes. A typical driver to solve equations in conservative form implements several boundary communication related tasks that are split on purpose. These tasks include (a) initializing/resetting the individual MPI handles, (b) starting and receiving flux correction (with mesh refinement enabled after calculating block local fluxes), (c) filling communication buffers with the updated data (e.g., after calculating the flux divergence), (d) start sending communication buffers (via MPI_Start), and (e) fill ghost cells from buffers already received. These tasks can be run for individual blocks and variables and, thus, allow to hide communication related walltime (e.g., latency) behind computations. In other words, while buffers of some blocks are filled in a compute kernel executed on a device, already filled buffers of other blocks can already be communicated in parallel in the background.

The second (and more specific to GPU-accelerated simulations) strategy is filling more than one communication buffer in a single kernel. In ATHENA++ each buffer is filled independently in small pack and unpacking routines. However, the work done in these buffer filling kernels is very small, for example, just copying 8 numbers for a corner buffer of a 3D block with 2 ghost zones in each direction, making the actual kernel runtime significantly smaller than the kernel launch time (typically a couple of μs). Given that some vendor APIs (e.g., when running with the CUDA backend) are inherently serial for launching kernels, no significant performance increase can be expected even when multiple kernels can be executed in parallel on the device. For this reason, we implemented a flexible “fill-in-one” approach that allows us to fill all buffers of one or more Variables on one or more blocks in a single kernel, see Figure 2 for an illustration. The performance in practice of this approach is shown in Section 5.1.

With the block structured AMR adopted in PARTHENON, prolongation and restriction of data only occurs during communication of data between neighboring MeshBlocks at different levels of refinement, and therefore these steps are functionally part of the boundary communication design. Data sent from fine-to-coarse levels are first restricted and then communicated to reduce message sizes. Data sent from coarse-to-fine are packed into special coarse buffers on the target MeshBlock. Once all communication has completed, the data in these coarse buffers are then interpolated (prolongated) to the fine resolution. Details of the multi-level communication and interpolation algorithms for cell- and face-centered data are given in Sections. 2.1.3 and 2.1.5 of Stone et al. (2020). Again, in order to reduce the number kernel launches restriction is now handled within the “fill-in-one” machinery in contrast to ATHENA++ where each restriction is a separate kernel.

Finally, contrary to the ATHENA++ design each Variable uses a unique MPI communicator rather than the default communicator and individual buffers use MPI tags created sequentially rather than globally. The key advantage is to circumvent the minimum upper bound of at least 32,767 defined by the MPI standard. This bound is easily
reached when running 3D mesh refinement simulations with small block sizes on modern devices where a single rank can (computationally) easily handle 100s–1000s of blocks.

### 3.8. Load balancing and mesh refinement

When new **MeshBlocks** are created or destroyed as part of the AMR, load balancing of the resulting workload across devices becomes important. Following the strategy in **ATHENA++** (see section 2.1.6 in Stone et al. (2020)), in **PARTHENON** **MeshBlocks** are redistributed across nodes whenever mesh refinement occurs and the tree is rebuilt. Generally some fractions of the **MeshBlocks** on each device will have to be moved to neighbors to achieve good balance. Nevertheless, the increase in performance associated with good load balancing outweighs the overhead of this communication. Note that mesh derefinement is only allowed periodically (controlled by a runtime parameter) to prevent regions very close to the criterion from refining and then derefining on subsequent cycles.

For performance, the new tree structure is always rebuilt first and that information is used to determine the meshblock distribution across ranks. Thus, only afterward the tree is populated with data either by (a) moving pointers to **MeshBlock** objects for same-level, same-rank blocks from the old to the new tree, (b) by creating or destroying blocks for same-rank, (de)refined blocks, or (c) by sending meshblock data to a different rank. For the latter, the data transfer is optimized for size, that is, if blocks can be derefined on the sending rank, this is done first before sending the data, and, similarly, if the block needs to be refined, the original data is being sent and the refinement occurs on the receiving rank.

### 3.9. IO

**PARTHENON** uses (parallel) **HDF5** to read and write simulation data. An arbitrary number of different outputs can be defined for a given simulation that can differ in the time interval for writing output, the variables contained, the precision (single or double precision floating point numbers) and the compression level. The latter is also enabled through the **HDF5** library and allows for inline compression, which is particularly useful for sparse variables. Several environment variables are processed by **PARTHENON** for a fine-grained control of both **HDF5** parameters as well as MPI-IO parameters. For performance, data locality, and (optional) compression **HDF5** chunking is used where each chunk corresponds to the meshblock data of a **Variable** component. The special “restart” output type forcibly includes all variables with the Independent or Restart Metadata flags and write output in double precision. They allow for a simulation to be restarted in a bitwise identical manner. Moreover, when restarting a simulation a different number of MPI ranks can be chosen, for example, to adapt to a changing number of **MeshBlocks** when using AMR. This is naturally handled by the load balancing mechanism as the tree is being rebuilt upon restarting a simulation.

**PARTHENON** also automatically writes **xdmf** files along the data files, which allows external (analysis) tools such as **PARAVIEW** or **VISIT** to directly read the output data. Finally, a **VT** frontend is currently being reviewed and expected to be merged soon.

### 3.10. Tasks and reductions

**PARTHENON** provides a simple infrastructure for exploiting task-based parallelism. Tasks are organized hierarchically in **TaskCollection**, **TaskRegion**, and **TaskList** objects. In typical usage, applications build and execute a **TaskCollection** object that encapsulates each stage of a calculation, which might correspond to a timestep or even a single Runge–Kutta integrator stage. Each **TaskCollection** is made up of one or more **TaskRegions**, each of which contains one or more **TaskLists**. At the lowest level of the hierarchy, tasks are added to **TaskList** objects by capturing the function to be executed, all of its arguments, and any dependencies that must be executed before the task can be launched. Tasks in a **TaskList** all operate on data at the same granularity, be that the data on a single “MeshBlock” or data across multiple “MeshBlocks.” Tasks in different **TaskList** objects within a **TaskRegion** can be executed concurrently, but **TaskRegions** are serialized within a **TaskCollection**. Figure 3 illustrates these relationships.

Many algorithms require the ability to do global reductions. In a task-based environment where each rank may be executing multiple tasks lists operating on independent sub-domains, orchestrating these reductions is nontrivial. **PARTHENON** provides task-based global reductions for typical datatypes encountered in downstream applications such as plain integers or floating point data, std::vectors thereof, and Kokkos::Views or parthenon::Par ArrayNDs. Reductions are realized by updating a shared rank-local variable from individual tasks in each **TaskList**. Those tasks are marked as a shared dependency within that **TaskRegion**. Only after all tasks with the shared dependency are completed a non-blocking MPI reduction operation is called from a single task on each rank.

### 3.11. Application driver

In **PARTHENON**-based applications, a driver orchestrates the execution of a computation by building and executing collections of tasks, calling I/O functions as needed, and calling into the load balancing and AMR capabilities, if desired. **PARTHENON** provides a basic set of driver classes from which applications can derive.
applications derive from the need only de-
Kutta integration. In this case, the downstream applica-
tions must de
function as appropriate for a multi-stage Runge-
Step function from within a loop that executes
is already de
when the dependencies of a given task can only be other tasks
operate on the same MeshBlock. Once all tasks in the
region are complete, the execution moves to the next region
where three tasks are launched that each operate on all four
MeshBlocks simultaneously. Finally, once these are complete,
execution moves to the final region which defines tasks that
operate on subsets of MeshBlocks. In this way, task
granularity is controlled at the task region level and overall
execution is controlled at the collection level.

At the most basic level, the Driver class gives access to
the mesh and I/O capabilities, but assumes nothing about the
type of calculation being performed. Downstream applica-
tions must define an Execute function that encapsulates
the entirety of the control flow and execution. The cal-
culate_pi example demonstrates a capability that de-

erives from Driver, namely, one that approximates the
value of \( \pi \) using AMR.

Deriving from Driver, the EvolutionDriver is
appropriate for applications that evolve a solution through
time. In this case, Execute is already defined. When
applications derive from EvolutionDriver they must provide a Step function that is responsible for evolving a
solution through a timestep. The EvolutionDriver calls this Step function from within a loop that executes until a specified amount of simulated time has elapsed,
calling the I/O, load balancing, and AMR capabilities as
appropriate.

Finally, PARTHENON provides a MultiStageDriver
which must build the TaskCollection object appro-
priate for a single stage of the integration. The advection
example demonstrates the usage of this driver class.

3.12. Machine dependent build configuration
While the hardware environment becomes more heterog-

eous (requiring performance portable approaches), the
software environment similarly adapts and becomes more heterogenous. For example, custom launchers like \( jsrun \) = on OLCF’s Summit are developed and used to allow for an
appropriate mapping of hardware resources to processes for parallel execution. At the same time, the user has to choose a
suitable mix of compiler, communication, and potentially
offloading libraries for configuring, compiling and running
a code.

For ease of use, PARTHENON ships with so-called machine
configuration files for various supercomputers. These files
contain default values, e.g. architecture specific flags or
parallel launch commands, as well as a recommendation for
the environment modules to load. The configurations are
regularly tested and updated to reflect the latest software
environment provided on a system. This allows (new) users
to readily compile and run the test suite without being
bothered by machine specific details.

4. Downstream applications
4.1. PARTHENON-HYDRO
PARTHENON-HYDRO\(^1\) is a minimal implementation of algo-
rithms solving the Euler equations. In contrast to the ex-
amples included in the PARTHENON repository, which are
mainly used to demonstrate and/or test individual features,
PARTHENON-HYDRO is considered a fully-fledged miniapp
consisting of just \( \approx 1400 \) lines of C++ code total. Its main
purposes are to both illustrate a possible use of various
PARTHENON features combined in practice as well as an
external integration and performance test. PARTHENON-HYDRO
supports 1D, 2D, and 3D compressible hydrodynamics on
uniform and (static and adaptive) multilevel meshes. Given
PARTHENON’s ATHENA++ origins, PARTHENON-HYDRO is also
based on a subset of the algorithms implemented in
ATHENA++. More specifically, PARTHENON-HYDRO uses a
second-order method consisting of a two-stage Runge–
Kutta integrator, piecewise linear reconstruction and
HLLE Riemann solver. For illustration purposes following
three problem generators are implemented: a linear wave
(which is also used to illustrate automated convergence
testing by reusing the PARTHENON infrastructure externally),
a spherical blast wave, and a Kelvin-Helmholtz instability to
illustrate adaptive mesh refinement. There are no plans to
further extend “physics” capabilities of PARTHENON-HYDRO
with the exception of demonstrating new features in
PARTHENON as hydrodynamics is also supported by other, more feature rich downstream applications such as ATHENAPK.

4.2. AthenaPK

AthenaPK (Athena-Parthenon-Kokkos) is a general purpose astrophysical magnetohydrodynamics code which serves as a performance-portable, AMR-capable conversion of ATHENA++ (Stone et al., 2020). It implements the hydrodynamics solvers from ATHENA++ and supplemented them with a divergence cleaning magnetohydrodynamics solver based on Dedner et al. (2002).

At present, AthenaPK is used for simulations of magnetized galaxy clusters with feedback from active galactic nuclei, cf., Meece et al. (2017); Glines et al. (2020); Prasad et al. (2020), cloud crushing in galactic outflows, and magnetohydrodynamic turbulence. To support these applications additional features implemented include various Riemann solvers, passive scalars, tabulated cooling, and (an)isotropic thermal conduction with support for 2nd-order Runge–Kutta–Legendre based super-time-stepping (Meyer et al., 2014), see Figure 4 for an example multi-physics simulation with AMR.

Development of AthenaPK is public and contributions are welcome.

4.3. PHOEBUS

PHOEBUS is a general relativistic neutrino radiation magnetohydrodynamics code, designed for modeling compact binary mergers and their aftermath. It uses the Valencia formulation of general relativistic hydrodynamics (Marti et al., 1991), with constrained transport for magnetic fields. Currently the cell-centered formulation of Tóth (2000) is utilized, but face-centered fields will be leveraged once the underlying data structures are implemented in PARTHENON. On the radiation side, PHOEBUS implements Monte Carlo transport as in Miller et al. (2019a), and a novel hybrid scheme first presented in Ryan and Dolence (2020) is in development. Currently PHOEBUS implements both arbitrary fixed spacetimes as well as self-gravity under the monopole approximation. Full dynamical numerical relativity is a planned improvement. PHOEBUS carries with it several challenges: a general relativistic background carries with it a very large state vector, with O(100) variables; the fluid primitives are no longer trivially solve-able from the conserved variables, and must be found via numerical root finding; the method requires the interweaving of grid and particle variables; and the general relativistic equations themselves are complicated and compute intensive. A code paper for PHOEBUS is in preparation.

Figure 5 shows an example problem run in PHOEBUS: a non-rotating neutron star. The top panel shows the density in a poloidal slice. Any small perturbation excites the natural oscillation modes in the star, shown in the bottom panel, where we plot the central density, normalized by its value at the initial time. These modes match those predicted from perturbation theory (Yoshida and Eriguchi 2001) and presented in numerical tests in, for example, Löffler et al. (2012).

Figure 6 shows another PHOEBUS example problem using Monte Carlo neutrino transport, leveraging the PARTHENON particles infrastructure. In this problem, an initially inhomogeneous electron fraction, the ratio of electrons to baryons, of the background material is homogenized by neutrino emission, transport, and absorption (neutrinos transport lepton number). Inside PHOEBUS, we use the

![Figure 4. ATHENAPK example: Passive scalar concentration in a supersonic cloud crushing simulation with magnetic fields, optically thin radiative cooling, and mesh refinement configured to follow the cloud material (as passive scalar).](image-url)
SINGULARITY-EOS (Miller, 2022a) library for a realistic equation of state (Skinner et al., 2019) and the SINGULARITY-OPAC (Miller, 2022b) library for realistic opacities (O’Connor and Ott, 2010; Steiner et al., 2013). Singularity libraries provide production-quality data in a performance-portable way.

4.4. RIOT

RIOT is an LANL-based multi-physics code designed to emulate a subset of the physics in the xRAGE code (Gittings et al., 2008) to allow for comparisons of cell-based and block-based AMR approaches. Currently it includes multi-material, compressible hydrodynamics with a pressure–temperature equilibrium mixed-cell closure, gray radiation diffusion, a sub-grid turbulence model, thermo-nuclear reactions, and high-explosives models. RIOT makes heavy usage of PARTHENON’s sparse datatype to represent material-based state variables.

Figure 7 shows results from a classic three material test problem called triple-point (Kucharik et al., 2010). At one end of the domain, an ideal gas at high pressure drives a shock into two distinct ideal gases that differ in their adiabatic index $\gamma$. The flow develops vorticity that leads to a well-developed roll-up. The problem was solved in a 3D geometry by revolving the traditional 2D setup about the y-axis and made use of three levels of refinement triggered by material interfaces. The figure shows slices of volume fraction for each material where blue indicates the absence of the material and red indicates a pure material, with white indicating material mixing. On the top slice, we also show the AMR grid to indicate how PARTHENON adapts the mesh to accommodate the evolving and nontrivial geometry of the materials.

Figure 5. Self-gravitating compact star as evolved in PHOEBUS (top) and oscillations in the central density (bottom). The star is stable for many cycles, and the oscillations match the expected quasinormal mode structure for a non-rotating neutron star.

Figure 6. Initial and final electron fraction material states of the leptonization neutrino transport problem. Electron fraction-dependent emissivities act to equilibrate the electron fraction across the simulation domain from the inhomogeneous initial conditions. The mean electron fraction of the material is lower at the final time due to the presence of neutrinos.
5. Results

Unless noted otherwise, all result presented in this section were obtained using PARTHENON-HYDRO (changeset 52fa13c with included KOKKOS and PARTHENON sub-modules), that is, using a two-stage, second-order method consisting of RK2 integration, piecewise linear reconstruction, and HLLE Riemann solver.

5.1. Block and communication buffer packing

To highlight the need for packing meshblocks and combining the communication buffer filling routines in order to improve the performance on GPUs, we measured the overhead associated with an overdecomposition of the mesh. In this idealized setup, the mesh size is kept fixed and the meshblock size is varied. With smaller and smaller meshblocks, the ratio of ghost cells to active cells increases, the number of buffers increases, and, generally, the overhead associated with managing the entire hierarchy of meshblocks increases. Figure 8 illustrates the relative performance on a single GPU (V100) and a single CPU core (Xeon Gold 6148) when going from using a single meshblock for the entire mesh to 4096 meshblocks.

On the CPU this overdecomposition results in an overhead of $\approx 3.5 \times$ independent of whether no packing ("original"), packing all buffers of a meshblock in a single kernel, or packing all buffers of all meshblocks in a single kernel is used. This is comparable to the original implementation in ATHENA++ with an overhead of $\approx 3.3 \times$, cf., Figure 36 in Stone et al. (2020).

On the GPU, the original implementation that launched one kernel per buffer resulted in a significant overhead and the performance drops by a factor of $\approx 82 \times$. This can be attributed to the kernel launch overhead ($\approx 5-7 \mu s$ on Summit) that is longer than the kernel runtime itself—especially when the communication buffers are small, for example, for small meshblock sizes or for corners (8 cells) in general. To alleviate this bottleneck, we first tried to use multiple streams and launching kernels from multiple threads. While the performance improved with multiple kernels running simultaneously, the results were not satisfactory because the kernel launch itself is inherently serial at the CUDA level. The second approach of reducing the number of kernel launches by filling all buffers of a meshblock in one kernel (see Section 3.7) and by packing multiple blocks (see Section 3.6) significantly reduced the additional overhead. As shown in Figure 8, filling buffers in a single kernel reduced the overhead from $\approx 82 \times$ to $\approx 13 \times$ at an overdecomposition of 4096 meshblocks. Combining this with also handling all meshblocks in a single kernel reduced the overhead further down to $\approx 3.5 \times$, which is now on par with the CPU result.

5.2. Pack sizes and overdecomposition

As already noted in the ATHENA++ method paper (Stone et al., 2020), some (limited amount of) overdecomposition,
that is using more than one block per computing device (e.g., a CPU core) resulted in higher performance as it allowed for additional overlapping of computation and communication. However, with an increasing number of blocks per device the block size itself decreases resulting in a smaller ratio of active to ghost cells that need to be communicated. Thus, an optimal mesh decomposition is problem and hardware dependent.

For PARTHENON with support for running on GPUs and packing multiple blocks into a MeshBlockPack that are handled simultaneously, finding an optimal decomposition is even more complex. This is illustrated in Table 1 where we list the performance per node of PARTHENON-HYDRO for uniform and multilevel mesh runs on 16 Summit nodes for various options to distribute the workload. Note, the example mesh and block sizes are chosen to illustrate a general direction and details will vary with other factors including (but not limited to) devices (and their features), interconnects, mesh hierarchy, or block sizes.

When using a single MPI rank per GPU the best performance is typically achieved when using just a single pack on each device containing all blocks. Moreover, in the uniform mesh case overdecomposing the mesh into 2 blocks per device increases performance from 10.8 × 10^8 zone-cycles/s/node to 11.7 × 10^8. This also holds for using 16 blocks per device on GPUs as the ratio of active to ghost cells is still large for block size of 128^3. In contrast, using 16 blocks per CPU core significantly reduces this ratio as the block size is reduced to 32^2 × 16 in the example given and the performance drops by ≈50% compared to using 2 blocks per CPU core, which is optimal (and similar to ATHENA++).

On GPUs the performance can be improved even further when using more than one rank per device. However, this needs to be supported by the GPU driver or software as the KOKKOS programming model currently supports a single device per process only. Both for the uniform and the multilevel mesh the performance is highest when using 4 ranks per device and splitting all blocks on each rank into two packs. On the uniform mesh, it peaks at 13.1 × 10^8 zone-cycles/s/node and for the multilevel mesh at 4.0 × 10^8. In contrast, the performance for the multilevel mesh is 4× lower when using a single rank per GPU handling 256 blocks each and using a separate pack for each block. In other words, both packing (i.e., reducing the number of kernel calls) and using more ranks per device (i.e., reducing the number of blocks per rank and, in turn, the block management overhead per host rank) each result in a performance increase of about 2× in this scenario. These potential performance gains/losses related to runtime parameters should encourage problem and application specific tuning for an optimal use of available computational resources.

5.3. On-node performance portability

To highlight the performance portability enabled at the higher level by the intermediate abstraction layer in PARTHENON and at the lower level by KOKKOS, we measured the performance of PARTHENON-HYDRO on individual devices across several architectures. These include x86 CPUs with AVX2 and AVX512 instruction sets, ARM CPUs with A64FX architecture, NVIDIA GPUs and AMD GPUs.

The results are shown in Table 2. A single V100 GPU is about 4× faster than a 40 core Intel Skylake system or ≈6× faster than a 28 core Intel Broadwell system, which matches the ratios measured for K-ATHENA (Grete et al., 2021a). Similarly, the Intel CPU performance of PARTHENON-HYDRO only about 20% lower than reported for the same algorithms in Athena++ (Stone et al., 2020) highlighting the low overhead of the abstractions provided by PARTHENON.

On a single MI250X GPU (using 2 GCDs) PARTHENON-HYDRO is about 2.6× faster than on a MI100 GPU and on an

| # blocks per dev | Uniform mesh | Multilevel mesh |
|------------------|--------------|-----------------|
|                  | 1            | 2               | 16              | 259 (GPU) & 37 (CPU) |
| # packs per rank | I            | B               | B               | B |
| 1 rank per GPU   | 10.8         | 11.7            | 10.7            | 2.2 |
| 2 ranks per GPU  | 11.7         | 11.3            | 11.0            | 2.2 |
| 4 ranks per GPU  | 12.6         | 12.2            | 11.6            | 2.2 |
| 1 rank per CPU core | 0.45 | 0.47 | 0.44 | 0.25 | 0.29 | 0.29 | 0.29 | 0.42 | 0.43 | 0.42 | 0.40 |
A100 GPU PARTHENON-HYDRO is about 55% faster than on a V100 GPU. This corresponds to the increased memory bandwidth in combination with the bandwidth limited algorithms implemented, cf., the roofline model shown in Grete et al. (2021a). While the relative performance of the MI100 GPU with ≈80% of a V100 GPU is still reasonable (despite the 57% increase in memory bandwidth), the A64FX CPU (≈13% of a V100) is slower than expected based on the device memory bandwidth. First tests indicate that some fraction of the lower performance can be attributed to difficulties of the compiler to (auto)vectorize the compute kernels, which is in agreement with similar results reported for the FLASH code (Feldman et al., 2022), and, thus, not intrinsic to the PARTHENON framework itself.

### 5.4. Scaling results

All scaling tests in this subsection have been performed with PARTHENON-HYDRO. Given the simplicity of the algorithms in the miniapp, PARTHENON-HYDRO is a well-suited proxy to gauge the performance of the PARTHENON framework itself. Table 3 lists an overview of the node configuration, software environment, and compiler flags of all machines used for testing.

Note that the individual mesh sizes used in the scaling tests on uniform meshes vary slightly between different machines and devices. We tried to keep the comparison as fair as possible by ensuring that the computational load per compute element is uniformly distributed, for example, each compute element (a CPU core or a GPU) handles the same number of MeshBlocks for a given test case so that there is no artificial load imbalance. Finally, the numbers reported correspond to the median performance of several tens of cycles to mitigate external effects (such as network congestion) as most of data was collected using non-exclusive allocations.

### 5.4.1. Weak scaling on uniform grids

The weak scaling of PARTHENON-HYDRO on various machines is illustrated in Figure 9. In general, we used problem sizes that used a large fraction of the available GPU memory (512 x 256^2 per 16G V100 GPU, 512^2 x 256 per 40G A100, and 512^3 per 64G MI250X GCD) and 64^3 per CPU core. At the largest scale, PARTHENON-HYDRO reaches a 92% parallel efficiency going from one to 9216 nodes (73,728 logical GPUs) on Frontier for a total of \(1.7 \times 10^{13}\) zone-cycles/s—in other words, effectively updating a 16, 384^3 mesh about four times per second. At the largest rank count, PARTHENON-HYDRO reaches a 93% parallel efficiency going from one to 8192 nodes (458,752 MPI ranks with one rank per core) on Frontera.

Overall, we see a significant speedups using GPUs over CPUs even at large node counts, for example, \(\approx 29\times\) on a 1024 Summit nodes. In addition, the parallel efficiency is generally comparable between CPUs and GPUs with the exception of Summit. This is in agreement with the scaling behavior of K-ATHENA (Grete et al., 2021a) and can be attributed to the improved node design of more recent machines. On Frontier and JUWELS Booster each GPU is directly connected to a separate interconnect card, whereas on Summit six GPUs share two InfiniBand cards per node connected to the CPU.

### 5.4.2. Strong scaling on uniform grid

The strong scaling on uniform grids of PARTHENON-HYDRO on various machines is illustrated in Figure 10. We used comparable problem sizes of \(\leq 1, 024\)^3 and started with the minimum number of nodes required on each machine. In general, the parallel efficiency using CPUs is slightly higher than using GPUs on the same machine, for example, on Summit remaining at \(\approx 80\%\) on CPUs for a \(32\times\) increase in node count (going from 4 to 128 nodes). While the parallel efficiency on Summit drops to \(\approx 35\%\) at 128 nodes using GPUs the raw performance of the GPU accelerated simulations is still more than 10× greater than using CPUs. The differences between CPU and GPU strong scaling parallel efficiency can be attributed to the significantly larger ratio of throughput and memory bandwidth to problem size on GPUs, resulting in a more challenging baseline on GPUs, cf., similar results for K-ATHENA (Grete et al., 2021a). Nevertheless, for a \(32\times\) increase in node count on Frontier the parallel efficiency remains high at 67% and 60% going from 1 to 32 or 64 to 2048 nodes, respectively.

### 5.4.3. Strong scaling with multilevel grids

In contrast to the scaling tests on uniform grids presented in the previous two subsections, Figure 11 show the strong scaling behavior of PARTHENON-HYDRO for a multilevel grid. The grid is the same as used in Section 5.2, that is, a block size of \(32^3\) is used on a 256^3 root grid with 3 additional levels of refinement resulting in 296, 1216, 1352, and 21,952 blocks on level 0, 1, 2, and 3, respectively. Therefore, this tests now includes the

| Device (Arch/Instr.) | Performance |
|----------------------|-------------|
| AMD MI250X GPU (ROCm, 2x GCD) | 5.7         |
| NVIDIA A100 GPU (CUDA Cap. 8.0) | 4.2         |
| NVIDIA V100 GPU (CUDA Cap. 7.0) | 2.7         |
| AMD MI100 GPU (ROCm)  | 2.15        |
| AMD EPYC 7H12 (2 x 64 C x86 AVX2) | 1.45       |
| Intel Xeon 6148 (2 x 20 C x86 AVX512) | 0.67       |
| IBM Power9 (2 x 21 C) | 0.51        |
| Intel Xeon E5-2680v4 (2 x 14 C x86 AVX2) | 0.43       |
| Fujitsu A64FX (1 x 48 C ARMv8.2-A) | 0.36       |
prolongation/restriction machinery for ghost zones across level boundaries as well as flux correction for faces across level boundaries.

The strong scaling parallel efficiency on CPUs is generally better than on GPUs on Summit reaching ≈97% and ≈59%, respectively, going from 8 to 128 nodes. Again, simulations on GPUs are significantly faster than on uniform grids, for example, ≈10 × on 8 nodes and ≈6 × on 128 nodes for the given setup. This difference stems from the small kernels sizes, for example, in the flux correction step, which currently is still follows a “one kernel per face” approach, and the associated overhead. We expect further improvements by also using the packing approach described in Section 3.6 for the flux correction. The (limited) super-linear speedup observed in the CPU runs on Summit can be attributed to the mesh management overhead where at the smallest scales (8 nodes) each rank handles ≈74 blocks, which is successively reduced with larger rank count, cf., Section 5.1 and 5.2. On GPUs this is not observed as the overhead is hidden by asynchronously running kernels over larger packs of blocks. Finally, on Frontier a 256× increase in resources still results in a parallel efficiency of 55% again highlighting the importance of the direct connection between interconnect and GPUs.

6. Software engineering

6.1. Development model

PARTHENON is an open, community-driven effort to create a performance-portable AMR framework applicable for a wide variety of applications. Developers come from several institutions, have access to different computational
resources, and have different application needs. In order to meet the needs of disparate interests within the community, we enforce sustainable collaborative software practices. These are also documented in the repository itself in the development guide.

Collaborative development is facilitated via the PARTHENON repository on GITHUB. Each contribution to the developmental branch is verified with a continuous integration pipeline, and reviewed and approved by developers from multiple downstream applications. A consistent code style is strictly enforced across the code base with each contribution using automated code style checking and formatting.

New features to the AMR framework are documented and demonstrated in examples contained within the repository. These examples are then used in continuous integration testing.

6.2. Testing

At the highest level, PARTHENON uses a cTEST-based testing environment that handles various test cases. A shorter test suite is triggered automatically for new commits and/or opened pull request. An extended test suite is executed nightly for the develop branch or be triggered manually. Similarly, the test suite can also be triggered locally during development and offers flexible options to adapt to local environments, for example, with respect to the number of
GPUs per node or the `mpilaunch` command. The test infrastructure contains the following three building blocks.

6.2.1. Simple, standard tests include unit testing, build testing, and coding style. For each new feature, developers are encouraged to provide separate unit tests that are ideally independent of other components in PARTHENON. PARTHENON uses `CATCH2` for these tests to automatically create descriptive test cases that integrate with `CTEST`.

Given the various hardware architectures PARTHENON targets and their respective recommended compilers, the automated build testing covers several combinations. These include `Release` and `Debug` builds for NVIDIA GPUs with `NVCC`, x86 CPUs with `G++`, and AMD GPUs with `HIPCC`. The builds are tested in `DOCKER` containers that are maintained and published through the main repository so that they are easily available for developers and users.

Finally, consistent code style is automatically enforced using `CLANG-FORMAT` and `CPPLINT`.

6.2.2. Regression tests. Regression tests also include integration tests as they cover more complex use cases. The majority of regression tests use the examples available in PARTHENON to verify correctness either against the analytic/exact solution or against a good known previous reference solution.

In contrast to the simple tests, which are directly called from `CTEST`, we develop a `PYTHON` based framework for the regression tests. This framework allows to create complex tests that are tailored to PARTHENON, for example, with respect to calling a PARTHENON based executable (i.e., one of the examples) with a given input file. The latter can also be modified from within the testing framework. Moreover, the “analysis” step of each test case also allows to process the test results (including the data written to disk or the terminal output) to create artifacts for easy visual inspection.

The testing framework is fully documented and can easily be reused in downstream codes. This allows for a seamless integration of PARTHENON and downstream code testing with a unified approach.

6.2.3. Performance testing. Performance testing and reporting is also realized through a separate framework: the PARTHENON Performance Metrics App (PPMA). It is a custom `GITHUB` application whose source is maintained in the main repository. It allows to run multi-node performance regression tests on internal machines and can only be triggered manually manually after code review for security reasons. For each run `JSON` file is created containing information about time and date of the test, the branch, the commit hash, and various performance metrics. The results are automatically compared and plotted against the previous five commits of that branch and against develop.

7. Current limitations and future enhancements

In the active, ongoing development of PARTHENON, we already identified several areas and features that can be further improved and/or need to be implemented motivated by a downstream code requirement.

For example, PARTHENON itself currently only supports Cartesian coordinate systems with fixed mesh spacing. Nevertheless, all coordinate related functions are already abstracted and contained in in a separate class. Similarly, all functions provided by PARTHENON are already making use of those abstraction, for example, when calculating the divergence of a flux or during flux correction in simulations with mesh refinement. Therefore, the addition of other coordinate systems is straightforward.

Similarly, the `Variables` class is already prepared to handle additional variable types such as face centered or edge centered variables. While basic support for face variables is already implemented (covering allocation and index handling), the boundary and communication routines are not fully refactored yet.

From a performance point of view, we are currently evaluating further improvements in the ghost zone communication routines. For example, while overlapping computation and communication is already supported through the tasking infrastructure in combination with asynchronous MPI routines, all ghost zones are currently handled in the same way. This is not ideal as ghost zones with neighbors on the same rank, that is, ones that are directly copied to the receiving buffer, are handled in the same kernels as those who are first copied into a buffer in preparation for being sent via MPI. We expect that a split of the kernel into handling remote ghost zones and rank-local ones separately (in that order) to be more efficient because rank-local buffers would be copied while all remote buffers are already being transmitted. The same pattern also applies to the unpacking of the receiving buffers in reverse order.

Independently, first tests indicate that the optimal loop pattern for these buffer handling kernels depend on many factors including overall simulation setup (e.g., `MeshBlock size` or `ghost zone width`), implementation details (e.g., number of components in a `Variable` vector), or device architecture. The results are not yet conclusive, but we expect to eventually provide both an architecture specific default pattern as well as a general simulation/algorithm dependent guideline. This similarly applies to other runtime parameters such as the `MeshBlockPack size` or the number of ranks per device, cf., Section 5.2.
8. Conclusions

In this article, we presented the performance portable block-structured adaptive mesh refinement framework PARTHENON. Performance portability is achieved through the use of the Kokkos library in combination with an intermediate abstraction layer. The mesh refinement machinery is based on Athena++.

The overall design philosophy follows a device-resident approach, that is, all simulation data is only allocated on the computing device to reduce data movement. Moreover, PARTHENON is designed for shared capabilities between various downstream application codes by exposing granular interfaces to the application developers. At the same time, we strive to keep PARTHENON simple enough to be easily extensible.

Key features includes abstractions for packages, which can be considered as disparate components containing, for example, a hydrodynamics solver or a radiation transport solver, abstractions for multidimensional variables including vectors and tensors with support for sparse allocation, and a task-based applications driver with support for asynchronous, dependency-based task execution.

From a performance point of view, the key features include the packing of variables and blocks into larger logical structures so that they can be handled within a single kernel. This is particularly relevant for kernels pertaining to filling communication buffers and when using small block sizes as the number of individual kernel launches can be significantly reduced. Similarly, asynchronous, one-sided MPI communicators are used directly from buffers in device memory to allow for an overlap of compute kernels and data transfer between nodes.

We demonstrated the success of these design decisions and features in various scaling test using the hydrodynamics miniapp PARTHENON-HYDRO reaching a total of $1.7 \times 10^{13}$ zone-cycles/s on 9216 Frontier nodes (73,728 logical GPUs) at $\approx92\%$ weak scaling parallel efficiency (starting from a single node). Moreover, we demonstrated performance portability across different CPU and GPU architectures including AMD and NVIDIA GPUs, Intel and AMD x86 CPUs, IBM Power9 CPUs, and Fujitsu A64FX CPUs. In general, simulations employing GPUs are significantly faster compared to using the CPU resources on the same node for both uniform grids (and weak and strong scaling) as well as for multilevel grids, that is, setups that require prolongation/restriction and flux correction.

Several downstream applications are in active development ranging from compressible magnetohydrodynamics to general relativistic neutrino radiation magnetohydrodynamics to multi-material compressible hydrodynamics exemplifying the diverse application scenarios enabled by PARTHENON. In addition, we also introduced the PARTHENON-HYDRO miniapp supporting full 3D compressible hydrodynamics with adaptive mesh refinement using PARTHENON’s capabilities in just over 1000 lines of code. This also highlights the use of PARTHENON as basis for rapid prototyping and testing of new algorithms.

Finally, we emphasize that PARTHENON is an open, collaborative project and that new members/contributions are always welcome!

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Notes
1. https://github.com/parthenon-hpc-lab/parthenon-hydro
2. https://github.com/parthenon-hpc-lab/athena
3. https://github.com/lanl/phoebus
4. https://github.com/parthenon-hpc-lab/parthenon

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