A performance portable library in support of future aerothermodynamics simulation software

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Atmospheric Reentry Context

Physics and Numerics

- Hypersonic flow around spacecraft
- Quantities of interest: heat flux on the object wall and aerodynamic coefficients
- RANS (Reynolds Averaged Navier-Stokes) simulations with turbulence models
- Real gas chemistry
- Heat transfer for ablation and pyrolysis simulation

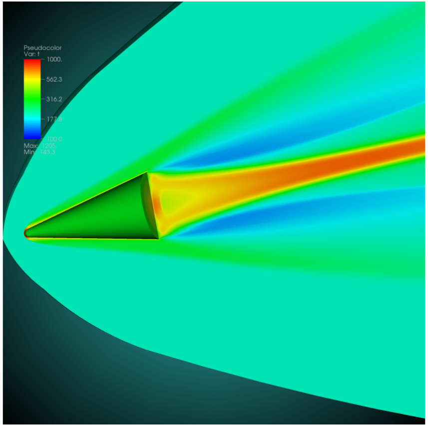


Figure 1: Slice of the flow temperature during reentry [1]

Atmospheric Reentry Context

Software

- In-house Fortran 90 production code at CEA/CESTA, ∼20yo, expected to run for the next 10 years
- Finite Volume scheme
- Capable of 2D, 2D axi, and 3D simulations
- Multiblock Structured Mesh
- Parallelized using MPI and OpenMP
- Some evolutions: neural nets to replace costly chemistry computation

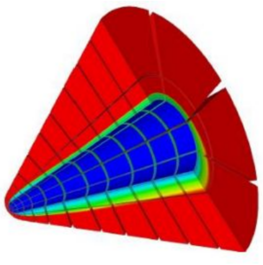


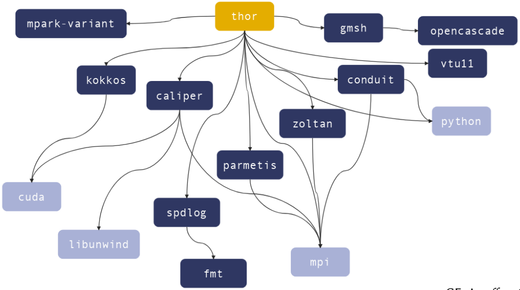
Figure 2: Blocks around a sphere-cone type object

Preparing for future needs

- A next-generation 3D code will be needed
- More complex geometries ⇒ generate unstructured meshes take less engineering time
- Innovative numerical schemes
  - Agnes Chan thesis (2023): *Innovative numerical schemes for 3D supersonic aerodynamics on unstructured mesh*
  - Vincent Delmas thesis (2026): *Design and development of innovative numerical methods to solve the 3D Navier-Stokes equations to model hypersonic flows on hybrid meshes*
- Ensure performance portability on future hardware
  - EXA1 (CEA-HF) with NVIDIA A100 nodes
  - EXA1 with NVIDIA GH200 nodes
  - What about the future systems ?

The Thor library: overview

- C++20 library started from a working group in 2022
- Fork/extension of Axom [3] with additional features, with ideas taken from Parthenon [2] and others
- Relies on Kokkos for performance portability
- Targets unstructured meshes first
- Collection of components: mesh reading, writing, partitioning, dataset parsing, logging, ...



The Thor library: components

Core

- Abstractions for Kokkos and MPI: `thor::ScopeGuard` wrapping init/finalize
- Wraps `Kokkos::parallel_for` if Kokkos enabled

```
template<class ExecutionSpace = DevExecSpace, class UnaryFunction>
void for_each(const std::string& label, int is, int ie, UnaryFunction function,
ExecutionSpace exec_space = ExecutionSpace()) {
  #if defined(THOR_ENABLE_KOKKOS)
  Kokkos::parallel_for(...);
  #else
  #pragma omp parallel for
  for (int i = is; i < ie; ++i) { function(i) };
  #endif
}
```

- Utilities (string, filesystem, etc.)

The Thor library: components

Mesh

- Data structures for 3D unstructured meshes with multiple cell types supported
- Reduced mesh connectivity: store the cell-to-node connectivity only, others can be computed if needed

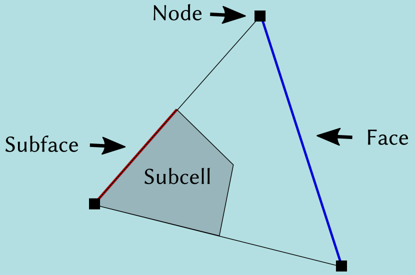


Figure 3: Cell with its connected entities

The Thor library: components

Mesh

- Variables attached to the mesh, using `Kokkos::DynRankView` as the underlying container

```
auto md_cell = Metadata({Metadata::Cell, Metadata::Output, Metadata::SyncGhosts});
std::vector<std::string> prim_labels = {"PrimDensity", "VelX", "VelY", "VelZ", "Pressure"};
auto prim = mesh->create_field<double>("Primitive", md_cell, {NUM_PRIM}, prim_labels);
auto some_matrix = mesh->create_field<double>("Mat", Metadata({Metadata::Face}), {3, 3});
```

- Metadata flags:
  - `None`,`Cell`,`Face`,`Subface`,`Node`: associate a variable with a topological element
  - `Output`: Mark field to be written to output files
  - `SyncGhosts`: Mark field ghost cells to be synchronized between MPI partitions

The Thor library: components

Mesh

- Parallel execution interface on mesh elements

```
// Loop over all cells, default execution space is DevExecSpace
for_all_cells("InitSod", mesh, THOR_LAMBDA(int cell_i) {...});
// Loop over all faces, with cell neighbors info
for_all_faces<SomeOtherExecSpace, xargs::cellids>("ComputeFluxInnerFaces", mesh,
  THOR_LAMBDA(int face_i, int left_cell_i, int right_cell_i) {...});
// Loop over all faces, with face nodes coordinates
for_all_faces<xargs::coords>(mesh,
  THOR_LAMBDA(int face_i, const FaceNodeCoords& nodes, const FaceNodeIds& node_ids) {...});
```

Loops on a subset of faces: `for_internal_faces`, `for_external_boundary_faces`

The Thor library: components

Mesh

- Partitioning using ParMetis or Zoltan, handling multiple ghost cell layers

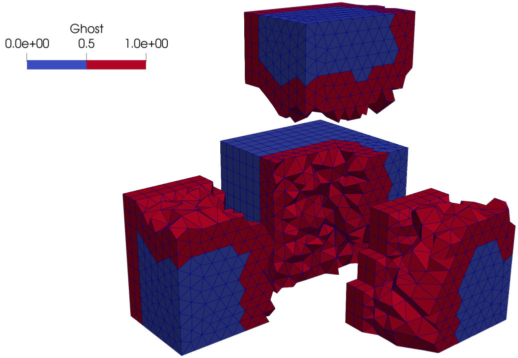


Figure 4: 2 layers of ghost cells on a 3D hybrid mesh

The Thor library: components

Mesh

- IOs: Gmsh reader, legacy VTK and (P)VTU writers
- Interested in ADIOS2, and PDI, especially for in transit analysis

Linalg

- Backport some C++26 `std::linalg` functions, e.g. `matrix_vector_product`

Input

- Read and verify input datasets in YAML, JSON, or Python (wip)

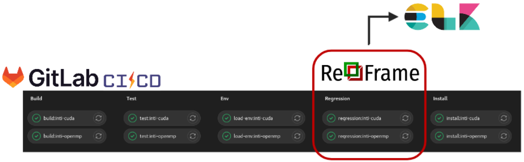
Profiling and Performance Monitoring

Profiling

- Score-P (OpenMP backend) and Nsight Systems and Compute (CUDA backend)

Automated Performance Monitoring

- Caliper (`https://github.com/llnl/caliper`) annotations in the code
- GitLab CI pipelines submitted nightly on EXA
- These nightly tests are automated with ReFrame
- Performance metrics are parsed from the tests output and visualized in a Kibana dashboard



MiniEuler

- CFD Miniapp using Thor
- Based on A. Chan and V. Delmas developments
- Classical and multi-point finite volume schemes
- Used for Thor integration and performance regression testing

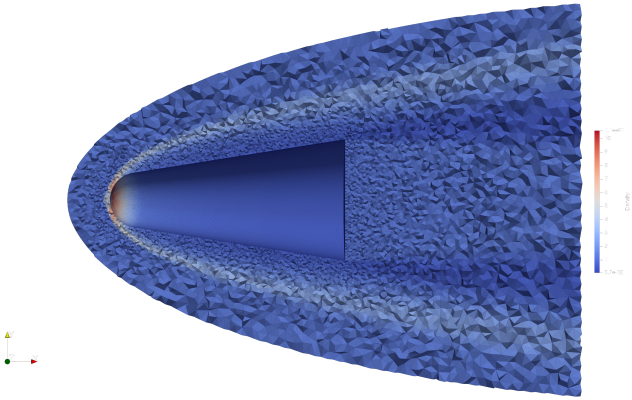
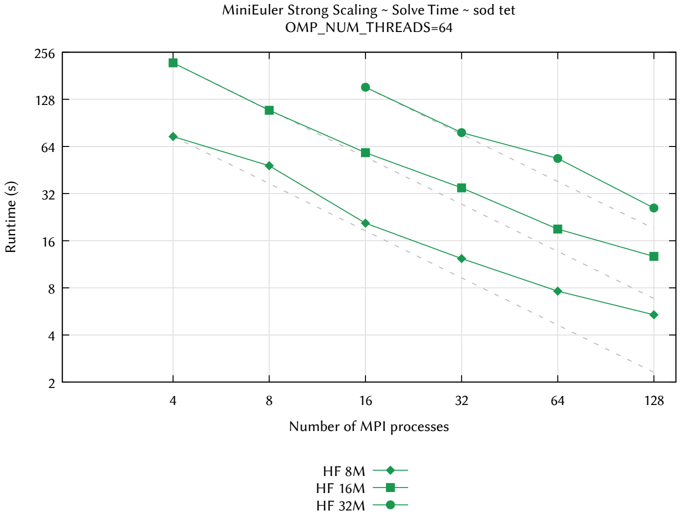


Figure 5: Density around RAM-C II vehicle

Strong Scaling benchmarks



Sod shock tube on tet mesh

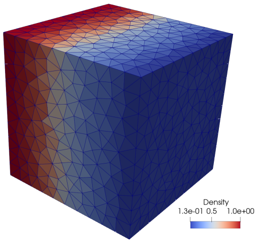
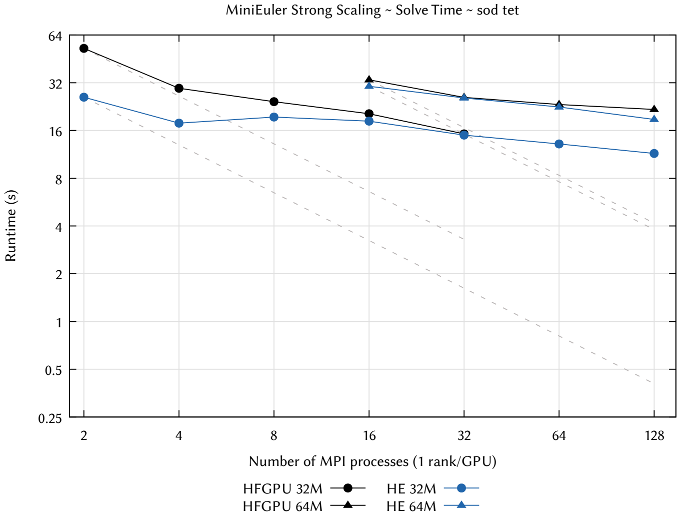


Figure 6: Density at t=0.2s

Strong Scaling benchmarks



Sod shock tube on tet mesh

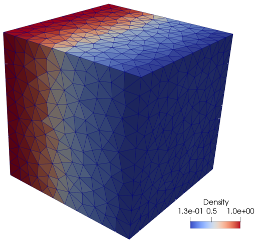
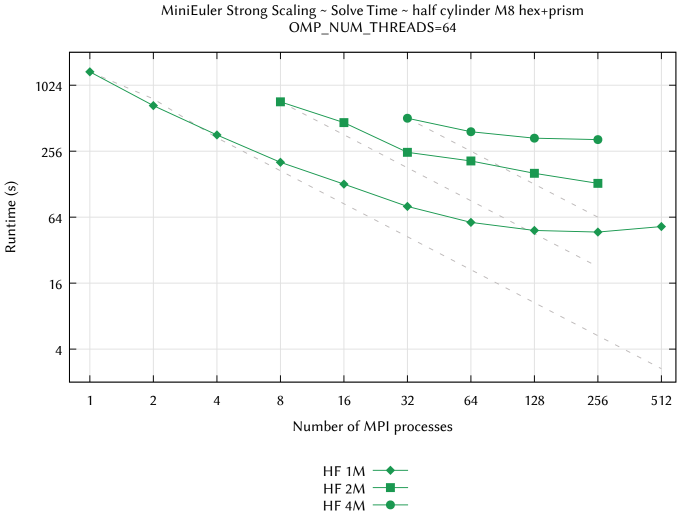
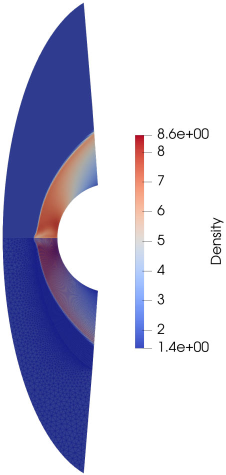


Figure 7: Density at t=0.2s

Strong Scaling benchmarks



Half cylinder @Mach 8 (hex+prism mesh) using the “two-point” solver



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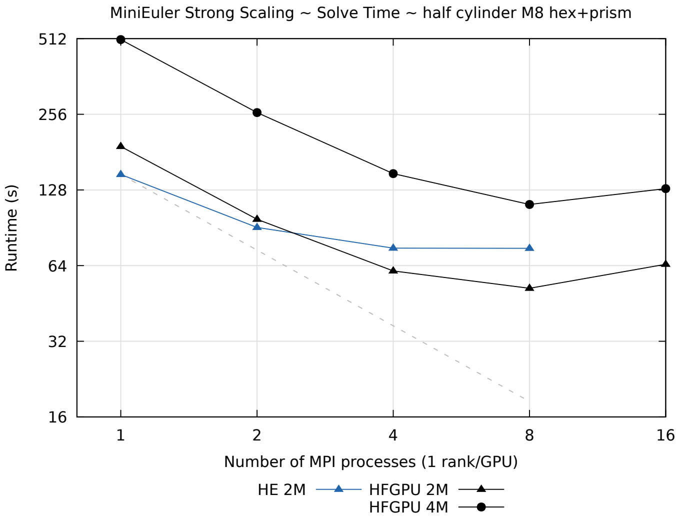

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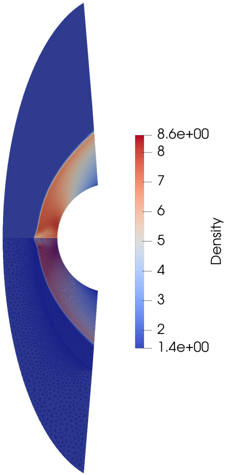

Conclusion and future work

- Working library prototype, successfully used for creating the C++ version of the Fortran code by V. Delmas
- Runs with the OpenMP, CUDA and HIP backends
- Nice to have: Kokkos interop with MPI, to pass Views directly and pack/unpack behind the scenes

- Working on improving acceptance from Fortran developers
- No magic to hide complexity - training on C++, Kokkos, and GPU stuff is essential

Thanks! Any questions?

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