HARD: Leveraging FleCSI for Heterogeneous Multi-Material Hydrodynamics

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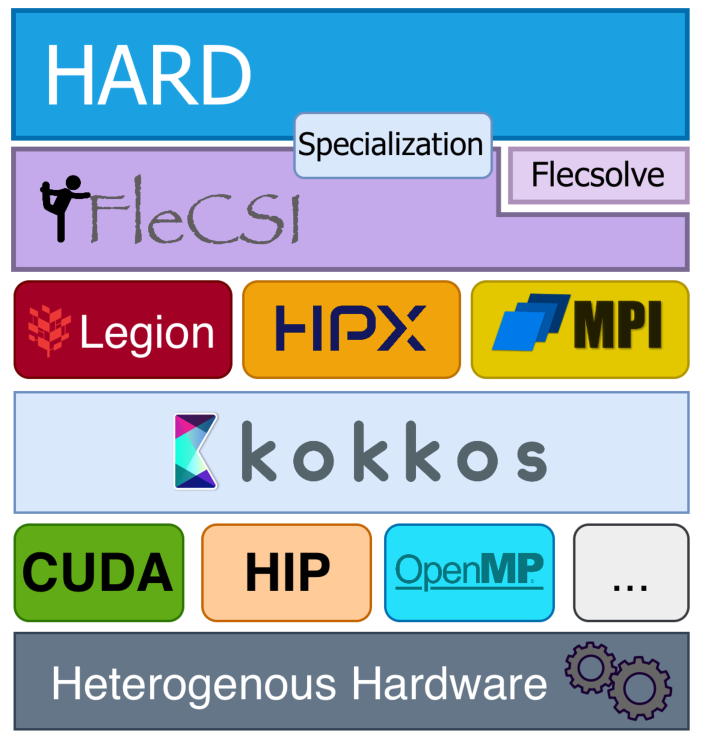
Background

HARD (**H**ydrodynamics **A**nd **R**adiation **D**iffusion) [1] is a radiation hydrodynamics code built upon **FleCSI** to efficiently target modern heterogenous architectures.

- **FleCSI** (**Fle**xible **C**omputational **S**cience **I**nfrastructure) [2] is a C++ framework for developing performance-portable scientific applications. It supports multiple distributed-memory backends and on-node parallelism via Kokkos.
- **Multi-material hydrodynamics** is critical in many fields, such as high-energy-density physics, reactive flows, and inertial confinement fusion, where accurate material tracking is needed.



Compressible Euler

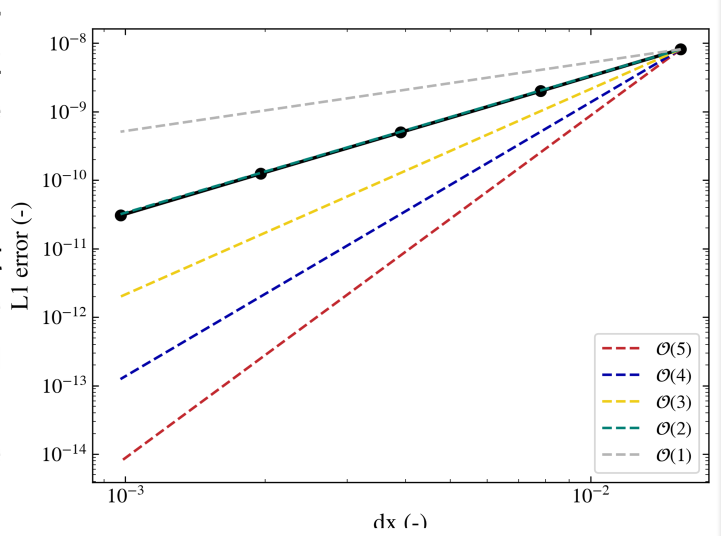
$$\partial_t \begin{bmatrix}\rho\\ \rho\mathbf{v}\\ E\end{bmatrix} + \nabla\cdot\begin{bmatrix}\rho\mathbf{v}\\ \rho\mathbf{v}\mathbf{v}^T + p\mathbb{I}_d\\ \mathbf{v}(E+p)\end{bmatrix} = \begin{bmatrix}0\\ 0\\ 0\end{bmatrix}$$

\+ **Ghost Fluid Method**

Project Goal: Implementing a multi-material hydrodynamics model in HARD to accurately simulate immiscible materials by preserving sharp interfaces.

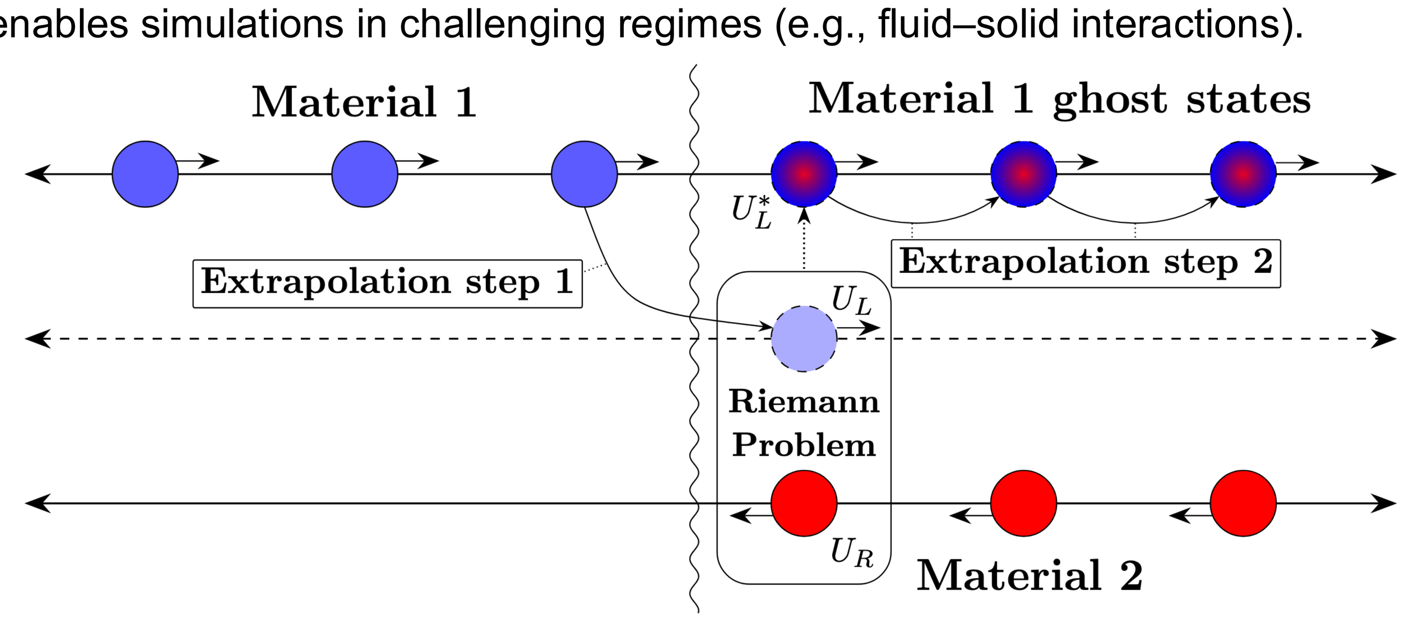
Numerical Methods

- **Hydrodynamic equations:** Explicit finite-volume method (FVM) using WENO5z spatial discretization with Heun's RK2 time integrator, leveraging FleCSolve [3] abstractions.
- **Interface tracking:** High-order level-set method with WENO5m finite-difference scheme and strong stability preserving RK3 integrator.
- **Extrapolation:** First-order finite difference scheme for linear pseudo-time PDE



Ghost Fluid Method (GFM)

Sharp interface tracking between immiscible materials and coupling fluid flow across an interface by defining "**ghost states**" [4]. This work improves on the original GFM by solving a Riemann problem to construct the ghost states. This enables simulations in challenging regimes (e.g., fluid–solid interactions).



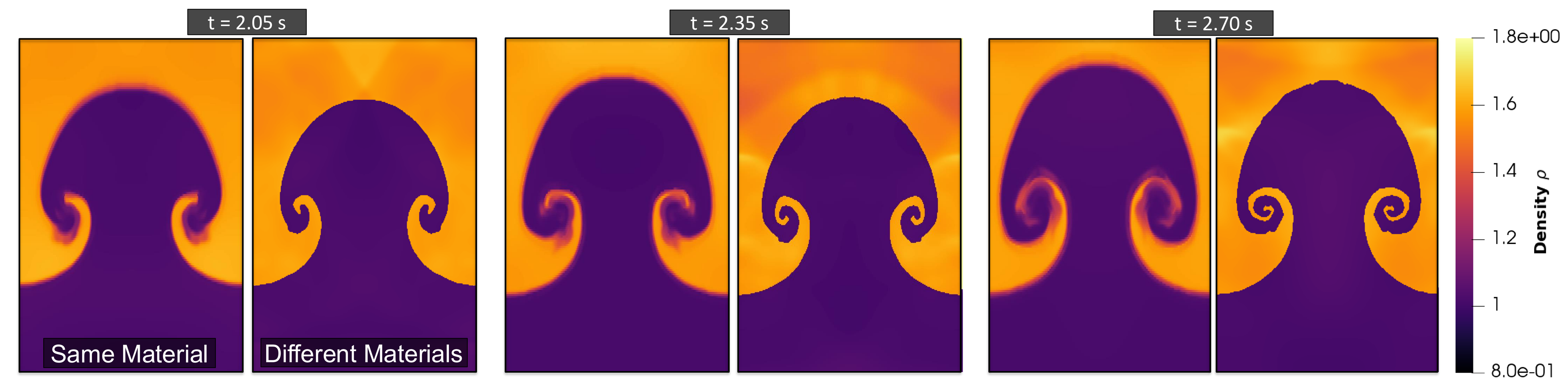
Modified GFM update is more robust than original GFM:

- Riemann problem ensures the ghost states are valid states for both materials.
- Prevents nonphysical states from crashing simulations.

Rayleigh-Taylor Instability

Rayleigh-Taylor (RT) Instability occurs at the interface of fluids with different densities, where the system is accelerated (i.e. by gravity) towards the denser fluid.

- With the same material test, diffusion between the fluids occurs.
- With different materials, there is **no diffusion** proving our methods are correct for **immiscible materials**.

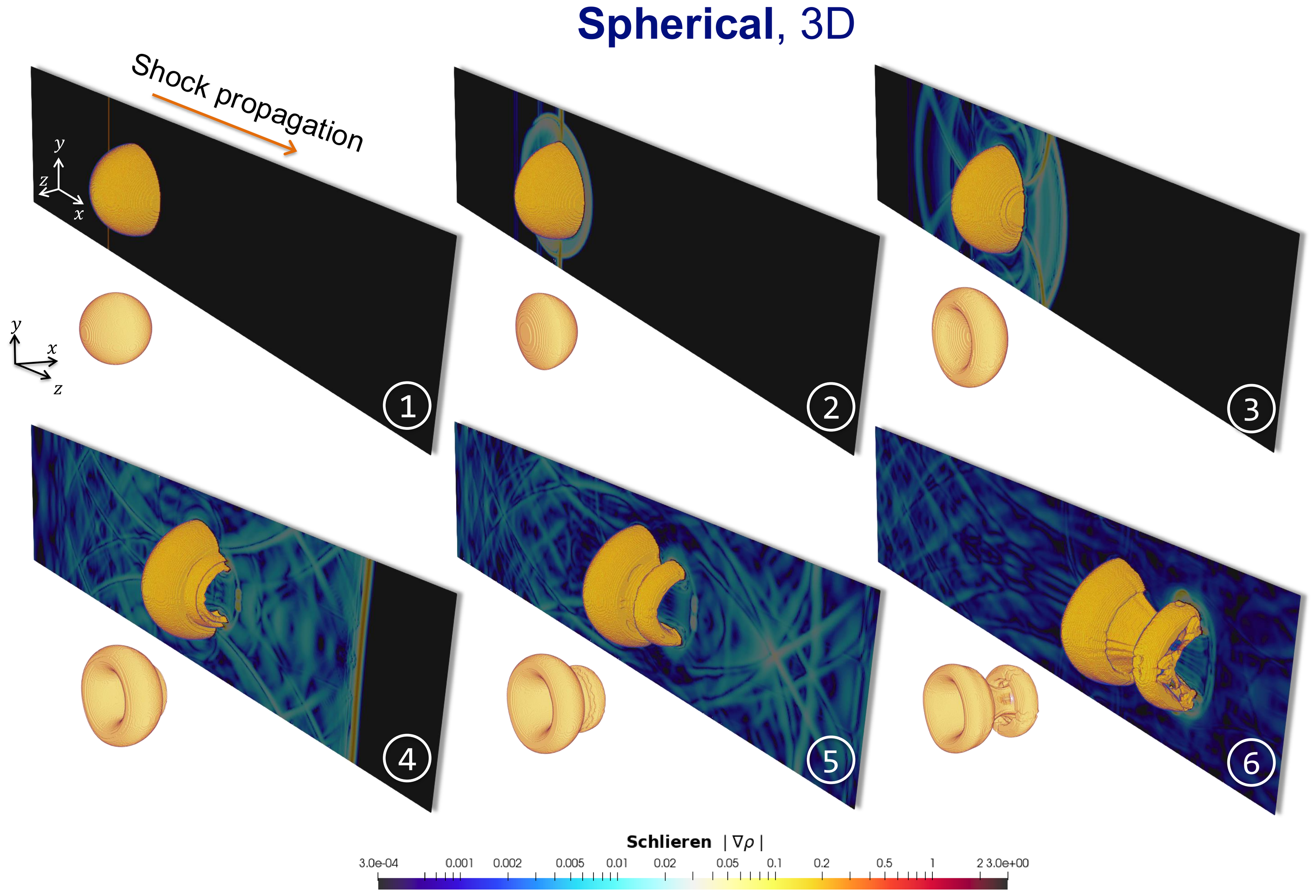


Shock-Helium Bubble Interaction

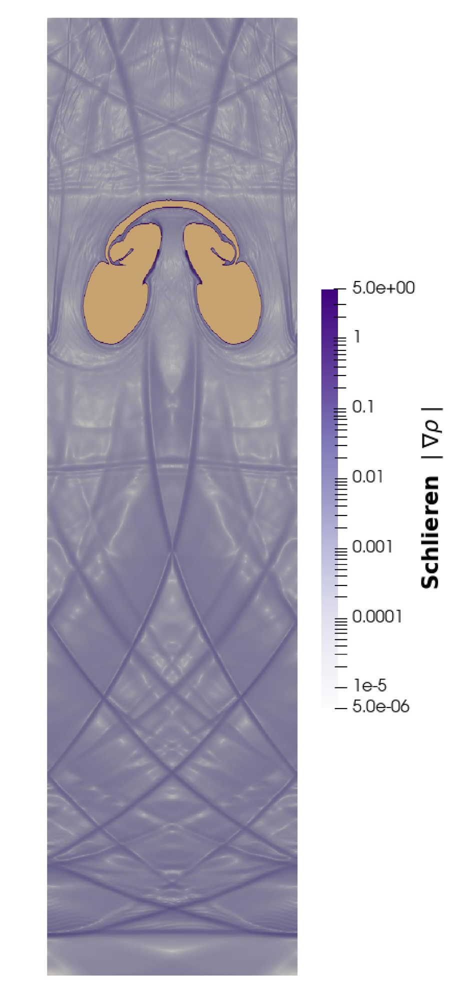
A helium bubble is in hydrodynamic equilibrium with surrounding air (with no gravity). A planar shockwave travels through the air and impacts the bubble, producing further shocks.

- Grid size: [512, 256, 256] for 3D case, [1024, 512] for 2D case.
- Runtime for 3D case: ~4h on 16 NVIDIA A100 GPUs.
- **Results agree with experimental results** [5], both for spherical (left) and cylindrical bubble (right).

Spherical, 3D



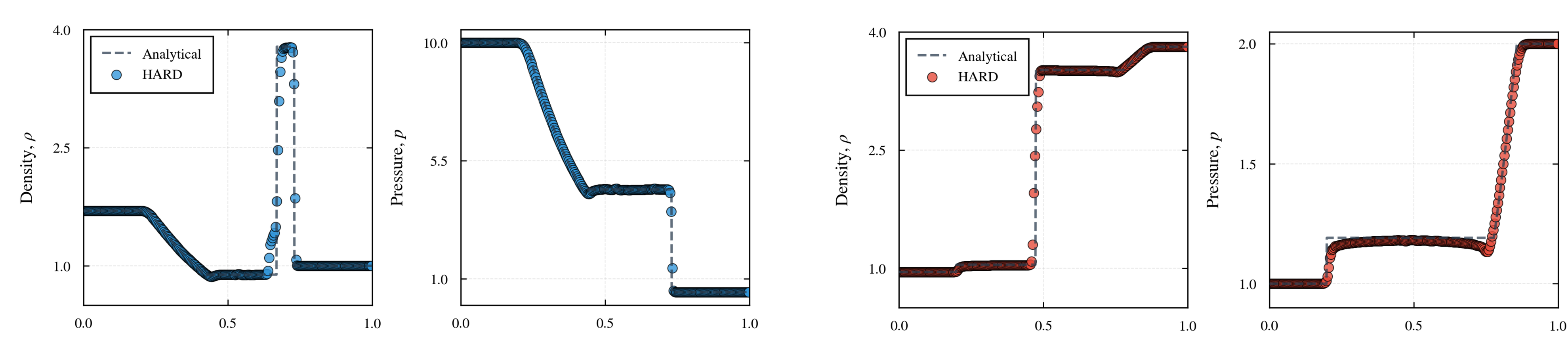
Cylindrical, 2D



Shyue and Lee Shock Tubes

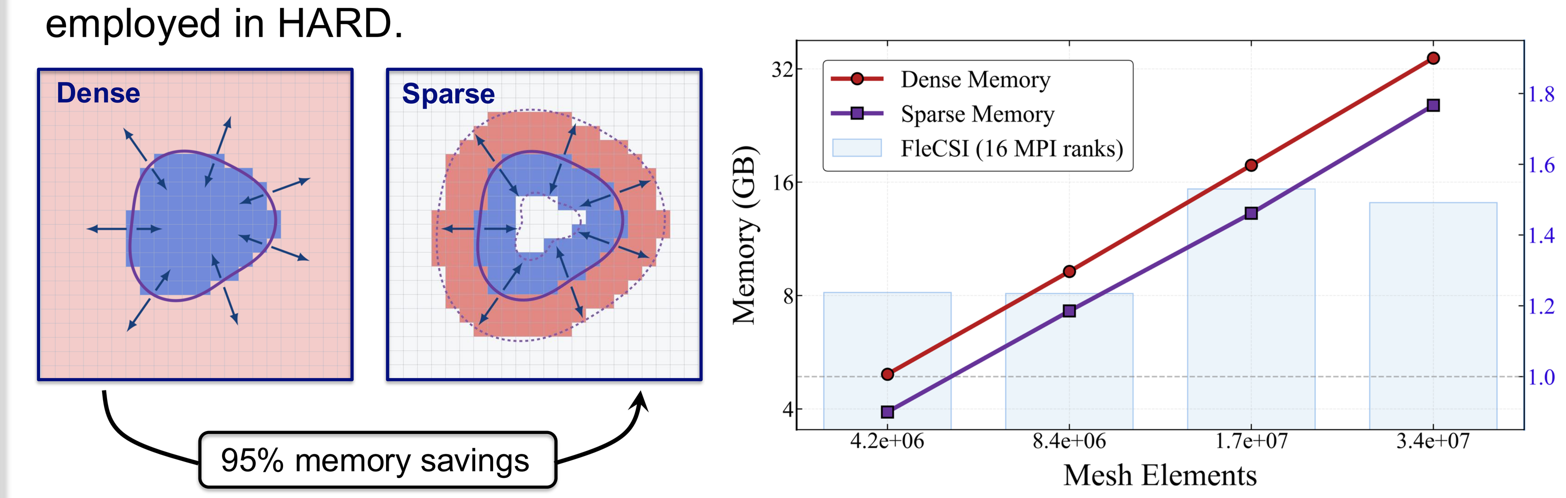
Multi-material physics often requires an equation of state other than the ideal gas equation like the **Jones-Wilkins-Lee (JWL) equation of state (EOS)**, which describes high-energy, reactive materials.

Two JWL-EOS Riemann problem shock tubes are studied in 1D space: Shyue (left) and Lee (right).



Optimizations

Memory usage is critical as it constrains simulation problem size and vastly increases MPI communication overhead, creating a major bottleneck. Hence, **sparse data structures** and **FleCSI's native MPI optimizations** for GPUs are employed in HARD.

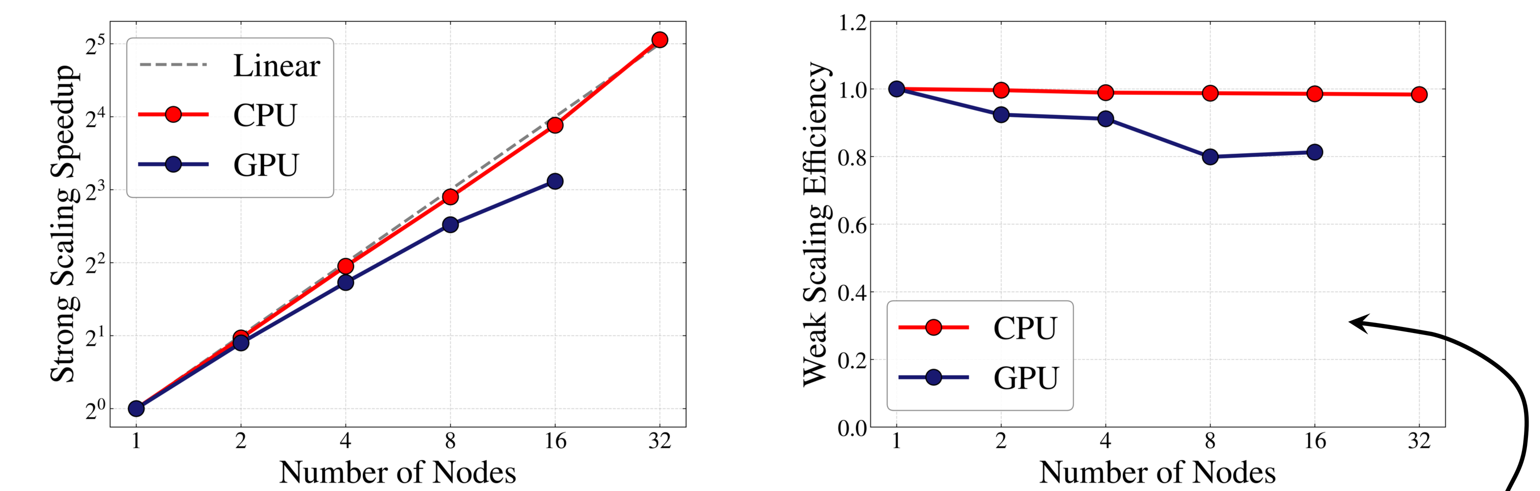


Sparse data structures decrease by ~95% the memory required in GFM extrapolation, yielding a 25% reduction of the total simulation memory footprint.

Parallel Performance

Parallel performance is evaluated on the **LANL Chicoma supercomputer** for both CPU (AMD EPYC 7H12) and GPU (NVIDIA A100) nodes, using **MPI** as distributed-memory backend. Each node is fully populated with 128 CPU cores or 4 GPUs.

- Single node performance GPU vs CPU: **12.2× speedup**
- Weak scaling GPUs: 81.3% efficiency at 16 nodes (right)
- Strong scaling GPUs: 8.67× speedup at 16 nodes (left)



Baseline helium bubble test setup:

- Grid: [16384, 8192].
- Memory: 107 GB.

	CPU Runtime	GPU Runtime	Speedup
1 node	1668 s	136.5 s	**12.2×**
4 nodes	1687 s	149.8 s	**11.3×**
16 nodes	1693 s	167.9 s	**10.1×**

Future Work

- Kernel fusion inside HARD to reduce data movement.
- Bring FleCSolve-style time integration for ghost-state extrapolation.
- Leverage sparse data structures to perform concurrent material extrapolation.

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