Design, development, and analysis of a compressible fluid dynamics solver capable of exceeding one quadrillion degrees of freedom

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Collaborative effort


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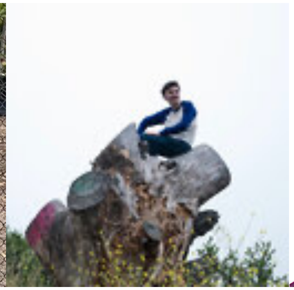
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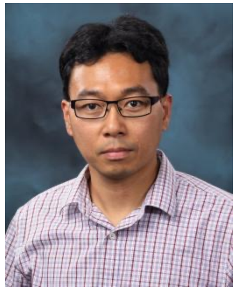
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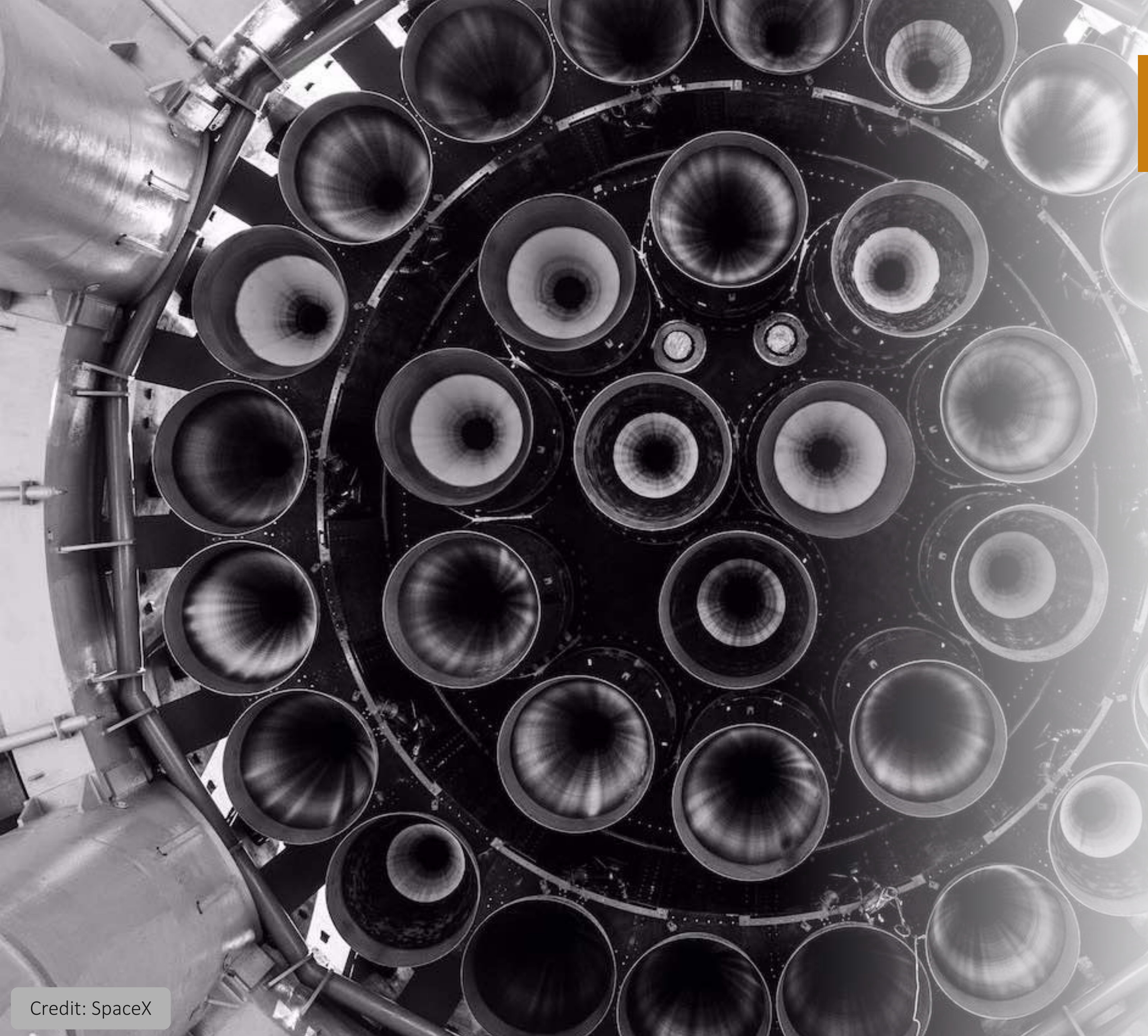
Introduction



Credit: SpaceX

- Large arrays of small rockets are the new standard
- Interactions between nearby rockets produce new problems
- Simulation resolution is limited by available GPU memory
- More resolution = more rockets
- Existing tools for shock-laden flows are poorly conditioned at lower precision
- Lower precision and linear numerics are faster

Timeline of biggest CFD simulations

2013[1]
(GB Winner)

- 10T grid cells on BlueGene/Q
- Enabled by susbstanial CPU memory
- Nonlinear state-of-the-art numerics
- Time to solution ~ 1 month for meaningful time scales

Sep. 2024[2]

- 35T grid cells on OLCF Frontier
- Incompressible flow
- Time-to-solution dominated by all-to-all communication
- Time to solution: hours to days

Oct. 2024[3]

- 10T grid cells on OLCF Frontier
- Nonlinear state-of-the-art numerics
- Time to solution: hours to days
- Compressible

Today

- 200T cells on OLCF Frontier
- 113T cells on LLNL El Cap
- 100T cells on JSC Jupiter
- Compressible flow solver
- Novel numerics
- Time to solution: hours to days

[1] Rossinelli et al. (2013) Proceedings of SC '13
[2] Yeung et al. (2025) CPC
[3] Sathyanarayana et al. (2025) JPDC

Summary of contributions

- Information geometric regularization foregoes nonlinear viscous shock capturing, enabling linear off-the-shelf numerical schemes and sequential summation of right-hand side contributions.
- Unified addressing on tightly coupled CPU–GPU and APU platforms increases total problem size with negligible performance hit.
- FP32 compute and FP16 storage further reduce memory use while remaining numerically stable, enabled by the algorithm's well-conditioned numerics.
- Reduce memory footprint 25-fold over state-of-the-art. Improve time and energy-to-solution factors of 4 and 5.4, compared to an optimized implementation of state-of-the-art methods.
- First CFD simulation exceeding 200T grid points and 1 quadrillion degrees of freedom, improving on previous largest simulations by a factor of 20.

How big is a quadrillion???

$$1 \text{ quadrillion} = 1,000,000,000,000,000 = 1 \times 10^{15}$$

$$1 \text{ quadrillion seconds } \approx 31.7 \; \textit{million} \text{ years}$$

- Model and numerical method
- Basic implementation details
- System-specific design
- Performance and results

Model and numerical method

Navier-Stokes equations for a single fluid

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0,$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + p\mathbf{I} - \mathbf{T}) = \mathbf{0},$$

$$\frac{\partial E}{\partial t} + \nabla \cdot [(E + p)\boldsymbol{u} - \boldsymbol{u} \cdot \mathbf{T}] = 0,$$

Old solution method:

- High-order finite volume solver
- HLLC Riemann solver
- WENO spatial reconstructions
- Requires converting between conservative and primitive variables for stability
- Expensive, nonlinear, and ill-conditioned at lower floating-point precisions

Model and numerical method

Navier-Stokes equations for a single fluid

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0,$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + p\mathbf{I} - \mathbf{T}) = \mathbf{0},$$

$$\frac{\partial E}{\partial t} + \nabla \cdot [(E + p)\boldsymbol{u} - \boldsymbol{u} \cdot \mathbf{T}] = 0,$$

New solution method (IGR):

- Add some terms to the equation
- Solve using linear numerics and in purely conservative variables

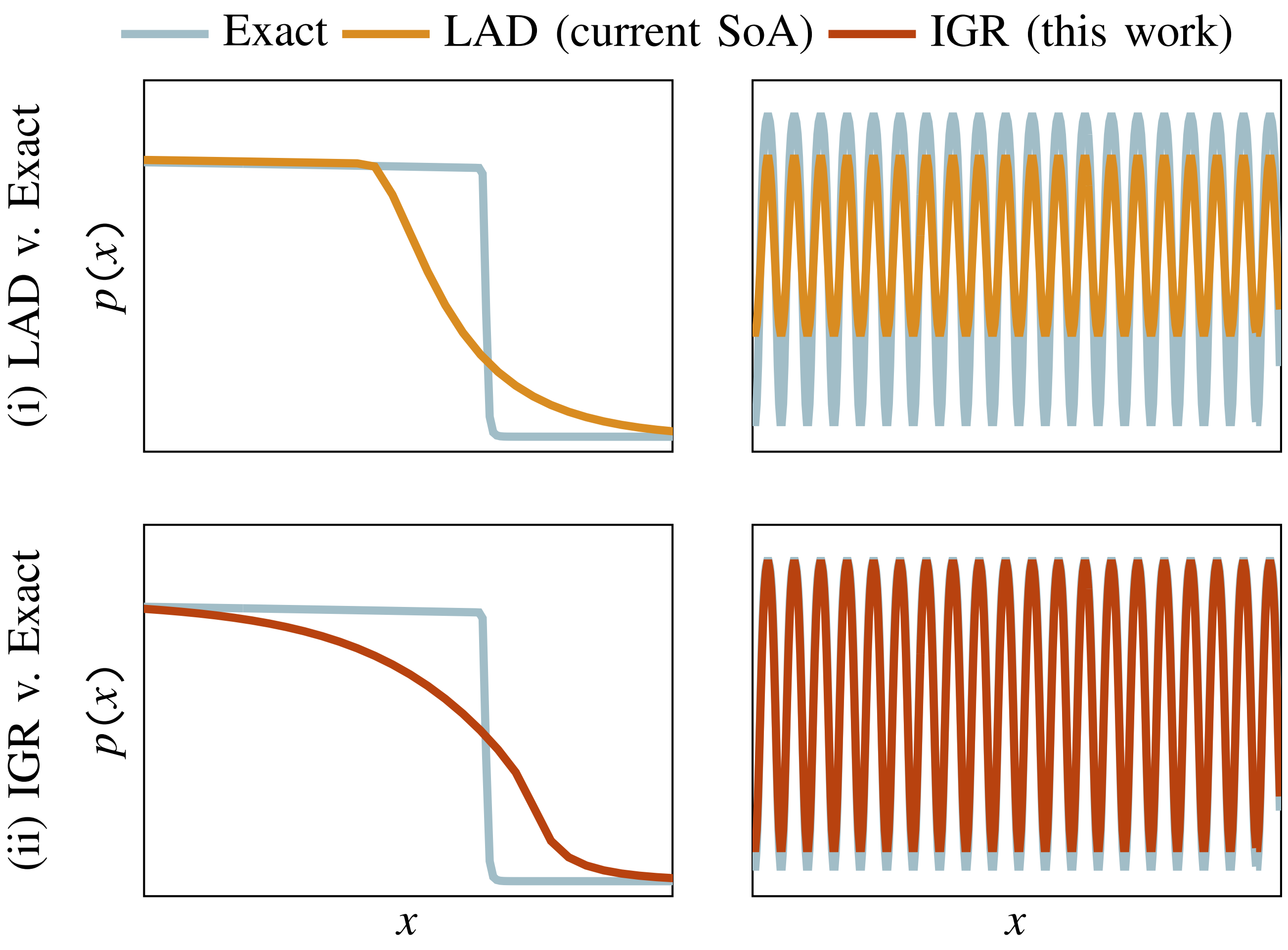
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0,$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + (p + \Sigma)\mathbf{I} - \mathbf{T}) = \mathbf{0},$$

$$\frac{\partial E}{\partial t} + \nabla \cdot [(E + p + \Sigma)\boldsymbol{u} - \boldsymbol{u} \cdot \mathbf{T}] = 0,$$

$$\alpha \left[\operatorname{tr}(\nabla \boldsymbol{u})^2 + \operatorname{tr}^2(\nabla \boldsymbol{u})\right] = \frac{\Sigma}{\rho} - \alpha \nabla \cdot \left(\frac{\nabla \Sigma}{\rho}\right)$$

Benefits of IGR



(a) Shock problem (b) Oscillatory problem

- Existing approach (LAD) yields solutions that are not smooth to higher orders
  - Can lead to spurious oscillations at discontinuities and dissipation of oscillatory features
- IGR replaces shocks with high-order smooth profiles to reduce oscillations near shocks and dissipation of oscillatory features

Credit: Cao and Schafer, 2024

Solution overview

3rd order SSP TVD Runge-Kutta

$$\boldsymbol{q}^{(2)} = \boldsymbol{q}^{(1)},$$

$$\boldsymbol{q}^{(1)} = \boldsymbol{q}^{(1)} + \Delta t \frac{\partial \boldsymbol{q}^{(1)}}{\partial t},$$

$$\boldsymbol{q}^{(1)} = \frac{3}{4}\boldsymbol{q}^{(2)} + \frac{1}{4}\boldsymbol{q}^{(1)} + \frac{1}{4}\Delta t \frac{\partial \boldsymbol{q}^{(1)}}{\partial t},$$

$$\boldsymbol{q}^{(1)} = \frac{1}{3}\boldsymbol{q}^{(2)} + \frac{2}{3}\boldsymbol{q}^{(1)} + \frac{2}{3}\Delta t \frac{\partial \boldsymbol{q}^{(1)}}{\partial t}$$

RHS Calculation

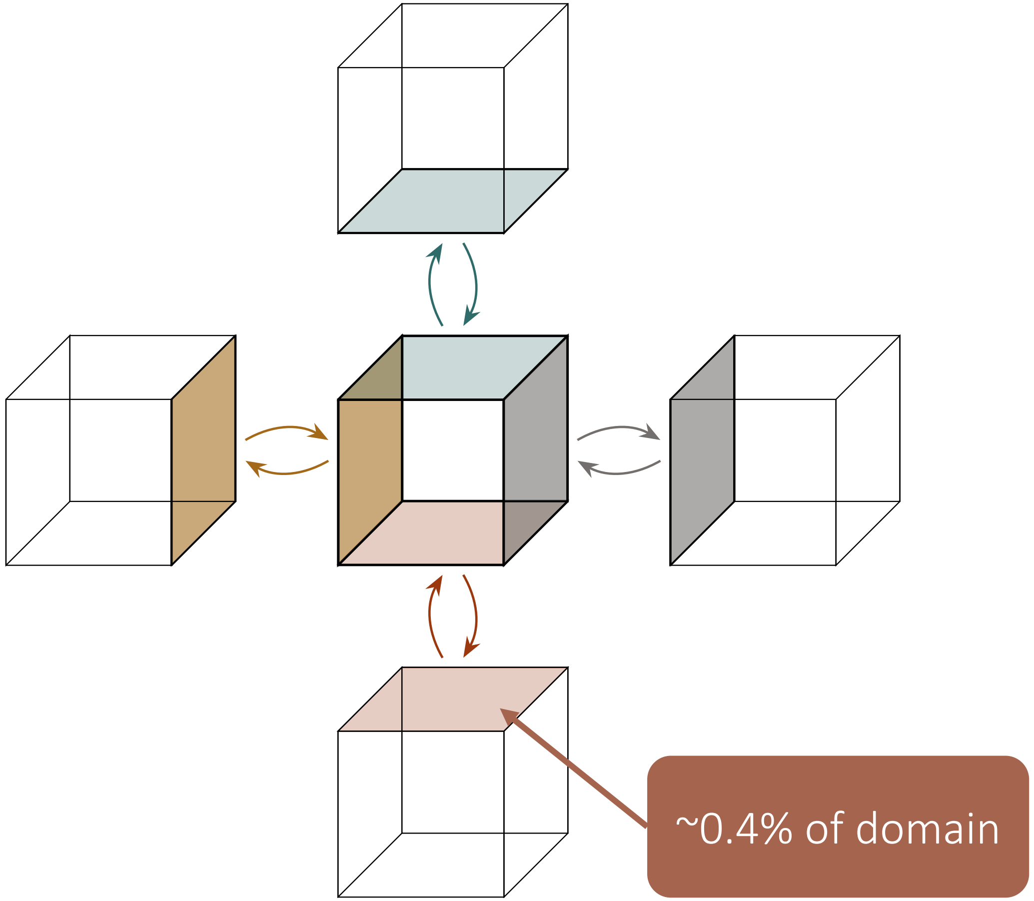
$$\frac{\partial \boldsymbol{q}}{\partial t} = \begin{cases} \frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{u}), \\ \frac{\partial (\rho \boldsymbol{u})}{\partial t} = -\nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + (p + \Sigma)\mathbf{I} - \mathbf{T}, \\ \frac{\partial E}{\partial t} = -\nabla \cdot \left[(E + p + \Sigma)\boldsymbol{u} - \boldsymbol{u} \cdot \mathbf{T} \right], \end{cases}$$

Elliptic solve for entropic pressure

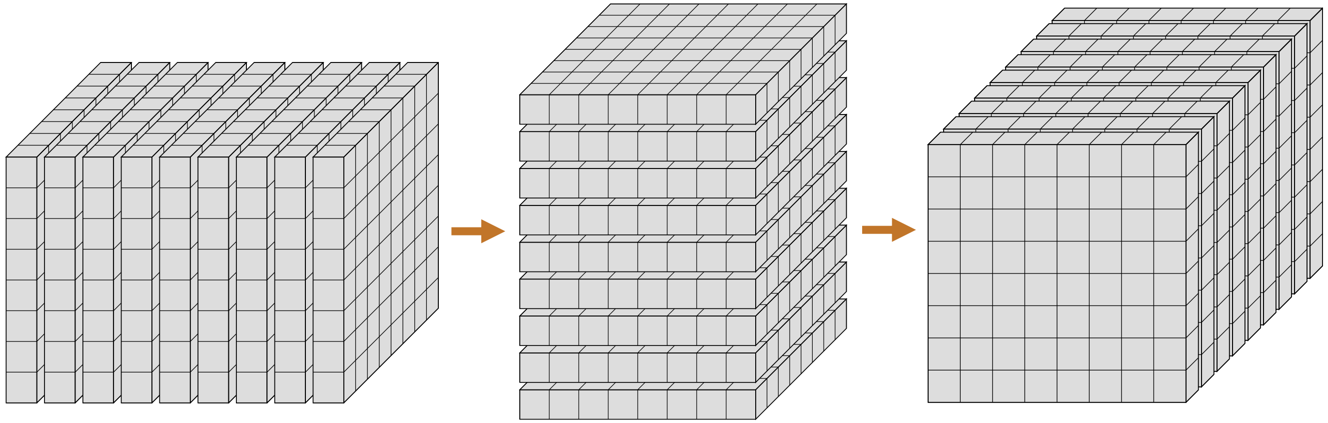
$$\frac{\Sigma}{\rho} - \alpha \nabla \cdot \left(\frac{\nabla \Sigma}{\rho} \right) = \underbrace{\alpha \left[\mathrm{tr}\,(\nabla \boldsymbol{u})^2 + \mathrm{tr}^2\,(\nabla \boldsymbol{u}) \right]}_{\Sigma_{\mathrm{rhs}}}$$

- Model and numerical method
- Basic implementation details
- System-specific design
- Performance and results

Domain decomposition and communication



Block decomposition communication pattern



Example max problem size decompositions

N_{proc}	Proc Disc.	Total (T)
128	$4 \times 4 \times 8$	0.340
384	$8 \times 8 \times 6$	1.02
1024	$16 \times 16 \times 8$	2.73
3072	$16 \times 16 \times 12$	8.18
8192	$32 \times 32 \times 16$	21.8
75264	$48 \times 49 \times 32$	200

Storage and I/O

```
restart_data
├── P1
│   ├── lusture_0.dat
│   ├── lusture_100.dat
│   └── ⋮
├── P2
│   ├── lusture_0.dat
│   ├── lusture_100.dat
│   └── ⋮
└── ⋮
```

Pros:

- Simple
- Fast

Cons:

- O(10^6) files for leadership scale simulation
- Lots of concurrent metadata creation

$$(1 \times 10^{15} \text{ scalars}) \times \left(16 \ \frac{\text{bits}}{\text{scalar}}\right) / \left(8 \times 10^{12} \ \frac{\text{bits}}{\text{terabyte}}\right) = 2000 \text{ terabytes} = 2 \ \boldsymbol{Petabytes}$$

GPU programming landscape

	OpenMP			OpenACC		
Compiler	NV GPUs	AMD GPUs	FP16 Atomics	NV GPUs	AMD GPUs	FP16 Atomics
AMD	❌	✅	✅	❌	❌	❌
CCE	✅	✅	❌	✅	✅	❌
NVHPC	✅	❌	?	✅	❌	✅*

- Modern supercomputers are procured from two hardware vendors, so portability is important!
- OpenMP is generally better supported, but OpenACC is generally faster when the necessary features are available
- If we want the best performance we can get on all hardware we need to support everything

Portable GPU offload using directive based programming and macros

Source code with macros

```
#:call GPU_PARALLEL_LOOP(collapse=3, private='[...]')
do l = 0, p            ! Z-direction
    do k = 0, n        ! Y-direction
        do j = 0, m ! X-direction
            !!> Core kernel,
            !!> O(1000) arithmetic operations
        end do
    end do
end do
#:endcall GPU_PARALLEL_LOOP
```

Preprocessor

OpenACC Code

```
!$acc parallel loop vector gange collapse(3) &
!$acc default(present) private(...)
do l = 0, Nz            ! Z-direction
    do k = 0, Ny        ! Y-direction
        do j = 0, Nx ! X-direction
            !!> Core kernel,
            !!> O(1000) arithmetic operations
        end do
    end do
end do
!$acc end parallel loop
```

OpenMP Code

```
!$omp target teams distribute parallel do simmd &
!$omp defaultmap(firstprivate:scalar) &
!$omp defaultmap(tofrom:aggregate) &
!$omp defaultmap(present:allocatable) &
!$omp defaultmap(present:pointer) &
!$omp collapse(3) private(...)
do l = 0, Nz            ! Z-direction
    do k = 0, Ny        ! Y-direction
        do j = 0, Nx ! X-direction
            !!> Core kernel,
            !!> O(1000) arithmetic operations
        end do
    end do
end do
!$omp end target teams distribute parallel do
```

- OpenMP and OpenACC are generated from one version of source code
- Developers don't need in depth understanding of directive tools

- Model and numerical method
- Basic implementation details
- System-specific design
- Performance and results

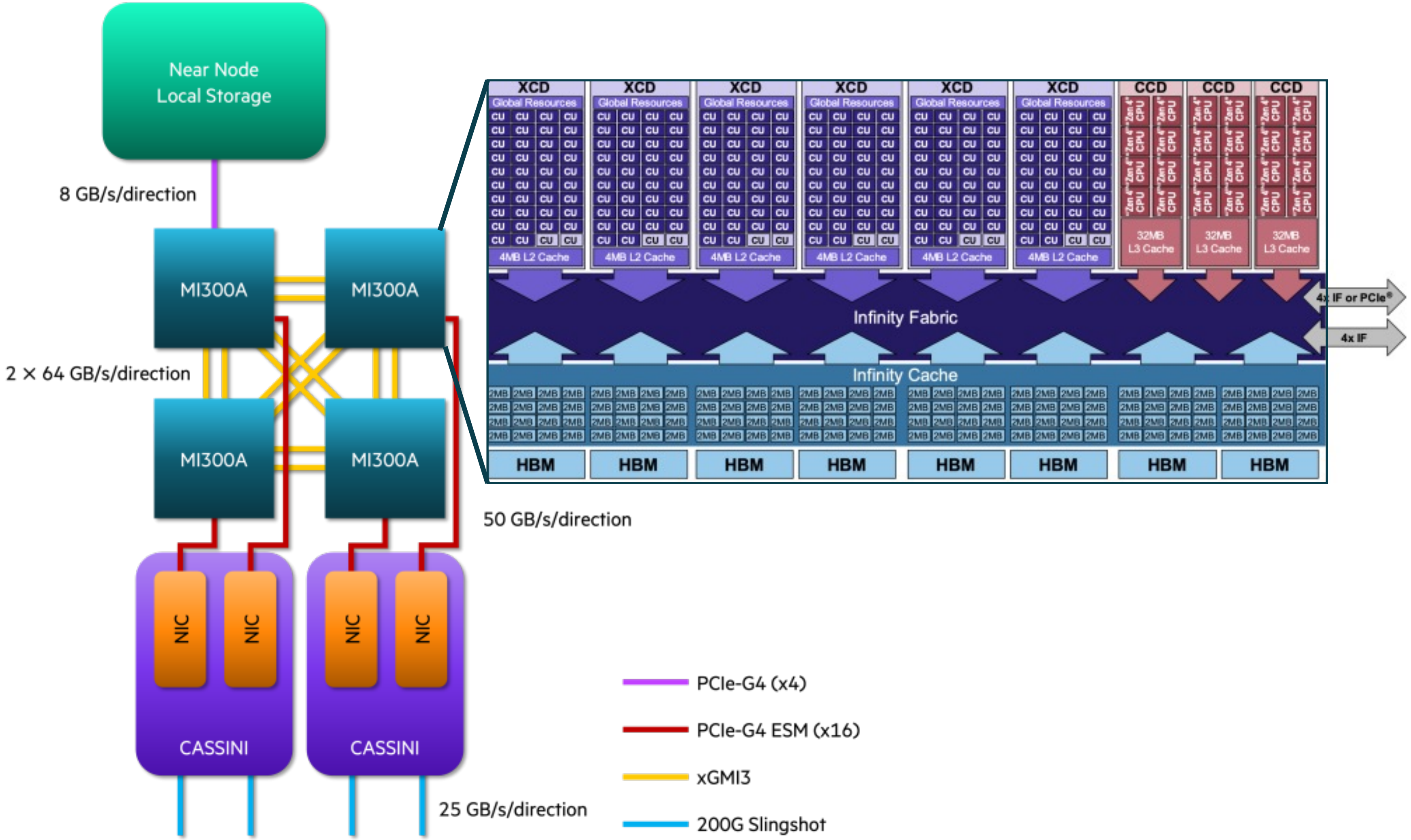
System Summary

	Node Configuration	# Nodes	Memory [Node, System]	Peak Power	Rmax	TOP500
LLNL El Capitan	4 AMD MI300A APU	11136	[512 GB, 5.6 PB] APU	34.8 MW	1742 PFLOPs	1
OLCF Frontier	4 AMD MI250X GPU 1 AMD Trento CPU	9472	[512 GB, 4.8 PB] GPU [512 GB, 4.8 PB] CPU	24.6 MW	1353 PFLOPs	2
CSCS Alps	4 NVIDIA GH200 (4 Grace CPU, 4 Hopper GPU)	2688	[384 GB, 1.0 PB] GPU [480 GB, 1.3 PB] CPU	7.1 MW	435 PFLOPs	8

- All systems of interest are within the top 10 fastest computers measured by the HPL benchmark
- CSCS Alps is “little brother” to 6k node JSC Jupiter which is ranked 3rd now
- >95% of total system memory is used on El Capitan and Frontier
- >85% of total system memory is used on Alps

- Shared critical features:
  - Ability to leverage unified address space between CPU and GPU
  - High performance networking and leadership class scale

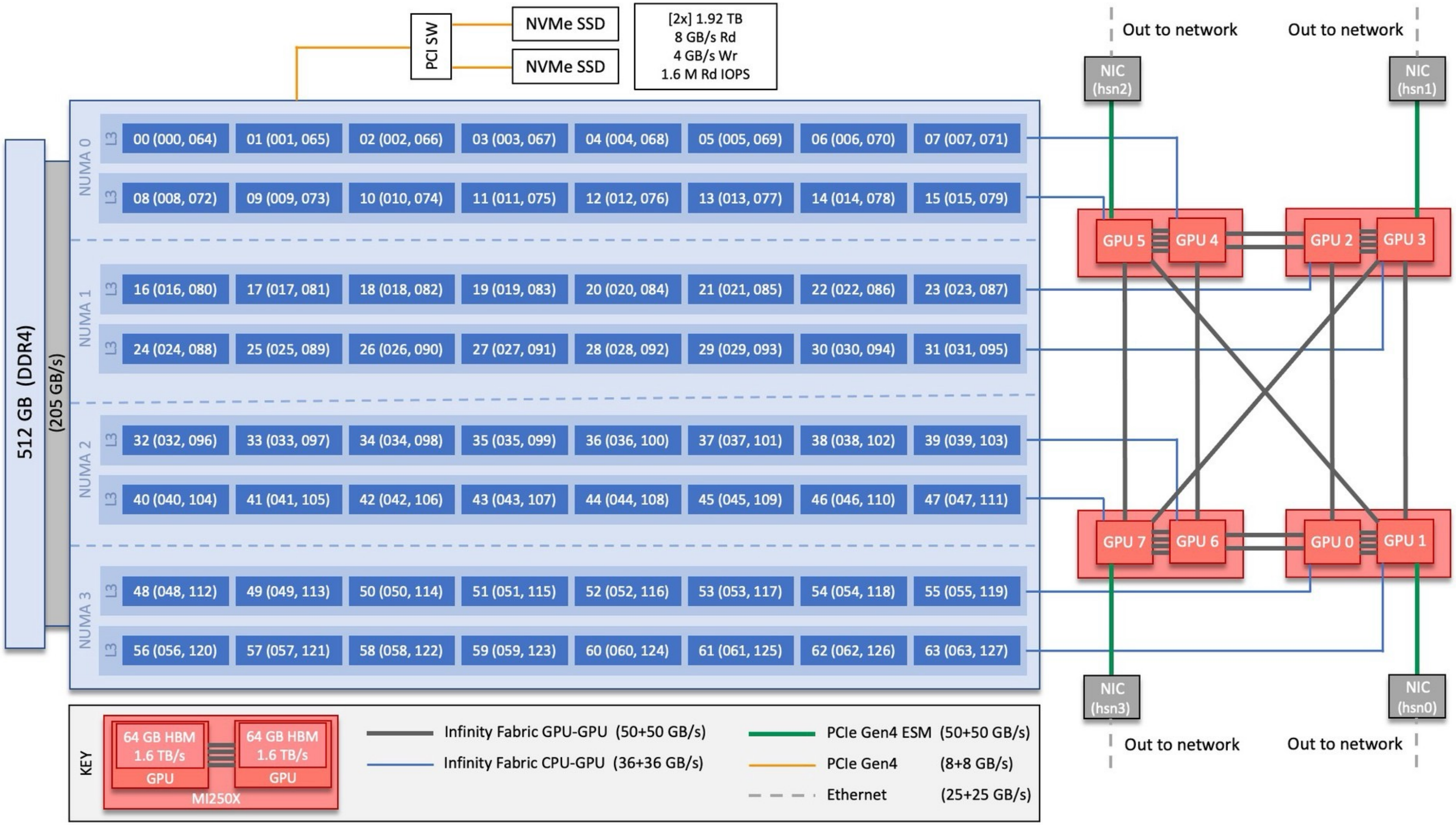
Tightly coupled GPU/APU architectures (AMD MI300A, LLNL El Capitan)



- 24 Zen4 CPU cores bonded to 6 AMD XCD chiplets
- 4 APUs per node
- Memory is universally addressable in address space and physical space
- Zero host-to-device transfers to perform because the host and device are one

Credit:https://hpc.llnl.gov/documentation/user-guides/using-el-capitan-systems/hardware-overview

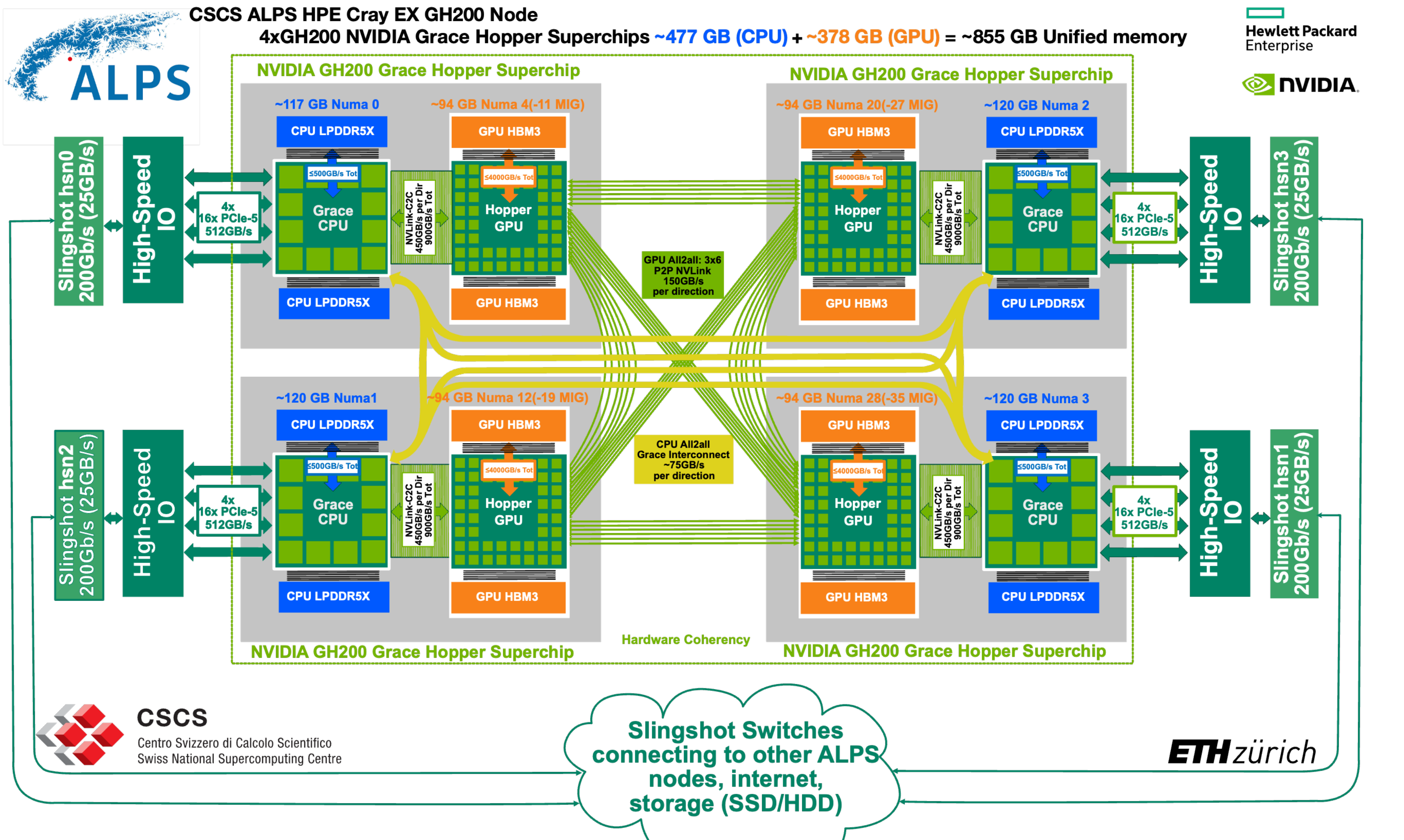
Tightly coupled GPU/APU architectures (AMD MI250X, OLCF Frontier)



- 4 Mi250X GPUs (8 GCDs) connected to one CPU via 36+36 GB/s links
- 1 CPU and 4 GPUs per node
- Each chip has its own memory
- Unified address space made possible through careful memory allocation and infinity fabric

Credit: https://docs.olcf.ornl.gov/systems/frontier_user_guide.html

Tightly coupled GPU/APU architectures (NVIDIA GH200, CSCS Alps)



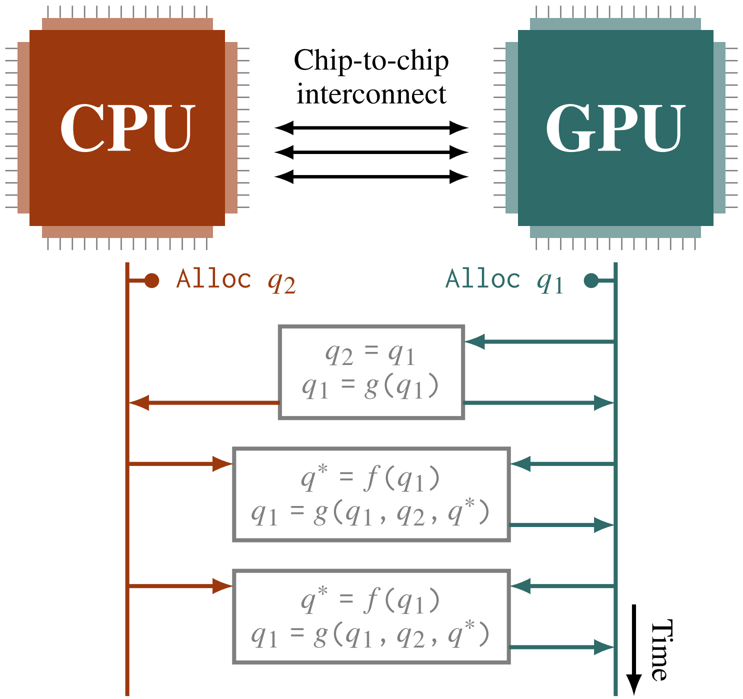
- Grace CPU and Hopper GPU connected via 900 GB/s chip-to-chip (C2C) link
- 4 CPUs and 4 GPUs per node
- Each chip has its own memory
- Unified address space made possible via high-speed interconnect, though memory regions are physically separate

Credit: https://docs.cscs.ch/alps/hardware/#nvidia-gh200-gpu-nodes

Unified memory strategy

MI250x - Allocate q_2 on the using **`hipMallocManaged`** and advise runtime *not* to make device copy

GH200 – Allocate q_2 and use **`cudaMemAdvise`** to keep memory on the host



MI250x - Allocate q_1 on the GPU using **`hipMalloc`** and advise runtime *not* to make a host copy

GH200 – Allocate q_1 and pin memory with **`cudaMemAdvise`**

- GH200's 900 GB/s link allows for storage of Σ and Σ_{rhs} on the host as well, further increasing problem size

- Model and numerical method
- Basic implementation details
- System-specific design
- Performance and results

Performance: Grindtime

Grindtime

Device	Baseline (in-core)	IGR (in-core)	IGR (unified)	
GH200	16.89	3.83	4.18	FP64
MI250X GCD	69.72	13.01	19.81	
MI300A	29.50	†—	7.21	
GH200	*N/A	2.70	2.81	FP32
MI250X GCD	*N/A	9.12	13.03	
MI300A	*N/A	†—	4.19	
GH200	*N/A	3.06	3.07	FP16/32
MI250X GCD	*N/A	22.63	24.71	
MI300A	*N/A	†—	17.39	

*Numerically unstable; †MI300A is always unified

Normalized by nanoseconds/grid cell/time step

- Baseline numerics unstable in lower precision
- AMD mixed precision slow due to using AMD's beta compiler and a pre-release of NVHPC SKD 25.9

- ~9% overhead in double precision on NVIDIA due to compiler regression
- <5% slowdown in single and mixed precision on NVIDIA thanks to 900 GB/s link
- 40-50% overhead in double and single precision on MI250x due to slower 36+36 GB/s link

- Up to 6x reduction in time to solution

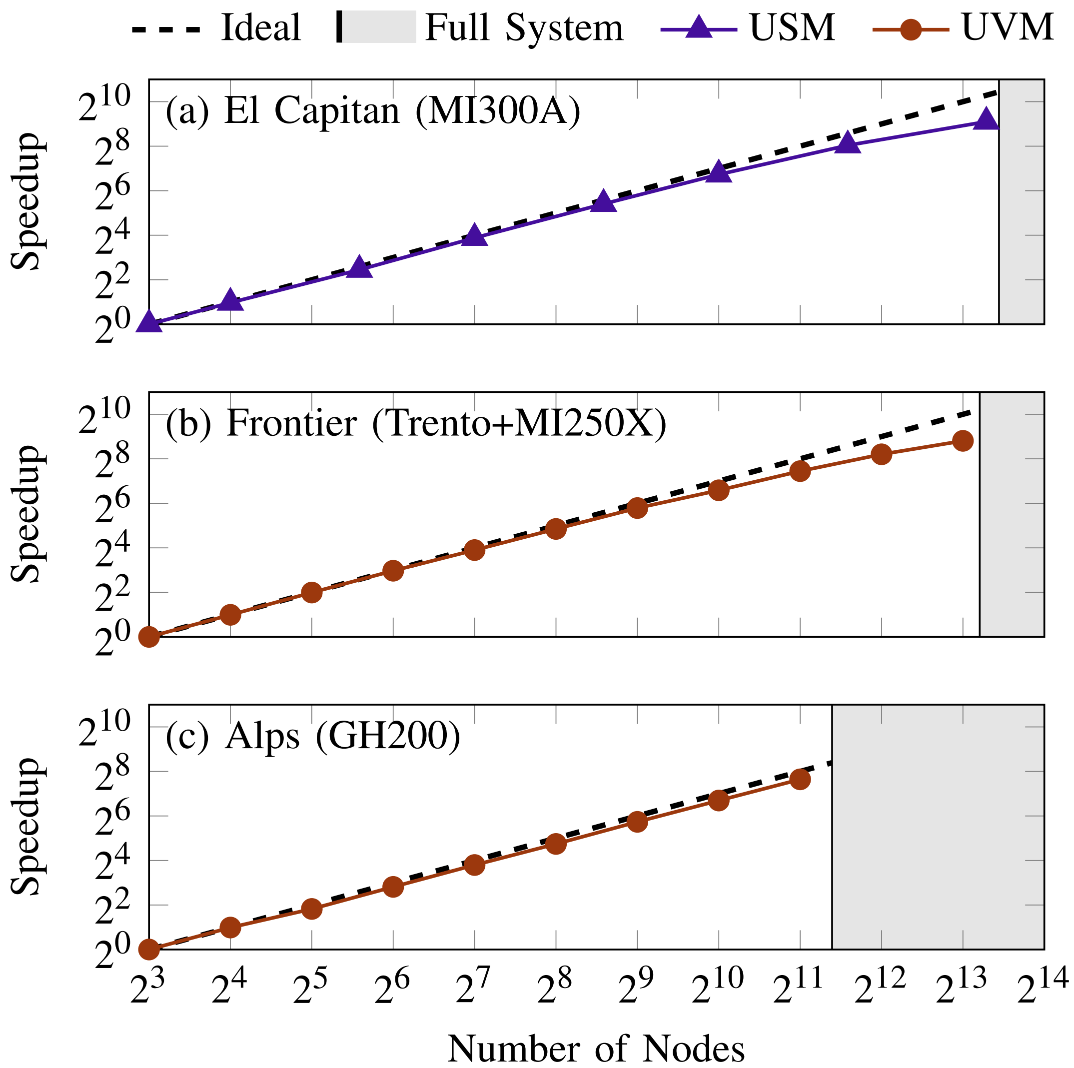
Performance: Power

Power

Energy (μJ)	El Capitan (MI300A)	Frontier (MI250X)	Alps (GH200)
Baseline	15.24	10.67	9.349
IGR	3.493	1.982	2.466

- Calculated by sampling `nvidia-smi` and `rocm-smi` to get a steady state wattage and then multiply by time
- Measured in in double precision for an apples-to-apples comparison
- Findings show power consumption is proportional to runtime as a first-order approximation
- GH200 uses more power with novel numerics than current state-of-the-art, but algorithm is faster

Performance: Strong scaling



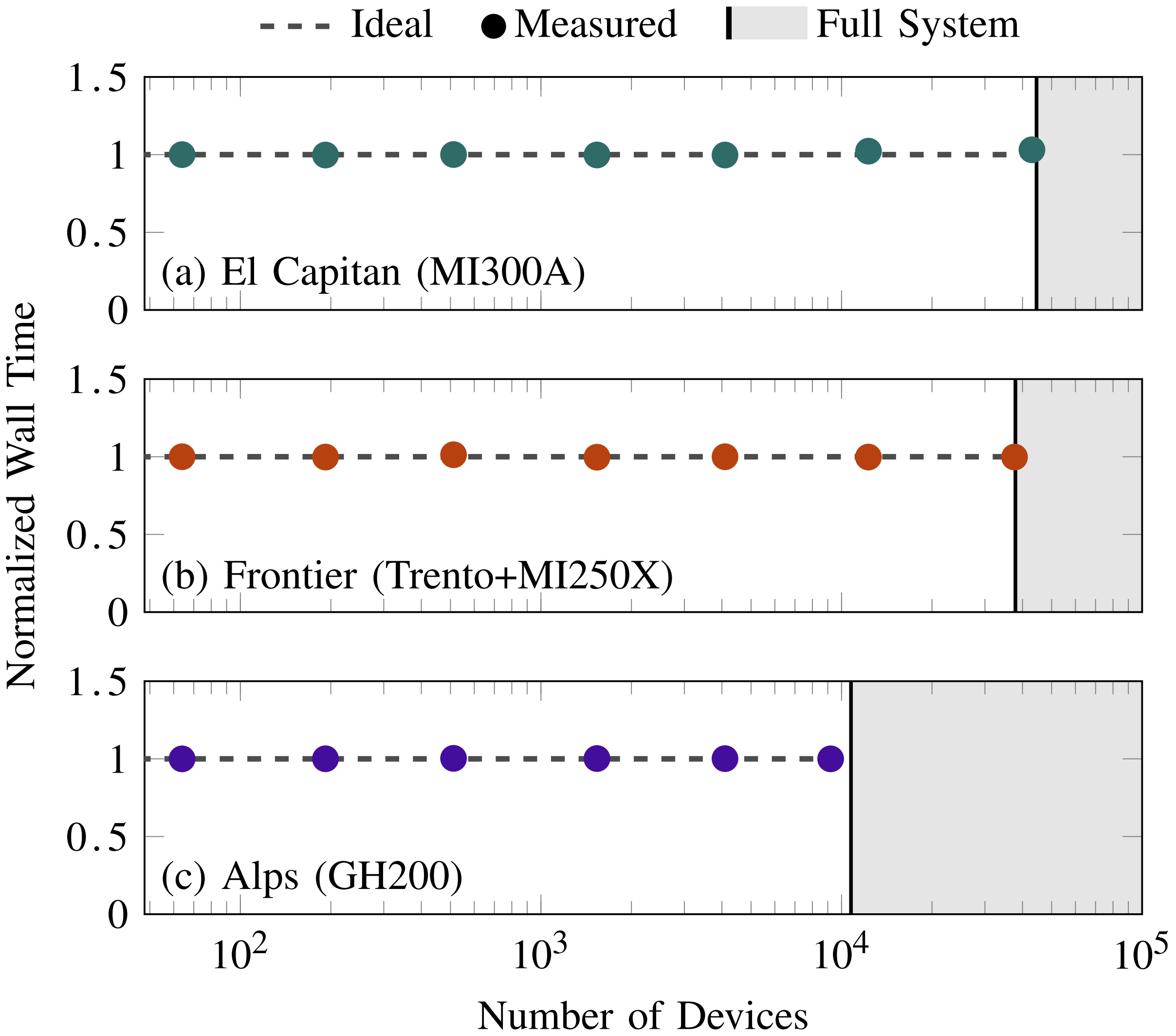
- 8-node base case does internode communication in all three physical dimensions
- Higher efficiency results in shorter time to solution for a given problem size

$$\text{Efficiency} = \frac{\text{Actual Speedup}}{\text{Ideal Speedup}}$$

Strong Scaling Efficiencies

Systemn	Base	32× Efficieny	Full System	
El Capitan	84 B	90%	10000 Nodes	44%
Frontier	170 B	90%	8192 Nodes	45%
Alps	134 B	86%	2048 Nodes	78%

Performance: Weak scaling



- 16-node base case does internode communication in all three physical dimensions (and makes for nice spacing)
- Efficiencies are all approx. 100%

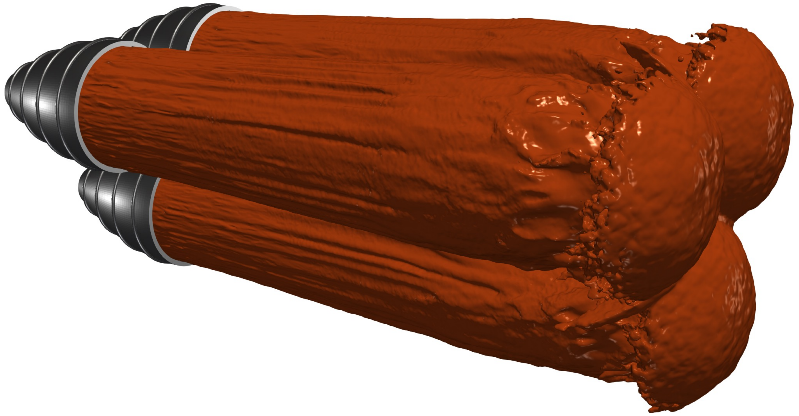
$$\text{Efficiency} = \frac{T_{\text{base case}}}{T}$$

Weak Scaling Efficiencies

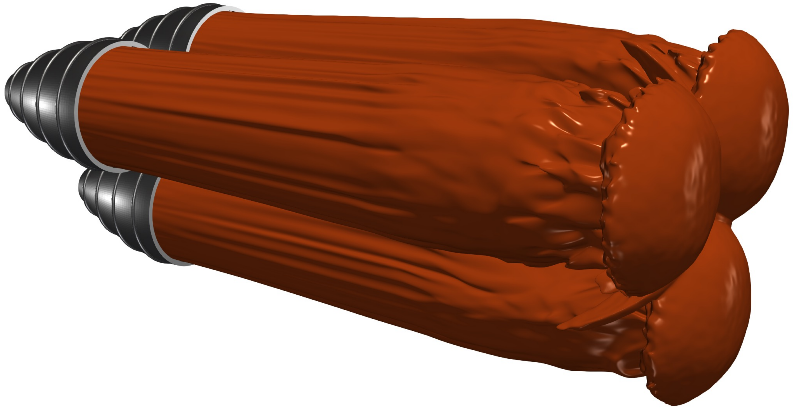
System	Base	Max	Increase	Efficiency
El Capitan	168 B	113 T	672×	97%
Frontier	341 B	200 T	588×	99%
Alps	268 B	38 T	143×	99%

Results: Precision comparison

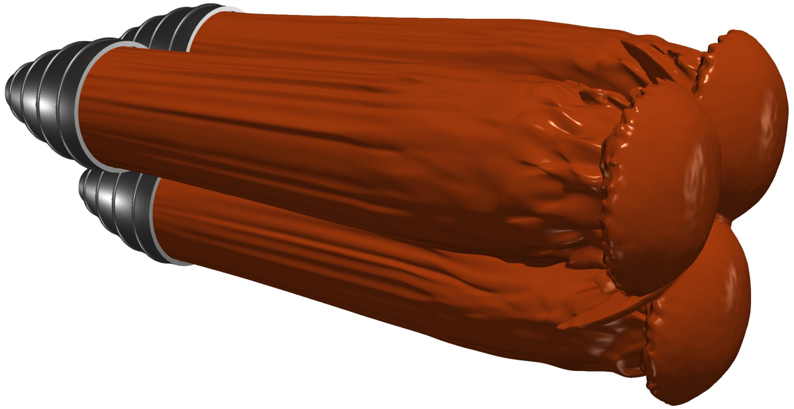
FP16/FP32



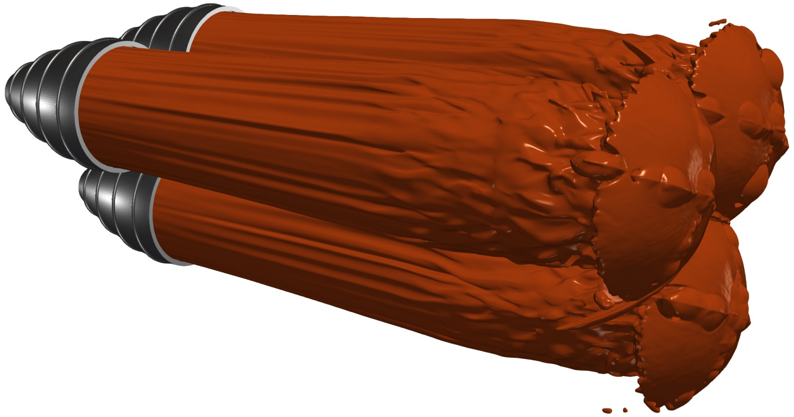
FP32



FP64



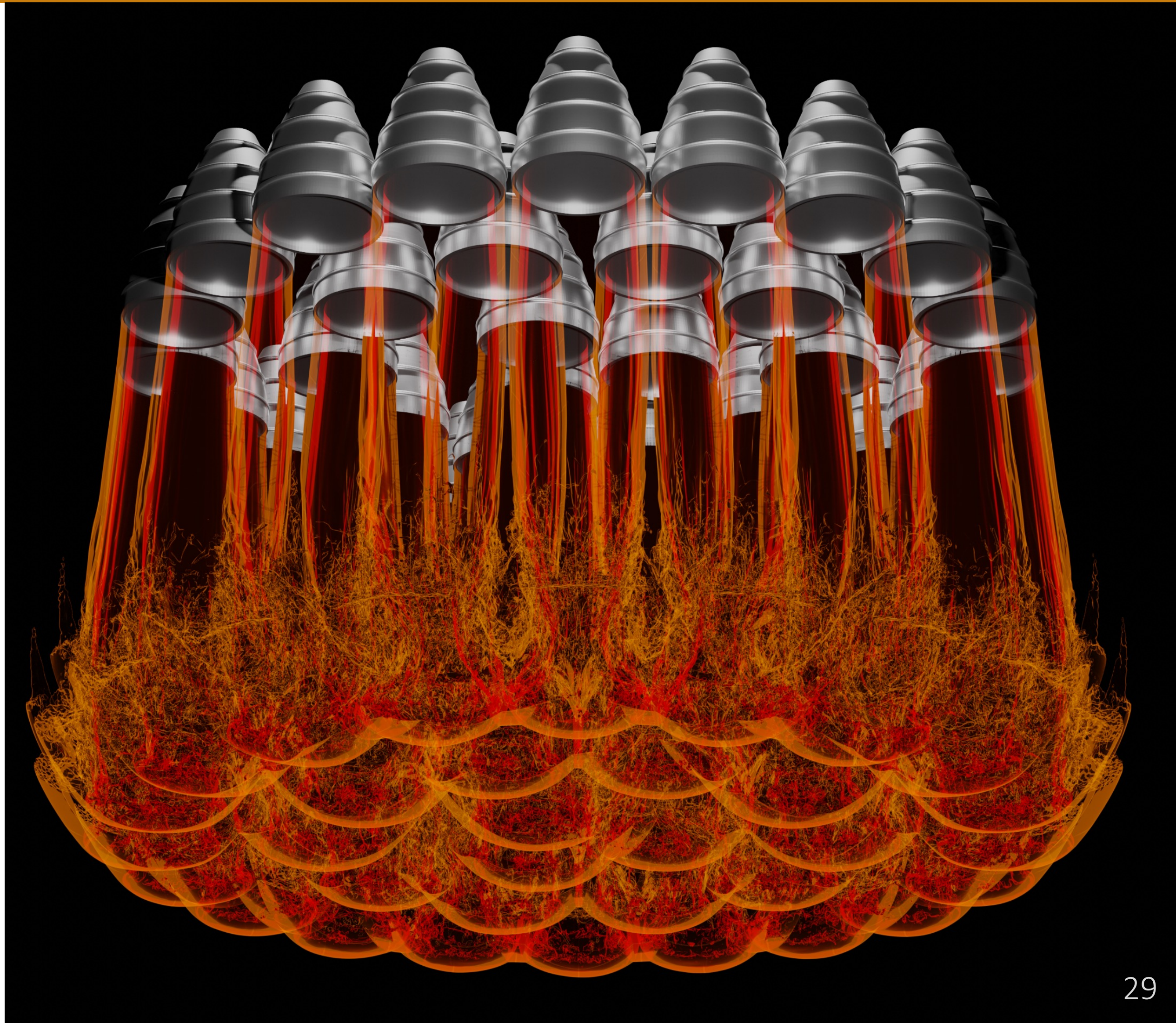
FP64 (baseline numerics)



- FP64 and FP32 visually indistinguishable
- FP16/FP32 is visually different, though the main flow features are captured
- Numerical error leads to early onset of hydrodynamic instabilities
- FP64 baseline has grid aligned artifacts due to gird aligned shock capturing

Results: Super heavy booster configuration

- 3.3 trillion grid cells
- 16.5 trillion degrees of freedom
- 16 hours on 9200 GH200 GPUs



Lessons learned

- NVIDIA compilers are great, but they let you do a lot of things that aren’t in the standards, so supporting new compilers can be challenging
- Compiler support for directive-based programming with lower floating-point precisions is still developing
- Heterogenous architectures are cool and allow you to do some interesting things
- Doing something no one has ever done before is difficult and time consuming

Code

Preprint

Questions?

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CSCS