Exploiting Thread Parallelism for Ocean Modeling on Cray XC Supercomputers

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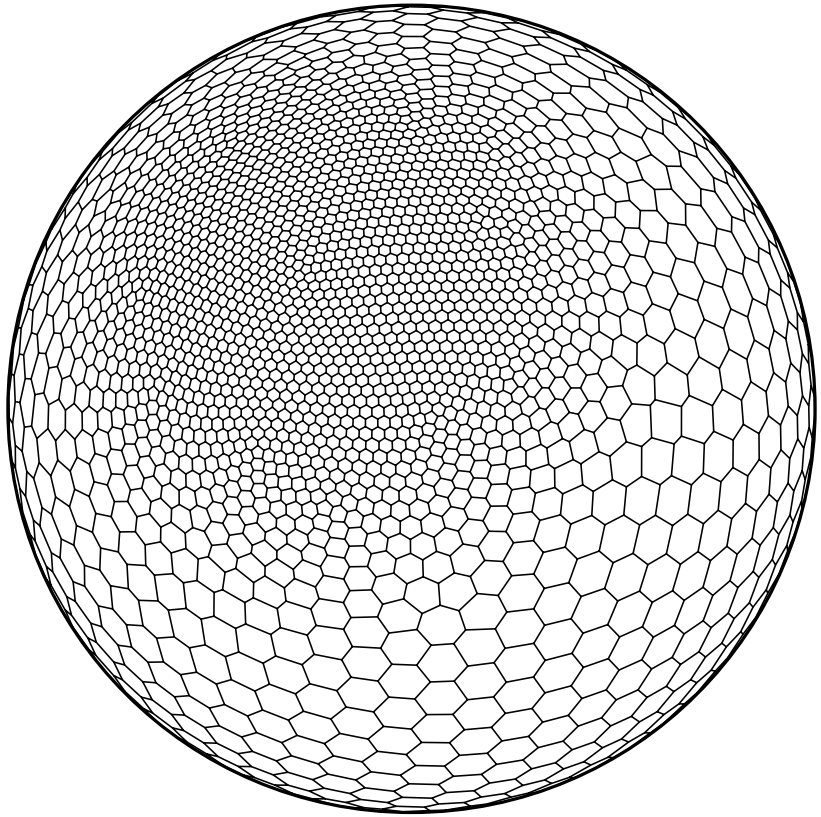
Ocean Modeling with MPAS-Ocean

- MPAS = **M**odel for **P**rediction **A**cross **S**cales. [LANL/NCAR]
- A multiscale method for simulating Earth's oceans.
- 2D Voronoi tessellation-based variable resolution mesh (SCVT).
- Structured vertical columns in third dimension represent ocean depths.



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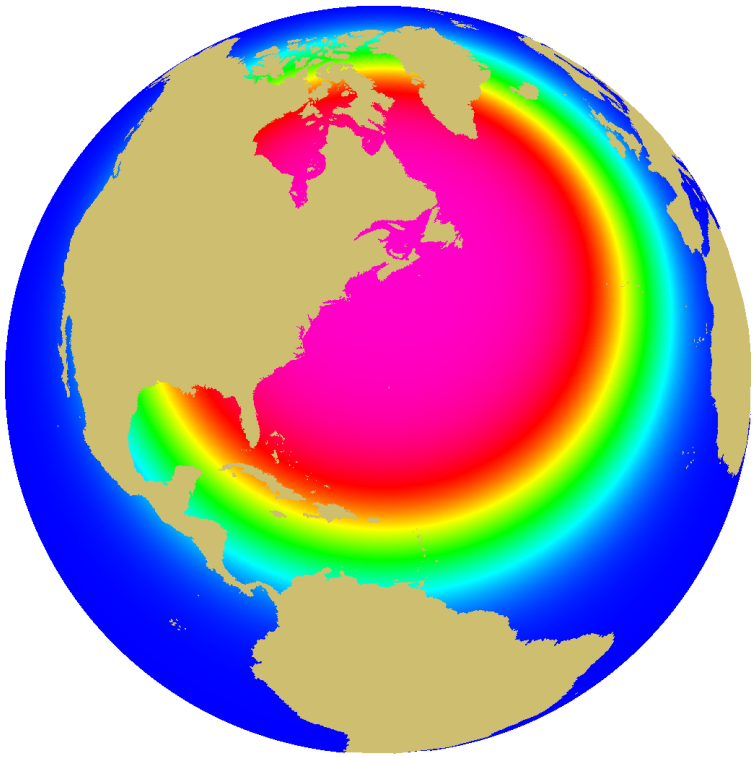
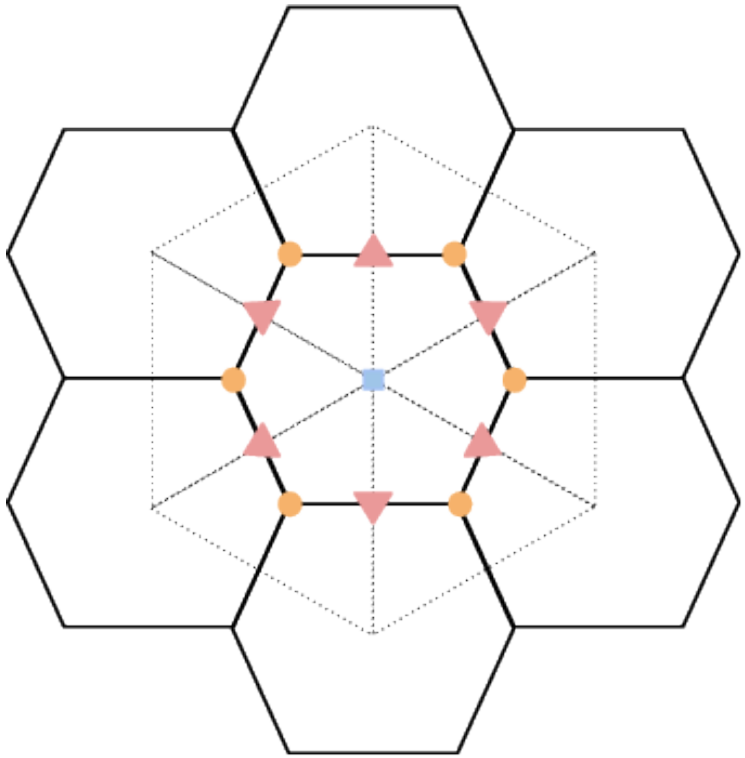


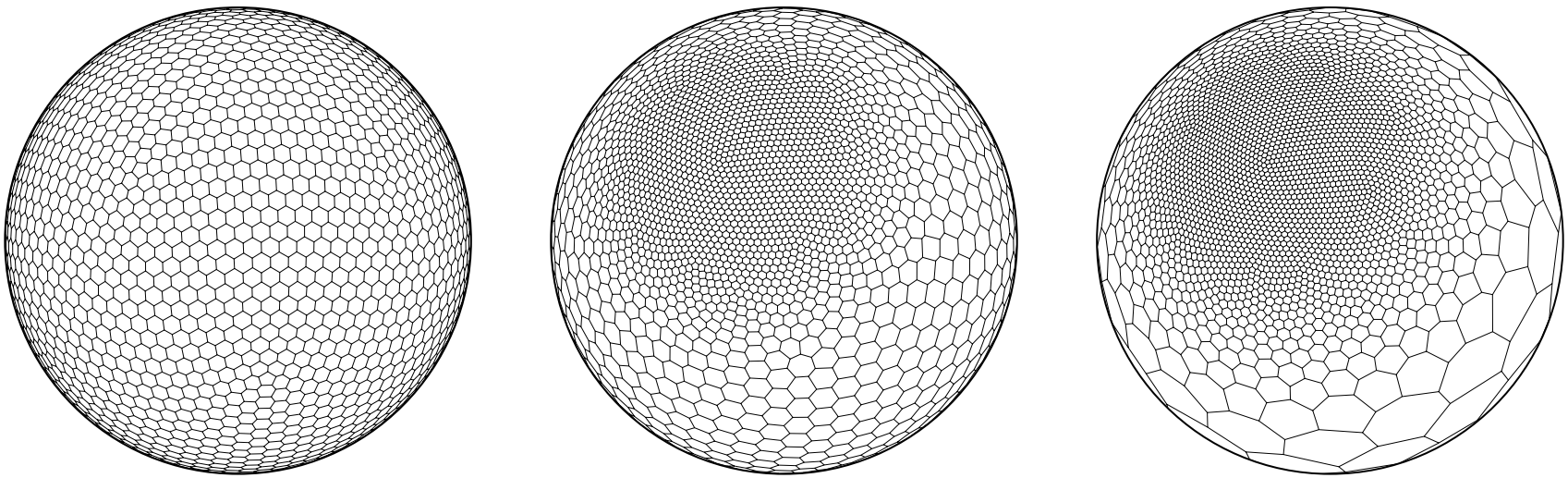
Variable Resolution Mesh



Mesh Elements

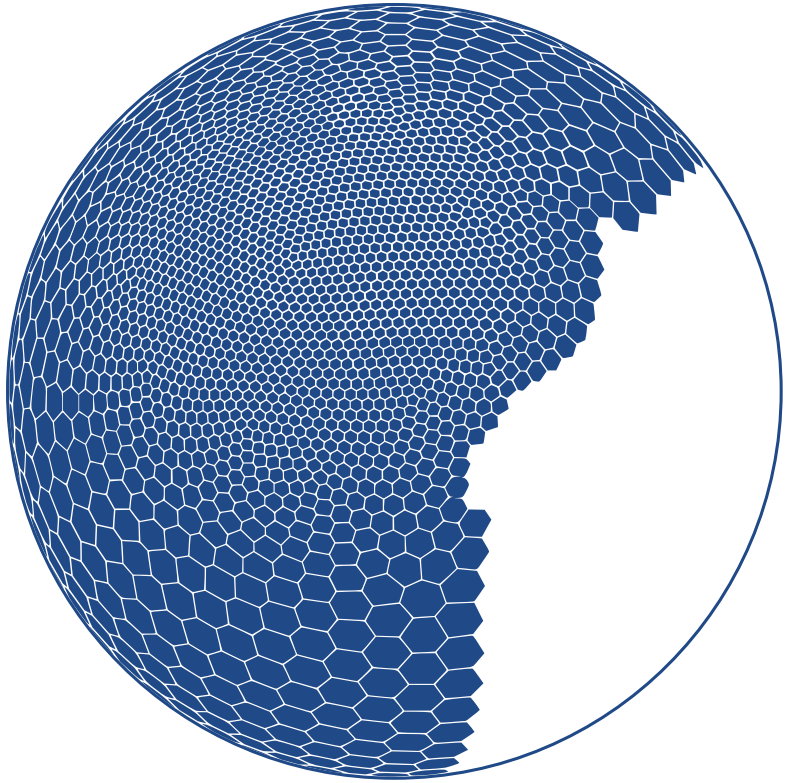
Ocean Modeling with MPAS-Ocean: Why Unstructured Meshes?

- Variable resolutions with any given density function.
- Straightforward mapping to flat 2D with effectively no distortions.
- Quasi-uniform (locally homogeneous) coverage of spherical surfaces.
- Smooth resolution transition regions.
- Preserve symmetry/isotropic nature of a spherical surface.
- Naturally allows unstructured discontinuities.



Background & Motivations

- Unstructured meshes in parallel environment.
- Challenging to achieve uniform partitioning unlike structured grids.
- Load balance depends on partitioning quality and element distributions.
- Data exchange between processes through deep *halo regions*.
- Threading motivated by increasing on-node core counts, with limited available memory per core.



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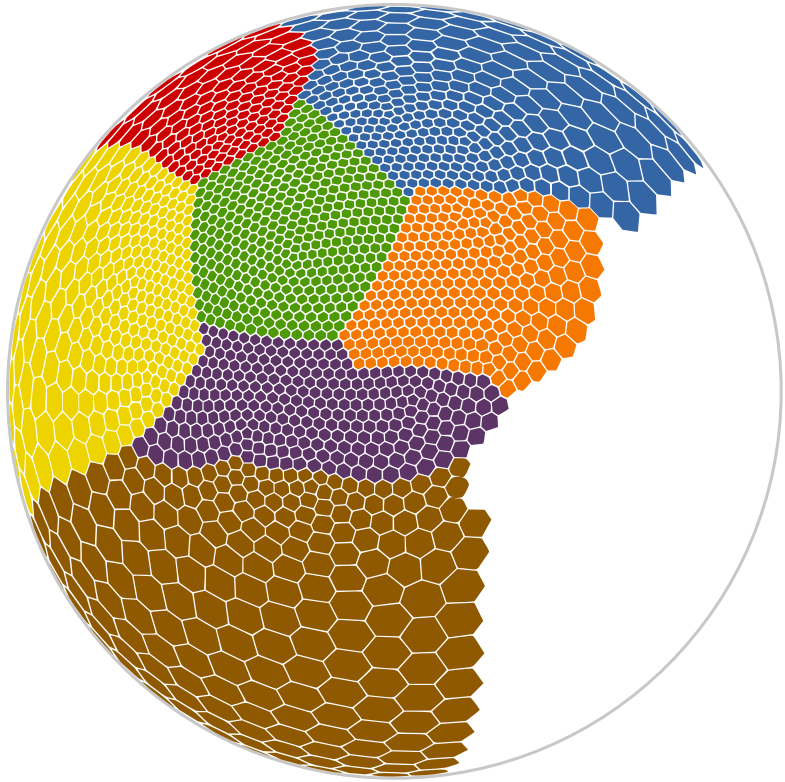

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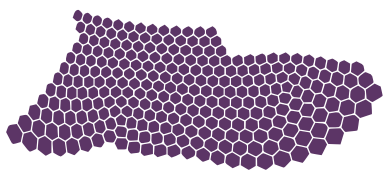

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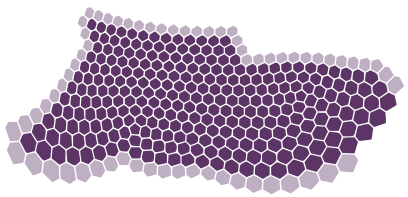

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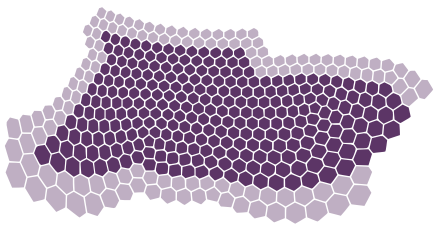

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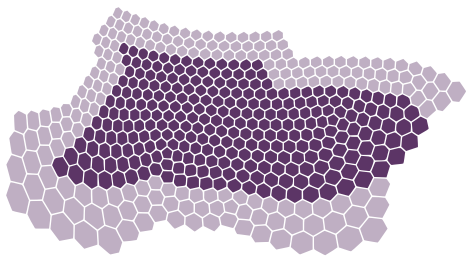

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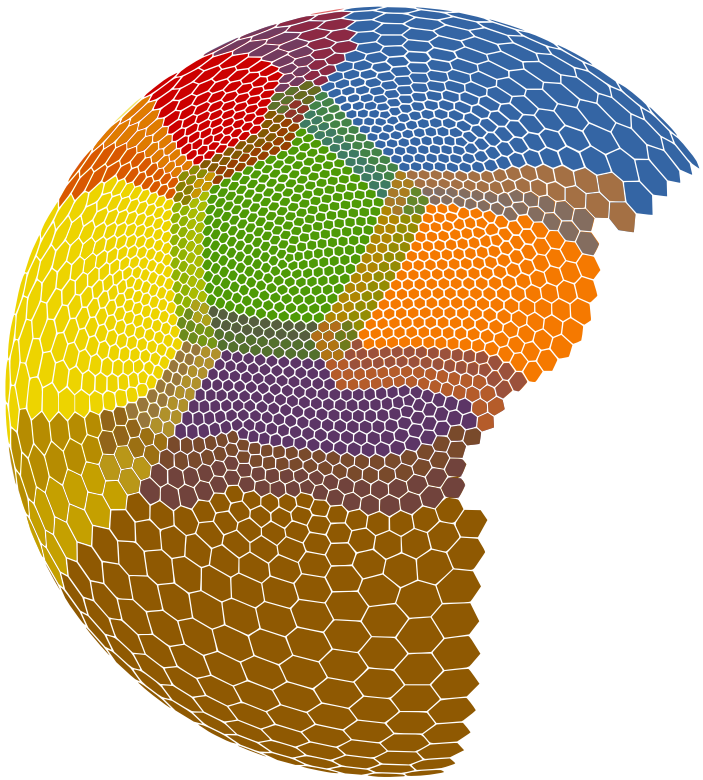

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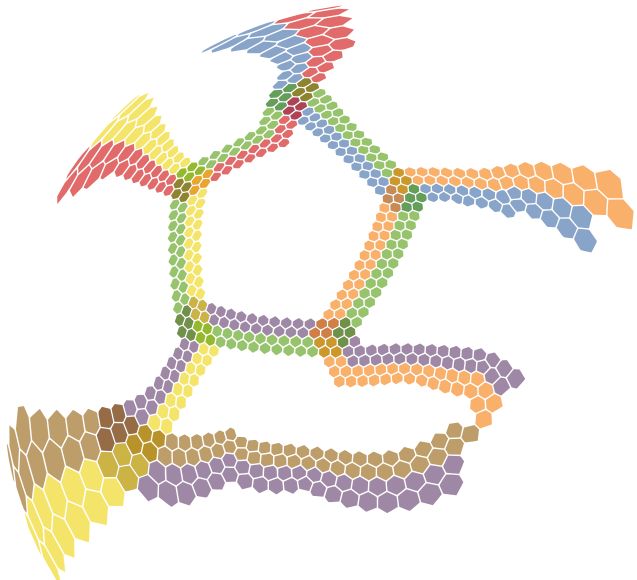

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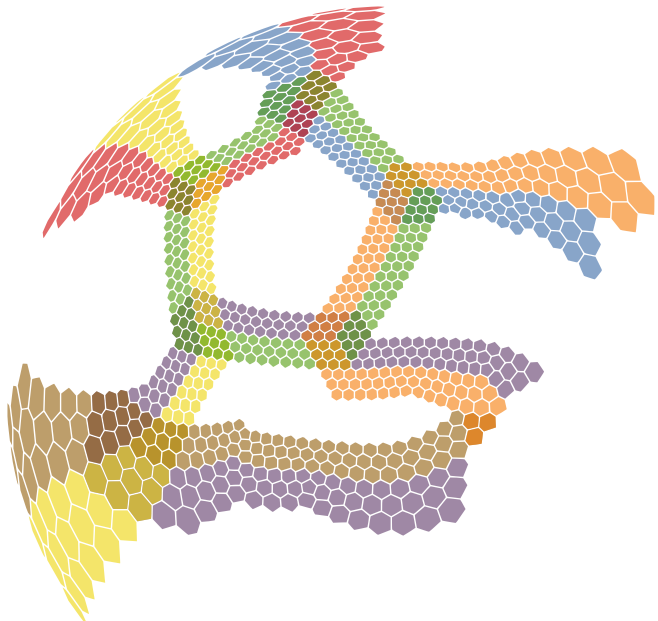
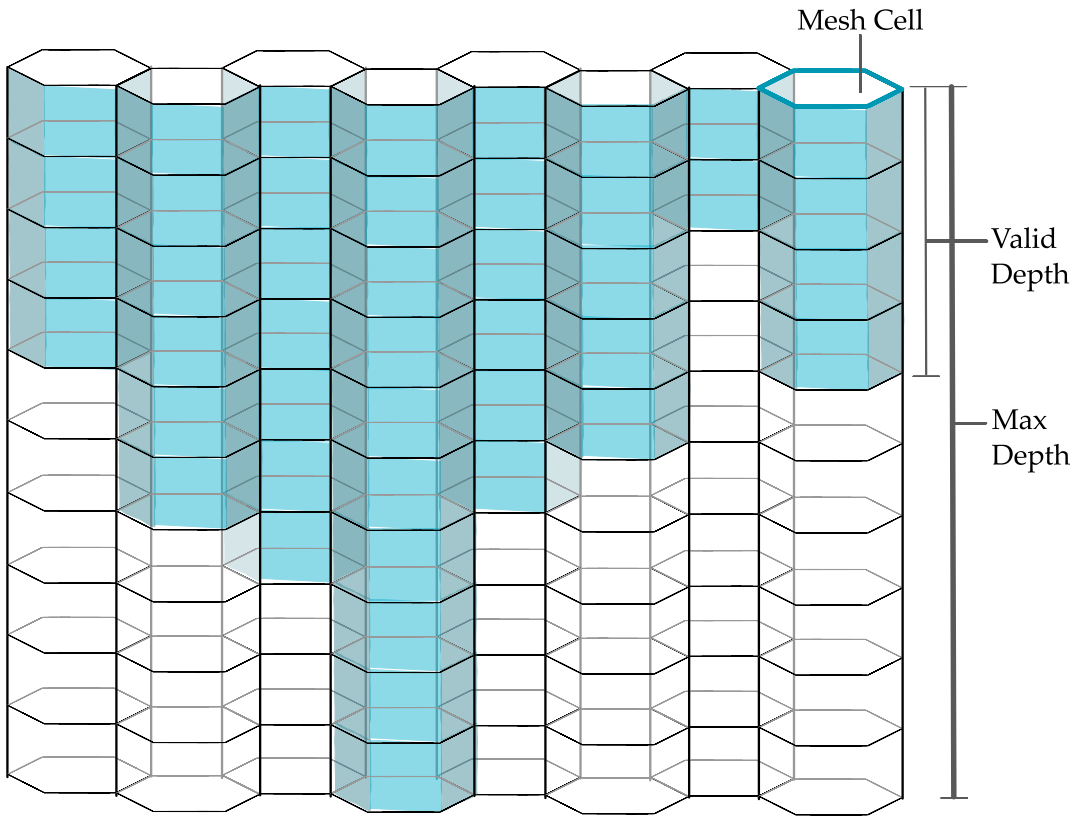


Background & Motivations

- Structured vertical dimension for ocean depth.
- Variable depth but constant sized buffers with maximum depth!



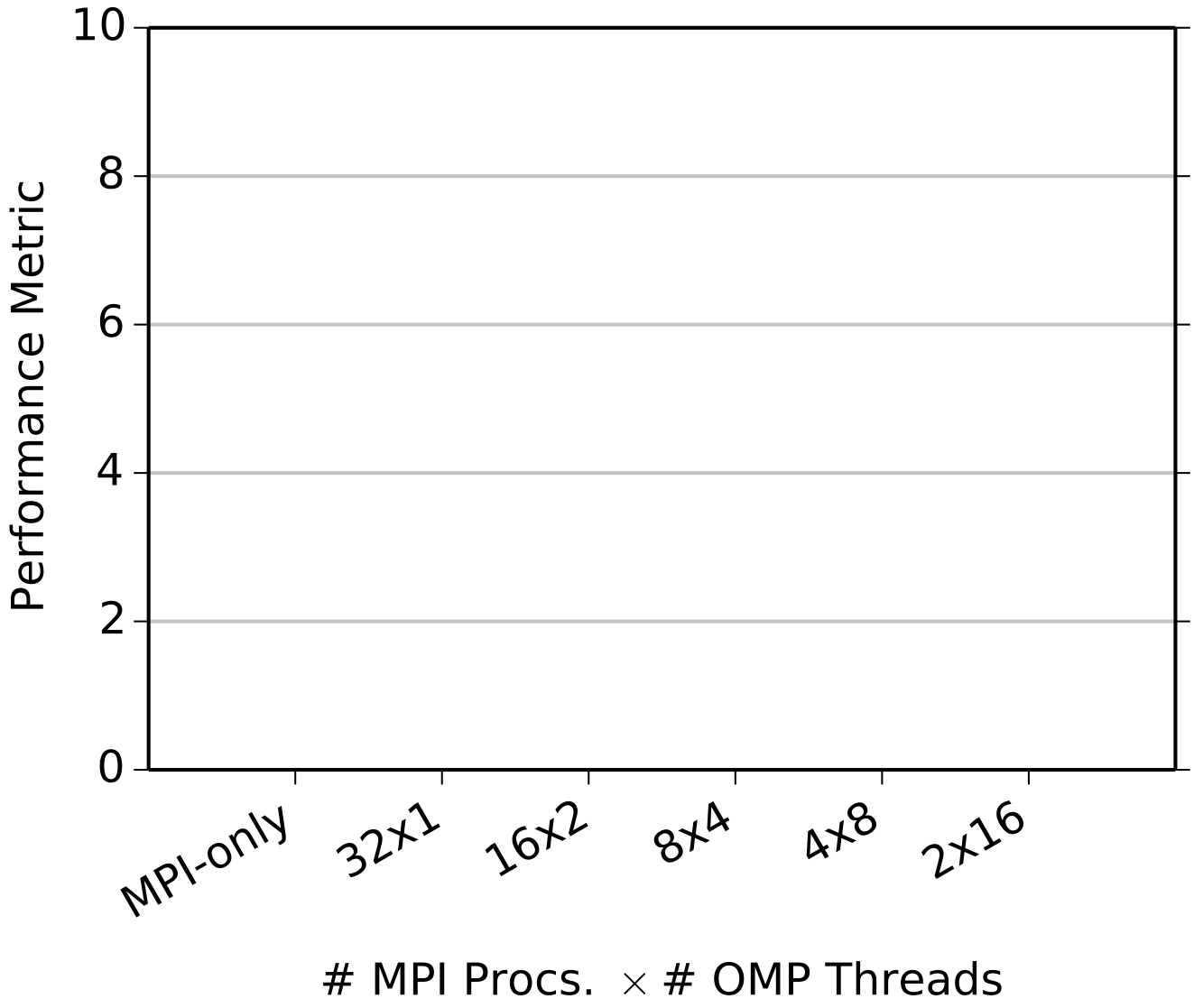
Developing a Hybrid MPI + OpenMP Implementation

Computational Environment

- Cray XC40: Cori Phase 1
  - 1,630 dual-socket compute nodes with Cray Aries interconnect
  - 16 core Intel Haswell processors
  - 32 cores per node
  - 128 GB DRAM per node

- Meshes:
  1. 60 kms uniform resolution:
     114,539 cells, maximum vertical depth of 40.
  2. 60 kms to 30 kms variable resolution:
     234,095 cells, maximum vertical depth of 60.

Performance Plots and Keys



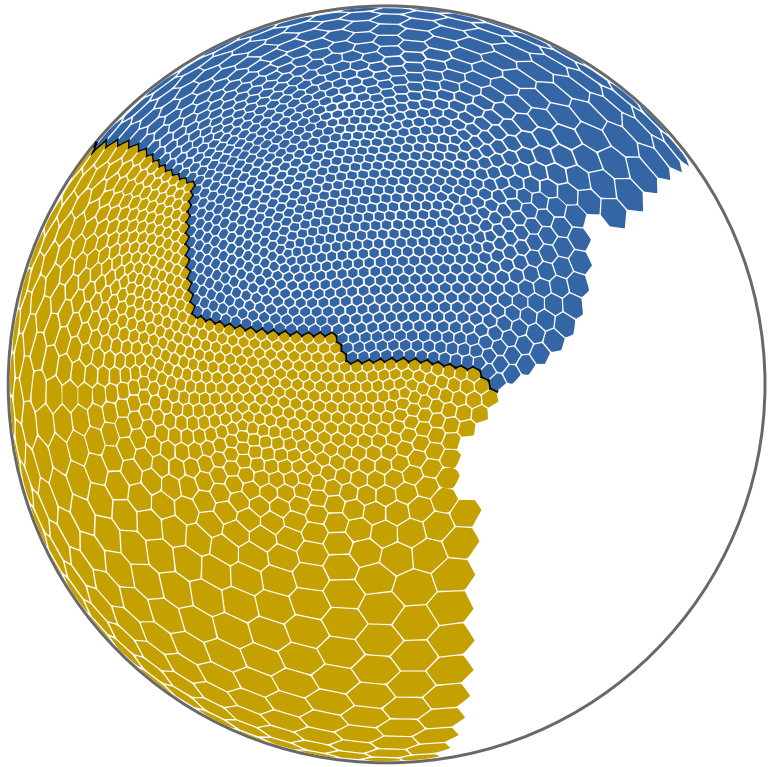
Performance Plots and Keys

Configurations = MPI procs. per node $\times$ OMP threads per MPI

Configuration	Decreasing	Increasing
1. 32×1	• Number of MPI processes per node	• Number of threads per process
2. 16×2	• Total halo region volume	• Amount of data sharing
3. 8×4	• Communication (number and volume)	• Threading overhead
4. 4×8	• *Extra* computations	• Inter-thread load imbalance
5. 2×16	• Memory requirements	
6. 1×32	• Inter-process load imbalance	

Threading Granularity: Block-Level

- Minimal implementation disruption to the code
- Simple intra-node halo-exchanges across threads without need for explicit communication
- Possibly insufficient parallelism
- Intra-block halo regions consume memory and require additional computations



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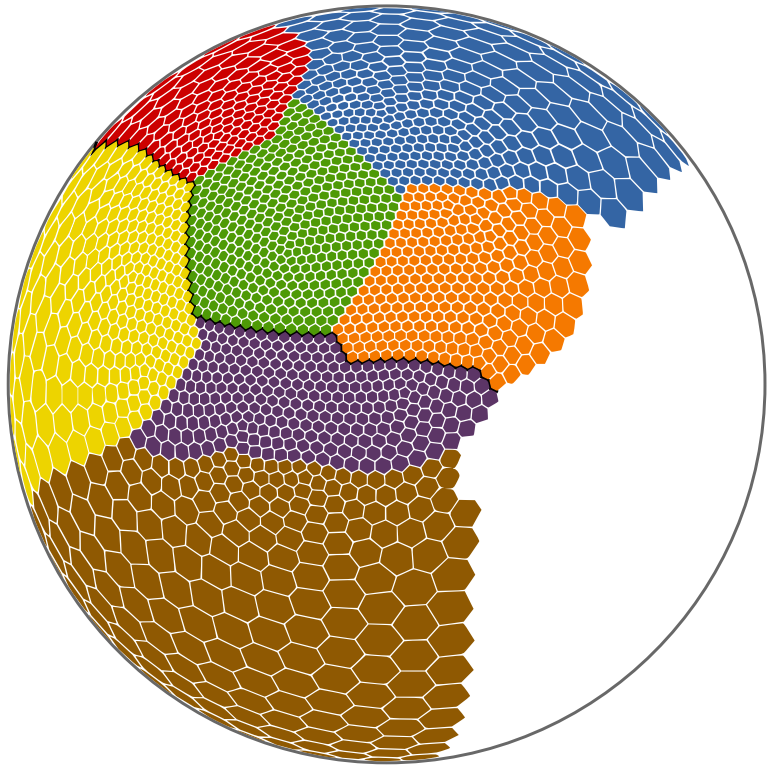

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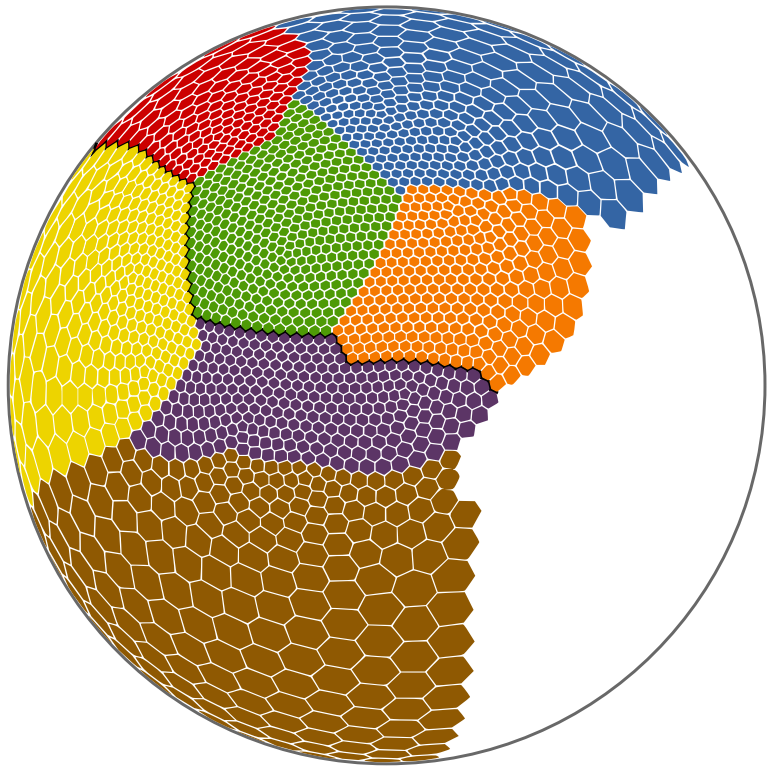
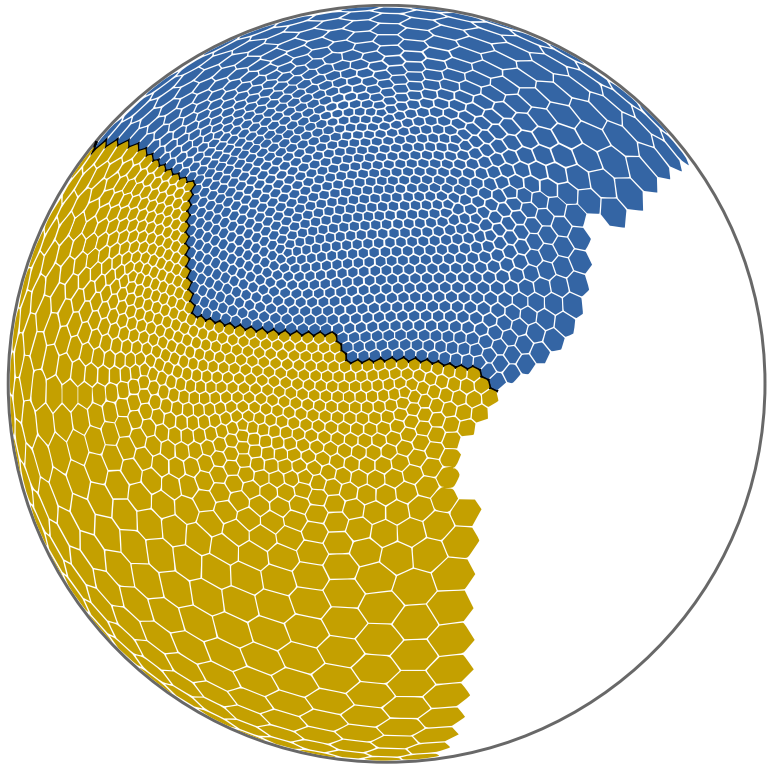


Threading Granularity: Element-Level

- Significant implementation disruption to the code
- Eliminates intra-process halo-exchanges and halo regions
- Computation and communication efficient



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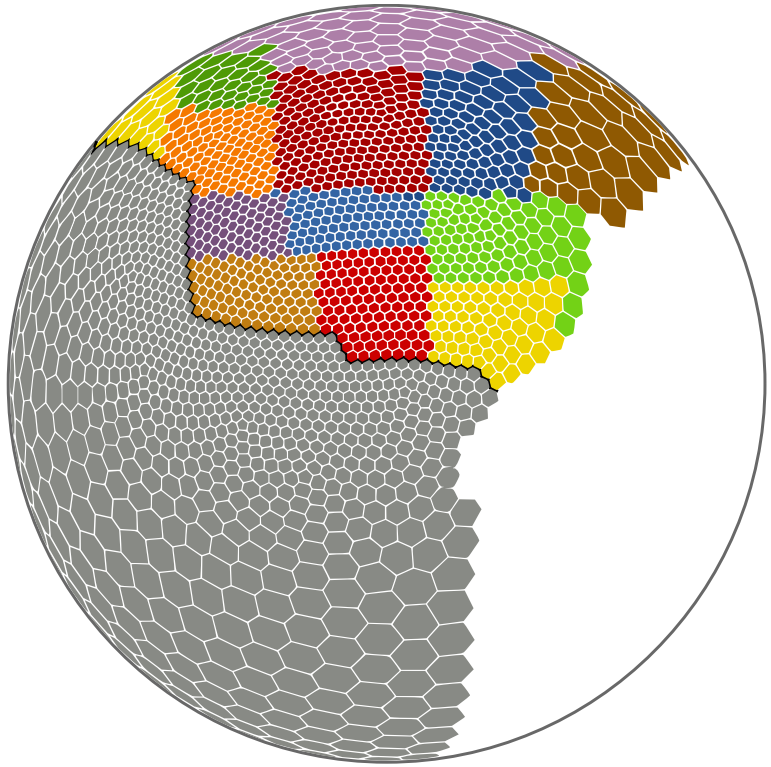

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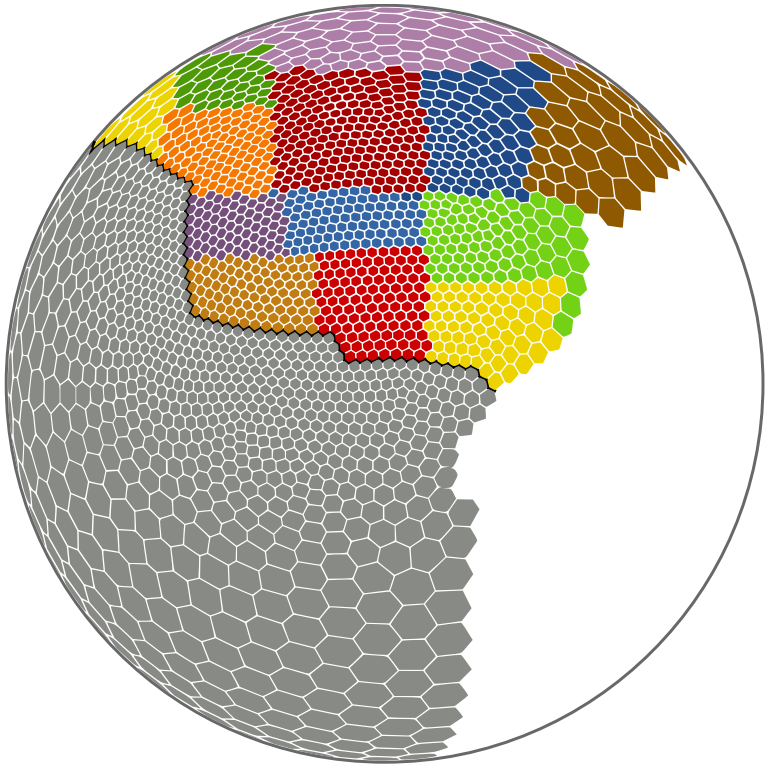

Element Distributions across Threads

Goal: What is the best approach to distribute mesh elements among threads?

1. Runtime distribution with explicit OpenMP loop directives.
2. Precomputed distributions.
   - Naive/Static.
   - Depth-Aware.

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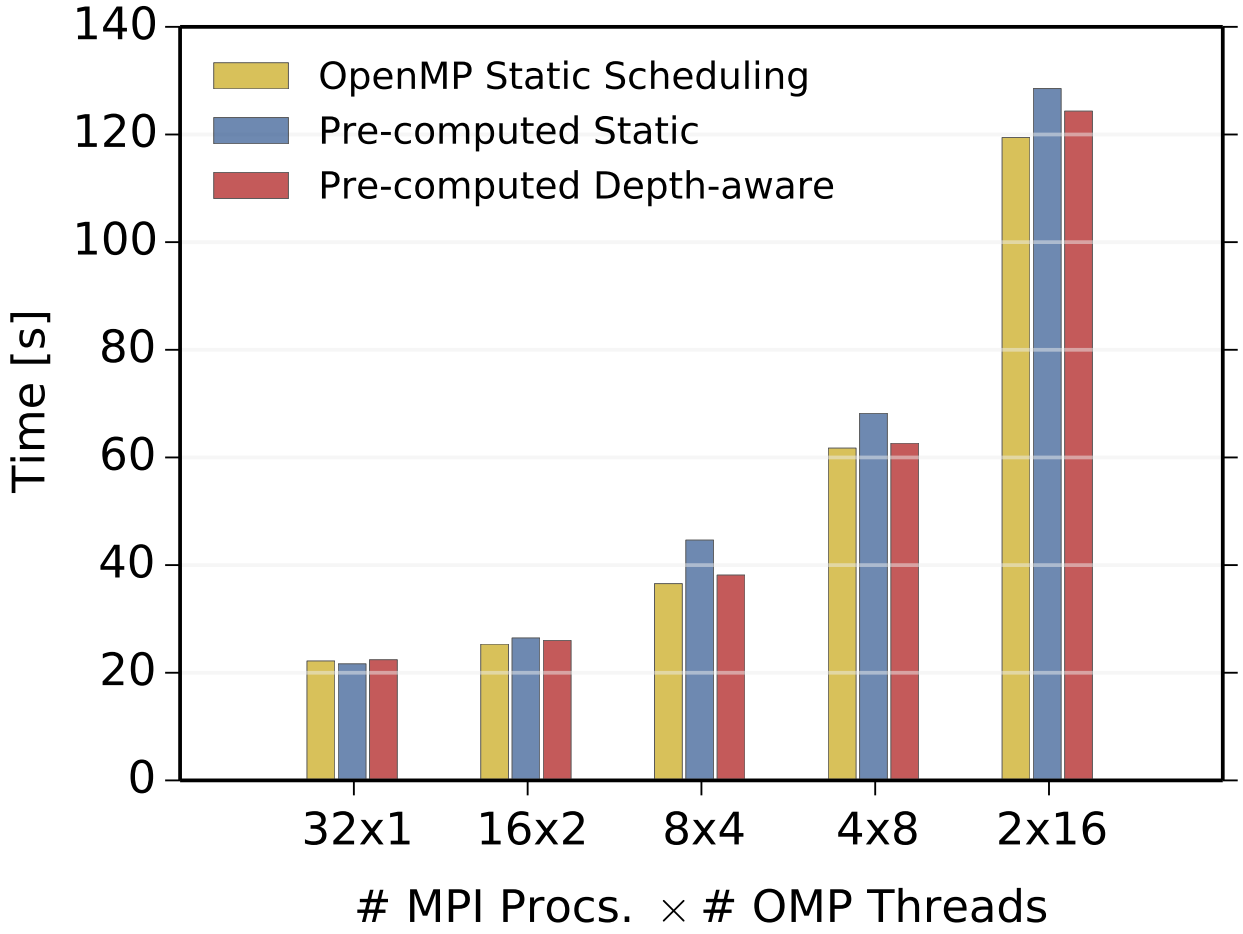

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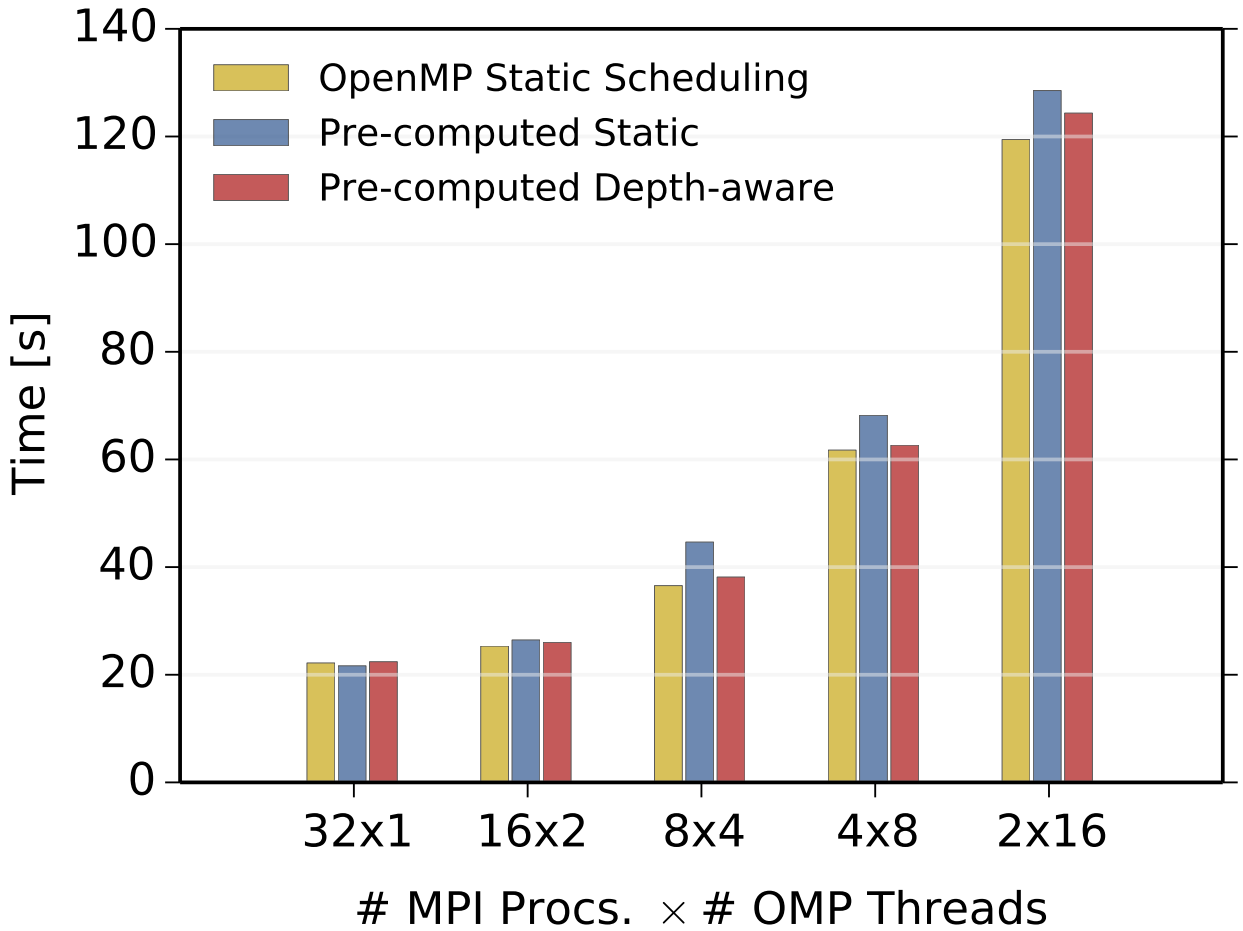

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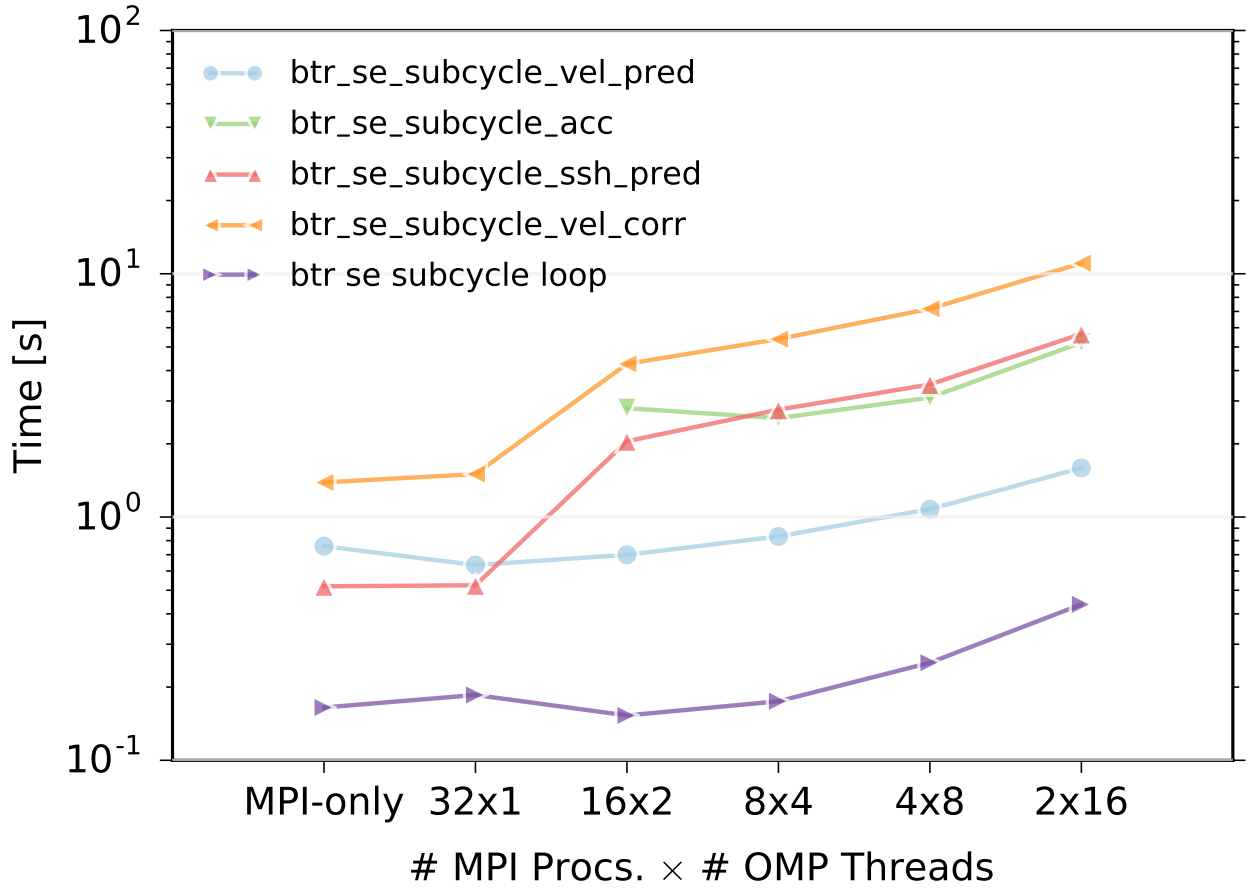
Thread Scaling Bottlenecks

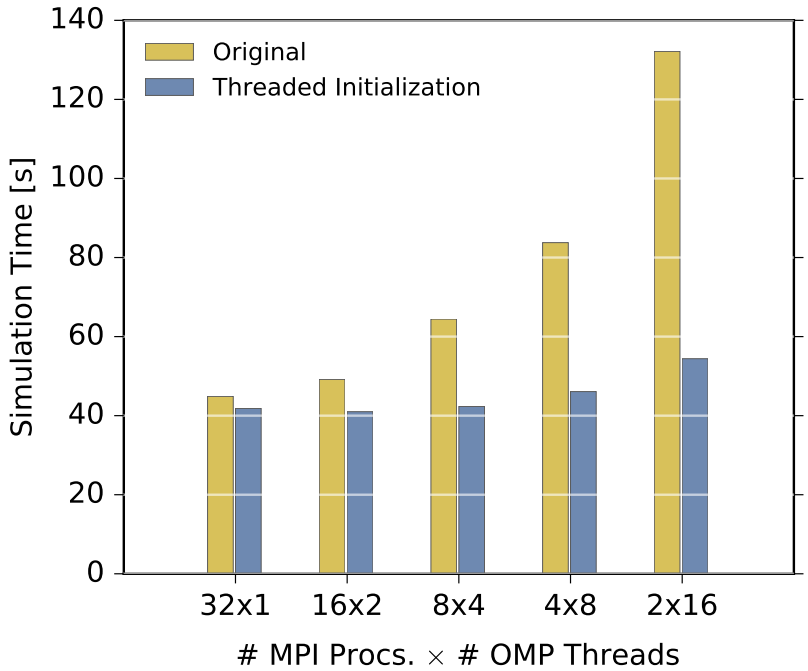


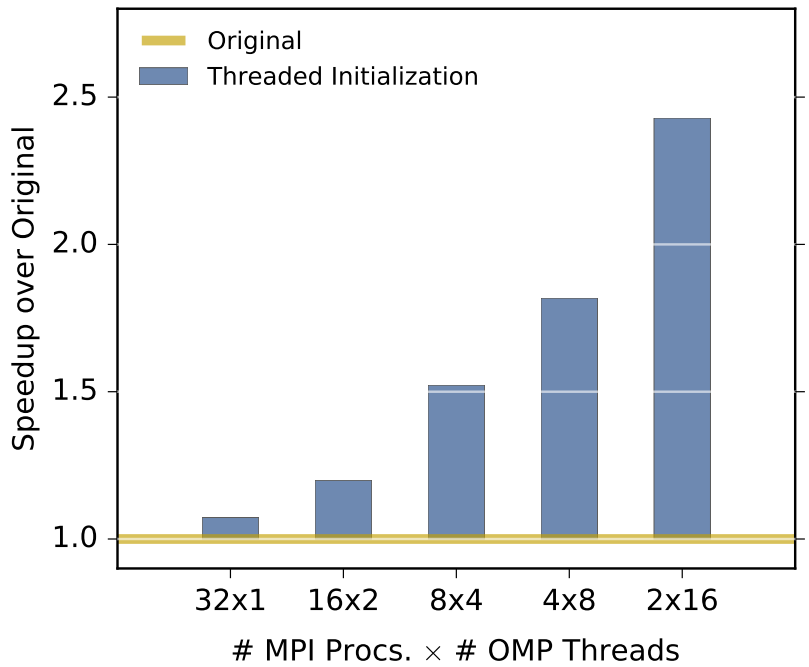
Memory Allocation and Initialization

Goal: Can the Amdahl bottlenecks be minimized?

1. Baseline code: Single thread for memory allocation and initialization.
2. Optimized code: All available threads for initialization.
3. Plus, reordered allocation and initialization events.

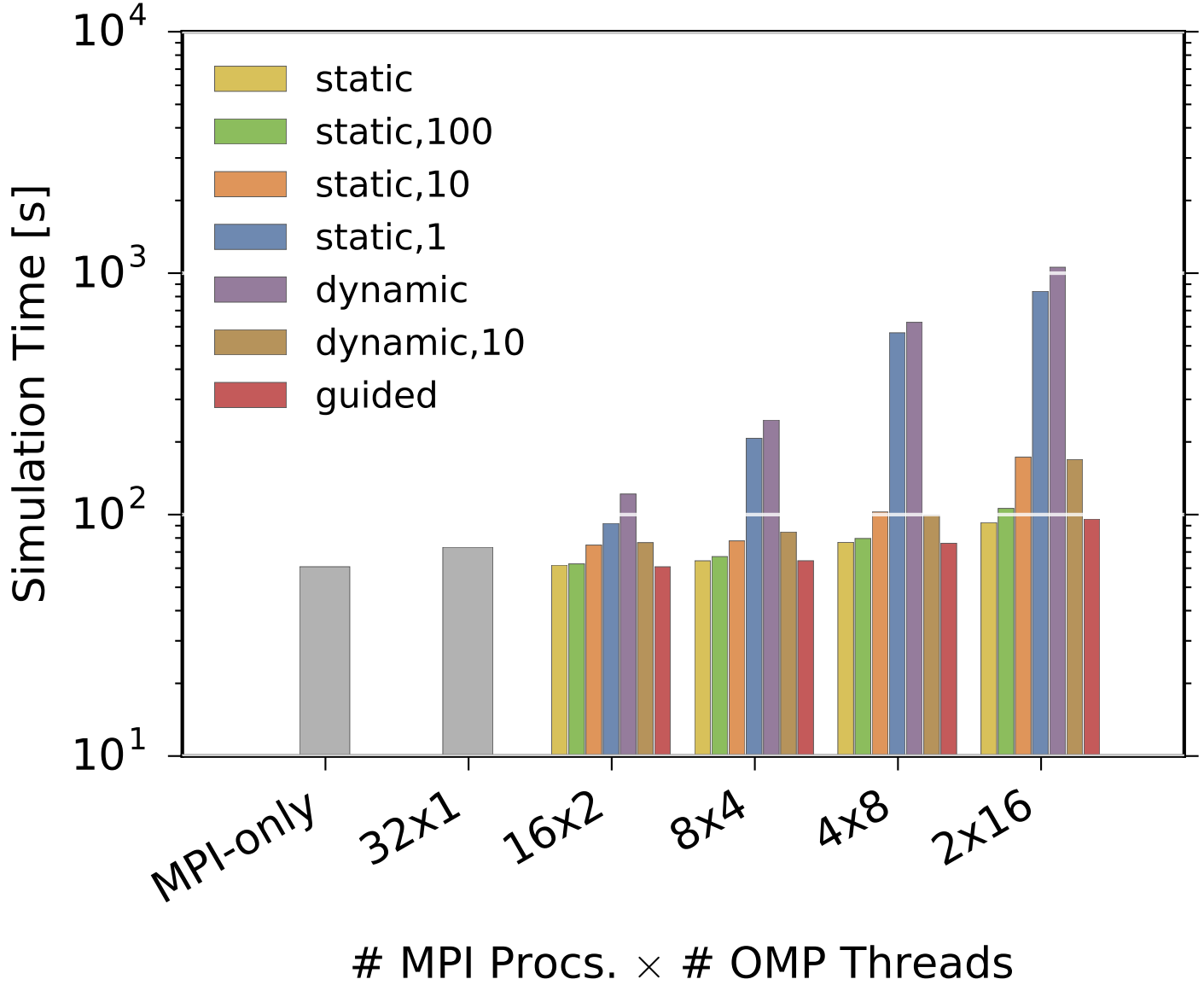
Memory Allocation and Initialization





Result: *Multi-threaded memory management.*

OpenMP Scheduling Policies



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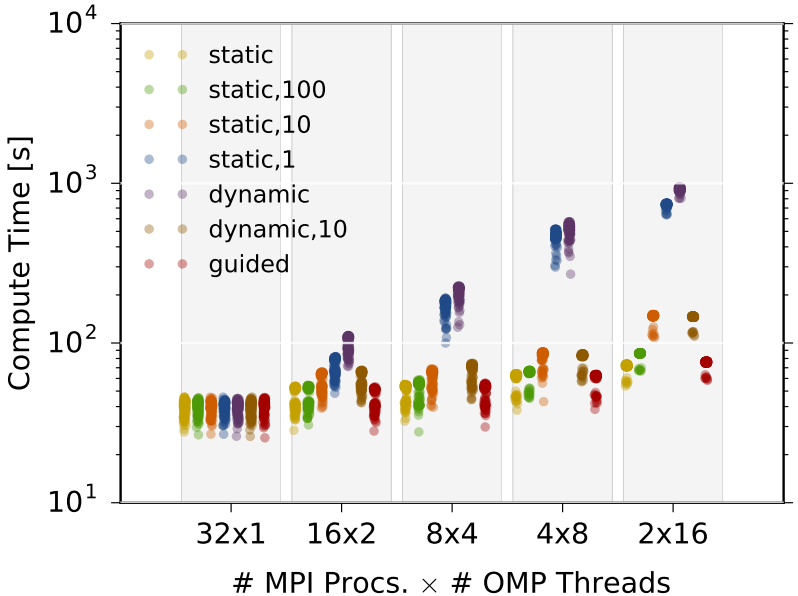

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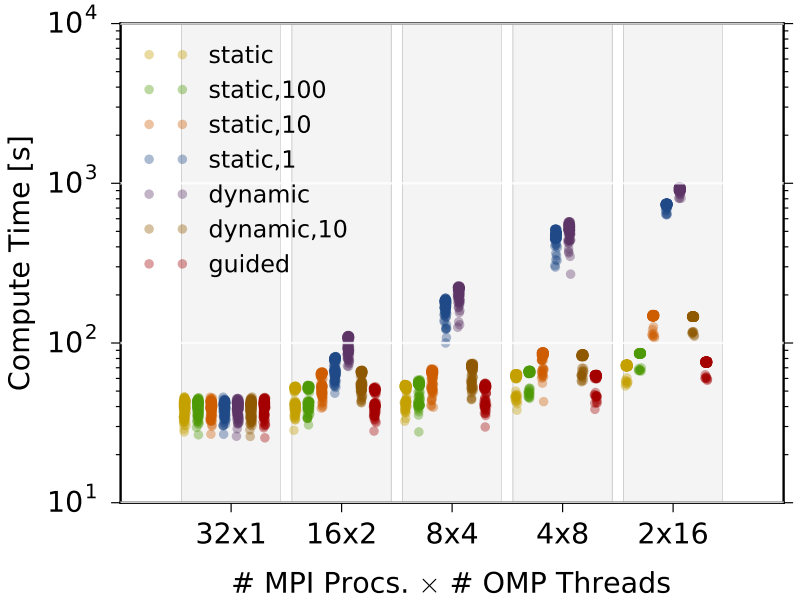

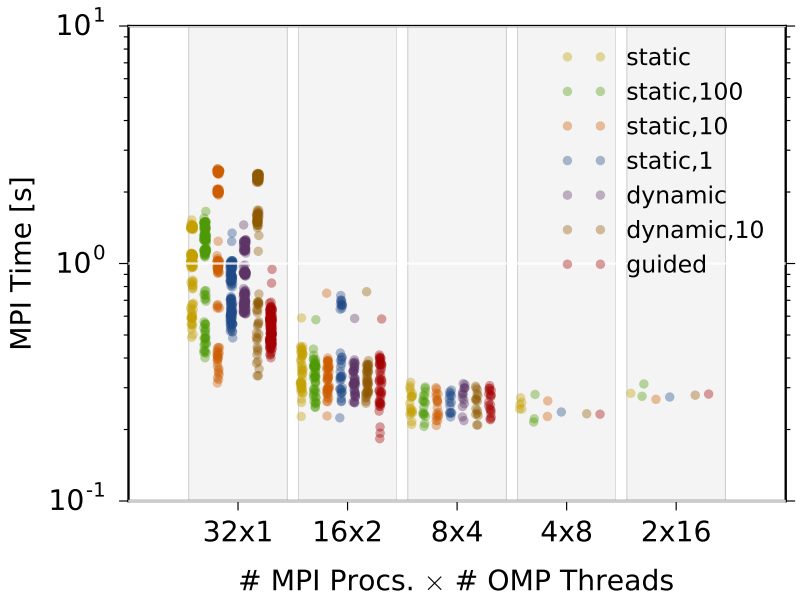

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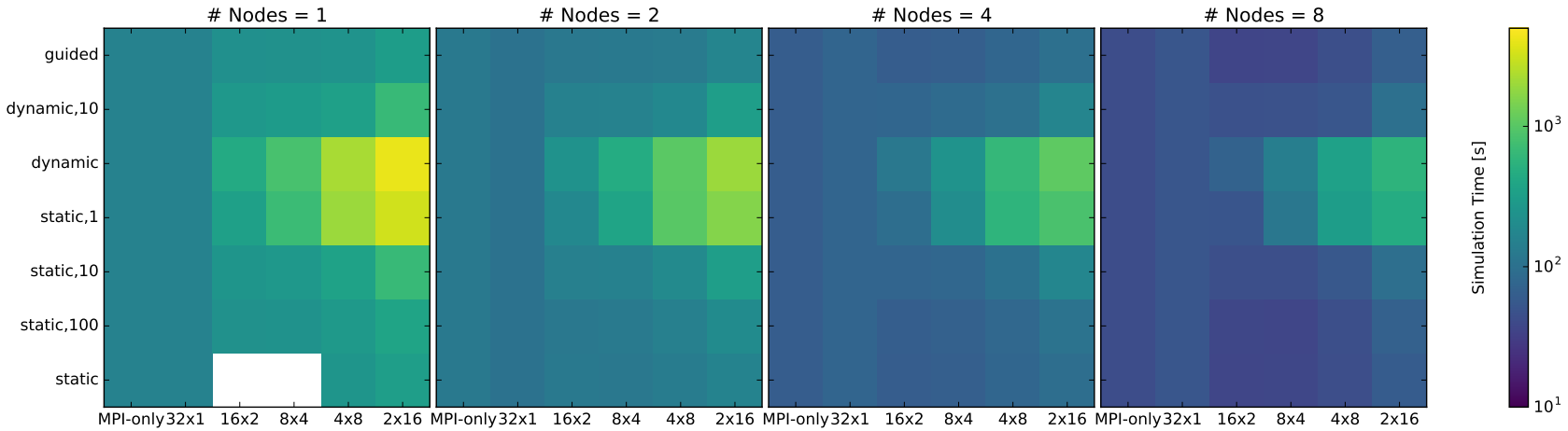

Result: *Select static or guided scheduling.*

Avoid small chunk sizes.

Balance number of MPI processes and threads: 16×2 *or* 8×4.

Vectorization?

Goal: Can we take advantage of the vector units?

1. None
   `-no-vec, -no-simd`
2. Compiler auto
   `-vec, -simd`
3. OpenMP SIMD only
   `-no-vec, -simd`
4. Full
   `-vec, -simd`
5. Full with aligned memory
   `-align, -vec, -simd`

Result: *Highly memory-bound, making vectorization unnecessary.*

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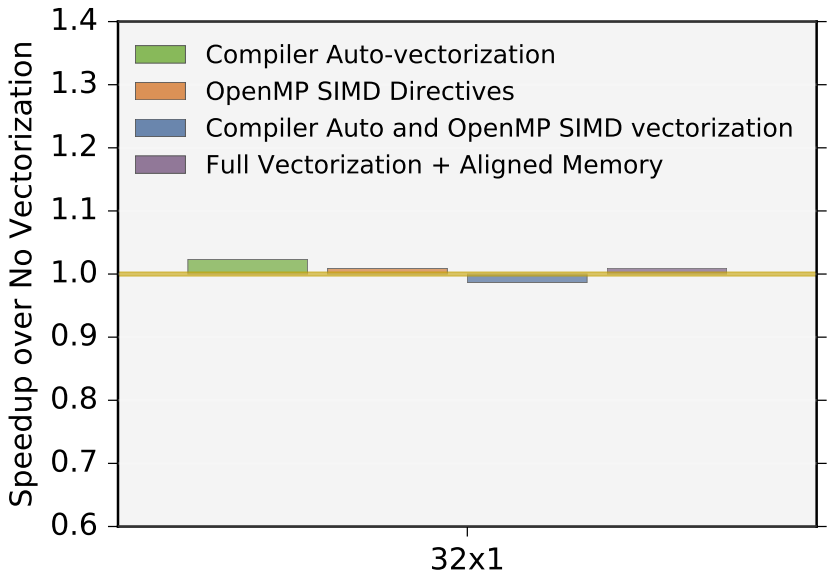

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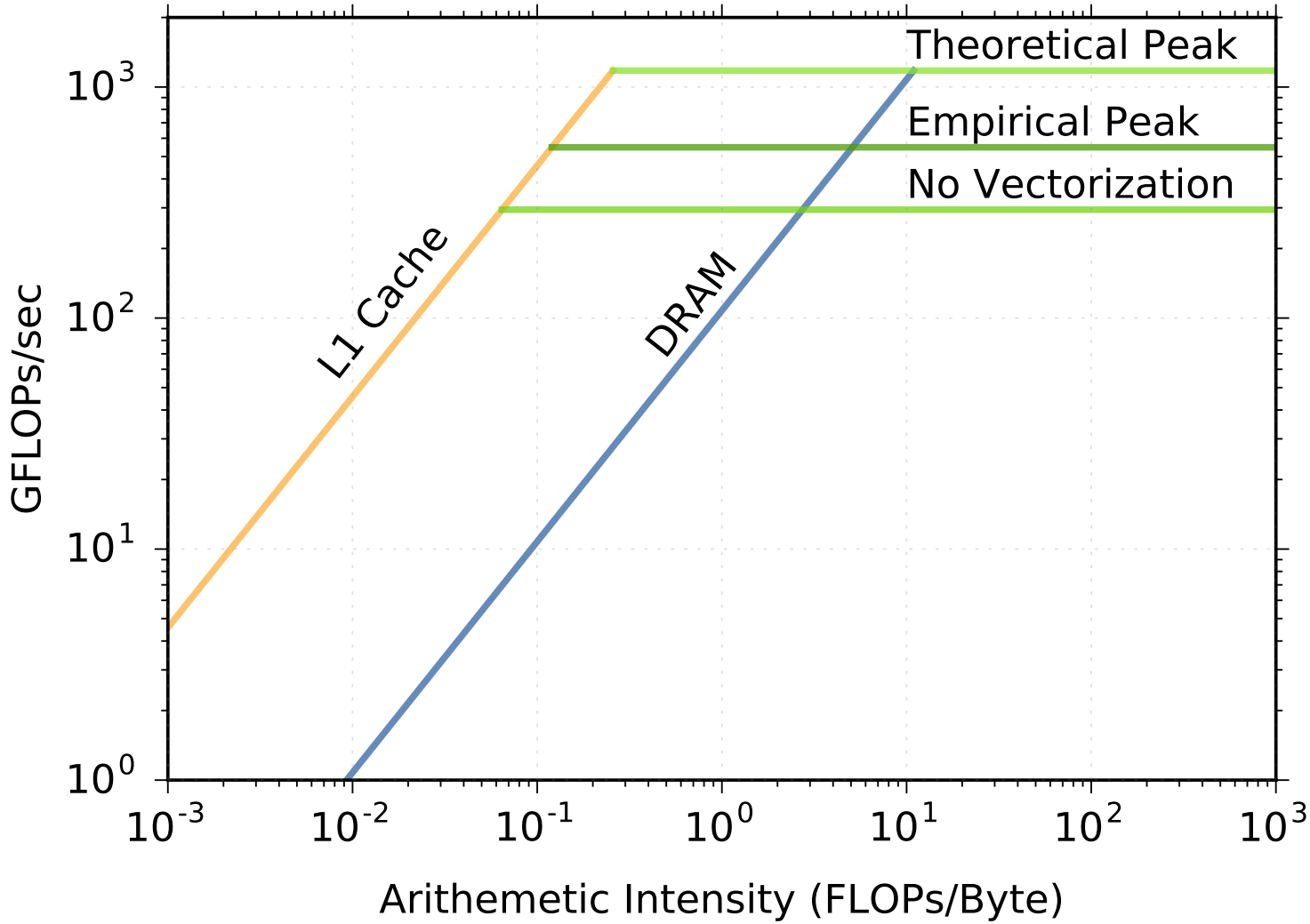

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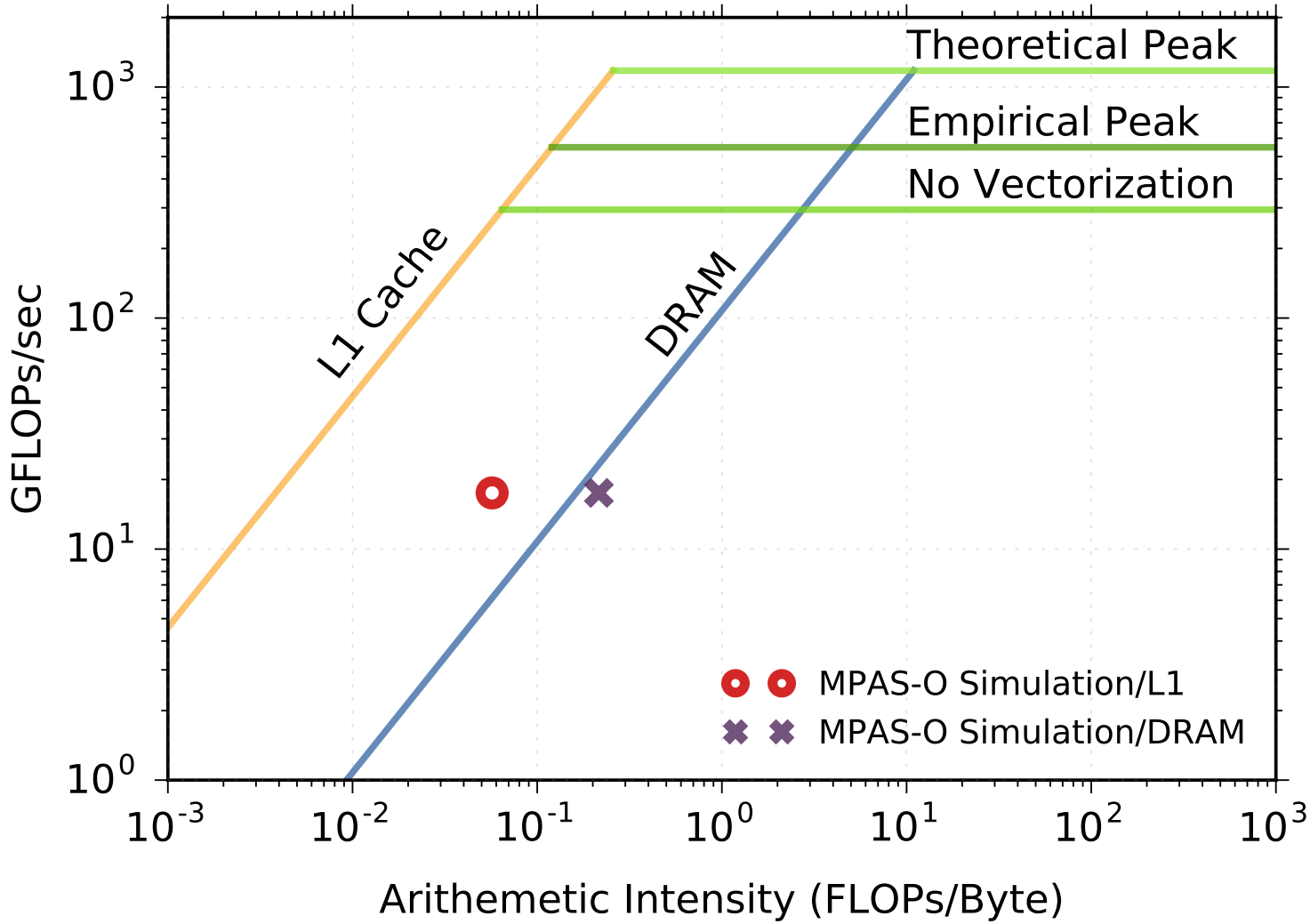
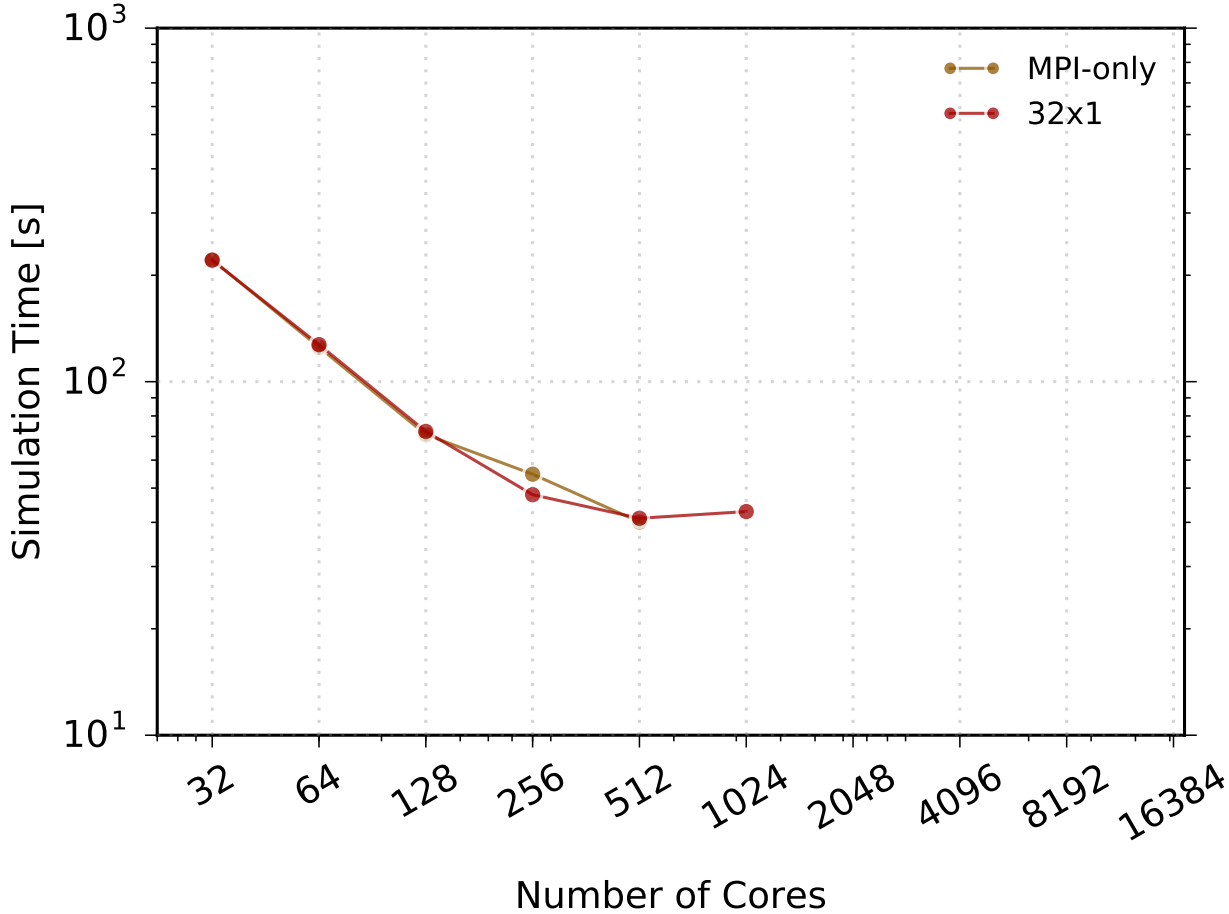


Strong Scaling: Performance

Goal: What is the optimal concurrency?



Result: $3\times$ *speedup for best hybrid* ($n = 64, 8 \times 4$) *w.r.t. best MPI-only* ($n = 16$) *runs.*
$2\times$ *speedup for best hybrid* (8×4) *w.r.t. best MPI-only runs at* $n = 16$.

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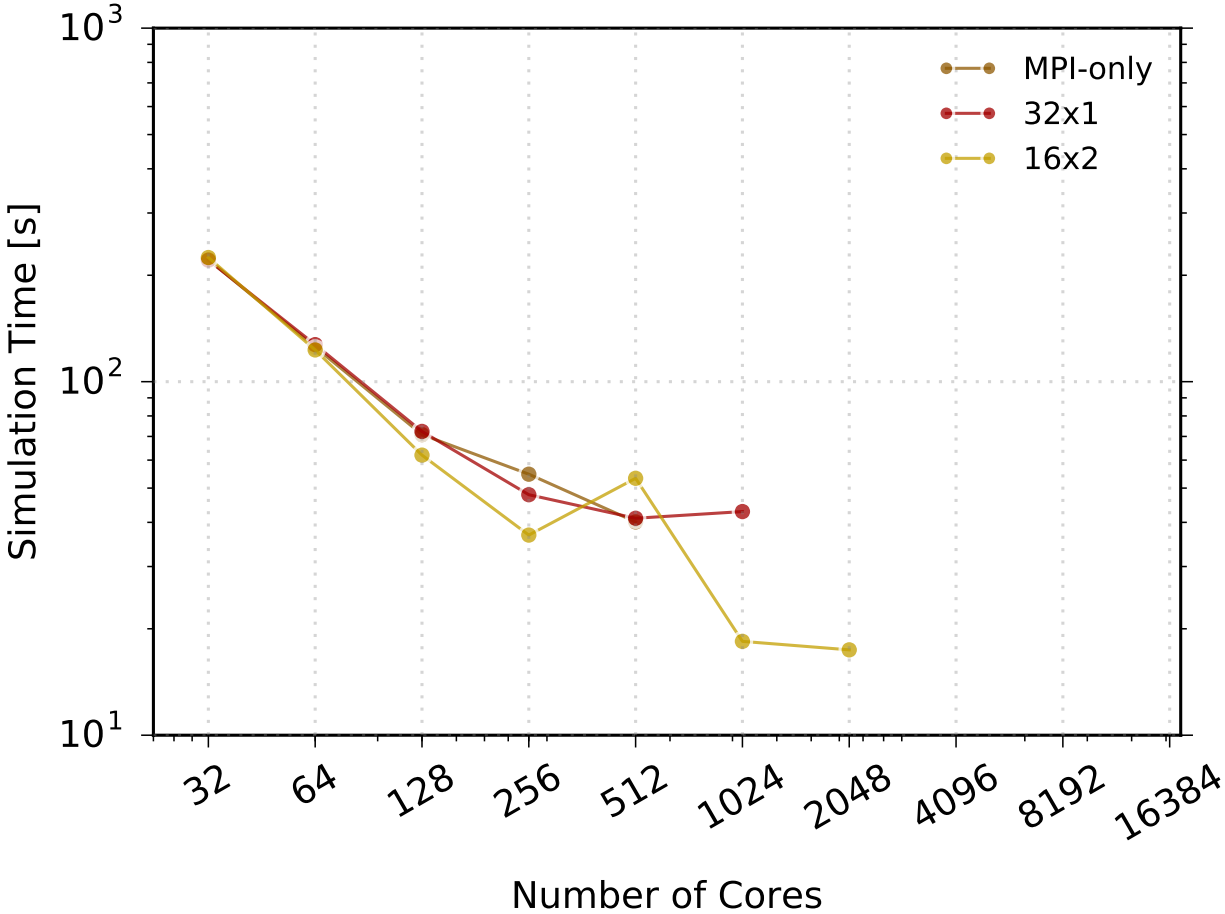

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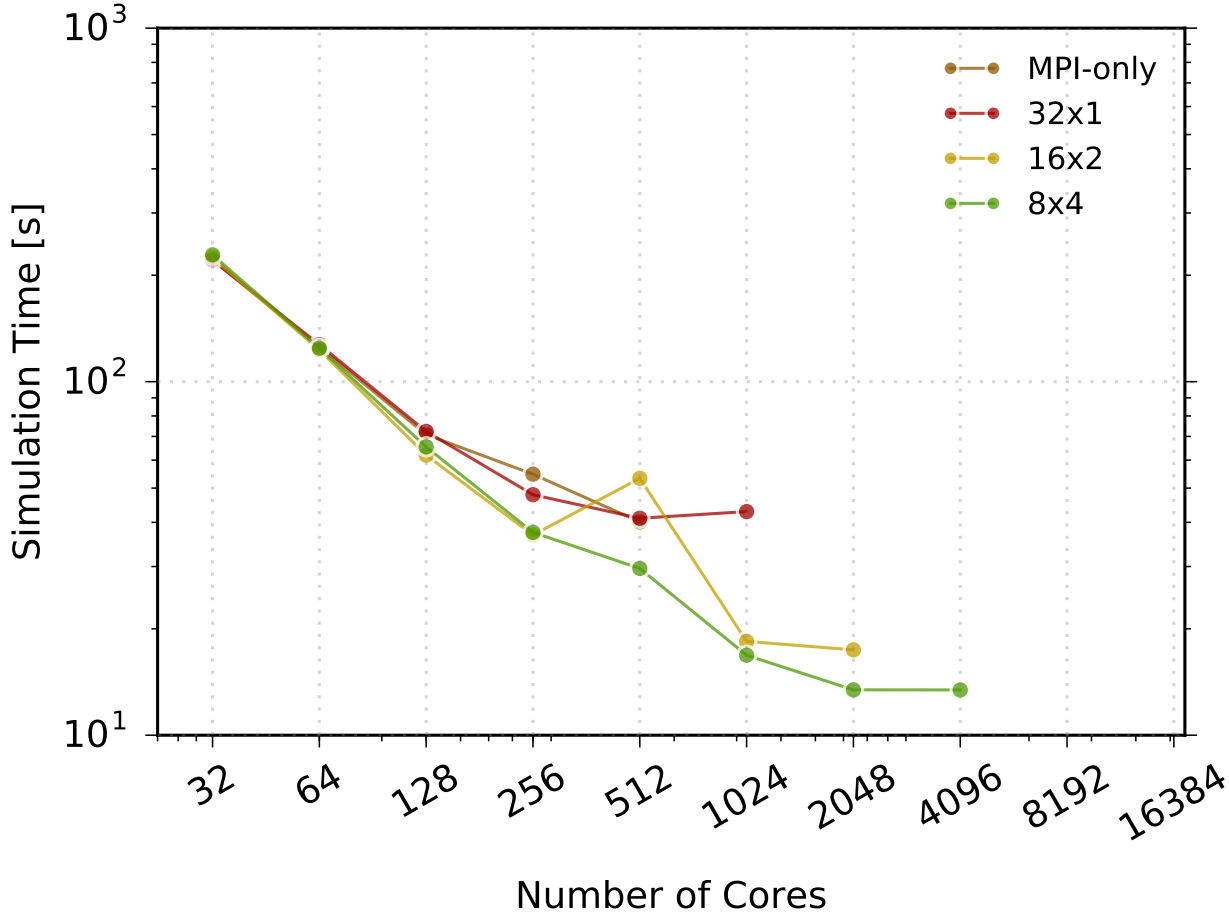

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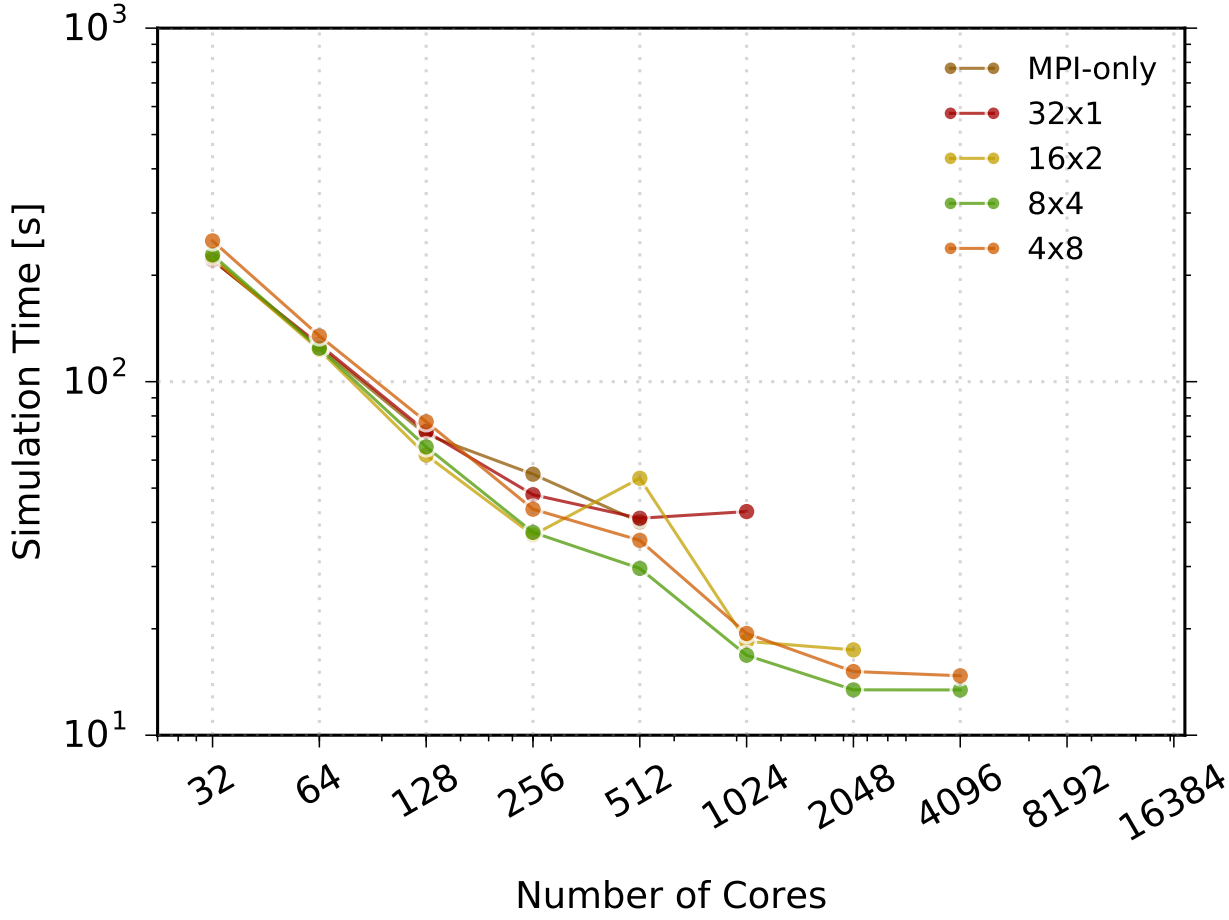

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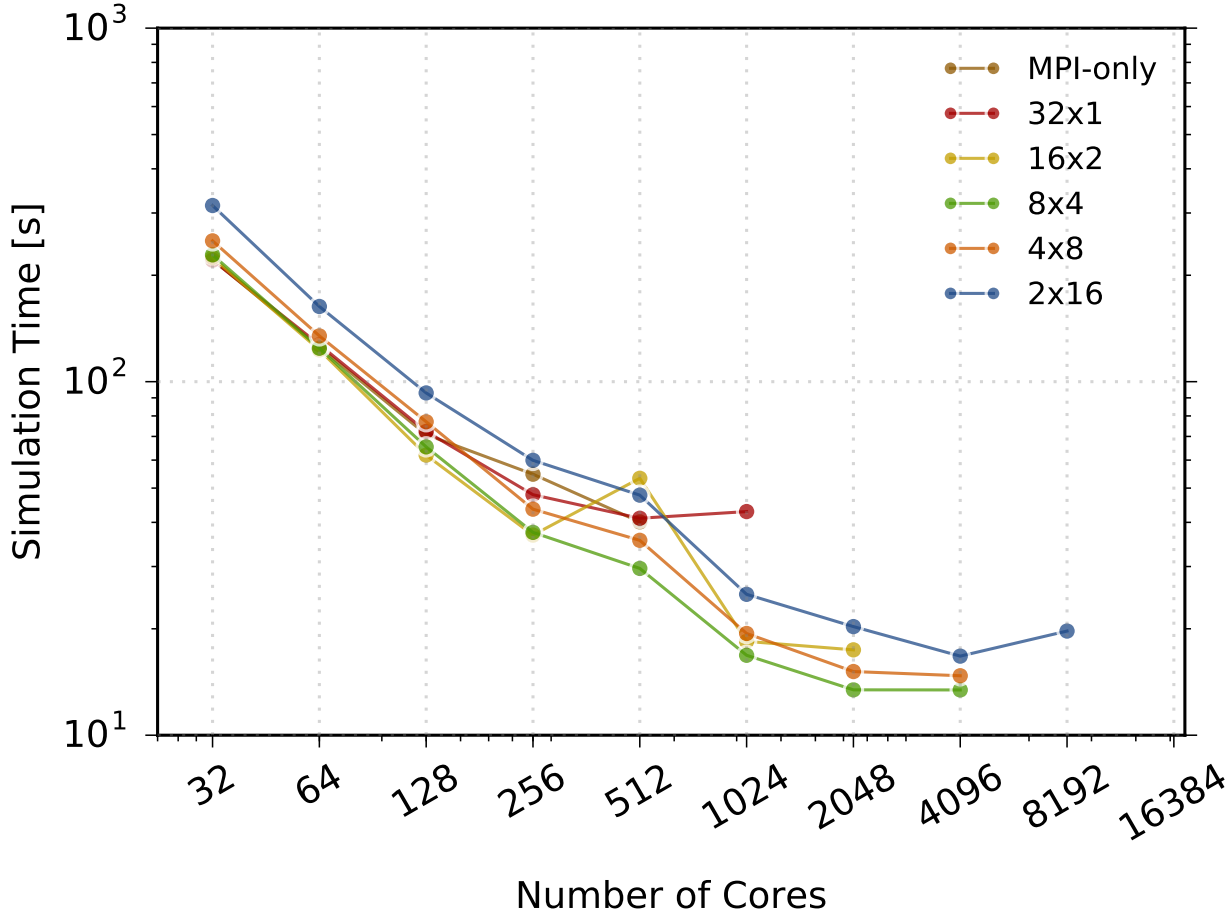

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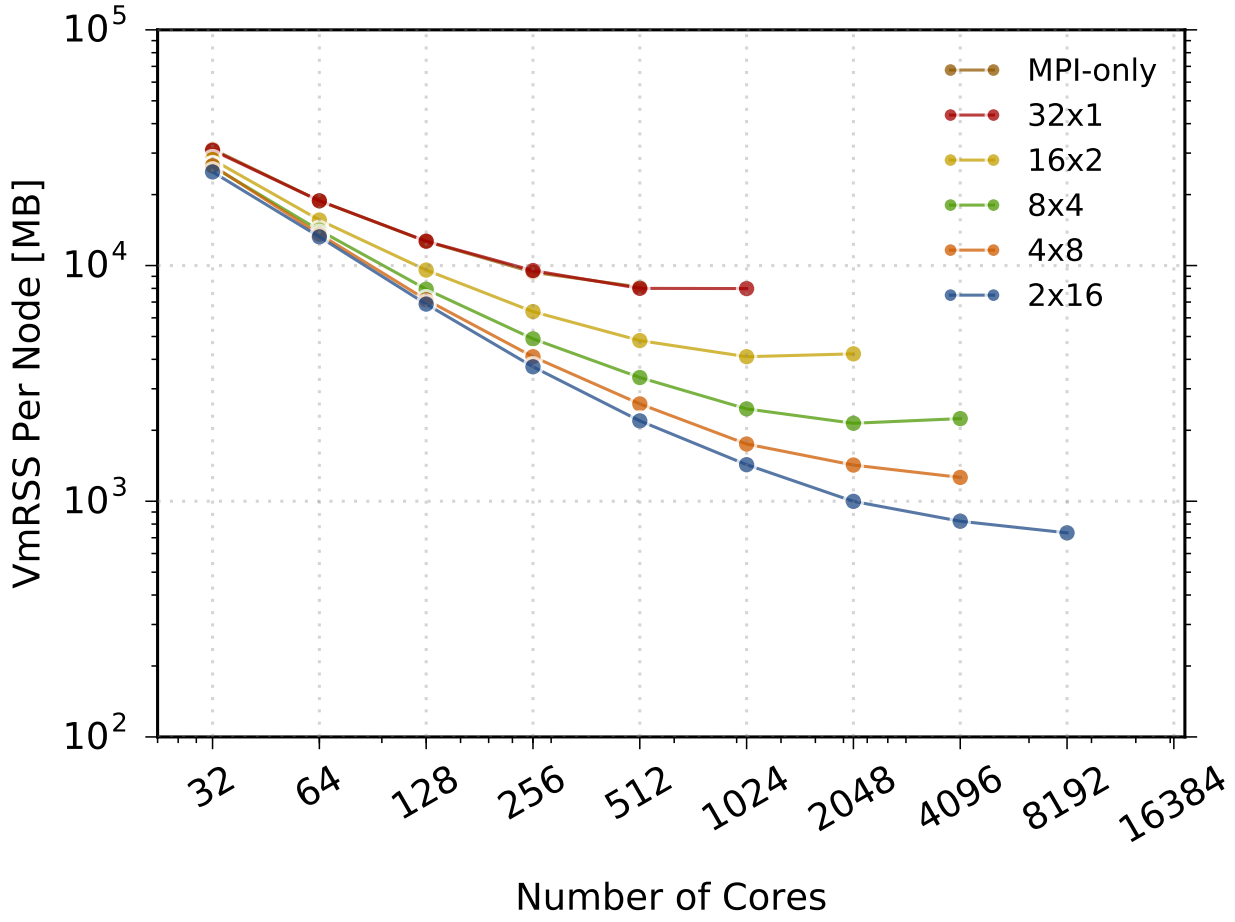
Strong Scaling: Memory Footprint



Minimum memory footprint per process ≈ 250 MB

The working set can possibly completely fit in the HBM on KNL.

End Notes

- Threaded buffer initialization necessary. Observed up to 2.5× speedup on a single node.
- Thread scheduling with larger chunk sizes, such as default static and guided policies, perform best with MPAS-Ocean. Single element chunk size degrades performance by up to an order of magnitude.
- Well balanced number of MPI processes and OpenMP threads (e.g. 8×4) showed best performance.
- Highly irregular memory accesses make depth-awareness redundant.
- Also, being memory bound, vectorization has no benefit.
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Thank you!