Parallel Performance Optimizations on Unstructured Mesh-Based Simulations

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Introduction

- *Structured* and *unstructured* meshes in real-world simulations.
- Parallel applications – Not straightforward to partition unstructured meshes.
- Load balance directly related to mesh partitioning quality.
- Data exchange between processes through partition *ghost* or *halo* regions.
- Two key parallelization challenges:
  - Load imbalance across processes – mesh partitioning.
  - Unstructured data access patterns – data organization.

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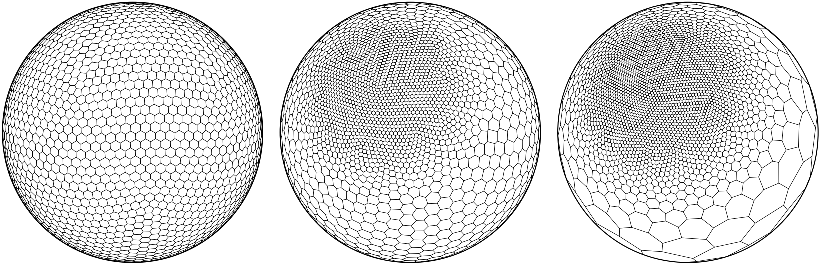
  - Unstructured data access patterns – data organization.

Ocean Modeling with MPAS-Ocean

- MPAS = **M**odel for **P**rediction **A**cross **S**cales. [Los Alamos]
- A multiscale method.
- Voronoi tessellation-based variable resolution mesh (SCVT).



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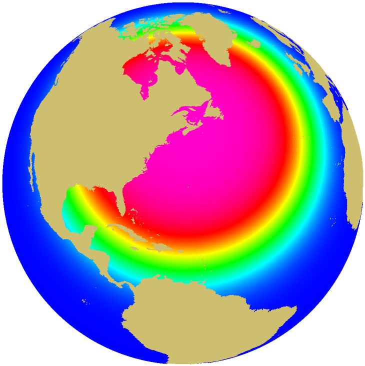

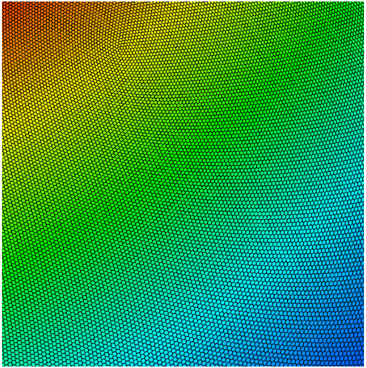

Ocean Modeling with MPAS-Ocean

- Major advantages of such unstructured mesh:
  - Offers variable resolutions. User defined density functions.
    - Focus on area of interest with high resolution.
    - Avoid unnecessary high-resolution computations in unwanted areas.
  - Smooth resolution transition regions.
  - Locally homogeneous/quasi-uniform coverage of spherical surfaces.
  - Preserve symmetry/isotropic nature of a spherical surface.
  - Naturally allows for discontinuities in the mesh.
  - Straightforward distortion-free mapping to 2D.
- A vertical quantization adds 3rd dimension, representing ocean depths.

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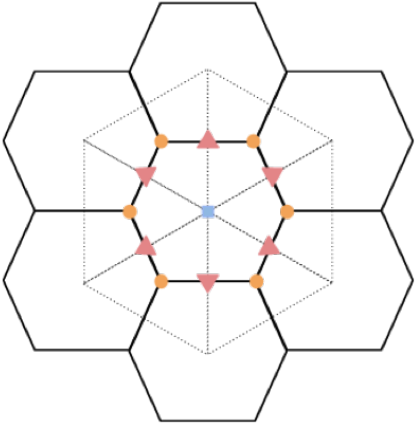
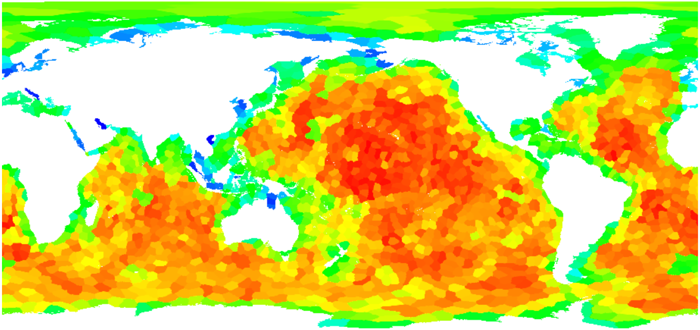


SCVT Cells and computed quantities.

Unstructured mesh partitioning ...

Mesh Partitioning and Load Imbalance

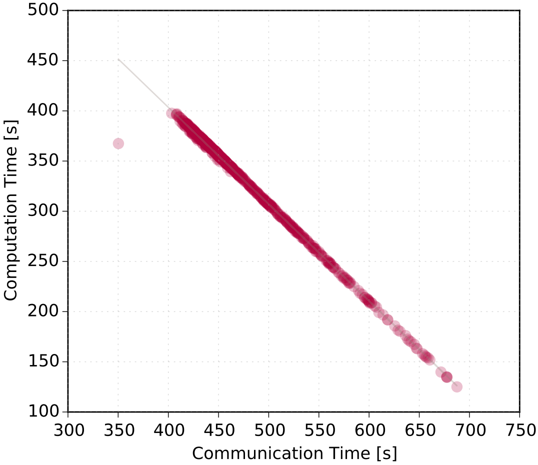
- Using a straight-forward graph partitioner, such as Metis.



Computational imbalance across partitions/processes

Mesh Partitioning and Load Imbalance

- High computation-communication imbalance across processes in a run with naive partitioning:



Mesh Partitioning and Load Imbalance

- Need for a better mesh partitioner.
- *Hypergraph* representations are known to model communication more accurately than graphs.
- Available partitioners generate a partitioning by,
  1. balancing the number of cells (or weights) across partitions, and
  2. minimizing the total number of edge cuts.
- Problem:
  - Cost due to halo cells is not considered.
  - Unstructured nature makes halo region costs highly variable across partitions.
  - *Deep* halo regions magnify the effects, making them an important factor for load balancing.

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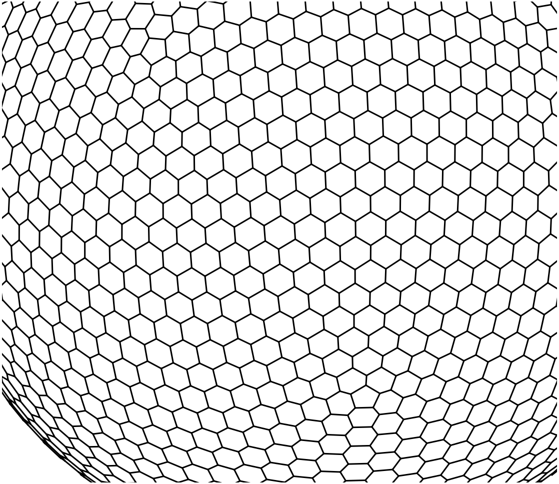
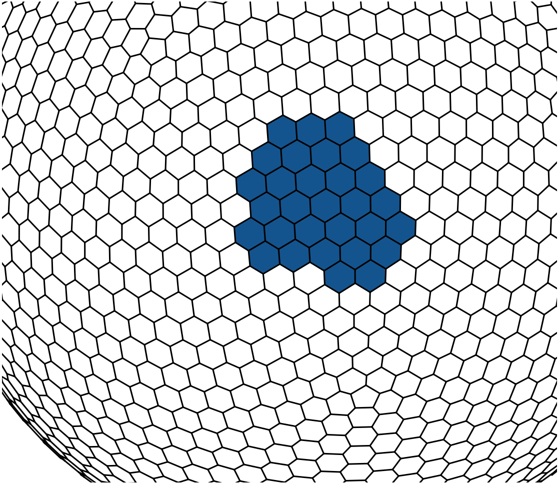
Mesh Partitioning and Load Imbalance

- Input mesh ...



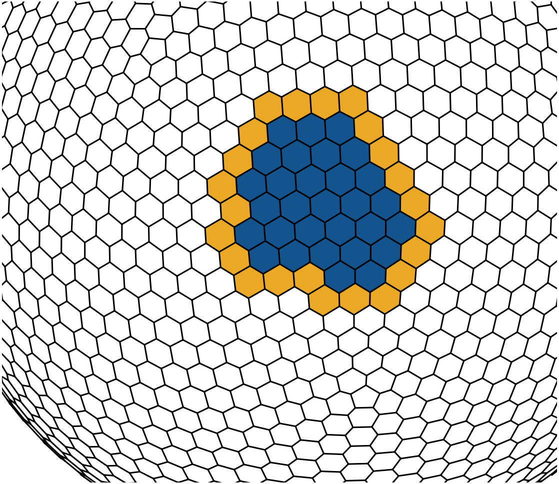
Mesh Partitioning and Load Imbalance

- A partition ...



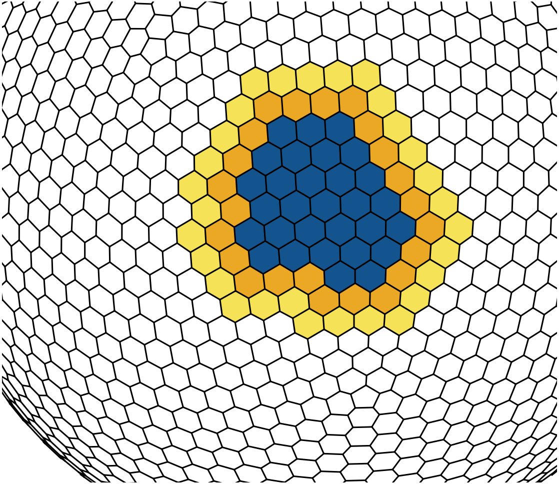
Mesh Partitioning and Load Imbalance

- 1-Halo region ...



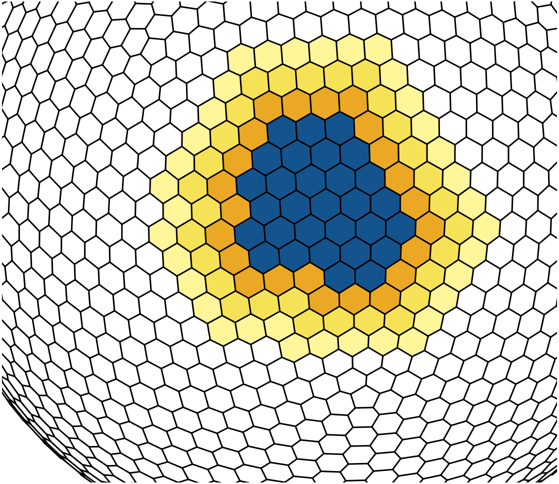
Mesh Partitioning and Load Imbalance

- 2-Halo region ...



Mesh Partitioning and Load Imbalance

- 3-Halo region ...



Partitioning-Based Cost Modeling

In a partitioning, for a partition k,

$$\text{computation cost, } C_\alpha = \frac{1}{F(p)}\left(\sum_{i}^{i\in N_k} w_i + a\sum_{i}^{i\in H_k} w_i\right)$$

$$\text{communication cost, } C_\beta = \frac{1}{F(p)}\frac{h_k}{b_k} + \left(\max_{i\in[1,p]}(c_i) - c_k\right)$$

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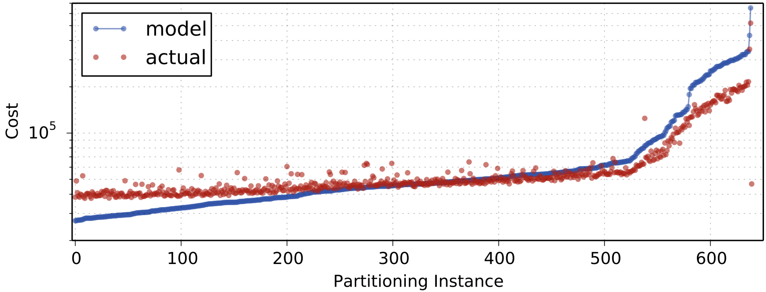

A Halo-Aware Partitioning Approach

```
procedure HaloAwarePartition(𝒢)
    Construct sparse matrix A representing 𝒢
    Compute A^2, ··· A^l, and A_{1...l} = Σ^l A^i
    Construct hypergraph ℋ_0 for A_{1...l}
    while not converged do
        Compute partitioning P_i of ℋ_i; construct halos for each partition in P_i
        Compute cost prediction for each partition k
        Assign weights to the cells, distributing halo cost equally among partition cells
        Compute total partition weights W_k
        Compute imbalance measure, f_i = (1 − min_k(W_k) / max_k(W_k))
        Accept P_i with probability m = min(1, e^((f_{i−1} − f_i)/2))
        if P_i is accepted then
            Update ℋ_i with the new cell weights to construct ℋ_(i+1)
        else
            Reject P_i by setting P_i = P_{i−1} and f_i = f_{i−1}
        end if
    end while
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end procedure
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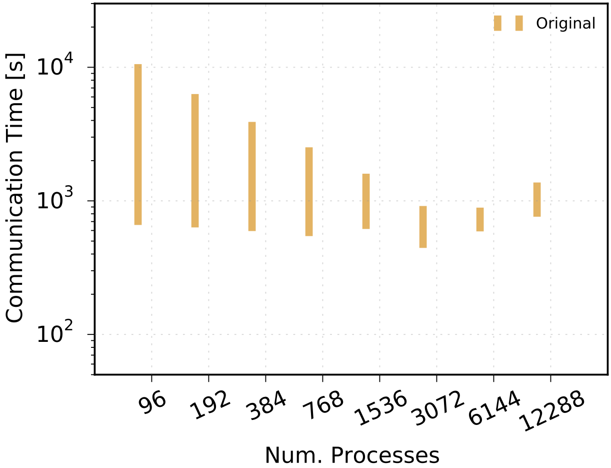
Performance Improvements with Better Partitioning



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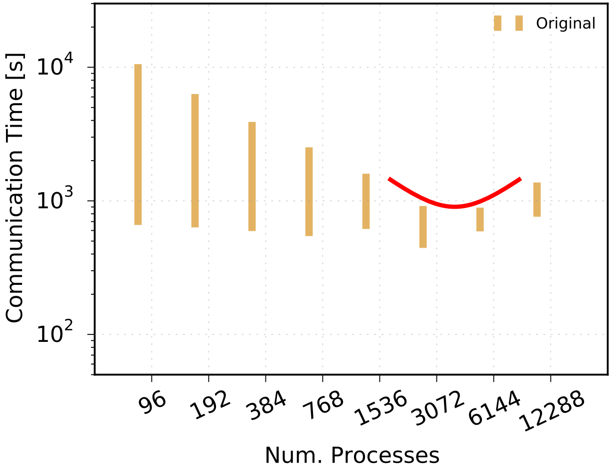

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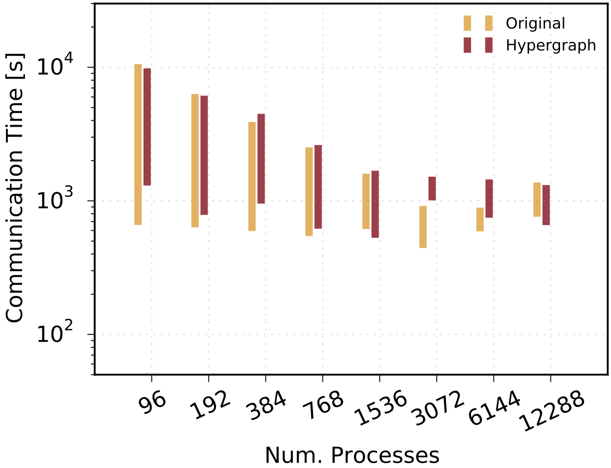

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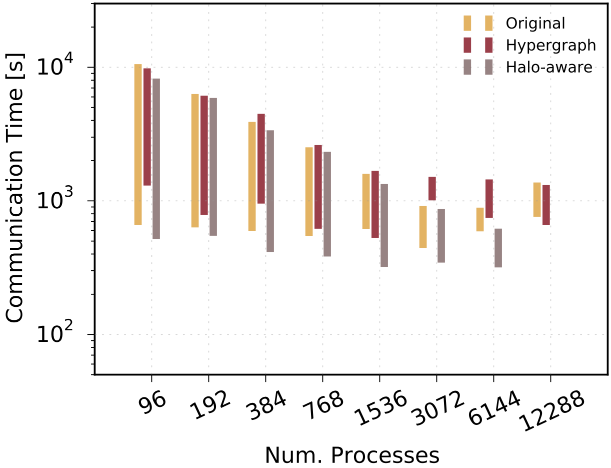

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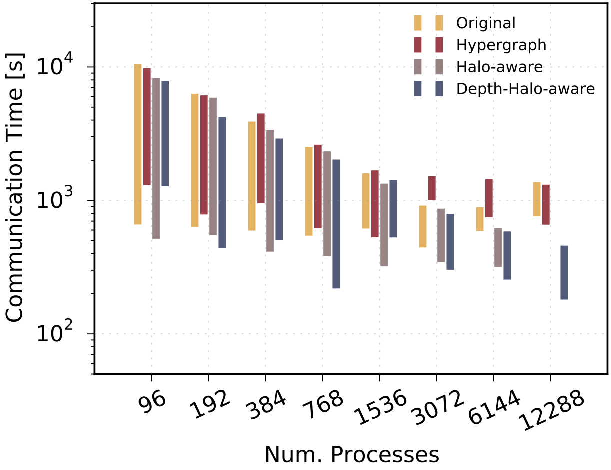

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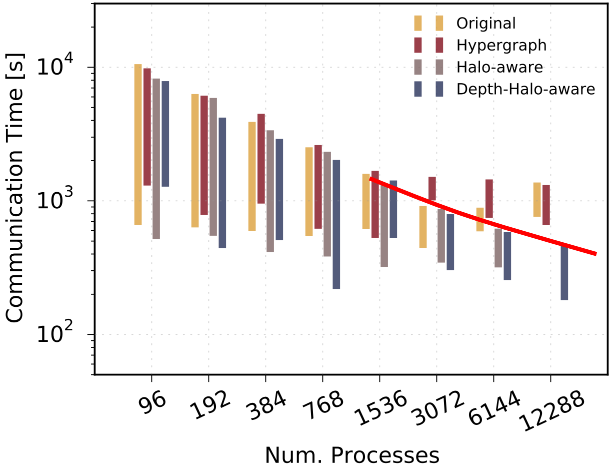

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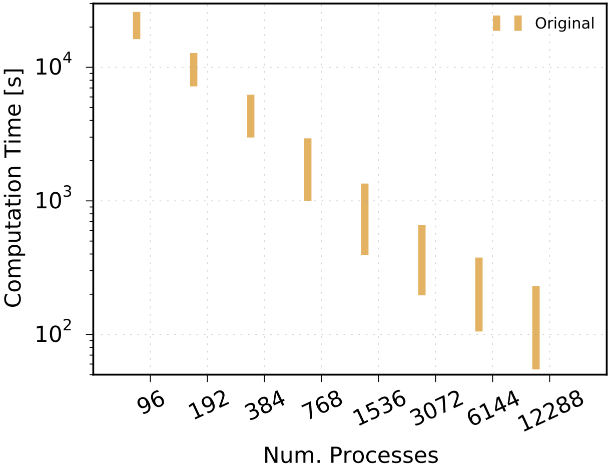

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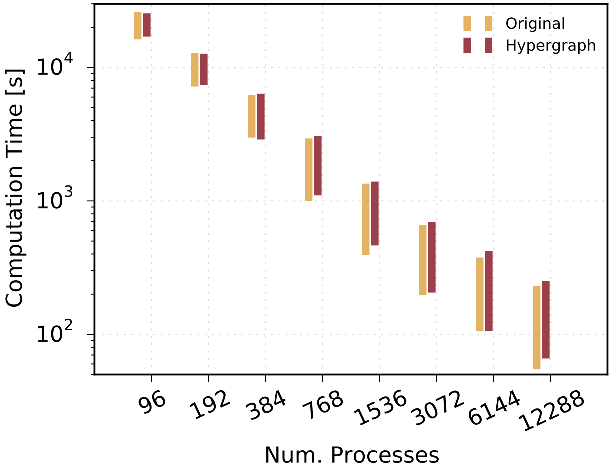

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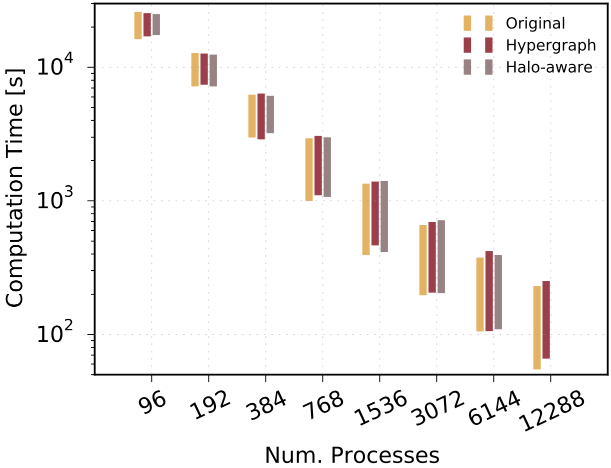

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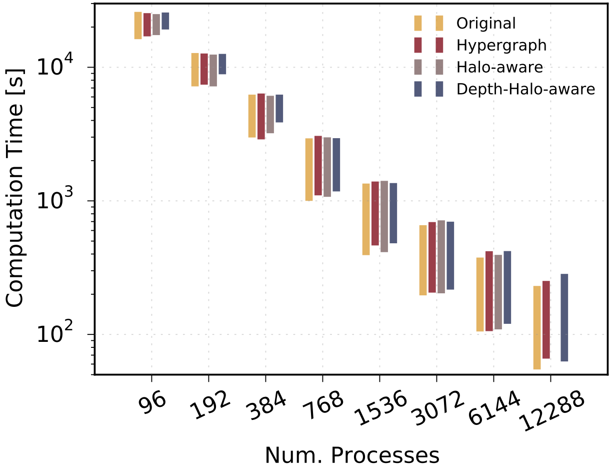

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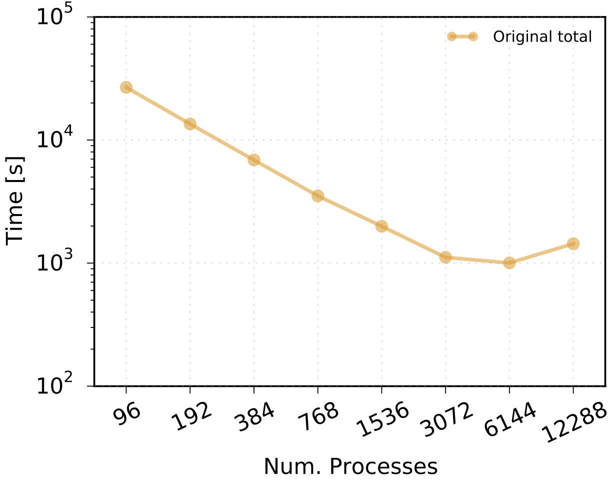

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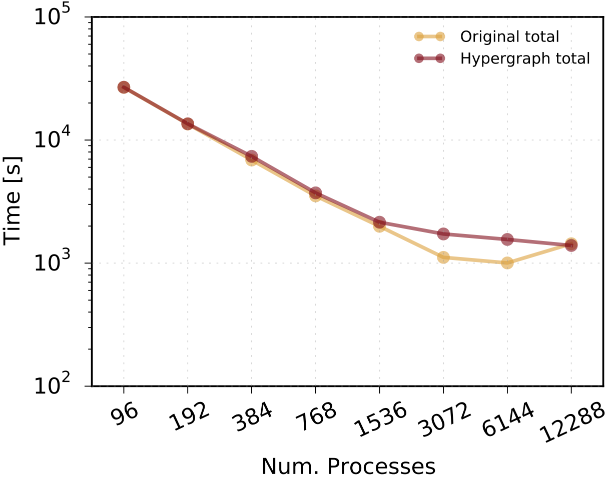

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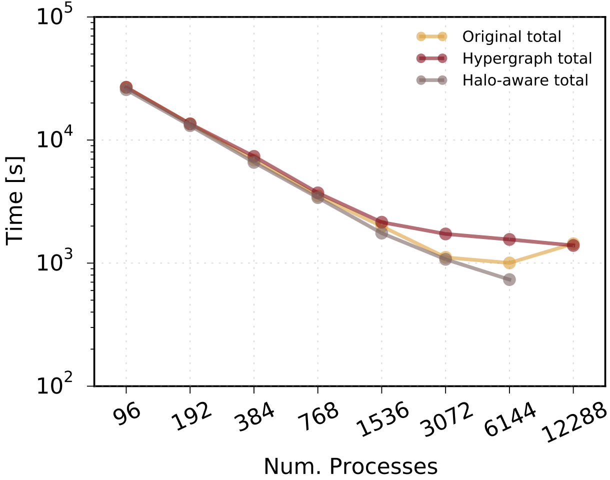

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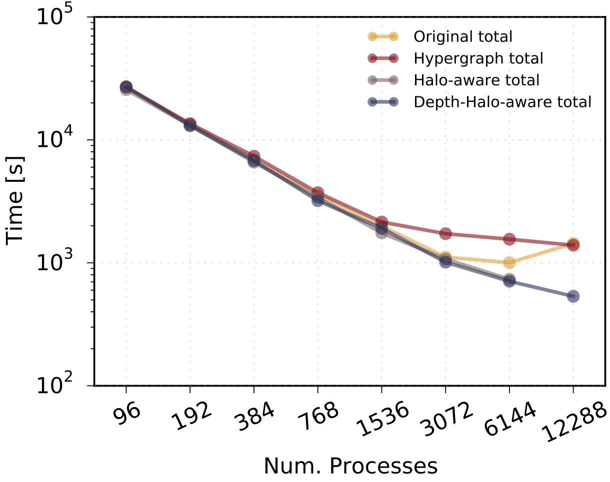

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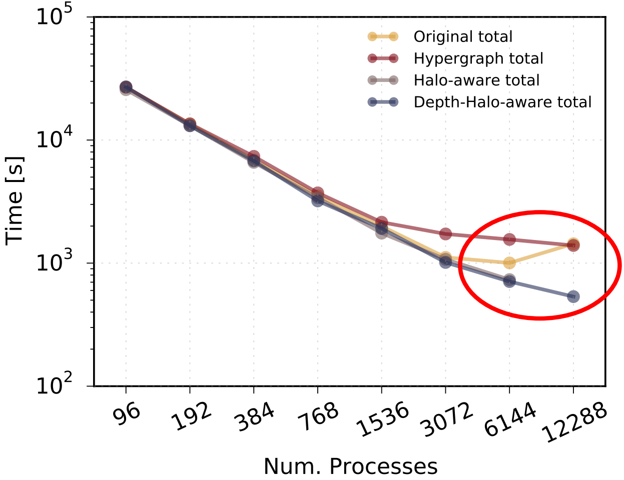
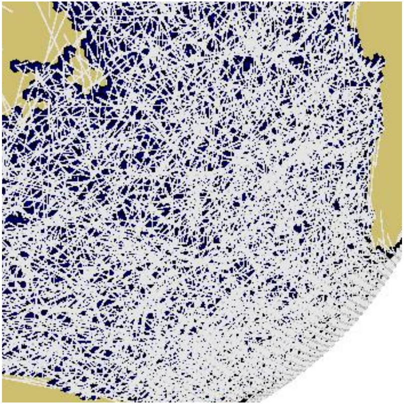
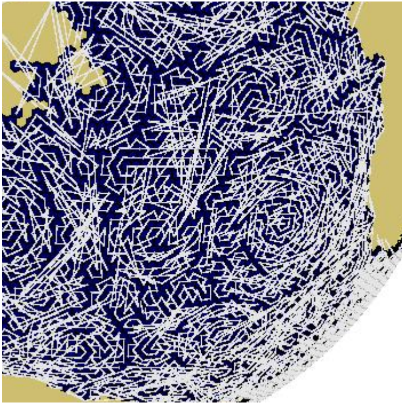


Unstructured data organization ...

Data Locality with Data Ordering

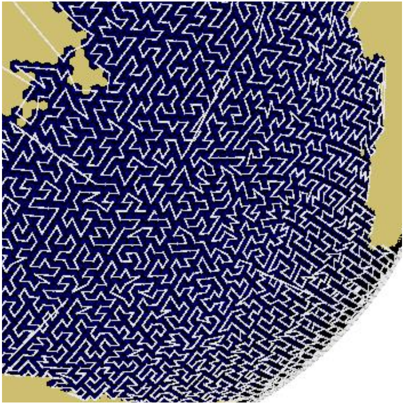


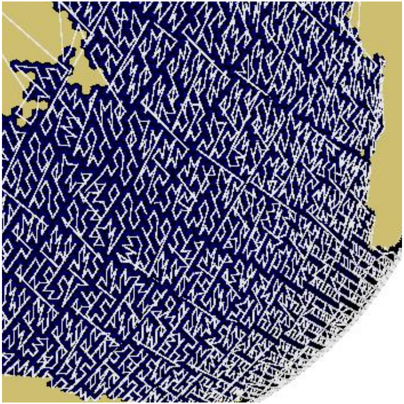
A complete random organization



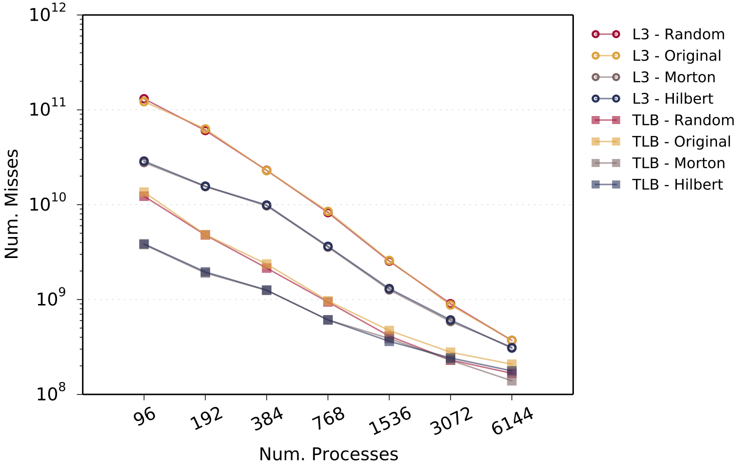
Original/Reverse Cuthill-McKee

Ordering Unstructured Data with Space Filling Curves


Hilbert SFC


Morton/Z-SFC

Performance Improvements with Data Re-ordering: Cache Usage



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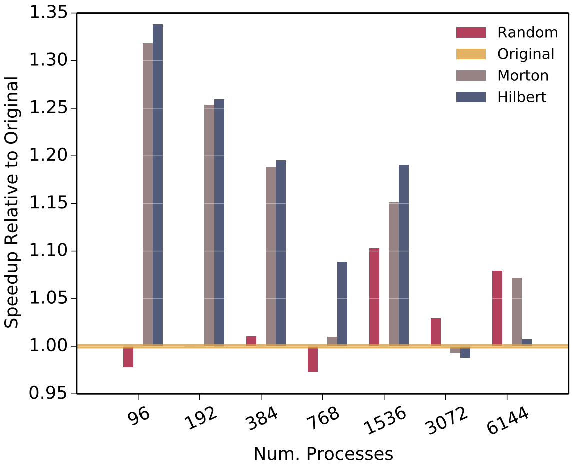

End Notes

- Overall improved performance by up to 2.2$\times$.
- Improved scaling.
- Enable increased resolution and throughput of high resolution meshes.
- Achieve high SYPD (Simulated Year Per Day.)
- Enable higher accuracy with high resolution.

- Partitioning and ordering methods are generic to apply to other unstructured meshes.
- Collaborations ... ?

Acknowledgements

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