Modular forest-of-octrees AMR: algorithms and interfaces

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Simula Research Laboratory, Norway

Additional Credits

Parallel AMR

- joint work with Lucas C. Wilcox, Tobin Isaac, Tiankai Tu (ICES, The University of Texas at Austin, USA)

Numerical methods and applications

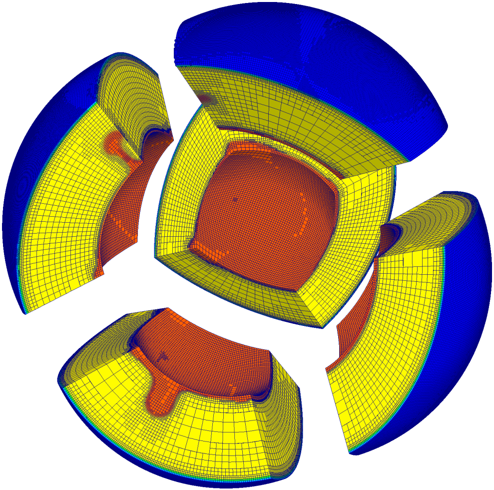
- joint work with Georg Stadler, James Martin (ICES), Mike Gurnis, Laura Alisic (CalTech, Pasadena, USA)

And most importantly

- Omar Ghattas (ICES)

Key points about AMR

AMR—Adaptive Mesh Refinement



- local refinement
- local coarsening
- dynamic
- parallel
- (element-based)
- (general geometry)

Key points about AMR

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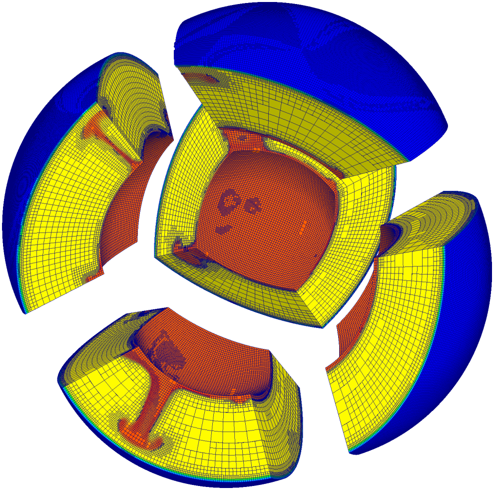

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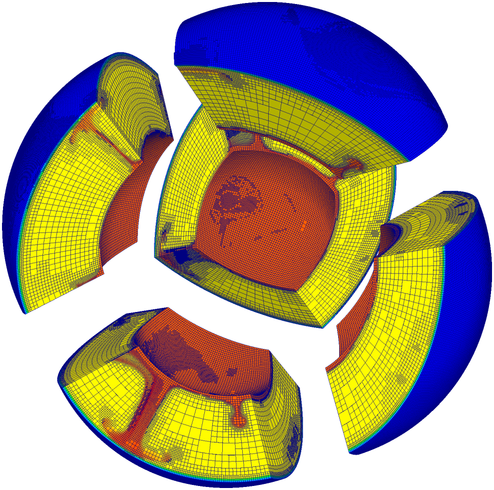

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Why (not) use AMR?

AMR—Adaptive Mesh Refinement

Benefits (problem-dependent)

- Reduction in problem size
- Reduction in run time
- Gain in accuracy per degree of freedom
- Gain in modeling flexibility

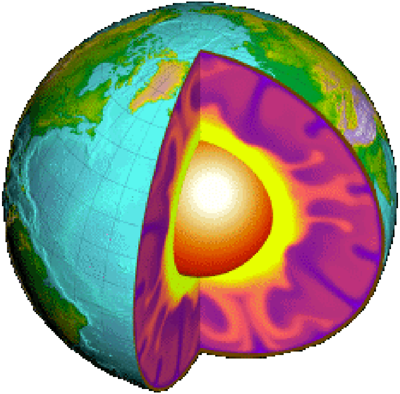
Challenges (fundamental)

- Storage: Irregular mesh structure
- Computational: Tree traversals and searches
- Networking: Irregular communication patterns
- Numerical: Horizontal/vertical projections

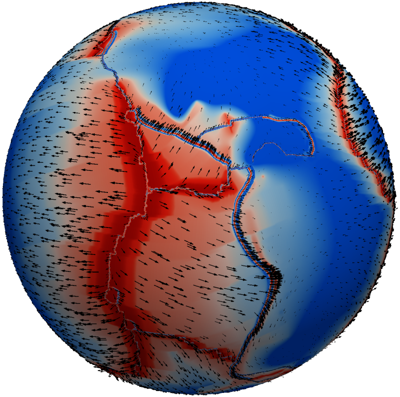
Geoscience simulations enabled by AMR

AMR—Adaptive Mesh Refinement

Mantle convection: High resolution for faults and plate boundaries



Artist rendering
Image by US Geological Survey

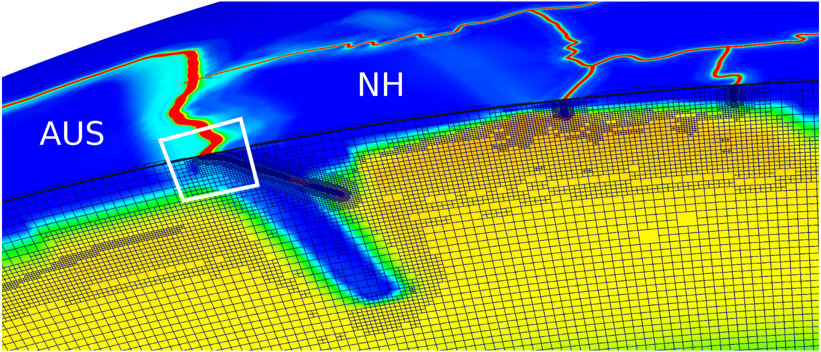


Simul. (w. M. Gurnis, L. Alisic, CalTech)
Surface viscosity (colors), velocity (arrows)

Geoscience simulations enabled by AMR

AMR—Adaptive Mesh Refinement

Mantle convection: High resolution for faults and plate boundaries

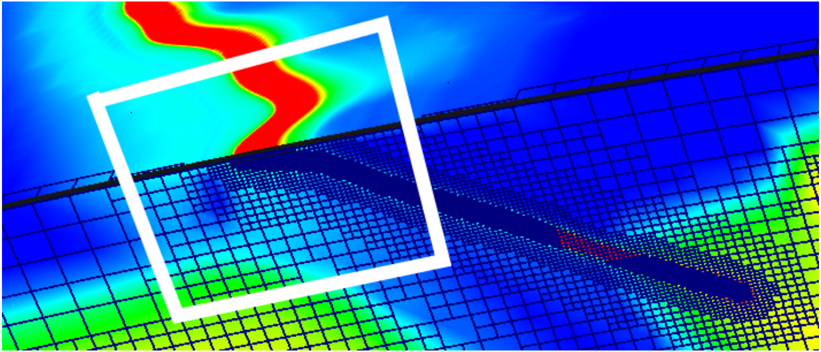


Zoom into the boundary between the Australia/New Hebrides plates

Geoscience simulations enabled by AMR

AMR—Adaptive Mesh Refinement

Mantle convection: High resolution for faults and plate boundaries

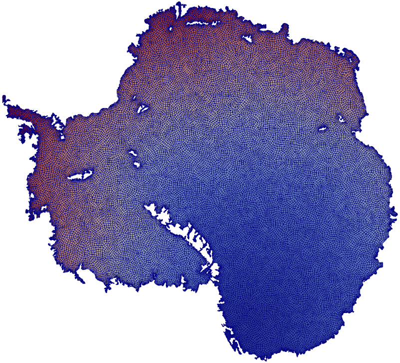


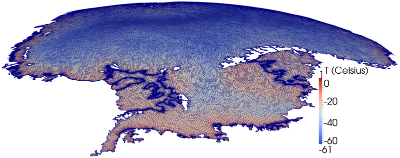
Zoom into the boundary between the Australia/New Hebrides plates

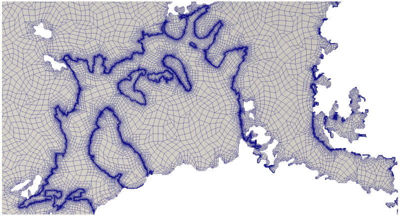
Geoscience simulations enabled by AMR

AMR—Adaptive Mesh Refinement

Ice sheet dynamics: Complex geometry and boundaries







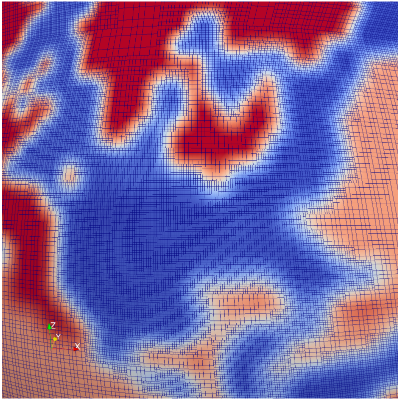
Antarctica meshes (w. C. Jackson, UTIG)
Adapt to geometry from SeaRISE data

Geoscience simulations enabled by AMR

AMR—Adaptive Mesh Refinement

Seismic wave propagation: Adapt to local wave length

Varying local wave speeds



Adapt to local wave length

Initial mesh

CSG description $\longrightarrow$ mesh generator $\longrightarrow$ XML file

- uniform element sizes
- finer resolution "where it matters"

$\boxed{\text{a-priori adaptation}}$

AMR

AMR—Adaptive Mesh Refinement

"Where it matters"

is sometimes known, often unknown beforehand

- emerging features
- moving fronts

$\boxed{\text{a-posteriori adaptation}}$

Common AMR cycle

$$\text{Solve} \longrightarrow \text{Mark} \longrightarrow \text{Refine} \longrightarrow \text{(repeat)}$$

- Mesh exists standalone (topology/geometry)

Common AMR cycle

Solve $\longrightarrow$ Estimate $\longrightarrow$ Mark $\longrightarrow$ Refine $\longrightarrow$ (repeat)

- Mesh exists standalone (topology/geometry)
- Fields (function space elements) are tied to a mesh

Solve $\longrightarrow$ Solution $\longrightarrow$ Indicator $\longrightarrow$ Flag $\longrightarrow$ Mark

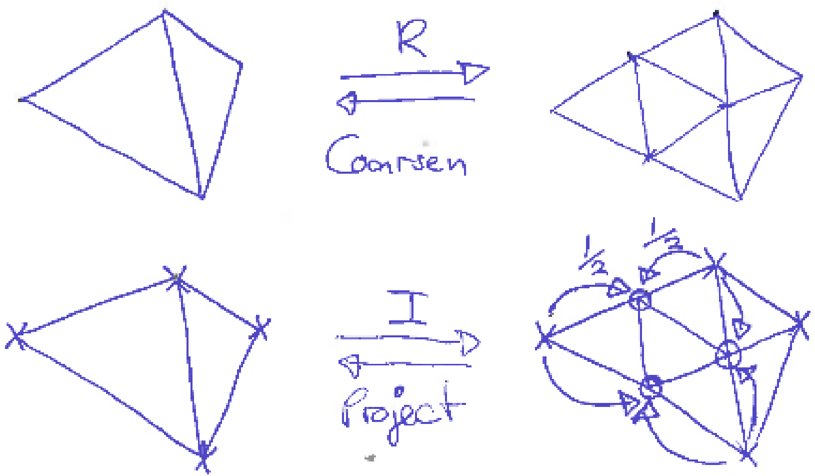
Common AMR cycle

$$\text{Solve} \longrightarrow \text{Estimate} \longrightarrow \text{Mark} \longrightarrow \text{Refine} \longrightarrow \text{(repeat)}$$

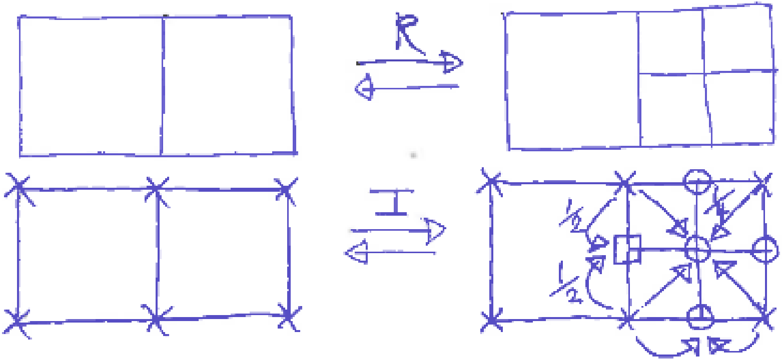
- Mesh exists standalone (topology/geometry)
- Fields (function space elements) are tied to a mesh

$$\text{Solve} \longrightarrow \text{Solution} \longrightarrow \text{Indicator} \longrightarrow \text{Flag} \longrightarrow \text{Mark}$$
$$\text{Solution} + \text{Refine} \longrightarrow \text{Interpolate} \longrightarrow \text{Solution}$$

Estimator, Flag, Interpolate: element-local (conforming)



Estimator, Flag, Interpolate: element-local (non-conforming)

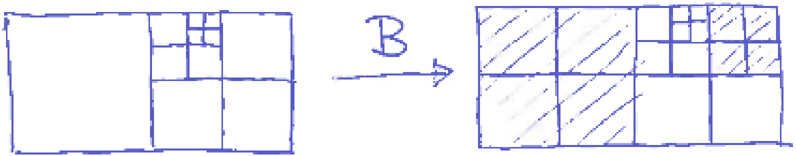


- Hanging node values are not part of Solution, never stored

Parallelization aspects

S $\longrightarrow$ E $\longrightarrow$ M $\longrightarrow$ R $\longrightarrow$ Balance $\longrightarrow$ Partition $\longrightarrow$ (repeat)

- 1. Balance: restore 2:1 non-conformity



Global split propagation

$\Rightarrow$ tricky algorithm (in serial)

$\Rightarrow$ extra tricky in parallel

Parallelization aspects

S $\longrightarrow$ E $\longrightarrow$ M $\longrightarrow$ R $\longrightarrow$ Balance $\longrightarrow$ Partition $\longrightarrow$ (repeat)

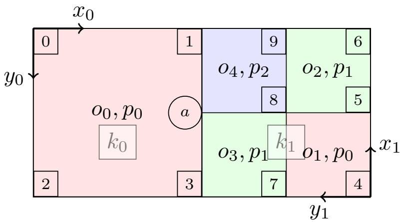
- 2. Partition: restore load balance
- Mesh $\equiv$ graph: partition is NP-hard $\lightning$

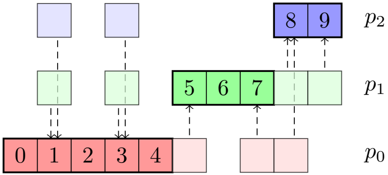
Add extra structure
($\Leftrightarrow$ reduce search space)
$\Rightarrow$ faster algorithms

Parallelization aspects

S $\longrightarrow$ E $\longrightarrow$ M $\longrightarrow$ R $\longrightarrow$ Balance $\longrightarrow$ Partition $\longrightarrow$ (repeat)

- 3. Nodes: create globally unique dof indices
- Nodes relevant to 2 or more processes $\Rightarrow$ ownership conflict





Add ghost elements
($\Rightarrow$ parallel algorithm)
$\Rightarrow$ resolve conflicts locally

Modular AMR

AMR—Adaptive Mesh Refinement

Yesterday's quotes on scalability

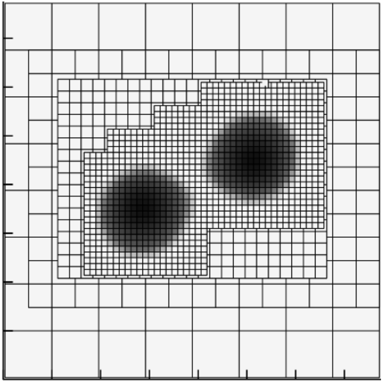
- "straightforward, but time required"
- "software engineering problem"
- Parallel AMR algorithms are neither

Modular tools available

- Outsource distributed mesh generation/modification
- Encapsulate algorithms, define interfaces
- Differ in scalability and speed/memory footprint

Types of AMR

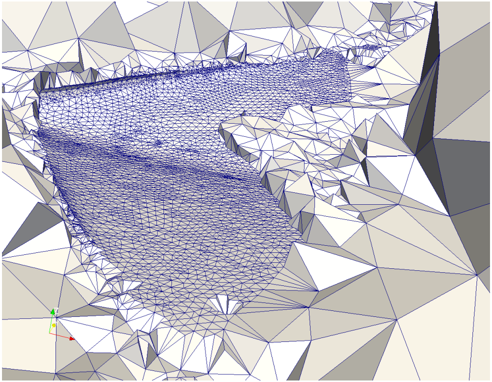
- Block-structured (patch-based) AMR



www.cactuscode.org

Types of AMR

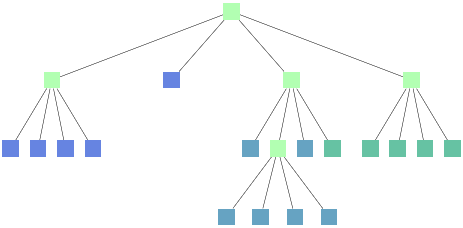
- Conforming tetrahedral (unstructured) AMR

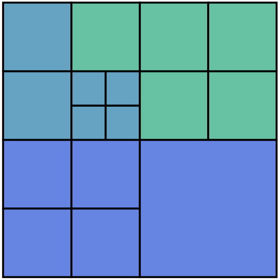


mesh data courtesy David Lazzara, MIT

Types of AMR

- Octree-based AMR





- Octree maps to cube-like geometry
- 1:1 relation between octree leaves and mesh elements

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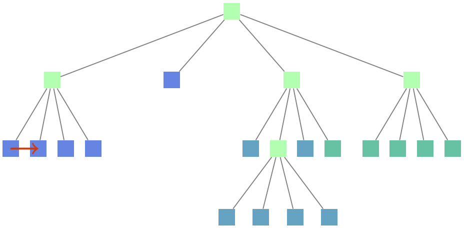

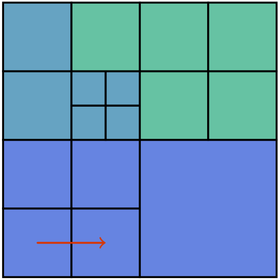

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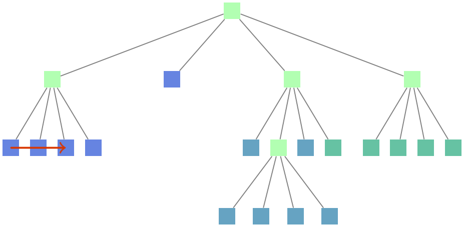

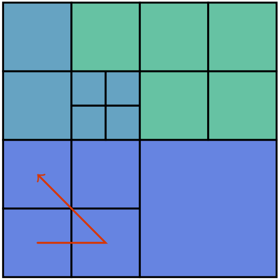

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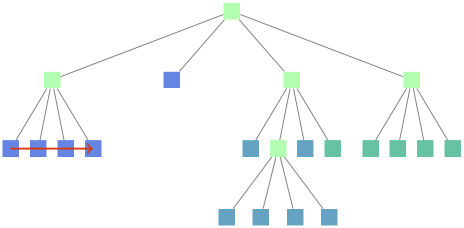

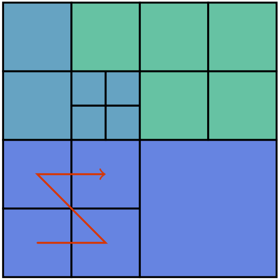

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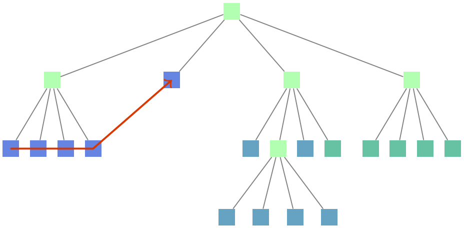

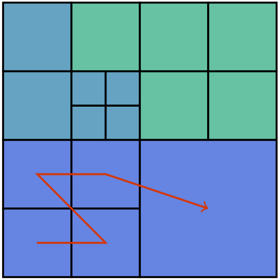

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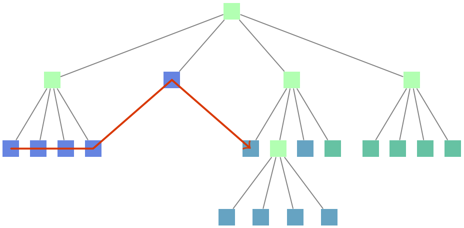

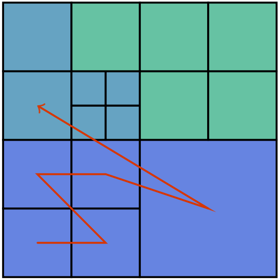

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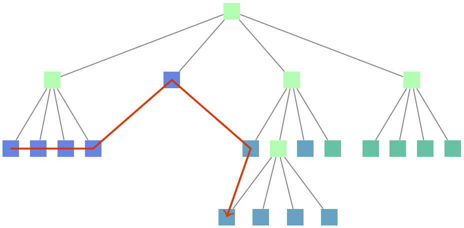

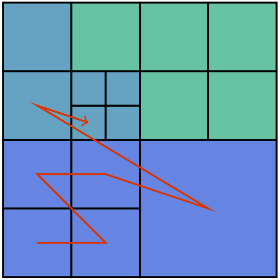

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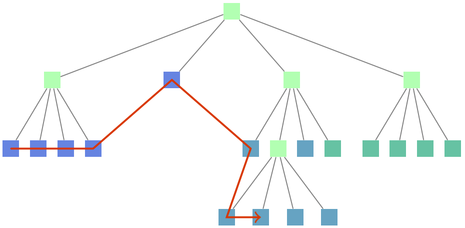

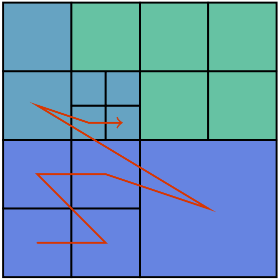

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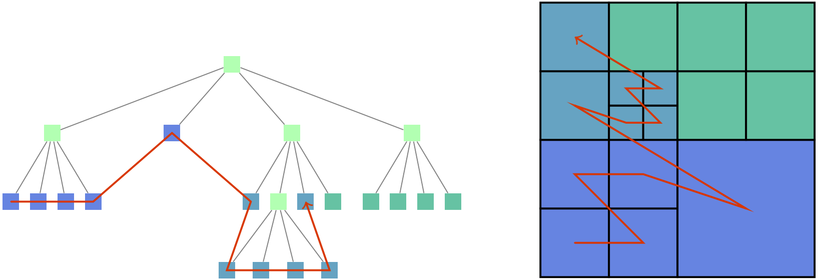

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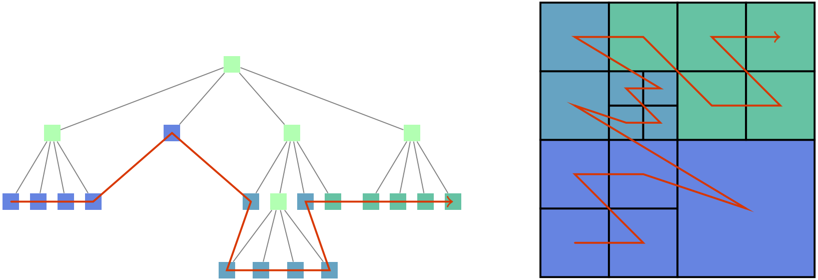

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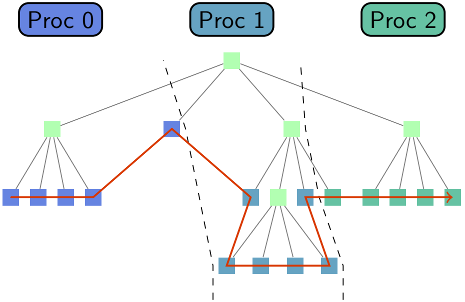
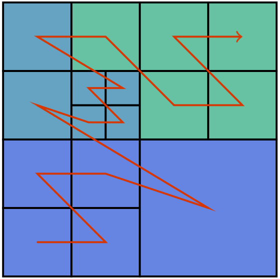
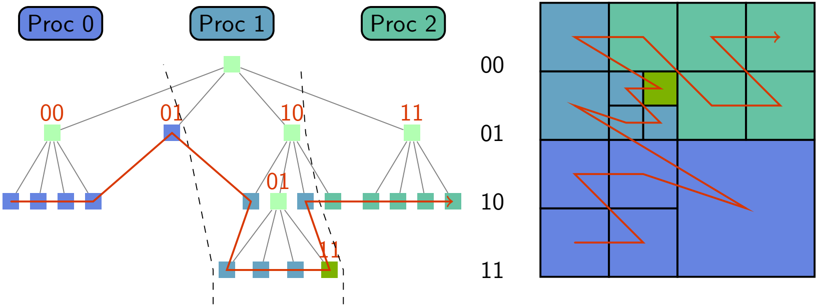




- Space-filling curve (SFC): Fast parallel partitioning
- Fast parallel tree algorithms for sorting and searching

Octree-based AMR

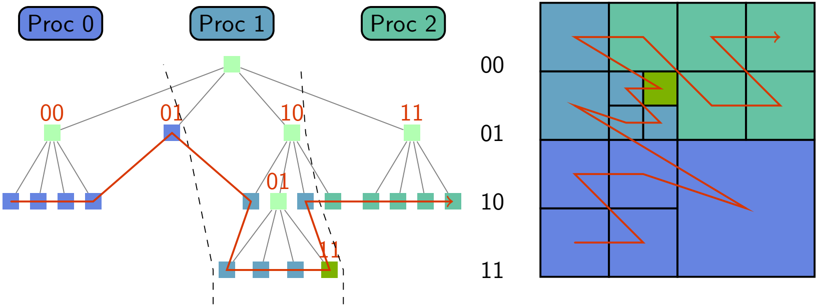
Efficient encoding and total ordering



- 1:1 relation between leaves and elements → efficient encoding
- path from root to node   10 01 11

Octree-based AMR

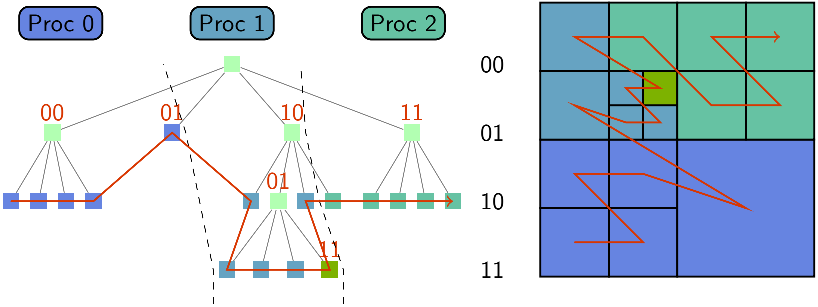
Efficient encoding and total ordering



- 1:1 relation between leaves and elements $\rightarrow$ efficient encoding
- path from root to node, append level `10 01 11 11` $\rightarrow$ `key`

Octree-based AMR

Efficient encoding and total ordering



- 1:1 relation between leaves and elements $\rightarrow$ efficient encoding
- path from root to node, append level `10 01 11 11` $\rightarrow$ `key`
- derive element x-coordinate `_0 _1 _1` $\rightarrow x = 3$

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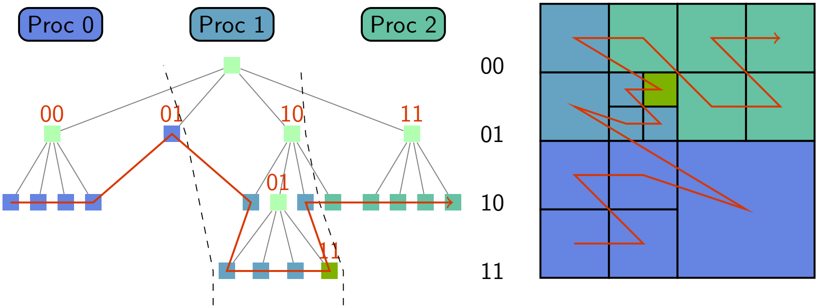
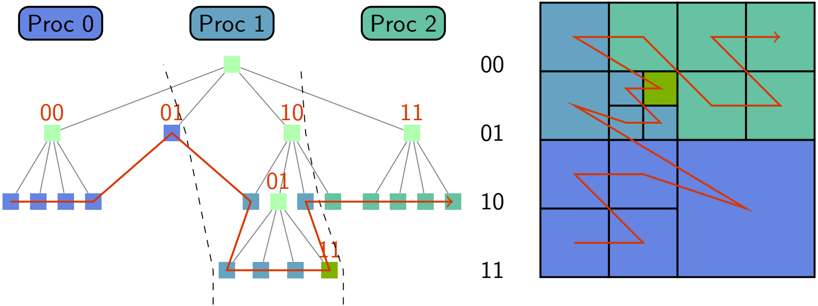
Efficient encoding and total ordering



- 1:1 relation between leaves and elements → efficient encoding
- path from root to node, append level   `10 01 11 11` → `key`
- derive element x-coordinate   `_0 _1 _1` → $x = 3$
- derive element y-coordinate   `1_ 0_ 1_` → $y = 5$

Octree-based AMR

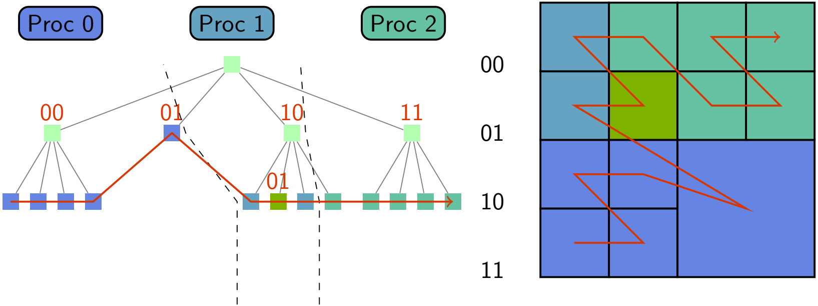
Fast elementary operations



- Construct parent or children → vertical tree step $\mathcal{O}(1)$
- path from root to node, append level `10 01 11 11` → `key`

Octree-based AMR

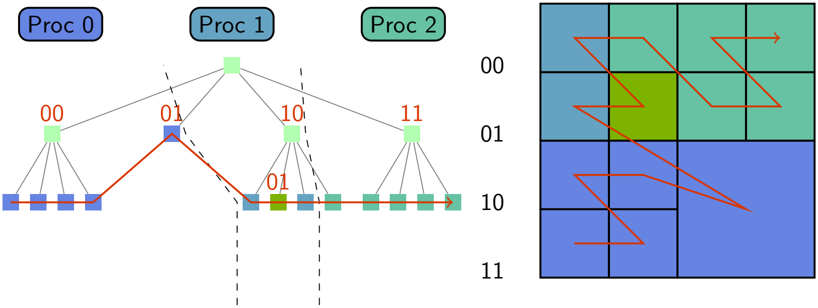
Fast elementary operations



- Construct parent or children $\rightarrow$ vertical tree step $\mathcal{O}(1)$
- path from root to node, append level `10 01 11 11`
- zero level coordinates, decrease level `10 01 00 10` $\rightarrow$ `key`

Octree-based AMR

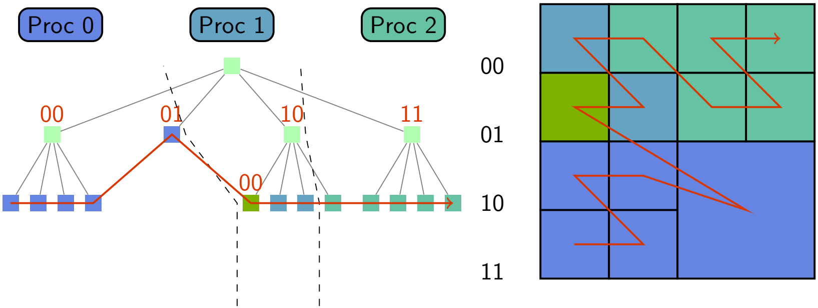
Fast elementary operations



- Construct neighbors → horizontal tree step/jump $\mathcal{O}(1)$
- path from root to node, append level `10 01 00 10` → `key`

Octree-based AMR

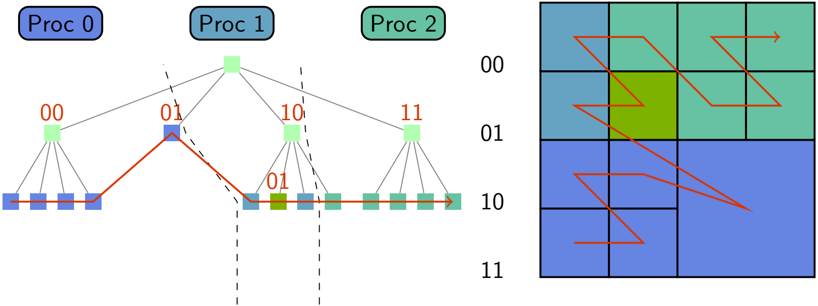
Fast elementary operations



- Construct neighbors $\rightarrow$ horizontal tree step/jump $\mathcal{O}(1)$
- path from root to node, append level   10 01 00 10
- Substract x-coordinate increment   10 00 00 10 $\rightarrow$ `key`
- Search on-processor element $\rightarrow$ tree search $\mathcal{O}(\log \frac{N}{P})$

Octree-based AMR

Fast elementary operations



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Octree-based AMR

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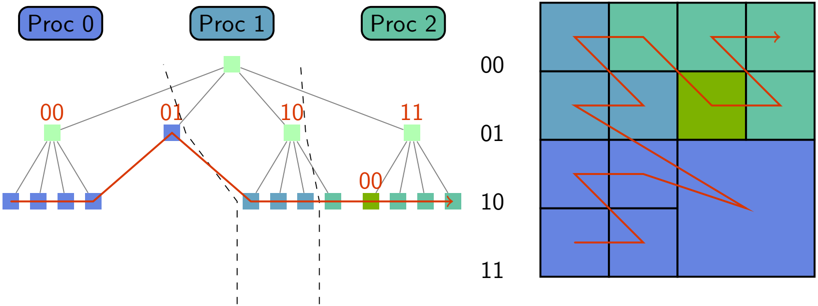
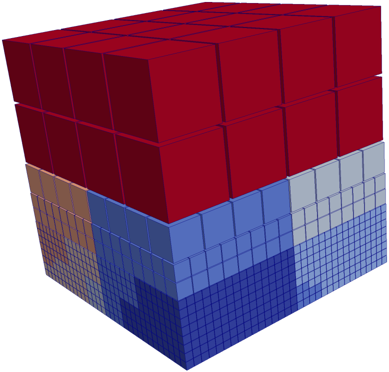


- Construct neighbors $\rightarrow$ horizontal tree step/jump $\mathcal{O}(1)$
- path from root to node, append level `10 01 00 10`
- Add x-coordinate increment `11 00 00 10` $\rightarrow$ `key`
- Search off-processor element-owner $\rightarrow$ search SFC $\mathcal{O}(\log P)$

Synthesis: Forest of octrees

From tree...

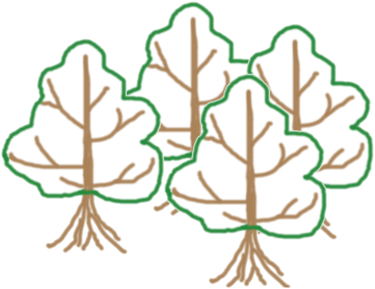
$=$



- Limitation: Cube-like geometric shapes

Synthesis: Forest of octrees

...to forest



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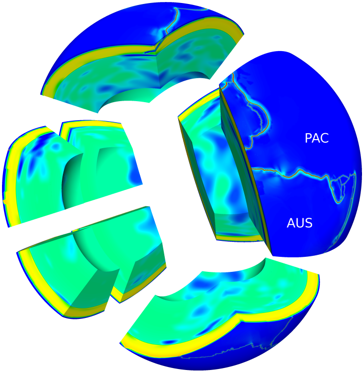
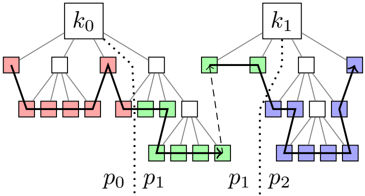
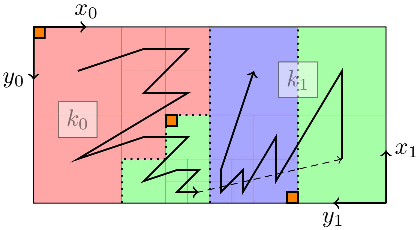


- Advantage: Geometric flexibility
- Challenge: Non-matching coordinate systems between octrees

“p4est”—forest-of-octrees algorithms

Connect SFC through all octrees





Minimal global shared storage (metadata)

- Shared list of octant counts per core $(N)_p$ $4 \times P$ bytes
- Shared list of partition markers $(k; x, y, z)_p$ $16 \times P$ bytes
- 2D example above $(h = 8)$: markers $(0; 0, 0), (0; 6, 4), (1; 0, 4)$

[1] C. Burstedde, L. C. Wilcox, O. Ghattas (SISC, 2011)

“`p4est`”—forest-of-octrees algorithms

`p4est` is a pure AMR module

- Rationale: Support diverse numerical approaches
- Internal state: Element ordering and parallel partition
- Provide minimal API for mesh modification

Connect to numerical discretizations / solvers (“App”)

- `p4est` API calls are like MPI collectives (atomic to App)
- `p4est` API hides parallel algorithms and communication
- App $\rightarrow$ `p4est`: API invokes per-element callbacks
- App $\leftarrow$ `p4est`: Access internal state read-only

“p4est”—forest-of-octrees algorithms

p4est core API (for “write access”)

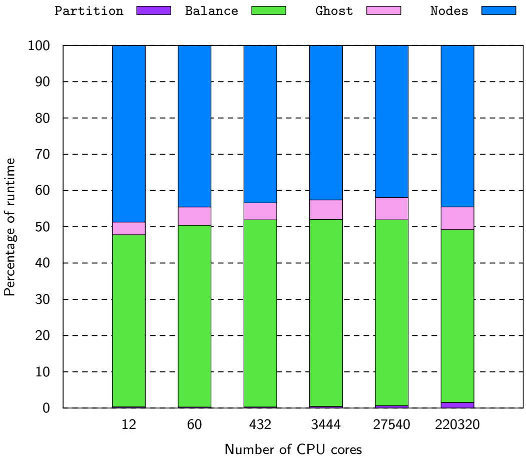
- p4est_new: Create a uniformly refined, partitioned forest
- p4est_refine: Refine per-element acc. to $0/1$ callbacks
- p4est_coarsen: Coarsen 2^d elements acc. to $0/1$ callbacks
- p4est_balance: Establish 2:1 neighbor sizes by add. refines
- p4est_partition: Parallel redistribution acc. to weights
- p4est_ghost: Gather one layer of off-processor elements

p4est “random read access” not formalized

- Loop through p4est data structures as needed

“p4est”—forest-of-octrees algorithms

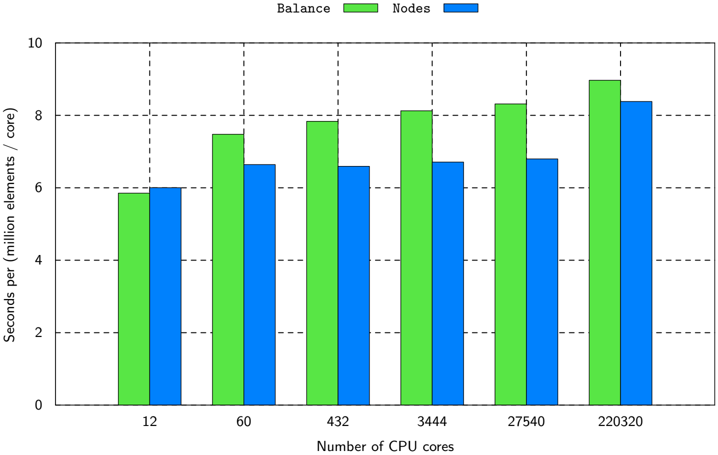
Weak scalability on ORNL’s “Jaguar” supercomputer



- Cost of `New`, `Refine`, `Coarsen`, `Partition` negligible
- 5.13×10^{11} octants; < 10 seconds per million octants per core

"p4est"—forest-of-octrees algorithms

Weak scalability on ORNL's "Jaguar" supercomputer



- Dominant operations: `Balance` and `Nodes` scale over 18,360x
- 5.13×10^{11} octants; < 10 seconds per million octants per core

“p4est”—forest-of-octrees algorithms

What is a p4est element? Anything!

- The App defines how it will interprete an element

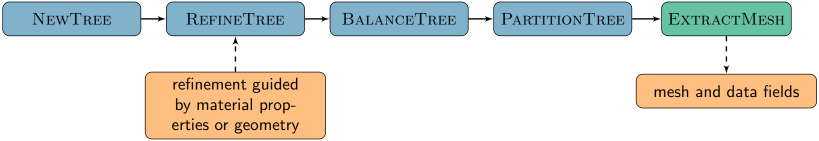
Examples

- Continuous bi-/trilinear elements
- High-order continuous spectral elements
- High-order DG elements with Gauss quadrature, LGL, ...
- An ijk subgrid optimized for GPU computation
- An M^d patch from PyClaw
- ...

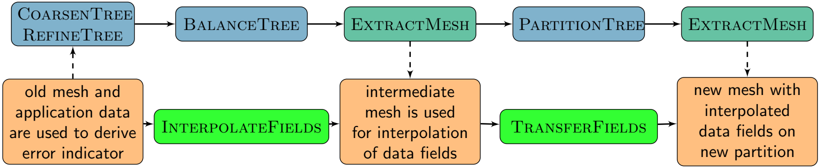
Parallel AMR

AMR—Adaptive Mesh Refinement

A-priori adaptation



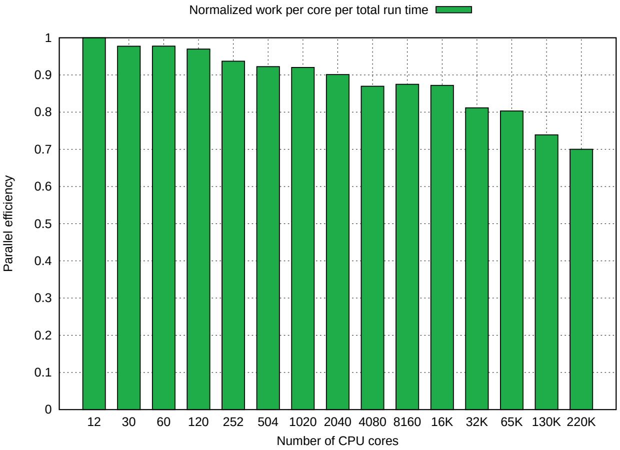
A-posteriori/dynamic adaptation



[2] C. Burstedde, O. Ghattas, G. Stadler, et.al. (TeraGrid, 2008)

App: Dynamic-mesh DG (3D advection)

Weak scalability on ORNL's "Jaguar" supercomputer



- 3,200 high-order elements per core from 12 to 220,320 cores
- Overall parallel efficiency is 70% over a 18,360x scale

Acknowledgements

Publications

- Homepage: `http://burstedde.ins.uni-bonn.de/`

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