Geometric Multigrid for Higher-order Discretizations

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Copper Mountain Multigrid 2013

Motivation

Scalable solution of large-scale linear systems

asymptotically optimal parallel solvers for elliptic PDEs

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variable coefficients

adaptive discretizations

arbitrary geometries

high-order discretizations

massively parallel

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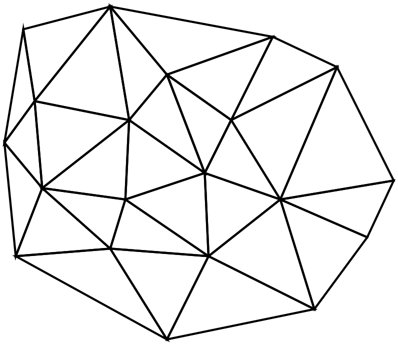
Parallel Geometric Multigrid

$$\mathcal{O}\left(\frac{N}{p} + \log N\right)$$ for elliptic PDEs with smooth coefficients

parallel multigrid

challenges

- geometric multigrid for arbitrary meshes
  - graph based partitioning (ParMETIS SC'98, SC'00)
  - scalability is challenging



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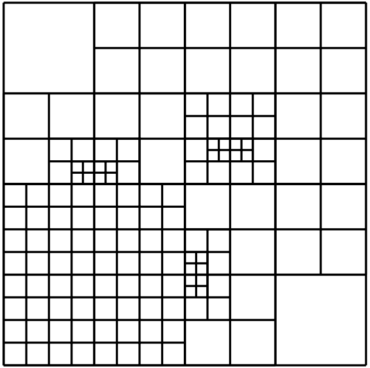
  - dendro (Sampath et al., SC'08)
  - limited to cubic domains



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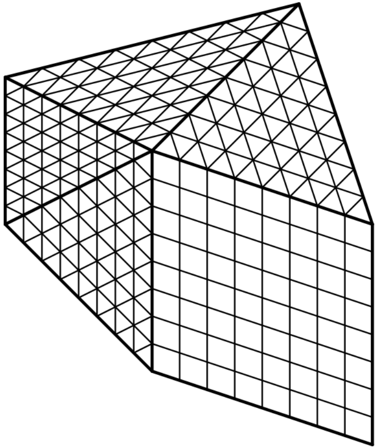
- two-tier meshes, macromesh + regular grid
  - HHG (Bergen et al., SC'05)
  - limited adaptivity



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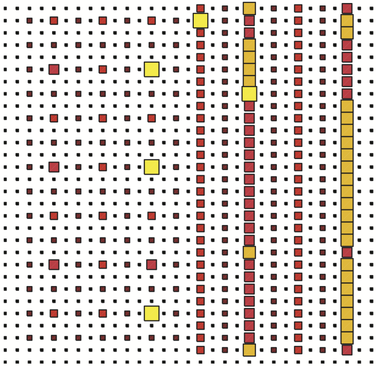
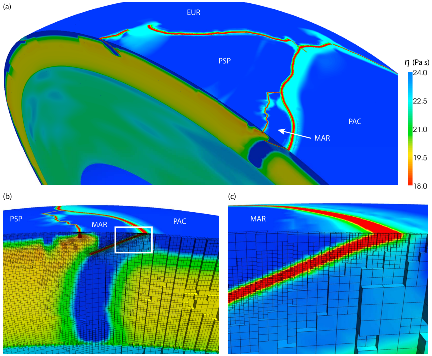
  - limited adaptivity
- algebraic multigrid
  - Adams et al., SC'04
  - Hypre(CHPC'10), `trilinos::ML`
  - graph based coarsening
  - need assembled matrix



Parallel Multigrid

Key Contributions

- GMG for complex geometries with adaptivity (macromesh + octrees)
- excellent strong and weak scalability
- low setup cost
- matrix-free implementation using non-blocking MPI calls
- $262K$ cores with single $\mathtt{MPI}$ process per core



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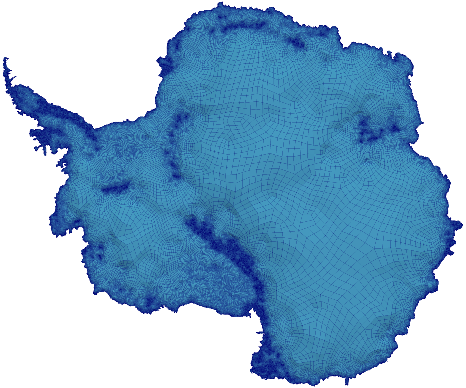
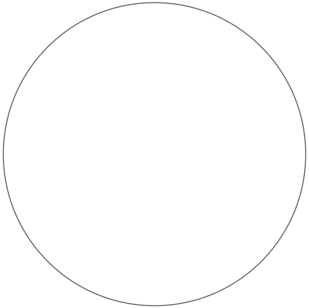


two-tier meshes

conforming macromesh of adaptive octrees



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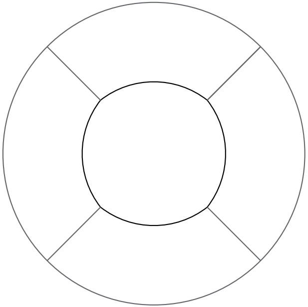
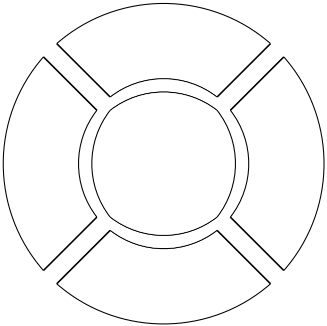


macromesh

two-tier meshes

conforming macromesh of adaptive octrees



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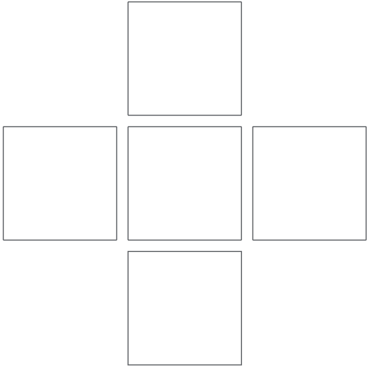
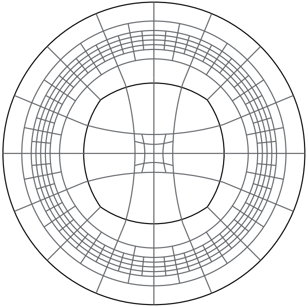


forest of octrees

two-tier meshes

conforming macromesh of adaptive octrees



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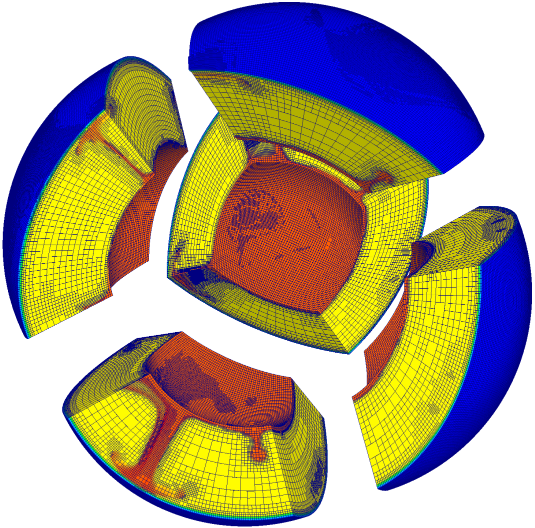
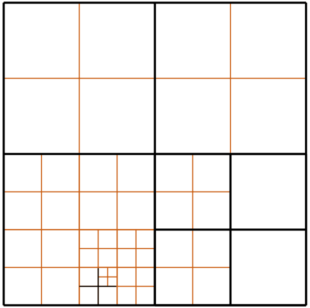


multigrid setup

coarsening

for octrees:

if all siblings exist, replace with parent



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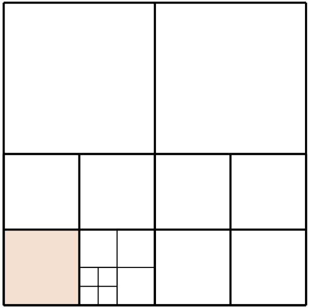
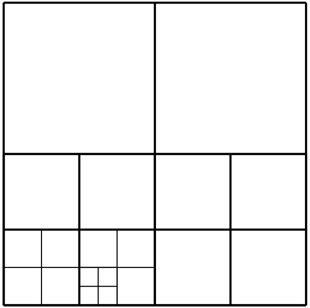


multigrid setup

coarsening

for octrees:

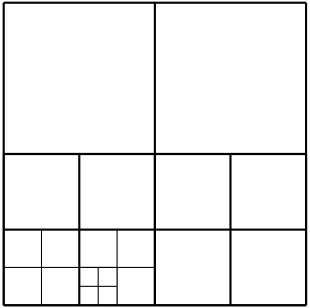
preserve 2:1 balance at all grids



multigrid setup

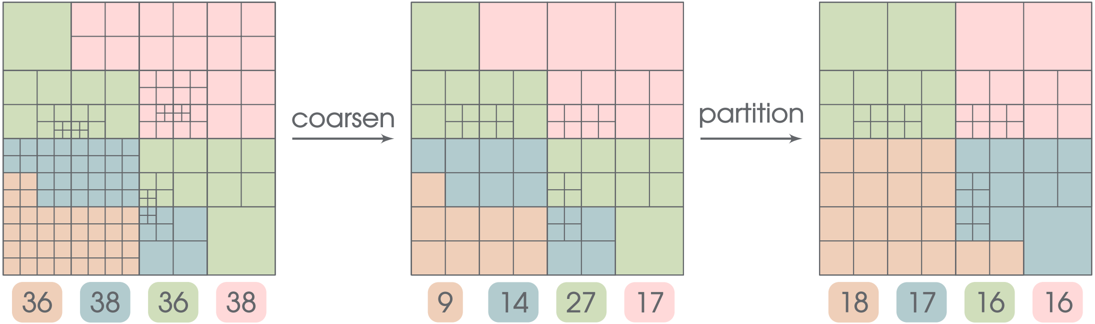
coarsening

for forests: cannot coarsen beyond first-tier macromesh



Multigrid Setup

Partitioning & load balancing



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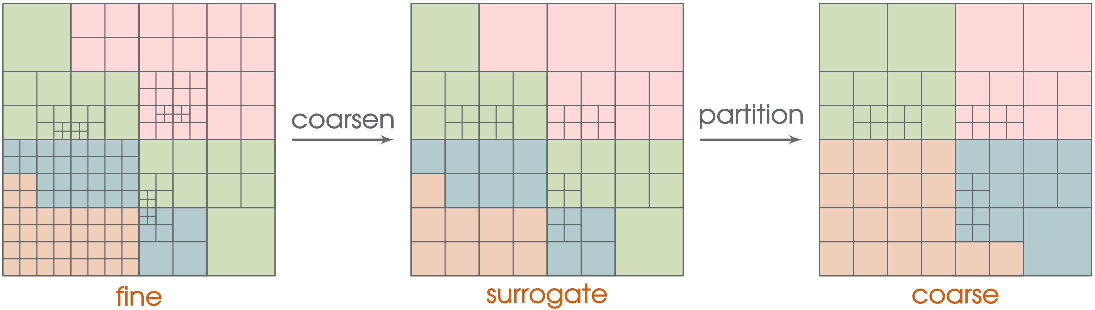

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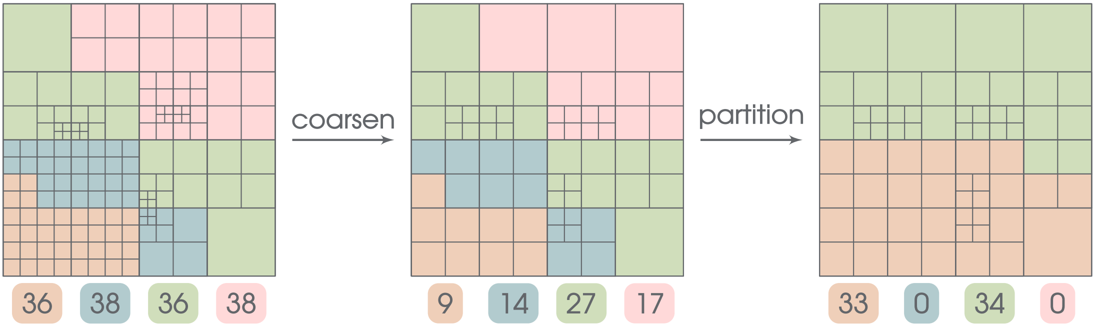

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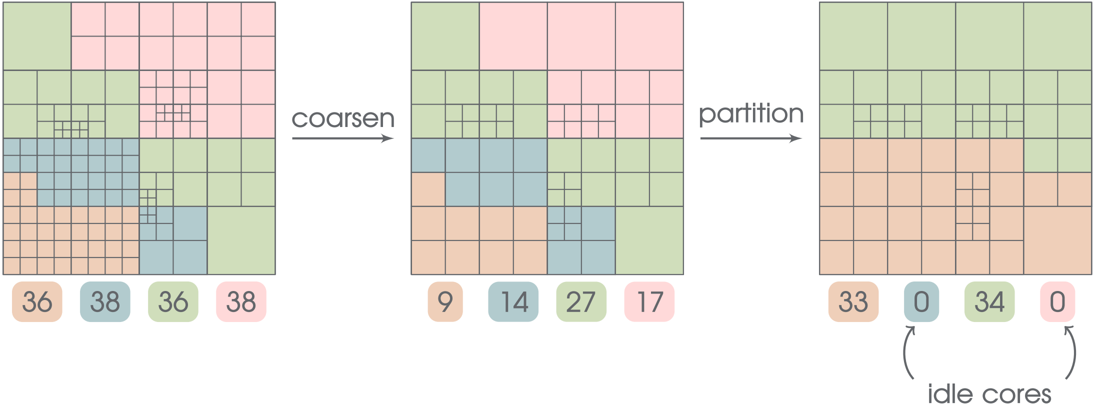
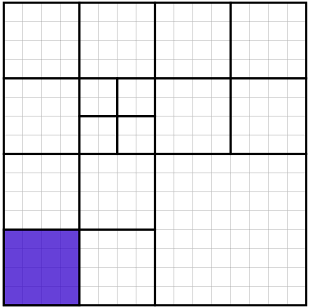
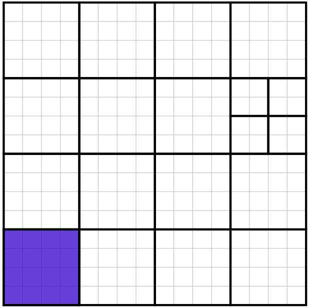


Inter-grid transfer operators

Simultaneous traversal over coarse and fine meshes

- matrix-free implementation
- P_{ij} - coarse grid shape function (ϕ_j) evaluated at the fine grid point (p_i)

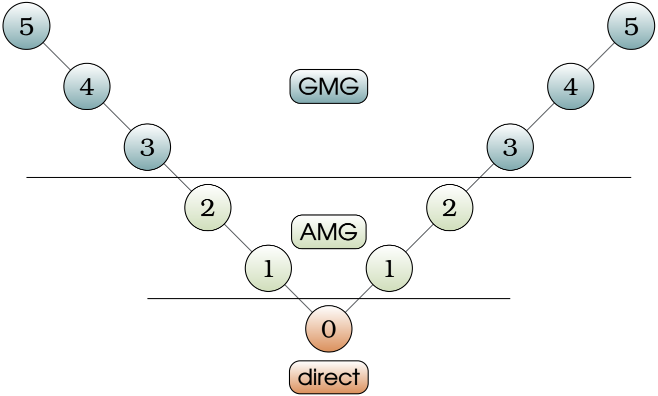




Multigrid Solve

Coarse grid solver

- smoothed aggregation algebraic multigrid (`trilinos::ML`)
- GMG-AMG approach matches our two-tier geometric decomposition of the domain
- AMG is used for small problem sizes on small process counts



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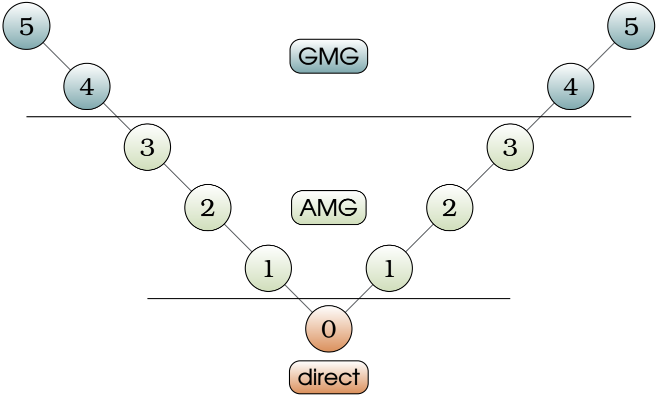


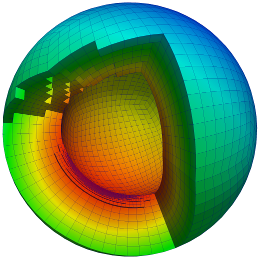
Results

Test problem

$$-\mathrm{div}(\mu(x)\nabla u(x)) = f(x) \qquad \forall x \in \Omega, \qquad u(x) = 0 \text{ on } \partial\Omega.$$

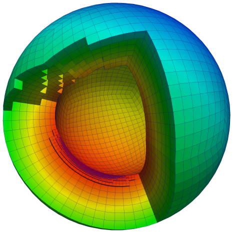
$$\mu(x) = 1 + 10^6\left(e^{-(x-x_1)^2/2\sigma_1^2} + e^{-(x-x_2)^2/2\sigma_2^2}\right)$$

- 3D Poisson problem
- Dirichlet boundary conditions
- isotropic spatially varying coefficient
- forest of 24 Octrees



Results

Strong scaling



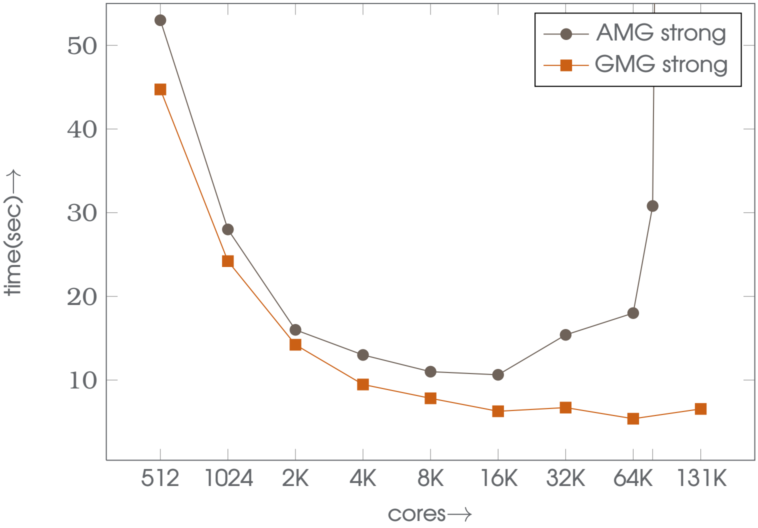
$124M$ elements

5 GMG levels

AMG* for Coarse solve

1 MPI process per core

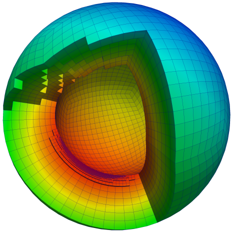
Jaguar $XK6$



*smoothed aggregation (ML)

Results

Weak scaling



$215K$ elements per process

AMG for Coarse solve

1 $\mathtt{MPI}$ process per core

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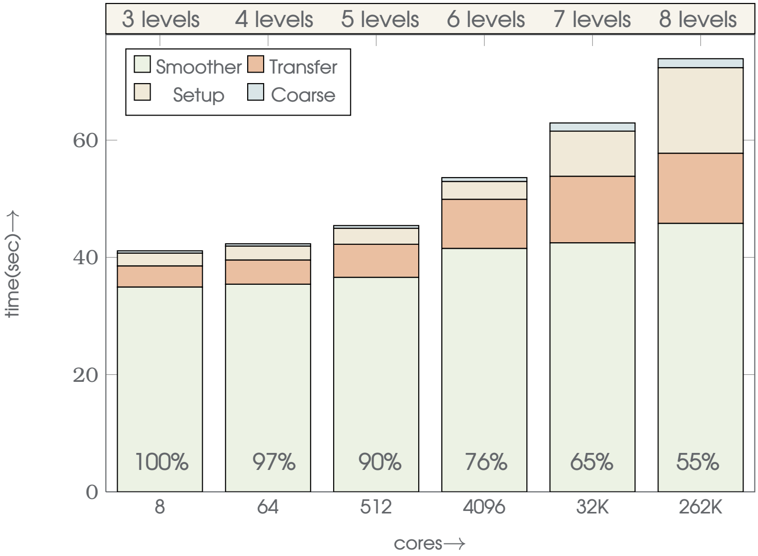

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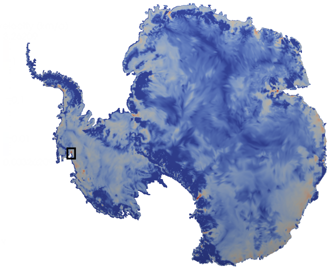
Weak scaling : Antarctica mesh



$45K$ Octrees

$400K$ elements per process

constant coefficient Poisson

Cores	64	512	4096	32768	262144
Setup	2.97	2.64	3.1	3.76	8.6
Smoother	**289.7**	**301.5**	**336.3**	**391.3**	**409.1**
Transfer	7.45	8.47	11.5	11.35	15.88
Coarse Setup	1.85	2.13	0.82	1.27	1.63
Coarse Solve	24.3	30.8	18.47	30.1	26.01
Total Time	326.3	345.5	370.2	437.8	461.2

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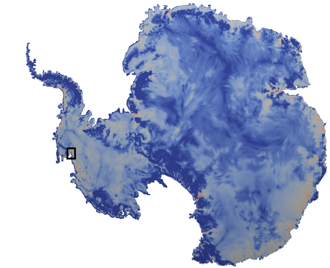

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100 Billion unknowns on $262K$ cores while sustaining 272 TFlops/sec.

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Scalable solution of large-scale linear systems

asymptotically optimal parallel solvers for elliptic PDEs

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adaptive discretizations

arbitrary geometries

high-order discretizations

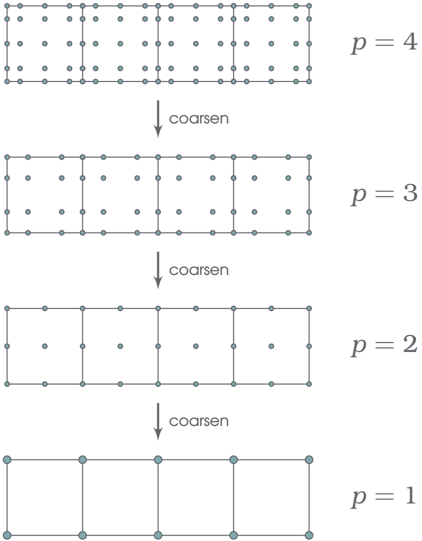
massively parallel

How to support high-order discretizations ?

high-order discretizations

challenges

- p-multigrid
  - coarse grid based on lower-order polynomials
  - Use GMG once $p = 1$ has been reached



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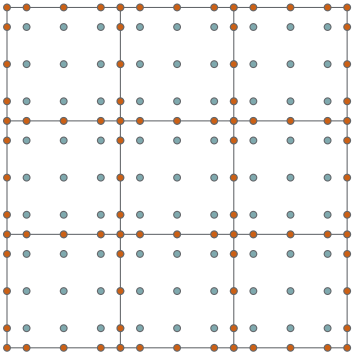
  - expensive local solves (deformed elements)
  - parallel scalability of coarse grid solve



Local Solve

Dirichlet boundary node

unknowns

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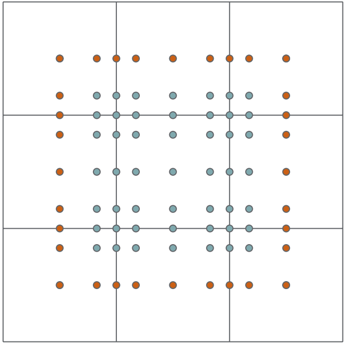
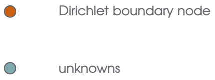


Schwarz Solve



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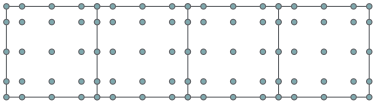
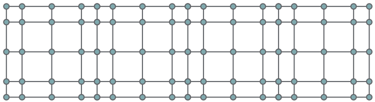
  - Spectrally equivalent
  - lower convergence at higher orders



$p = 4$



$p = 1$ collocated with $p = 4$

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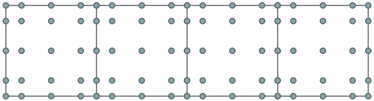
- h-multigrid using high-order discretizations
  - Use AMG (Heys *et al.*)



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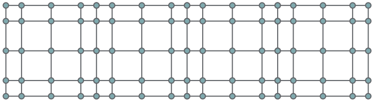

$p = 1$ collocated with $p = 4$

high-order discretizations

precondition using lower-order operator

Number of pCG iterations to converge to a relative tolerance of 10^{-8}

order	8×8	32×32	128×128	$8 \times 8 \times 8$
1*	4	4	4	5
2	14	14	14	25
3	21	21	21	45
4	30	30	30	79
5	43	43	43	144
6	64	65	65	260
7	98	99	99	465
8	142	146	148	840

high-order discretizations

h-multigrid using high-order discretizations

- Coarsening, inter-grid operators & coarse-grid solvers are straightforward

high-order discretizations

h-multigrid using high-order discretizations

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- Coarsening, inter-grid operators & coarse-grid solvers are straightforward
- Smoothers
  - Jacobi
  - chebyshev
  - Symmetric SOR

high-order discretizations

h-multigrid using high-order discretizations

- Coarsening, inter-grid operators & coarse-grid solvers are straightforward
- Smoothers
  - Jacobi
  - chebyshev
  - Symmetric SOR
- MG as a solver or with PCG

high-order discretizations

h-multigrid using high-order discretizations

Number of CG iterations/v-cycles to converge to a relative tolerance of 10^{-8}

order	Multigrid			MG pCG		
	Jacobi(3)	Chebyshev(3)	SSOR(2)	Jacobi(3)	Chebyshev(3)	SSOR(2)
1	5	6	4	4	4	4
2	6	10	4	5	6	4
3	8	24	5	6	11	4
4	-	54	8	-	16	6
5	-	178	13	-	28	8
6	-	-	24	-	51	12
7	-	-	70	-	105	19
8	-	-	270	-	204	36

high-order discretizations

h-multigrid using high-order discretizations

Number of CG iterations/v-cycles to converge to a relative tolerance of 10^{-8}

order	Multigrid			MG pCG			pCG
	Jacobi(3)	Chebyshev(3)	SSOR(2)	Jacobi(3)	Chebyshev(3)	SSOR(2)	linear
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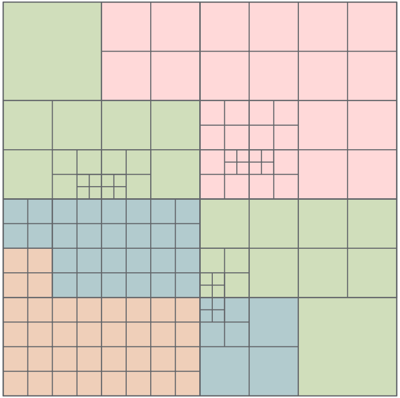
2	6	10	4	5	6	4	14
3	8	24	5	6	11	4	21
4	-	54	8	-	16	6	30
5	-	178	13	-	28	8	43
6	-	-	24	-	51	12	65
7	-	-	70	-	105	19	99
8	-	-	270	-	204	36	148

high-order discretizations

parallelizing SSOR - Octree Coloring

- block parallel SOR
- need coloring to define ordering
- Only boundary nodes need to be colored
- Coloring for balanced octree boundaries
  - Similar to Quadtree coloring
- Luby, LDF, SDL
- SDL $\longrightarrow$ 5 balanced colors



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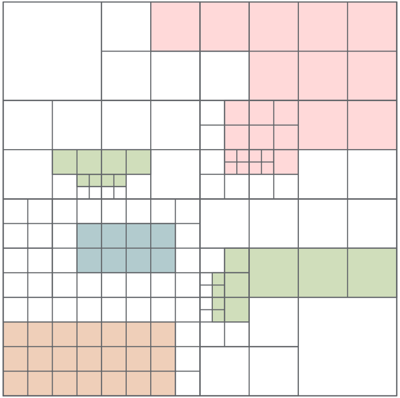

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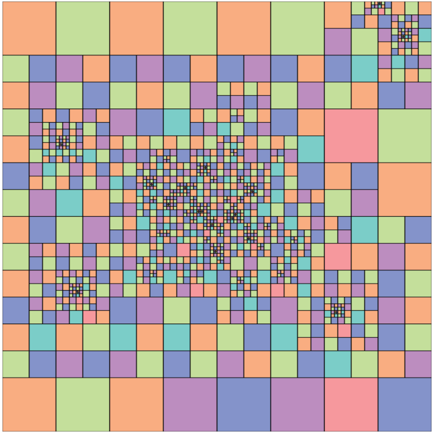

Summary

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- parallel, matrix-free multigrid method on geometry-conforming unstructured forests of octrees
- pCG using SSOR as a smoother capable of supporting high-order discretizations
- demonstrated strong scalability from 512 to $131K$ cores
- demonstrated weak scalability up to $262K$ cores using one MPI process per core
- largest solve was on a mesh with $45K$ octrees with 100 billion unknowns on $262K$ cores sustaining 272 TFlops/s
- Ongoing work to parallelize support for high-order discretizations

Thank you !