

A Strategy for Optimal Solvers in PyLith

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AMR Tutorial Workshop
Boulder, CO
Oct 24–27, 2007



“A very popular error – having the courage of one’s convictions: Rather it is a matter of having the courage for an attack upon one’s convictions.”
— Friedrich Wilhelm Nietzsche

Outline

- 1 Why Optimal Solvers?
- 2 Multigrid for Unstructured Meshes
- 3 Coupled Problems
- 4 Actual Work

Why Optimal Algorithms?

- The more powerful the computer, the **greater** the importance of optimality
- Example:
 - Suppose Alg_1 solves a problem in time CN^2 , where N is the input size
 - Suppose Alg_2 solves the same problem in time CN
 - Suppose Alg_1 and Alg_2 are able to use 10,000 processors
- In constant time compared to serial,
 - Alg1 can run a problem 100X larger
 - Alg2 can run a problem **10,000X** larger
- Alternatively, filling the machine's memory,
 - Alg1 requires 100X time
 - Alg2 runs in **constant** time

Linear Convergence

Convergence to $\|r\| < 10^{-9}\|b\|$ using GMRES(30)/ILU

Elements	Iterations
128	10
256	17
512	24
1024	34
2048	67
4096	116
8192	167
16384	329
32768	558
65536	920
131072	1730

Linear Convergence

Convergence to $\|r\| < 10^{-9}\|b\|$ using GMRES(30)/MG

Elements	Iterations
128	5
256	7
512	6
1024	7
2048	6
4096	7
8192	6
16384	7
32768	6
65536	7
131072	6

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Why not use AMG?

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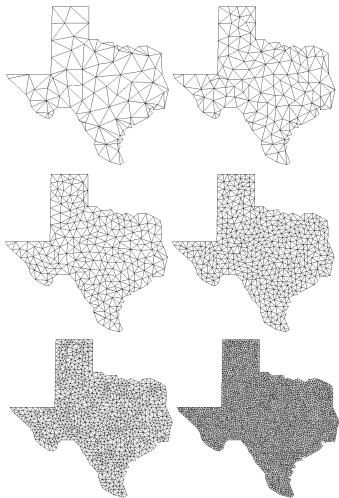
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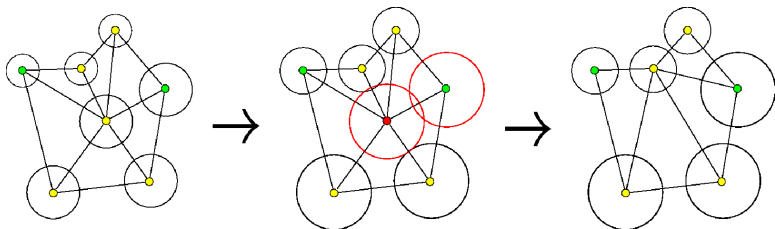
- Of course we will try AMG
 - BoomerAMG, ML, SAMG, ASA
- Problems with vector character
- Geometric aspects to the problem
 - Material property variation
 - Faults

Coarsening



- Users want to control the mesh
- Developed efficient, topological coarsening
 - Miller, Talmor, Teng algorithm
- Provably well-shaped hierarchy

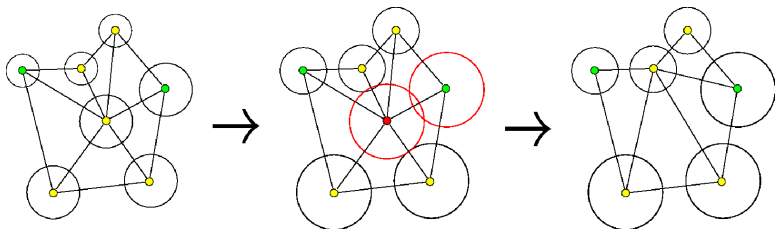
Miller-Talmor-Teng Algorithm



Simple Coarsening

- 1 Compute a **spacing function** f for the mesh (Koebe)

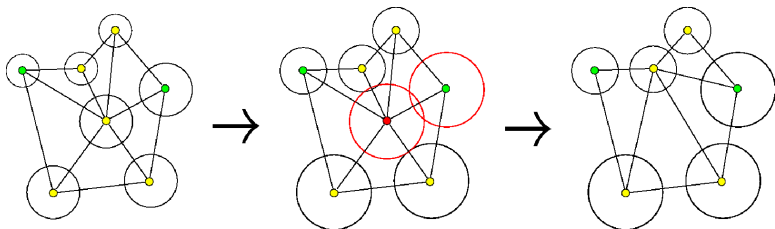
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Simple Coarsening

- 1 Compute a **spacing function** f for the mesh (Koebe)
- 2 Scale f by a factor $C > 1$

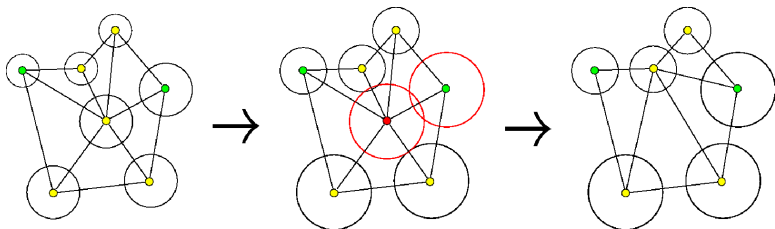
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- 1 Compute a **spacing function** f for the mesh (Koebe)
- 2 Scale f by a factor $C > 1$
- 3 Choose a maximal independent set of vertices for new f

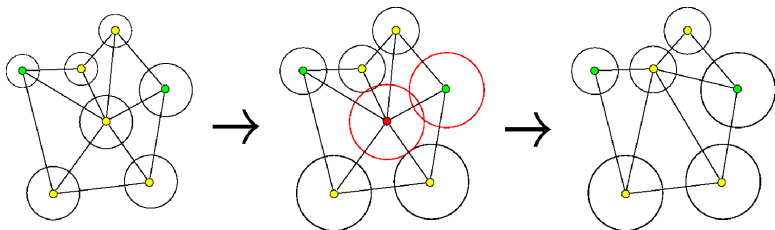
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Simple Coarsening

- 1 Compute a **spacing function** f for the mesh (Koebe)
- 2 Scale f by a factor $C > 1$
- 3 Choose a maximal independent set of vertices for new f
- 4 Retriangulate

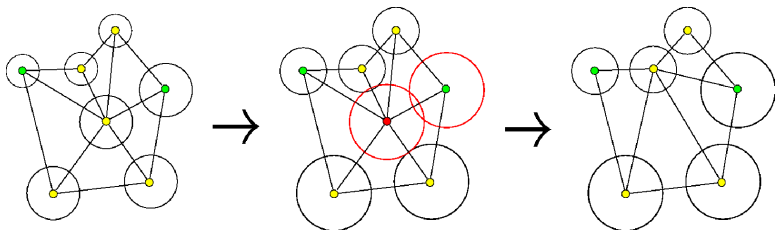
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Caveats

- 1 Must generate coarsest grid in hierarchy first

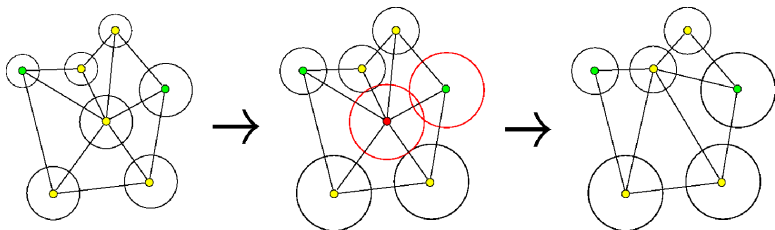
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- 1 Must generate coarsest grid in hierarchy first
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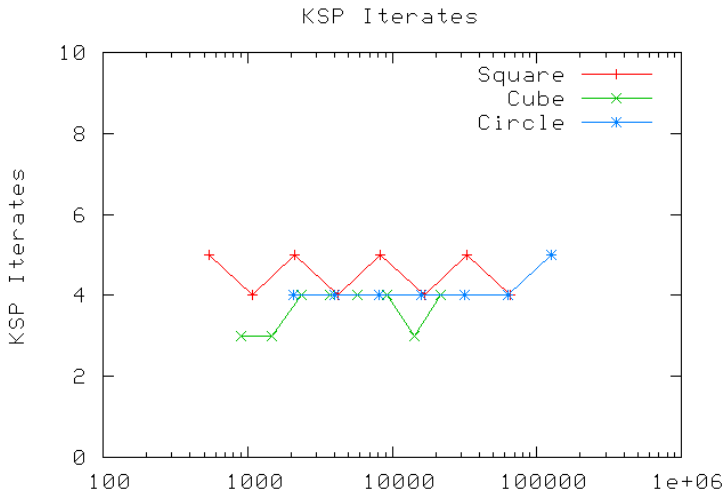
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- 1 Must generate coarsest grid in hierarchy first
- 2 Must choose boundary vertices first (and protect boundary)
- 3 Must account for boundary geometry

GMG Performance

For simple domains, everything works as expected:

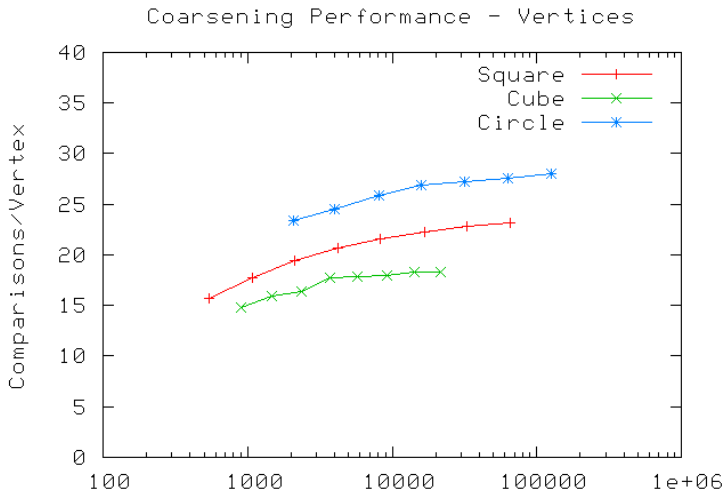
Linear solver iterates are constant as system size increases:



GMG Performance

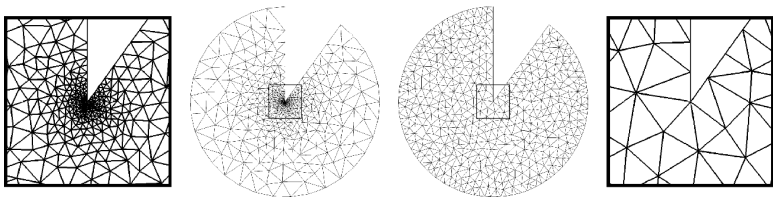
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Work to build the preconditioner is constant as system size increases:



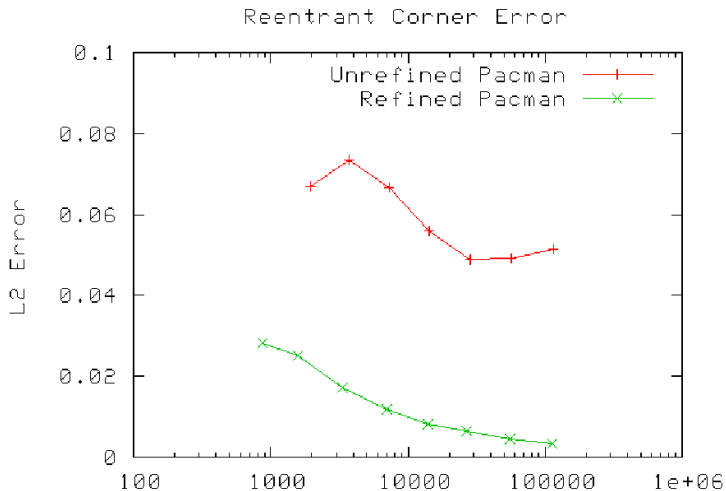
Reentrant Problems

- Reentrant corners need nonuniform refinement to maintain accuracy
- Coarsening preserves accuracy in MG without user intervention



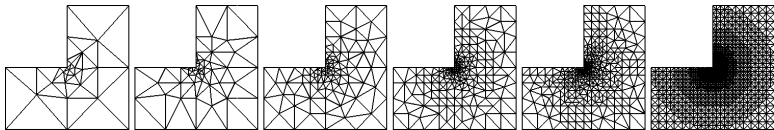
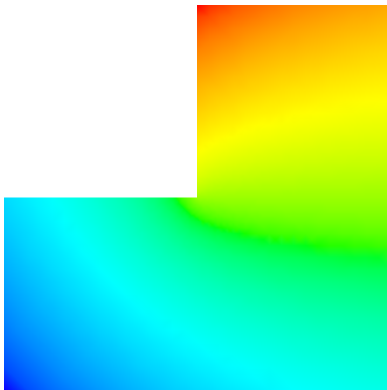
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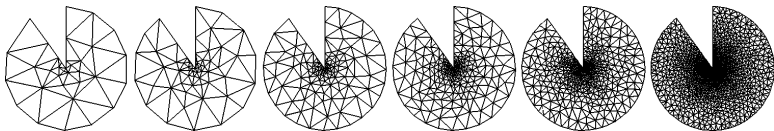
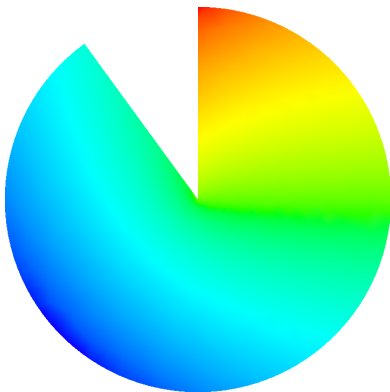
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Exact Solution for reentrant problem: $u(x, y) = r^{\frac{2}{3}} \sin(\frac{2}{3}\theta)$



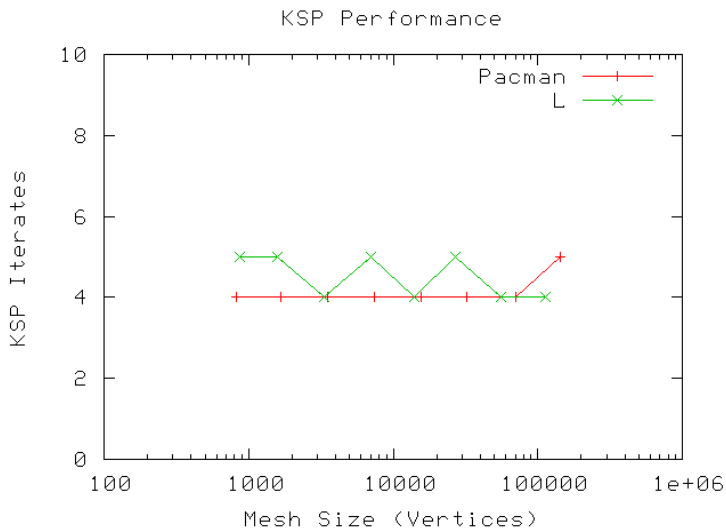
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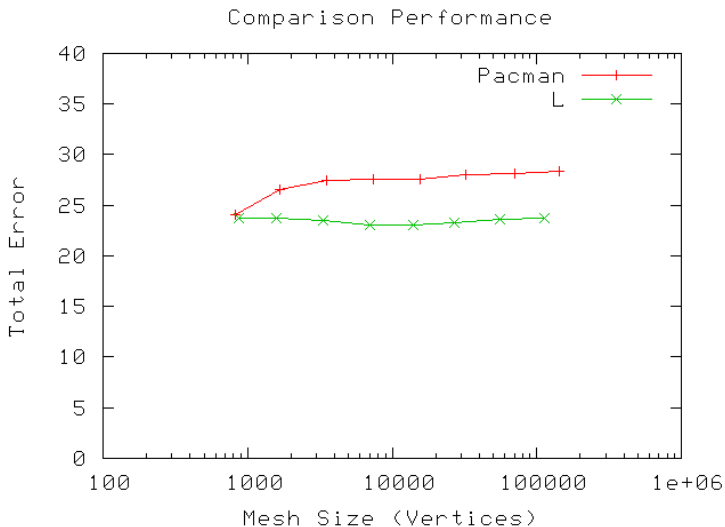
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Difficulties

We would like to couple

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However, we must cope with

- different length scales
- different time scales
- solving full algebraic system

Length Scales

We assume that

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- these meshes will change slowly during the simulation
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- 3 Solve each subproblem on its own hierarchy

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Our proposed solution is then

- 1 to formulate the problem as spacetime FEM
- 2 use Multi-Adaptive Galerkin timestepping

Multi-Adaptive Galerkin Methods for ODEs I,
Anders Logg, SISC, **24**, pp. 1879–1902, 2003.

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Jacobian-free Newton-Krylov methods: a survey of approaches and applications,
D.A. Knoll and D.E. Keyes, JCP, **193**, 2, pp. 357–397, 2004.

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PETSc Work

- New boundary protection scheme
 - Better preservation of embedded boundaries
- Replace mesh generator call with flips
 - Do not need point insertion

PyLith Work

- Replace KSP solver with DMMG
 - Enables GMG
 - Enables nonlinear solver
- Fix MG interpolation for cohesive elements
 - Collocation
 - Weighted average in a ball