hypre - High Performance Preconditioners

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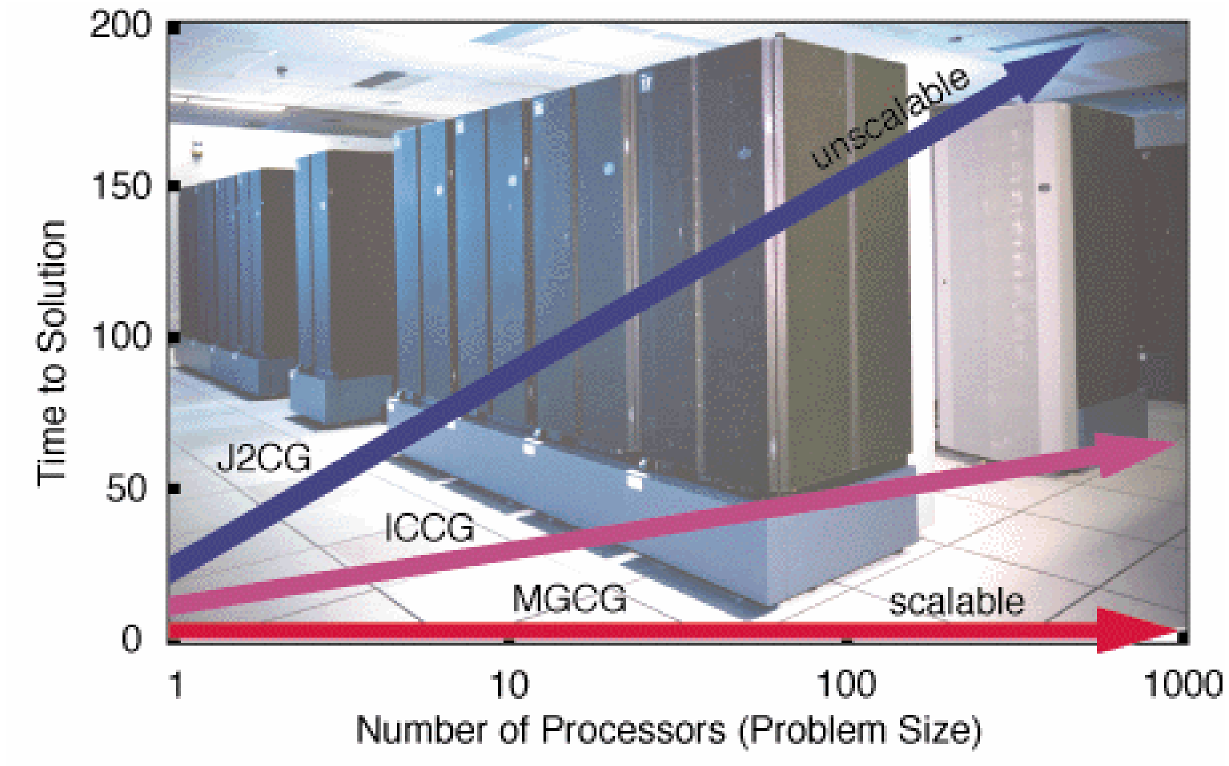
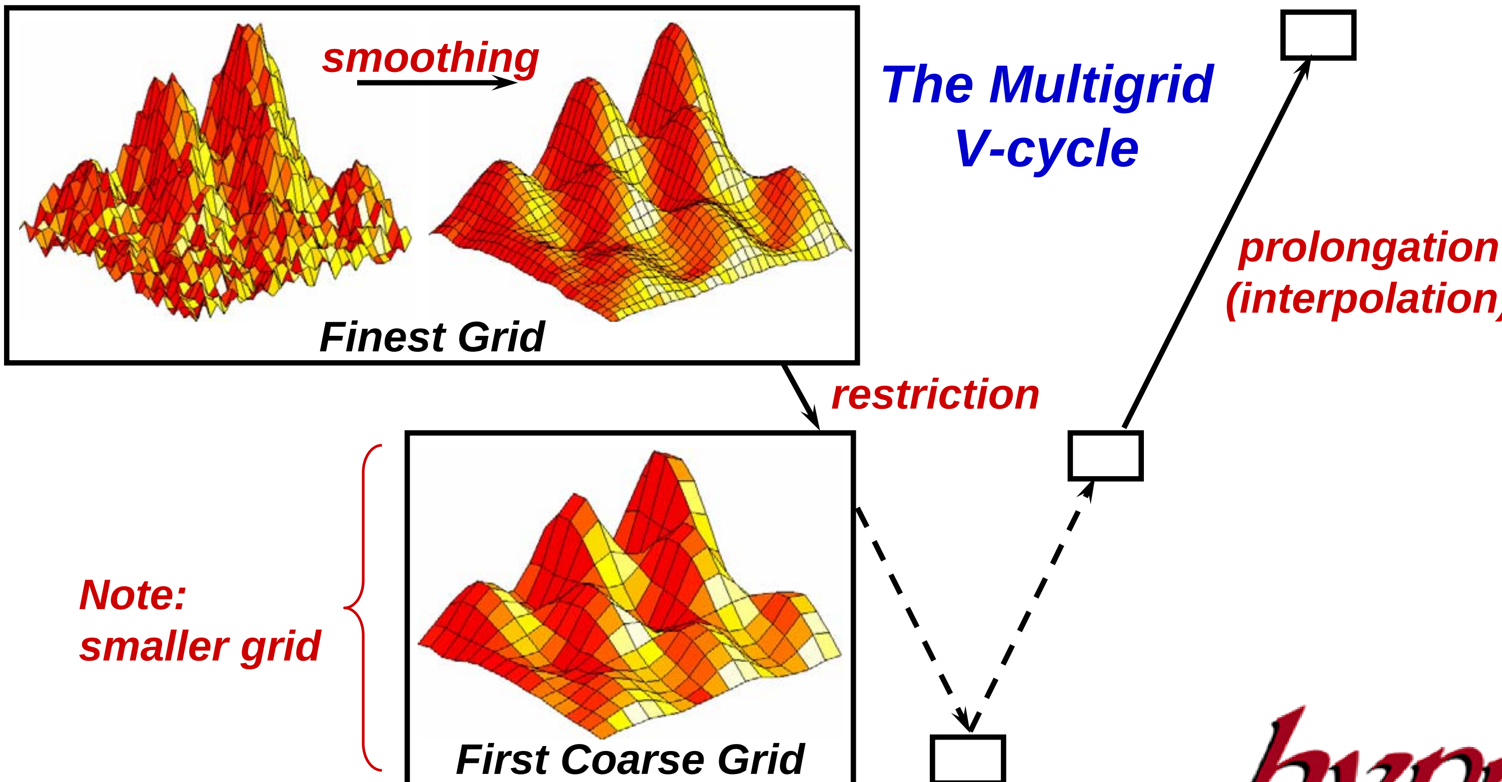
CIG Workshop
October 17, 2006

Scalability is a central issue for large-scale parallel computing

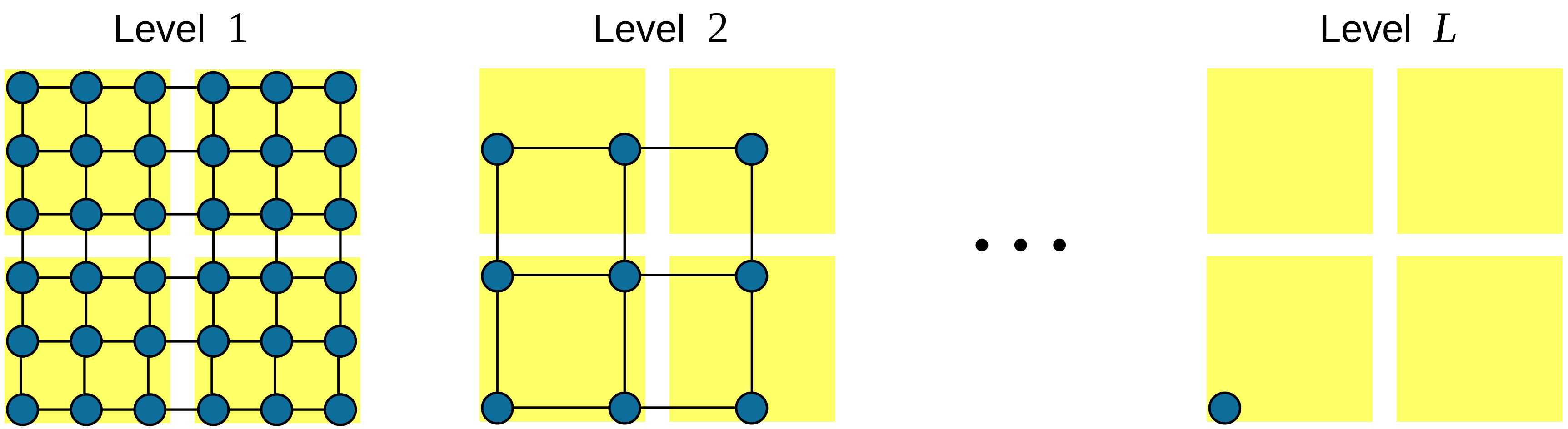


Want (nearly) constant solution time as problem size grows in proportion to the number of processors

Multigrid methods use coarse grids to efficiently damp out smooth error



Approach for parallelizing multigrid is straightforward data decomposition



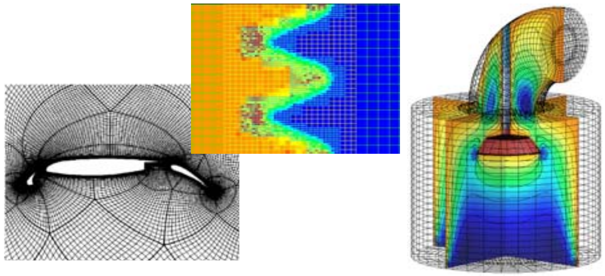
- **Basic communication pattern is “nearest neighbor”**
- **Time for doing relaxation in a *V*-cycle is**

$$T = O(\log\ N)\alpha + O(n)\beta + O(n^2)\gamma$$

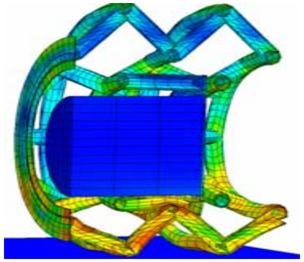
- **Primary difference between this and a simple matrix-vector multiply is the *log* term**

We are developing *MG* methods for a variety of application settings

- **Geometric multigrid for semi-structured grids**
  - — Grids highly structured, e.g., block-structured, structured AMR, overset
  - — Exploit structure where present



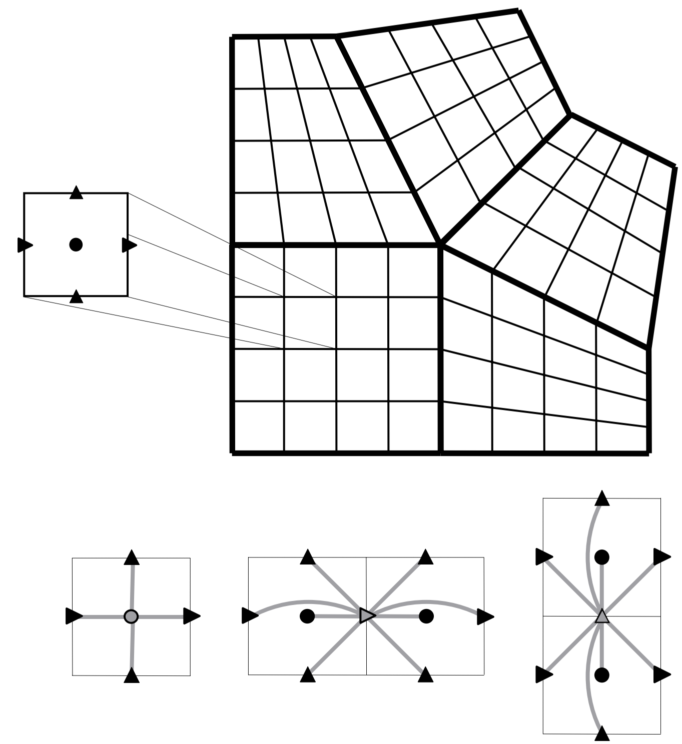
- **Algebraic multigrid (*AMG*) for unstructured grids**
  - — Assumes only the underlying matrix
  - — Automatically coarsens “grids”
  - — Characterizing smooth error is key



- **Our work ranges from…**
  - — longer-term fundamental research and theory, to
  - — shorter-term focused research and software development

Conceptual system interfaces supply “best” solvers

- **Example: *hypre*’s interface for semi-structured grids**
- **Appropriate for problems that are mostly structured**
  - **based on “grids” and “stencils”**
- **Allows for specialized solvers like *FAC* for structured AMR**
  - **First time in a linear solver library**
- **Also provides for more general solvers like *AMG***
- **This is unique to *hypre***

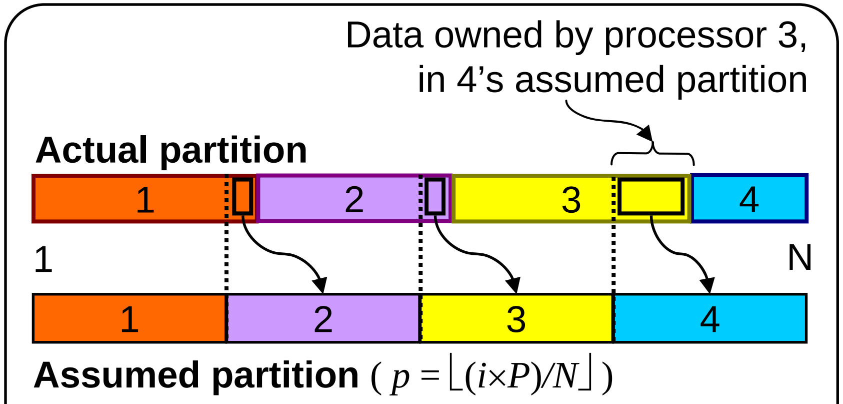


A block-structured grid with 3 variable types and 3 discretization stencils

New assumed partition (AP) algorithm enables scaling to 100K+ procs

- **Answering global data distribution queries currently requires $O(P)$ storage and computations (e.g., `MPI_Allgatherv`)**
- **On BG/L, storing $O(P)$ data is not always practical or possible**

- **New algorithm employs an assumed partition to answer queries through a kind of rendezvous algorithm**
- **Reduces storage to $O(1)$ and computations to $O(\log P)$**
- **Developed for *hypre*'s *IJ* and *SEMI* interfaces**
- **Assumed partition idea may help wherever there is a call to `MPI_Allgatherv`**



Actual partition info is sent to the assumed partition processors → distributed directory

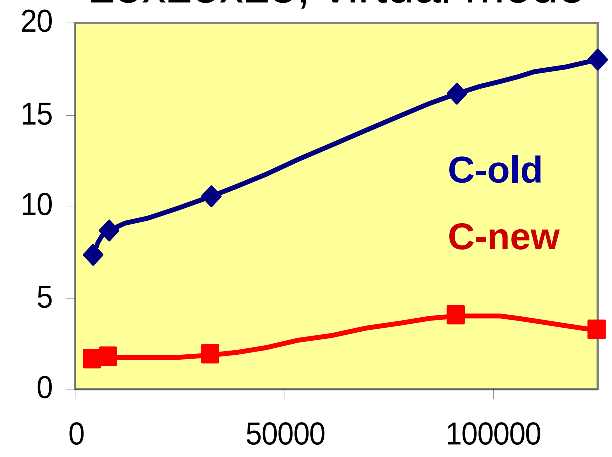
New AP and coarsening algorithms in *AMG* reduces memory and is 16x faster on BG/L

- ***BoomerAMG-CG*, total times in seconds**

Algorithms:	global partition (old)		assumed partition (new)	
# of procs	C-old	C-new	C-old	C-new
4,096	12.42	3.06	12.32	2.86
64,000	67.19	10.45	19.85	4.23

7pt 3D Laplacian; 30x30x30 unknowns per processor; co-processor mode

25x25x25; virtual mode

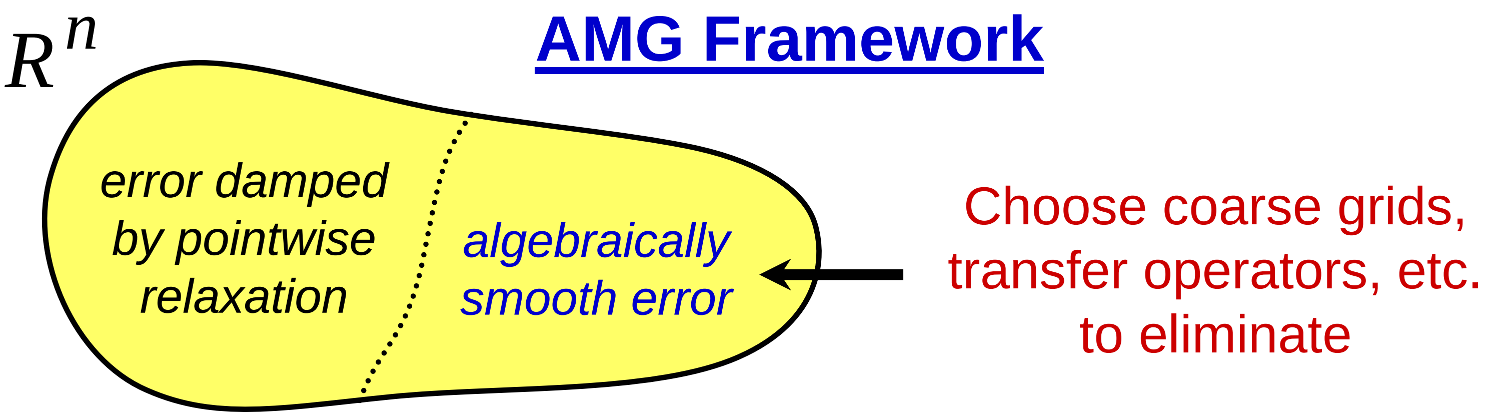


- **Coarsening algorithms:**
  - **C-old: *RS* with *CLJP* between procs**
  - **C-new: *HMIS* with 1 aggressive**
- **15x overall speedup on 64K procs!**
- **2 billions unknowns on 125K procs!**

Good local characterization of smooth error is key to *AMG*

- **Early *AMG* work assumed pointwise smoothers:**

AMG Framework



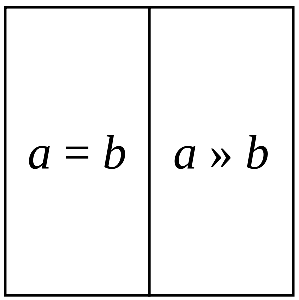
- ***Weak approximation property*: *interpolation must be more accurate on small eigenmodes***

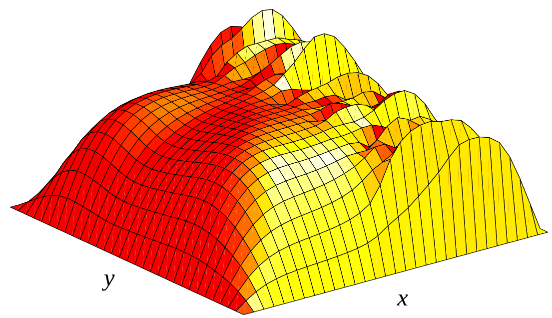
- **The near null space (kernel) is important!**

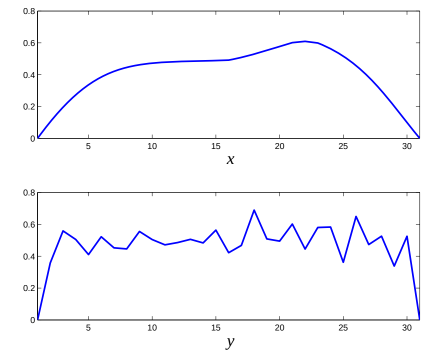
Algebraically smooth error can be geometrically oscillatory

- **7 GS sweeps on**

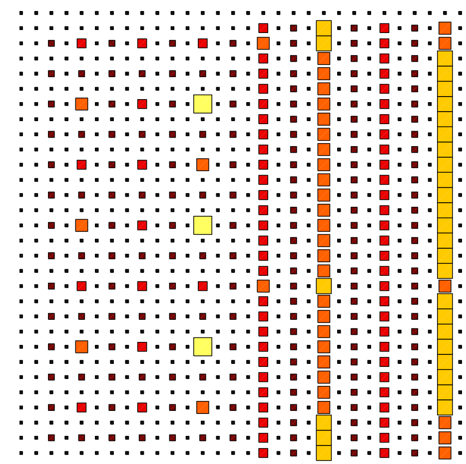
$$-au_{xx} - bu_{yy} = f$$







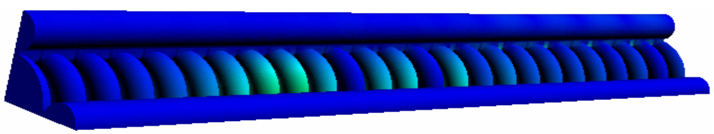
- **AMG can “follow physics”**
- **This example still targets geometric smoothness and pointwise smoothers**
- **Not sufficient for some problems!**



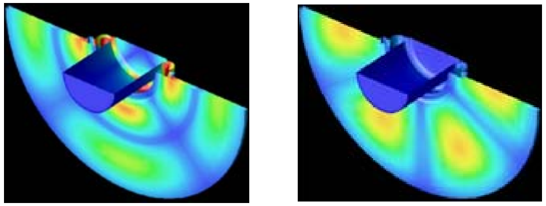
AMG coarse grids

We generalized the *AMG* framework to address new problem classes

- **Maxwell & Helmholtz problems have huge near null spaces and require more than pointwise smoothing**



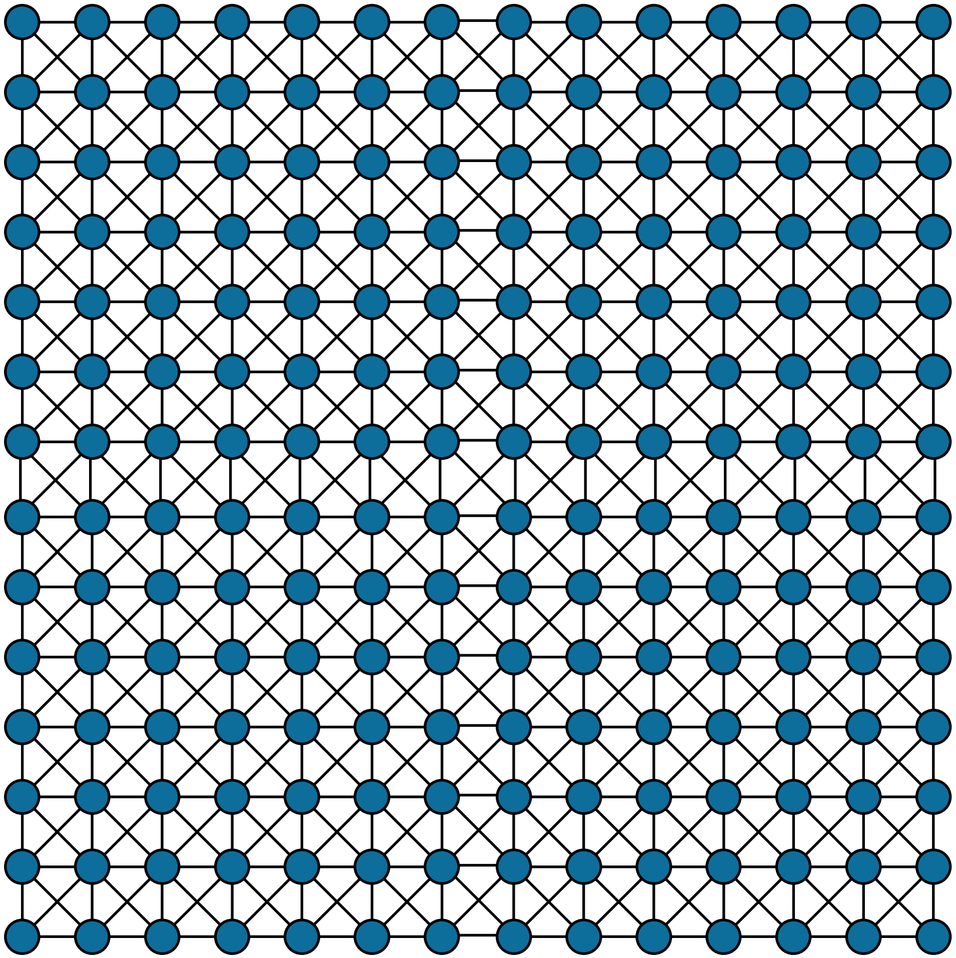
Model of a section of the Next Linear Collider structure



Resonant frequencies in a Helmholtz Application

- **Our new theory works for any smoother & formalizes idea of compatible relaxation (*CR*) (SINUM, 2004)**
  - **We defined several variants of *CR*, and proved that fast converging *CR* implies a good coarse grid**
  - ***CR* efficiently measures coarse grid quality!**
- **Developed *CR*-based coarsening algorithm**

CR to choose the coarse grid

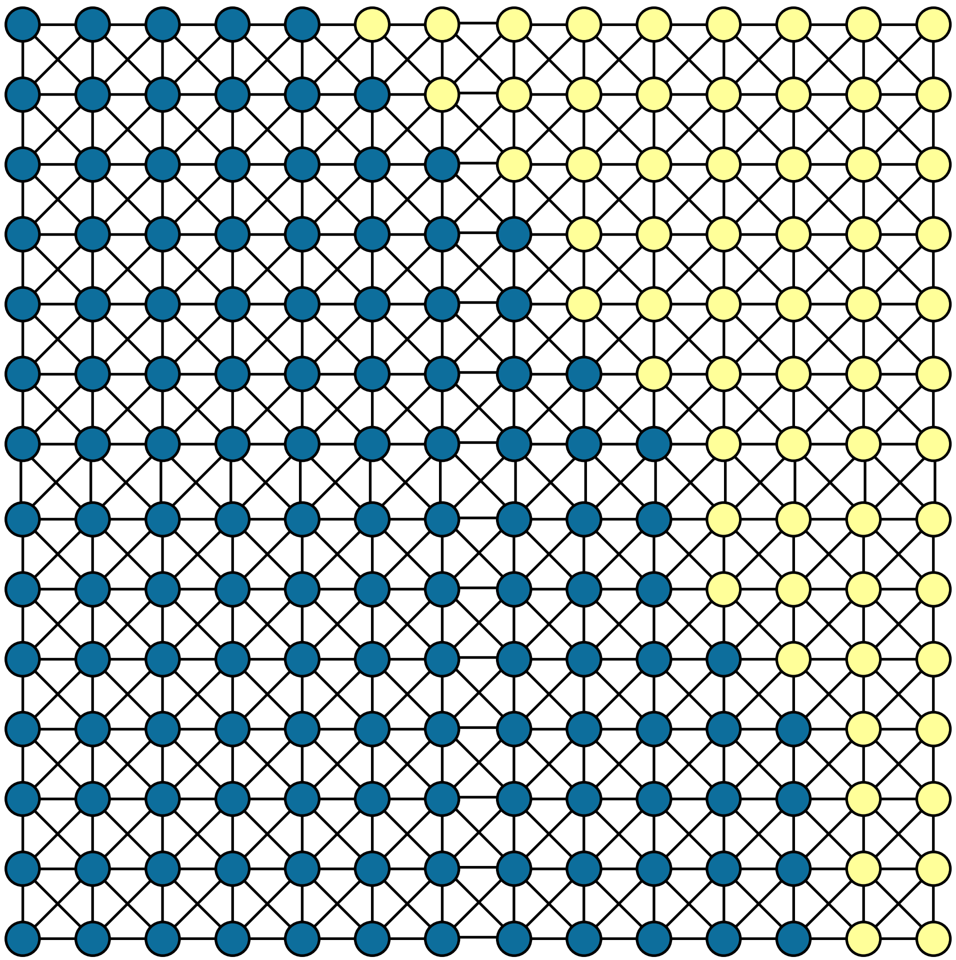


➔ Initialize U-pts

➔ Do *CR* on $Au=0$, and redefine U-pts

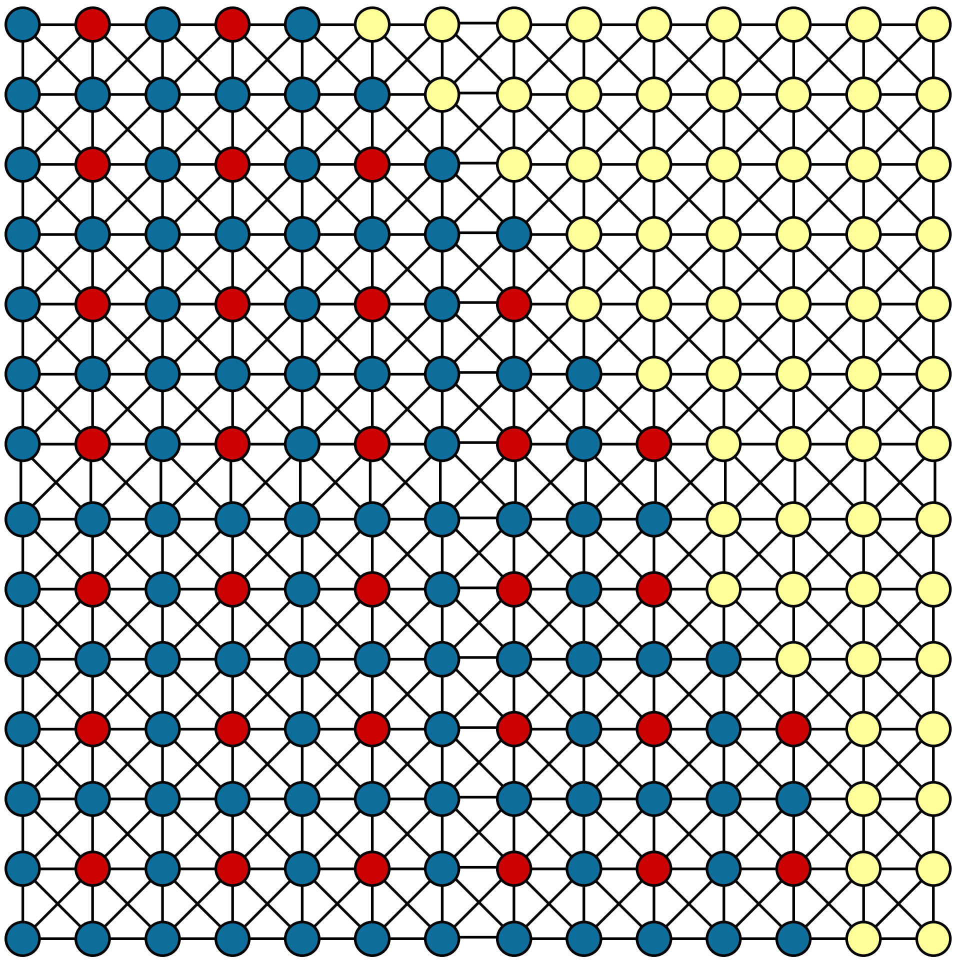
➔ Select new C-pts as indep. set over U

CR to choose the coarse grid



- ➔ Initialize U-pts
- ➔ **Do *CR* on $Au=0$, and redefine U-pts**
- ➔ Select new C-pts as indep. set over U

CR to choose the coarse grid



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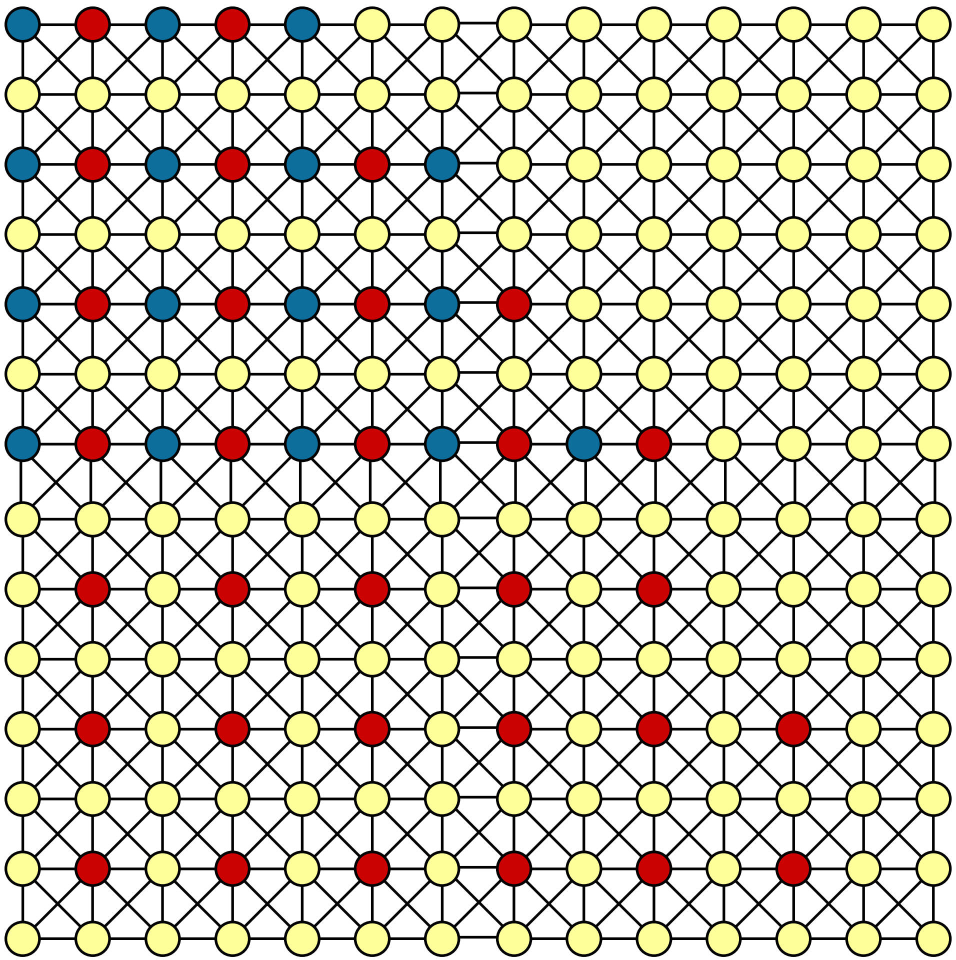
CR to choose the coarse grid



- ➔ Initialize U-pts
- ➔ **Do *CR* on $Au=0$, and redefine U-pts**
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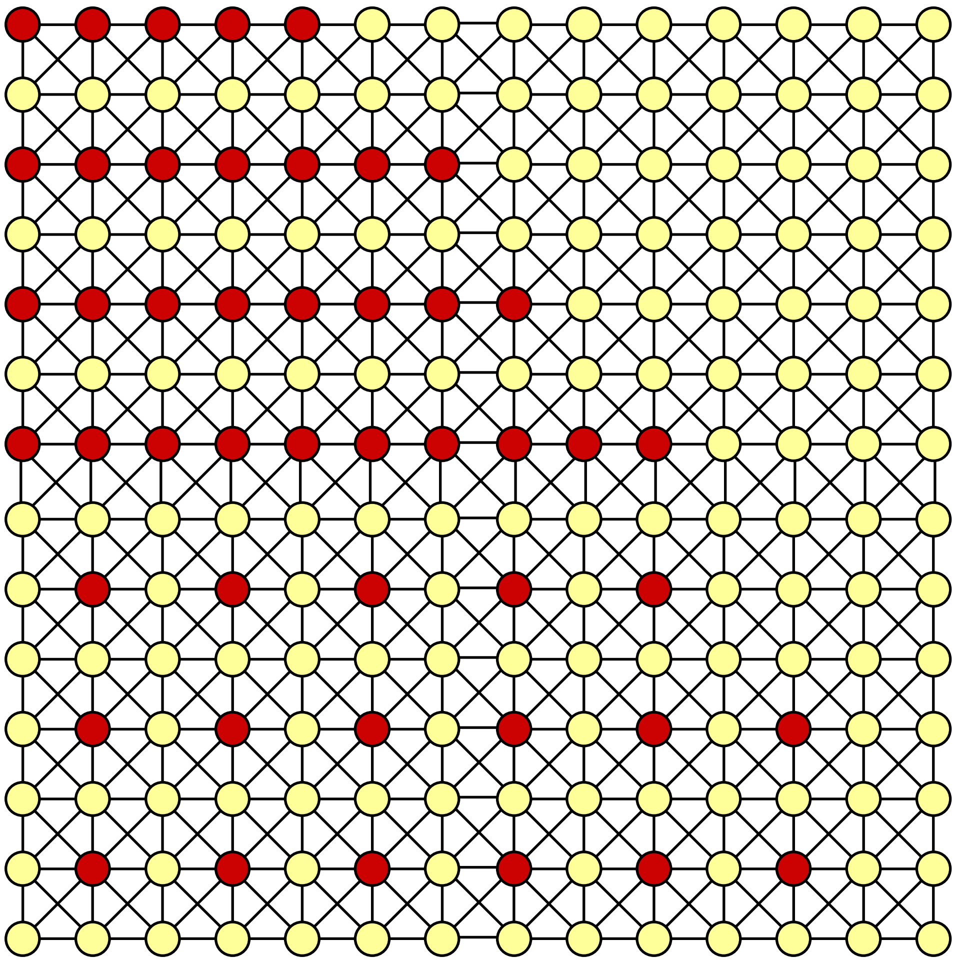
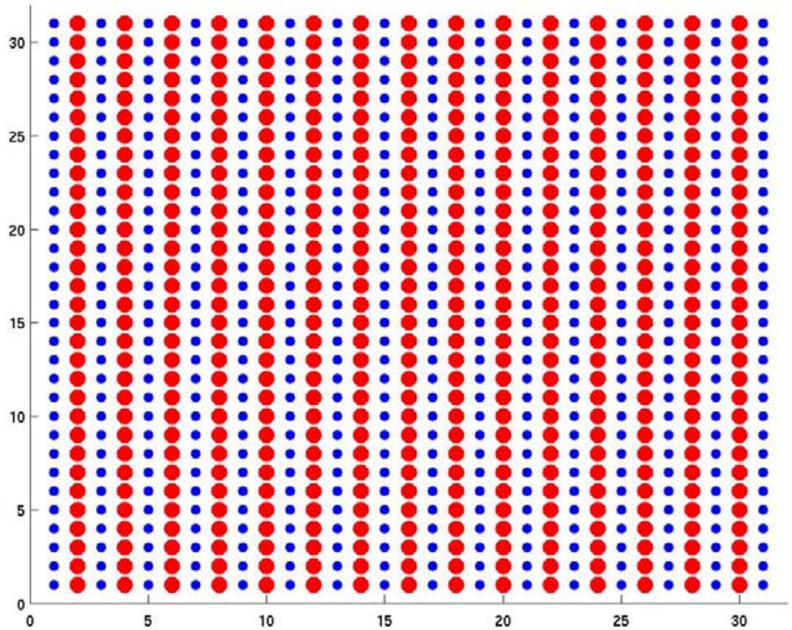
CR to choose the coarse grid

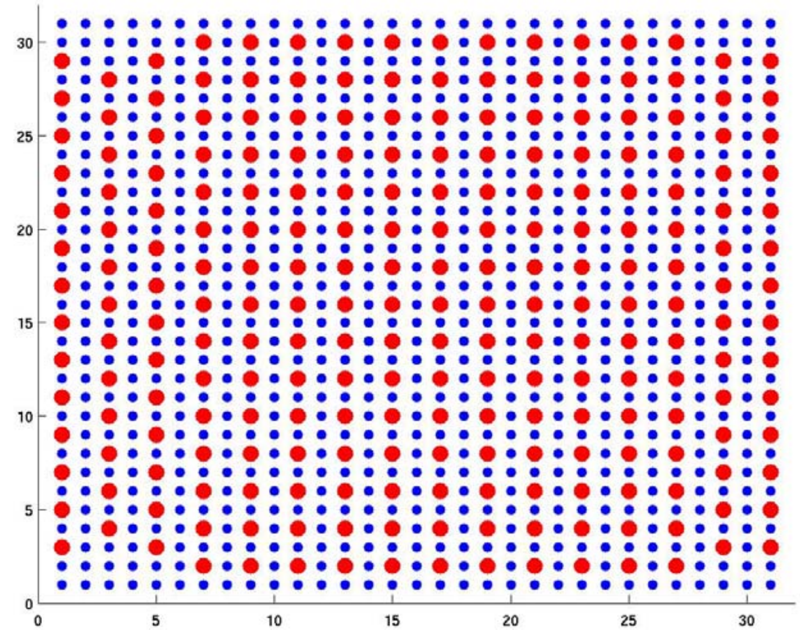


- ➔ Initialize U-pts
- ➔ Do *CR* on $Au=0$, and redefine U-pts
- ➔ **Select new C-pts as indep. set over U**

Anisotropic 9-pt FE: coarse grids reflect smoother used in *CR*

- **Pointwise Gauss-Seidel *CR***
- **Line Jacobi *CR***





- ***Not possible with other coarsening algorithms!***
- **Need new interpolation schemes to use in AMG**

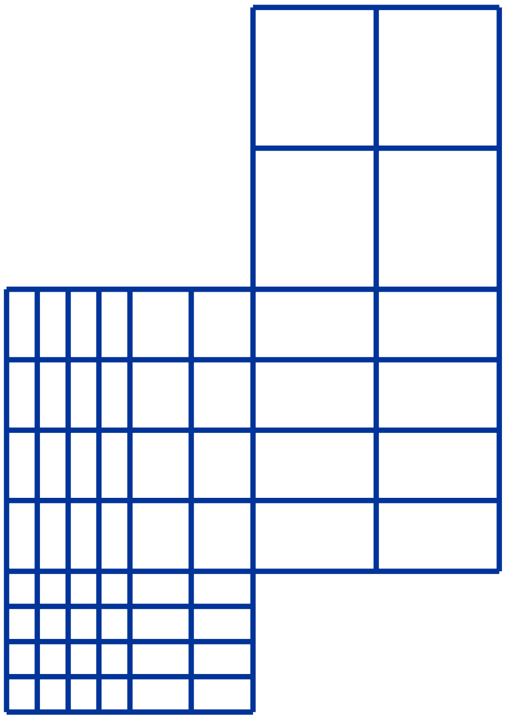
Current solver / preconditioner availability via *hypre*'s conceptual interfaces

Solvers	System Interfaces			
	Struct	SStruct	FEI	IJ
Jacobi	✓	✓		
SMG	✓	✓		
PFMG	✓	✓		
Split		✓		
SysPFMG		✓		
FAC		✓		
Maxwell		✓		
AMS		✓	✓	✓
BoomerAMG		✓	✓	✓
MLI		✓	✓	✓
ParaSails		✓	✓	✓
Euclid		✓	✓	✓
PILUT		✓	✓	✓
PCG	✓	✓	✓	✓
GMRES	✓	✓	✓	✓
BiCGSTAB	✓	✓	✓	✓
Hybrid	✓	✓	✓	✓

SMG and PFMG are semicoarsening multigrid methods for structured grids

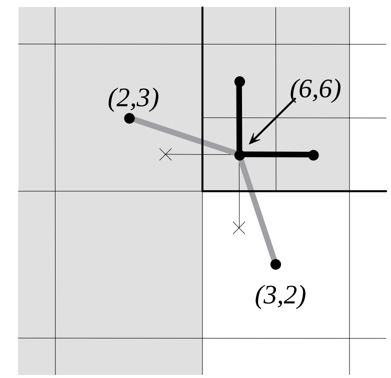
- Interface: `Struct/SStruct`
- Matrix Class: `Struct/SStruct`

- SMG uses plane smoothing in 3D, where each plane "solve" is effected by one 2D V-cycle
- SMG is very robust
- PFMG uses simple pointwise smoothing, and is less robust

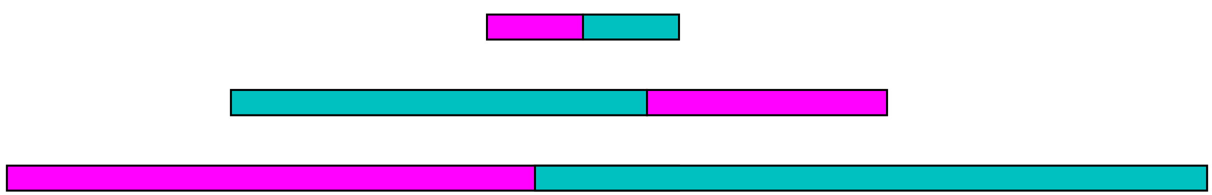


- Constant-coefficient versions!

FAC is an algebraic cell-centered fast adaptive composite grid solver in *hypre*



- **Interface: `SStruct`**
- **Matrix Class: `SStruct`**
- **Requires only the composite matrix**
  - no coarse underlying matrix needed
- **Does not require nested AMR levels in the processor distribution, e.g., 3 levels on 2 procs**
  - uses intra- and inter-level communication

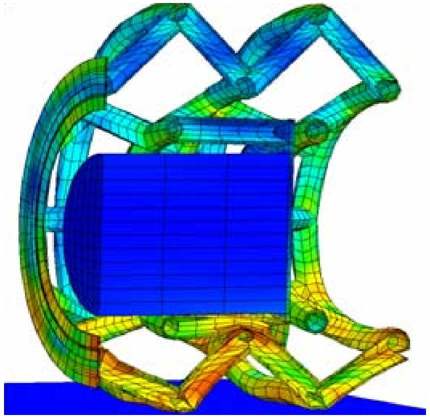


- **Designed for smooth-coefficient diffusion problems**

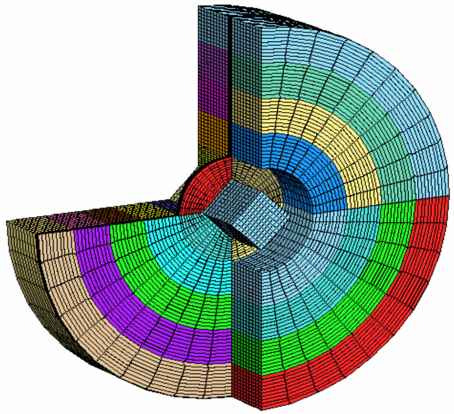
BoomerAMG is an algebraic multigrid method for unstructured grids

- Interface: `SStruct, FEI, IJ`
- Matrix Class: `ParCSR`

- Originally developed as a general matrix method (i.e., assumes given A, x, and b only)
- Uses various coarsening, interpolation and relaxation schemes
- Automatically defines coarse “grids”
- Can also be used for solving systems of PDEs if additional information provided

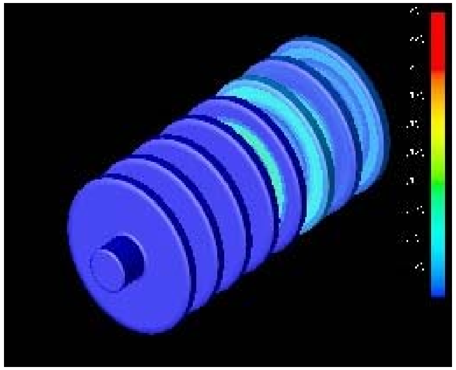


DYNA3D



PMESH

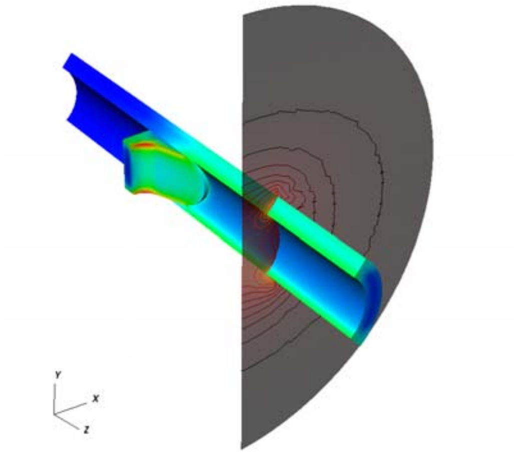
New: We have just released a Maxwell solver for (semi)-structured grids



- Interface: `SStruct`
- Matrix Class: `SStruct`

- Solves definite problems $\nabla \times \alpha \nabla \times E + \beta E = f, \ \beta > 0$
- Uses multiple coarsening and special relaxation, a coupled hierarchy to resolve different vector components of the correction
- Requires the linear system and a gradient matrix
- Only for edge finite element discretizations

New: AMS is an auxiliary space Maxwell solver for unstructured grids

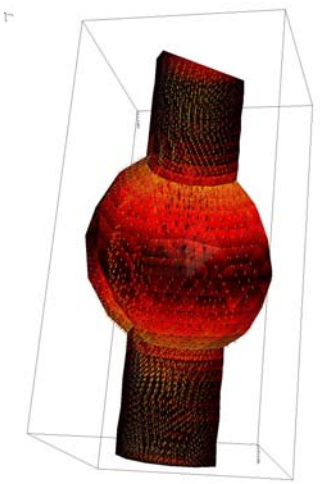


- **Interface: `SStruct, FEI, IJ`**
- **Matrix Class: `ParCSR`**

- **Solves definite problems:**

$$\nabla\times\alpha\nabla\times E+\beta E=f,\quad \alpha>0,\ \beta\geq 0$$

- **Requires the linear system, a gradient matrix, the coordinates of the mesh vertices**
- **Based on methods by Hiptmair and Xu**
- **Uses BoomerAMG**

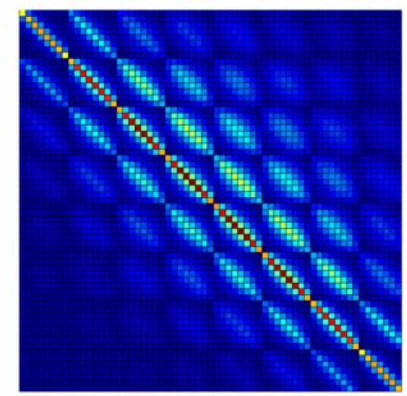


ParaSAILS is an approximate inverse method for sparse linear systems

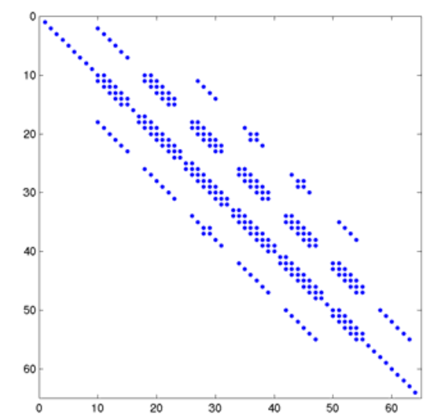
- Interface: `SStruct, FEI, IJ`
- Matrix Class: `ParCSR`

- Approximates the inverse of *A* by a sparse matrix *M* by minimizing the Frobenius norm of *I* - *AM*
- Uses graph theory to predict good sparsity patterns for *M*

Exact inverse

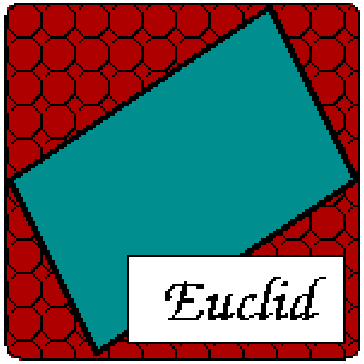


Approx inverse



Euclid is a family of Incomplete LU methods for sparse linear systems

- **Interface: `SStruct, FEI, IJ`**
- **Matrix Class: `ParCSR`**



- **Obtains scalable parallelism via local and global reorderings**
- **Good for unstructured problems**

- **`http://www.cs.odu.edu/~hysom/Euclid`**

The *hypre* library is LGPL open source

- **Download the source at:**

  http://www.llnl.gov/CASC/hypre/

  A short form must be filled out prior to download, just for our own records.

- **Send support questions, bug reports, etc. to:**

  hypre-support@llnl.gov

hypre Team

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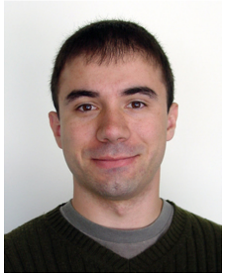
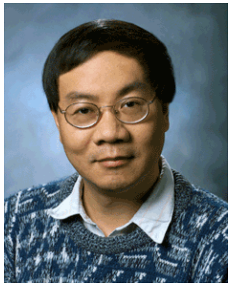


Tzanio Kolev

Jeff Painter



Charles Tong

Panayot Vassilevski

Ulrike Yang

Selected Publications

(see http://www.llnl.gov/casc/linear_solvers)

- "A Survey of parallelization Techniques for Multigrid Solvers," Chow, Falgout, Hu, Tuminaro, and Yang, *Parallel Processing For Scientific Computing*, Heroux, Raghavan, and Simon, editors, SIAM, series on Software, Environments, and Tools (to appear).
- "An Assumed Partition Algorithm for Determining Processor Inter-Communication," Baker, Falgout, and Yang, *Parallel Computing*, 32 (2006).
- "A Multigrid Method for Variable Coefficient Maxwell's Equations," Jones and Lee, *SIAM J. Sci. Comput.*, 27 (2006).
- "Adaptive Algebraic Multigrid," Brezina, Falgout, MacLachlan, Manteuffel, McCormick, and Ruge, *SIAM J. Sci. Comput.*, 27 (2006).
- "The Design and Implementation of *hypre*, a Library of Parallel High Performance Preconditioners," Falgout, Jones, and Yang, *Numerical Solution of Partial Differential Equations on Parallel Computers*, Bruaset and Tveito, editors, Springer-Verlag, 51 (2006).
- "Parallel Algebraic Multigrid Methods - High Performance Preconditioners," Yang, *Numerical Solution of Partial Differential Equations on Parallel Computers*, 51 (2006).
- "Conceptual Interfaces in *hypre*," Falgout, Jones, and Yang, *Future Generation Computer Systems*, Special Issue on PDE Software, 22 (2006).
- "Parallel Algebraic Multigrids for Structural Mechanics," Brezina, Tong, and Becker, *SIAM J. Sci. Comput*. 27 (2006).
- "Adaptive Smoothed Aggregation (αSA) Multigrid," Brezina, Falgout, MacLachlan, Manteuffel, McCormick, and Ruge, *SIAM Review: SIGEST*, 47 (2005).
- "On Two-Grid Convergence Estimates," Falgout, Vassilevski, and Zikatanov, *Numer. Linear Algebra Appl.*, 12 (2005).
- "On Generalizing the AMG Framework," Falgout and Vassilevski, *SIAM J. Numer. Anal.*, 42 (2004).

Thank You!

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

UCRL-PRES-225360