An Algebraic Multigrid Approach to PDE Systems with Variable Degrees-of-Freedom Per Node

Ray Tuminaro

David Noble

Sandia National Labs

Center for Computing Research

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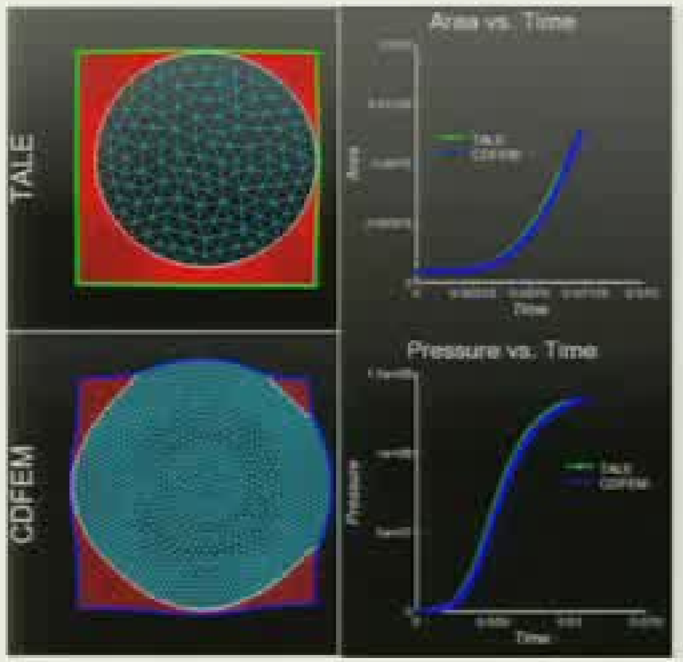
Outline

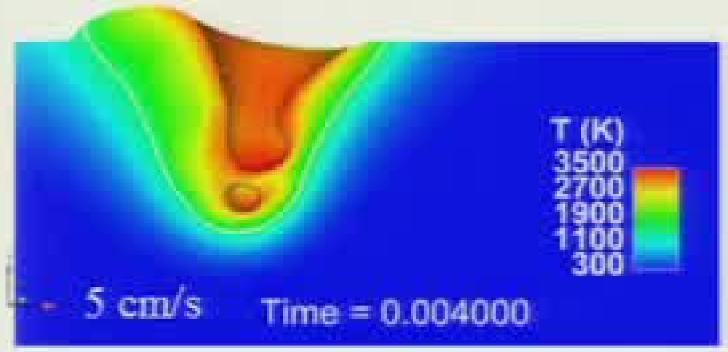
- Interfaces & CDFEM discretization
  - advantages: avoids re-meshing, captures interfaces (with discontinuities), leverages standard FE technology
  - concerns: bad elements, solution accuracy & matrix conditioning
- AMG challenges for PDE systems
  - interface problems with variable dofs/node
- An AMG strategy for variable dofs/node PDE systems
  - separate interpolation for different fields
  - interfaces & grid transfer sparsity patterns
- Numerical results

Motivation

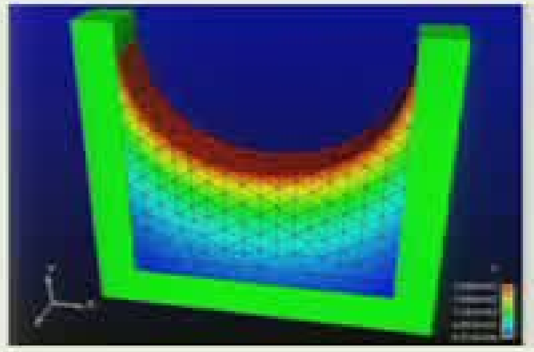
Applications with moving or complex interfaces & discontinuous physics/fields



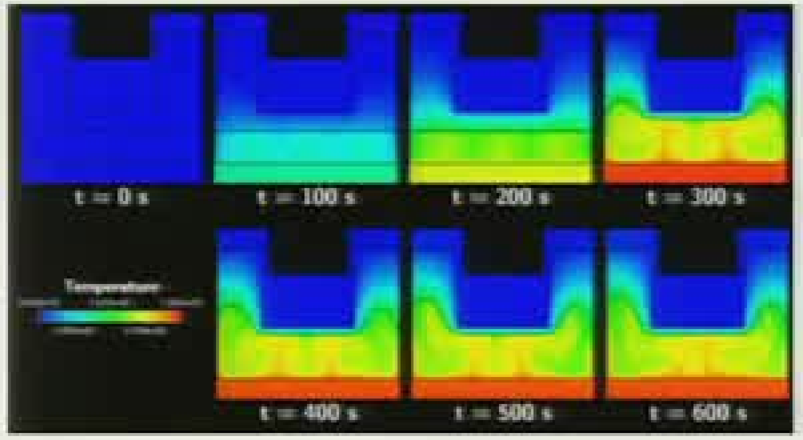
Conductive burn
of energetic materials



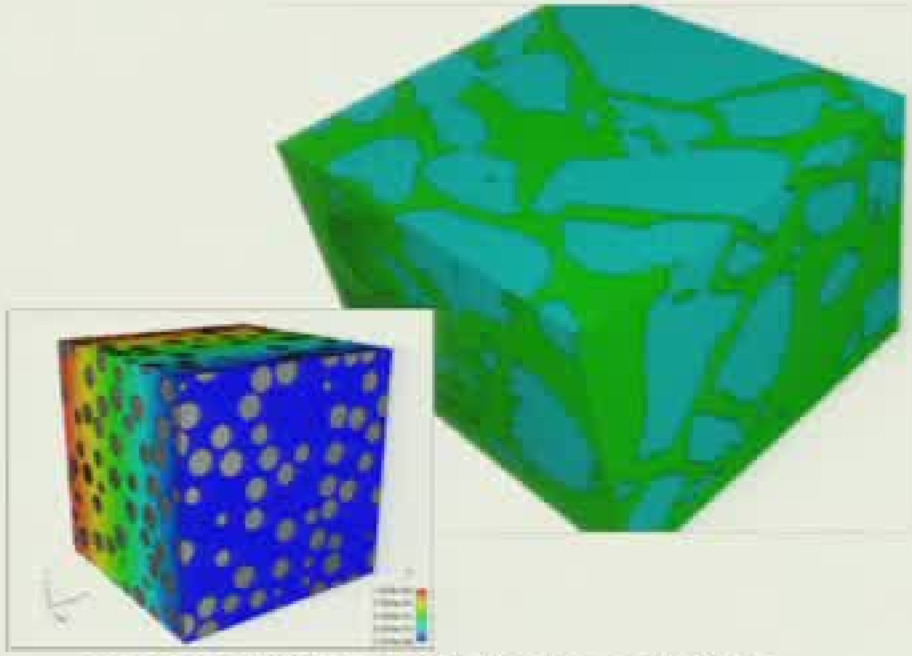
Laser welding



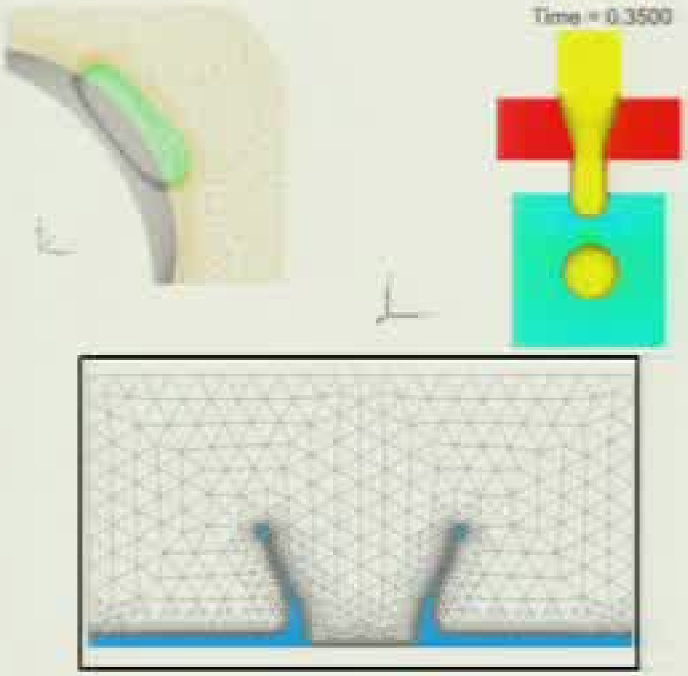
Material death



Organic Material Decomposition (OMD)
with coupled porous and low Ma flow



Transport in topologically complex
domains including composite
energetic materials and batteries



Capillary Hydrodynamics

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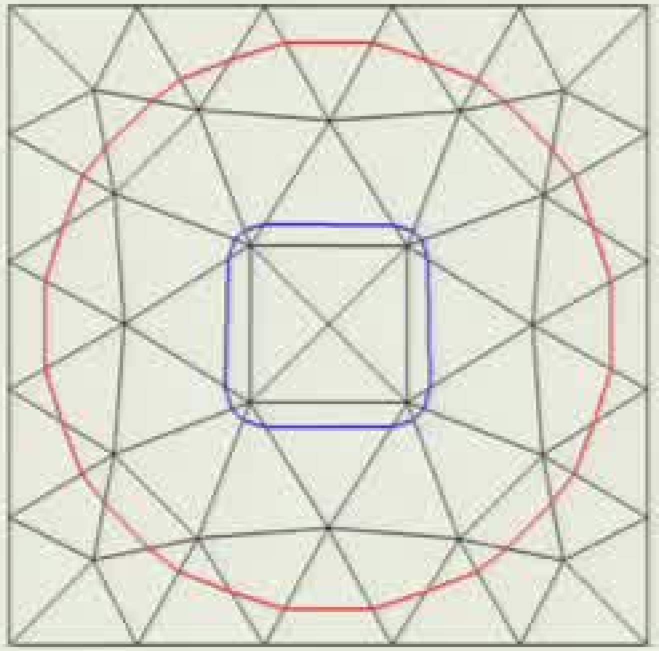
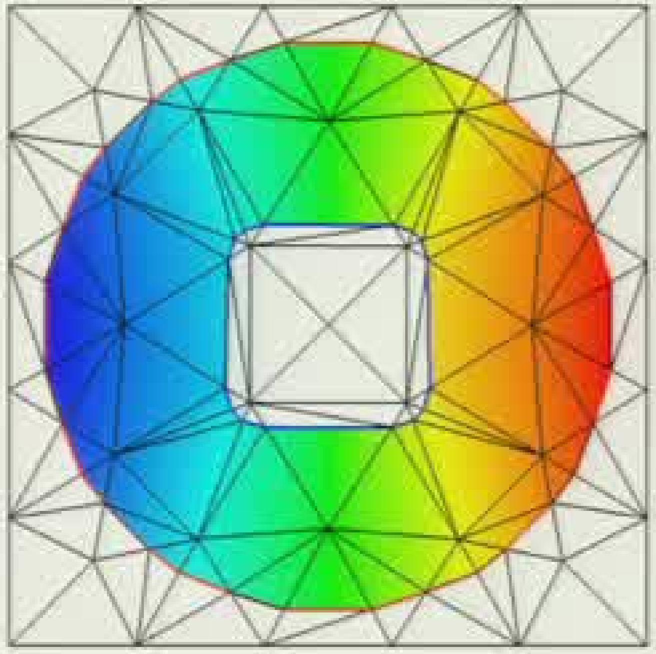
Conformal Decomposition Finite Element Method (CDFEM)

- Simple Concept (Noble, et al. 2010)
  - Use level sets to define materials or phases
  - Decompose non-conformal elements into conformal ones
  - Obtain solutions on conformal elements
- Related Work
  - Li et al. (2003) FEM on Cartesian Grid with Added Nodes
  - Ilinca and Hetu (2010) Finite Element Immersed Boundary
  - Soghrati, et al. (2011) Interface Enriched Finite Element
- Properties
  - Supports variety of interfacial conditions (identical to boundary fitted mesh)
  - Avoids manual generation of boundary fitted mesh
  - Supports general topological evolution (subject to mesh resolution)
- Similar to finite element adaptivity
  - Uses standard finite element assembly including data structures, interpolation, quadrature
- Connections to XFEM





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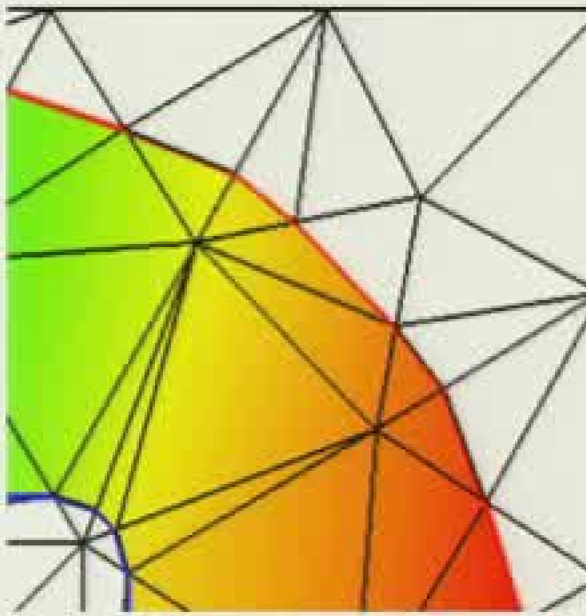
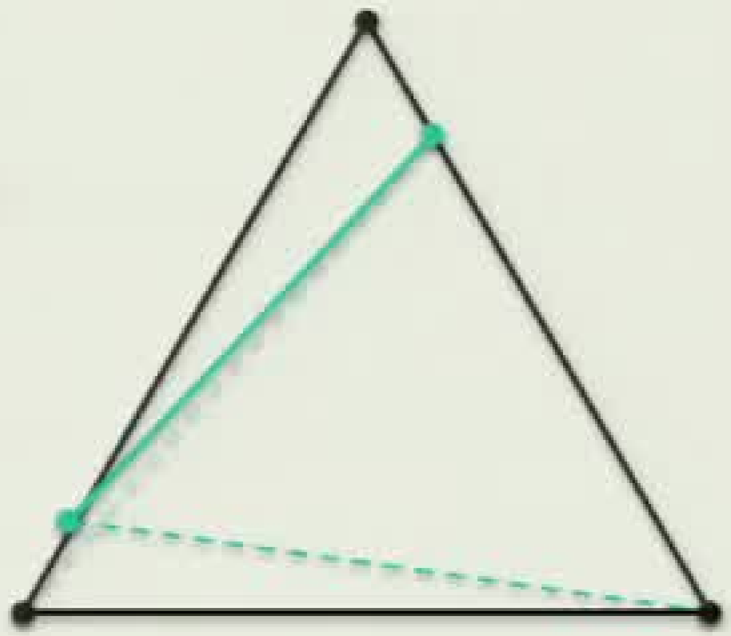
What About Element Quality?

- Meshing concerns
  - infinitesimal edge lengths
  - arbitrarily high aspect ratios (small angles)
  - obtuse angles. Depending on cutting strategy, large angles can approach 180^0



- Consequences
  - condition number of resulting matrix system
  - interpolation error
  - Other concerns: stabilized methods, suitability for solid mechanics, Courant number limitations, capillary forces



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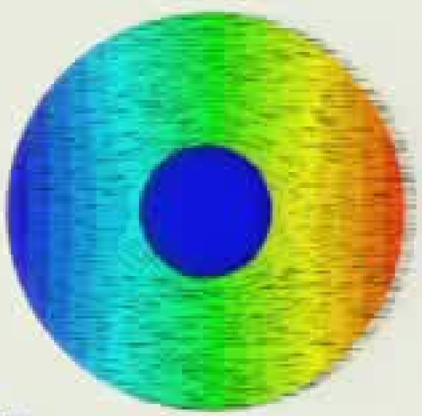
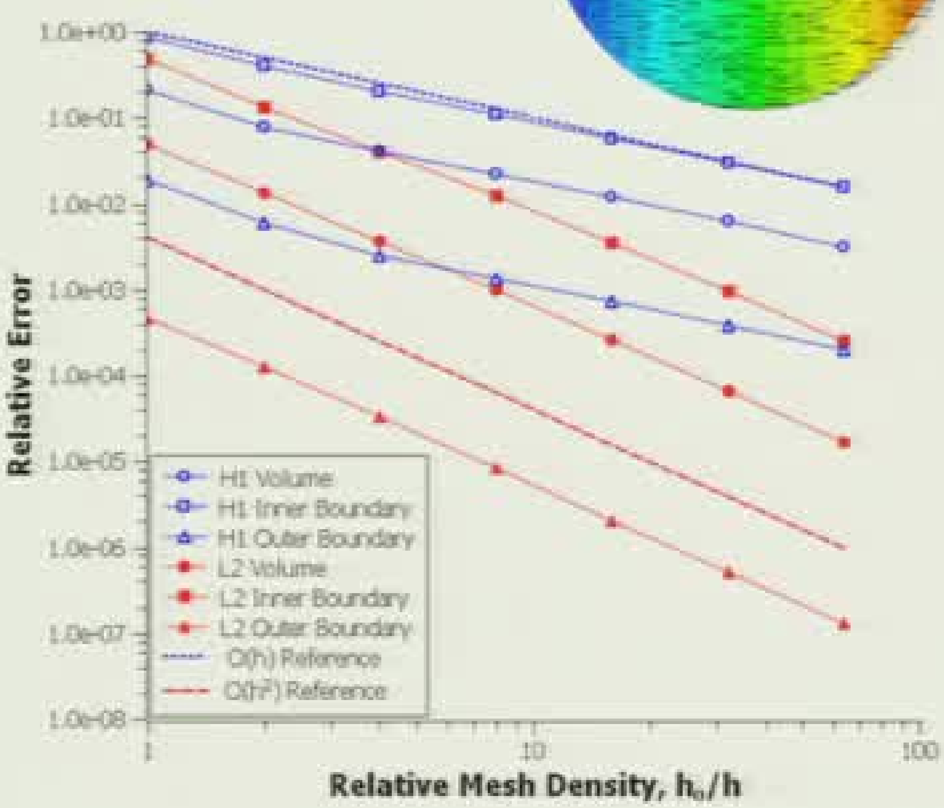
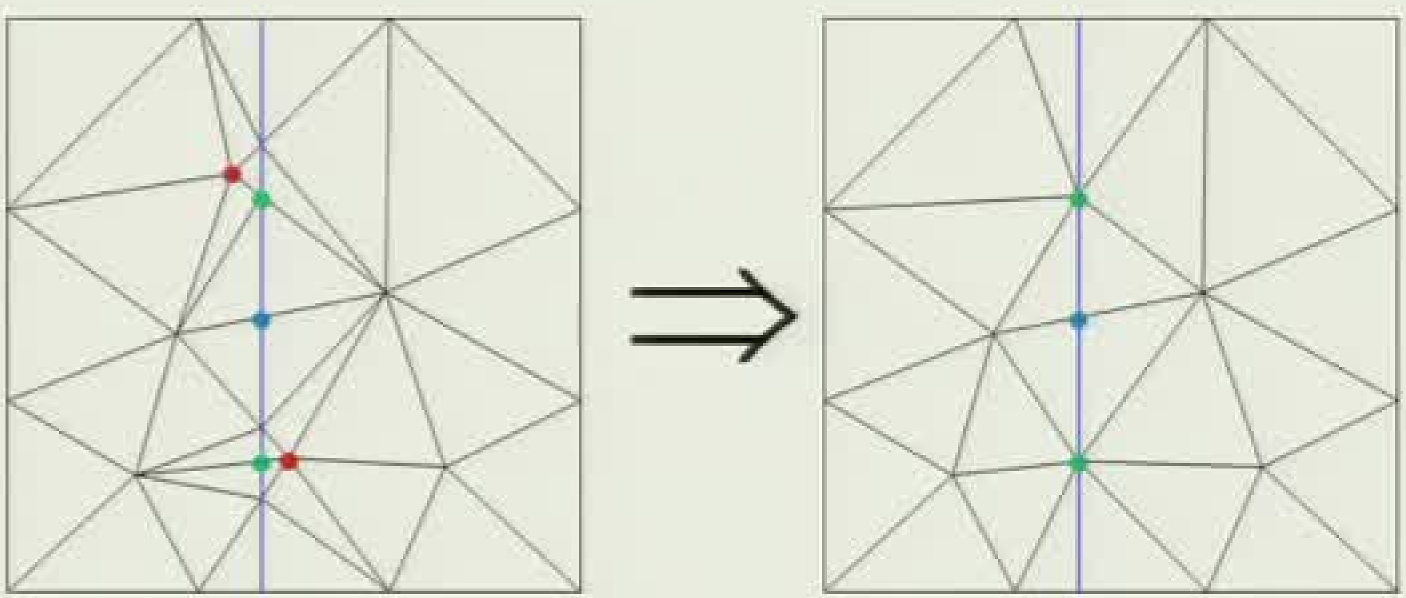
CDFEM Verification & Improvements

- Steady Potential Flow about a Sphere
  - Embedded curved boundaries
  - Dirichlet BC on outer surface, Natural BC on inner surface
  - Optimal convergence rates for solution and gradient both on volume and boundaries





- Snap "bad" nodes
  - Determine edge cut locations using level set
  - When any edges of a node are cut below a specified ratio, move the node to the closest edge cut location (snap background mesh nodes to interface, •→•)



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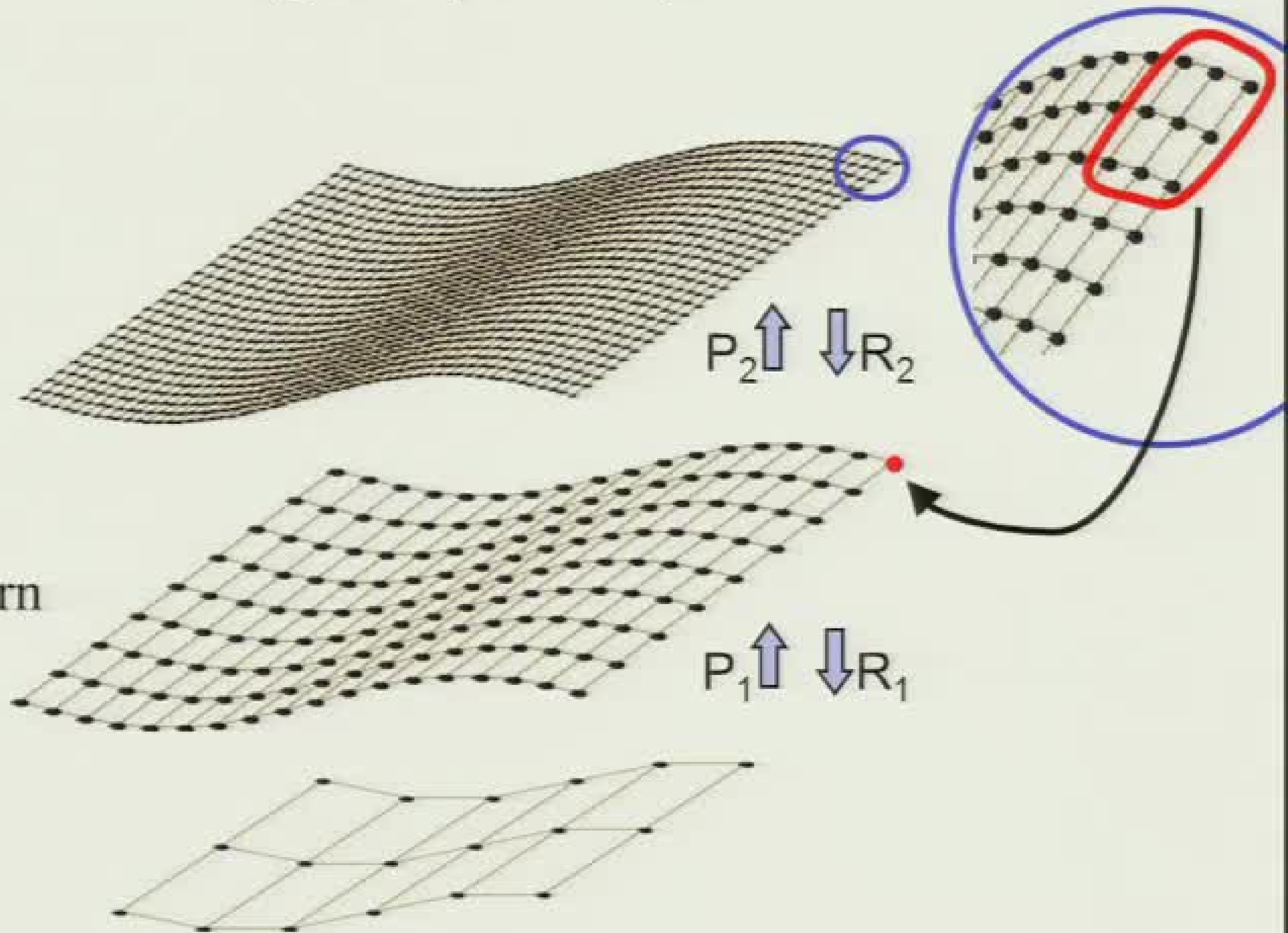
Algebraic Multigrid (AMG)

Solve $A_3 u_3 = f_3$

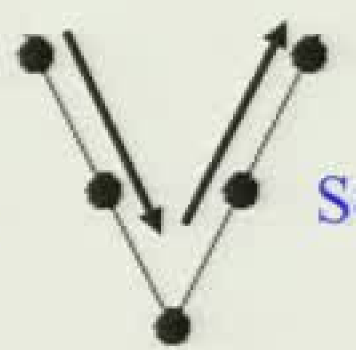


- Construct Graph & Coarsen
- Determine P_i & R_i sparsity pattern
- Determine P_i & R_i's coefs
- Project: $A_i = R_i A_{i+1} P_i$

Smooth $A_3 u_3 = f_3$. Set $f_2 = R_2 r_3$.

Smooth $A_2 u_2 = f_2$. Set $f_1 = R_1 r_2$.

Solve $A_1 u_1 = f_1$ directly.



Set $u_3 = u_3 + P_2 u_2$. Smooth $A_3 u_3 = f_3$.

Set $u_2 = u_2 + P_1 u_1$. Smooth $A_2 u_2 = f_2$.

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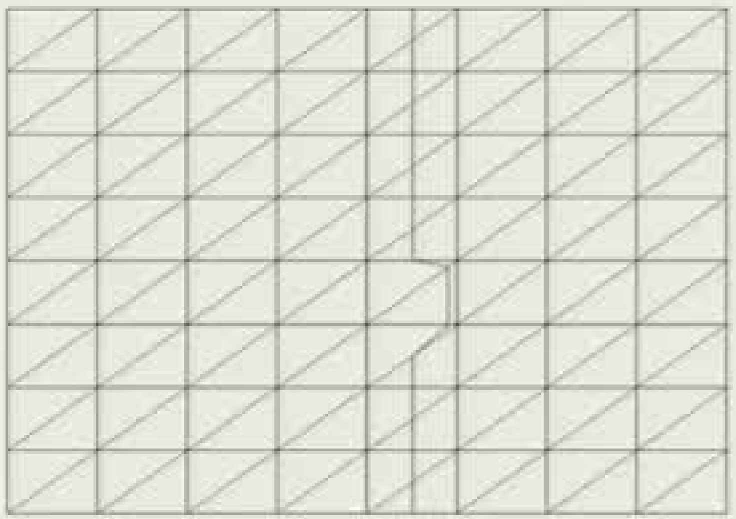
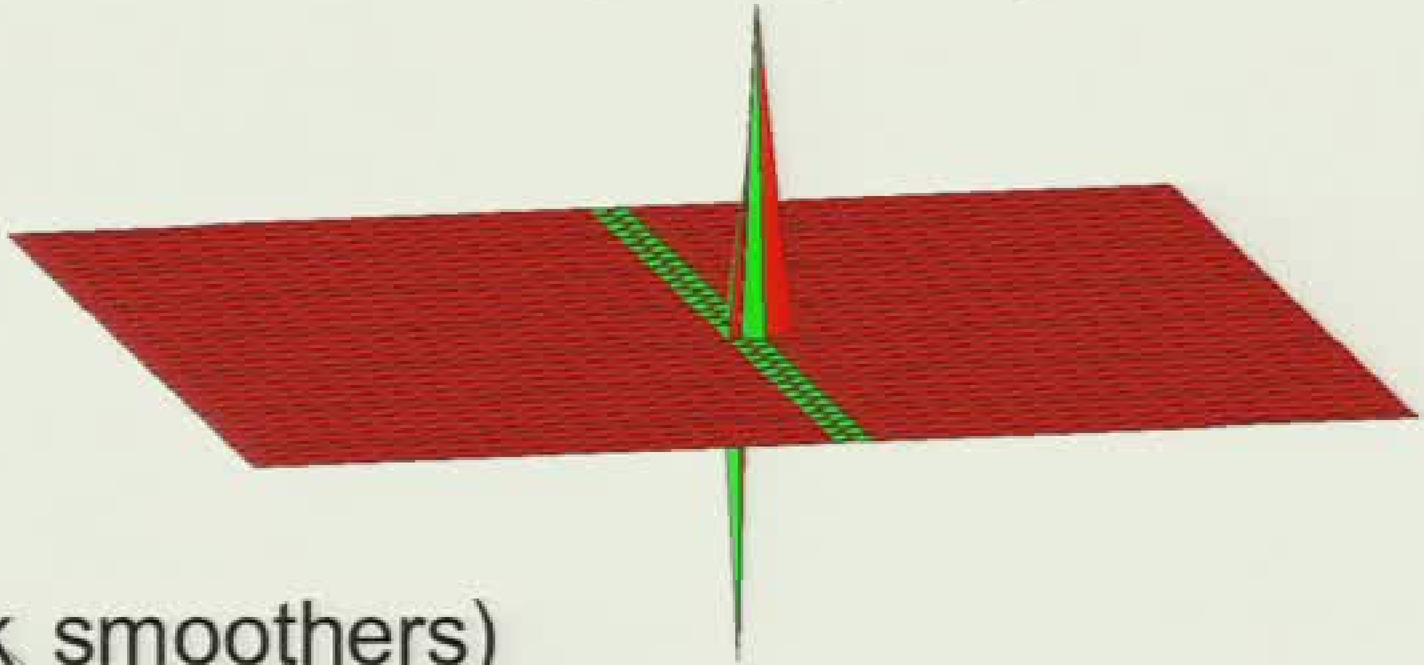
MG & CDFEM (scalar PDEs)

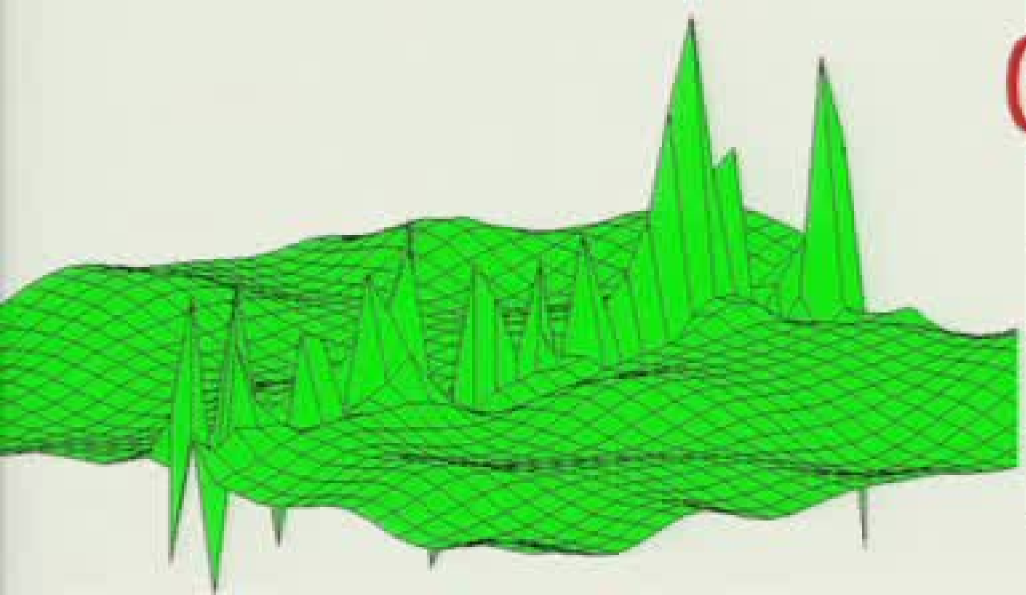
- CDFEM bad elements increase large λ values but not smallest
  - associated 'bad' eigenvectors are local & high frequency in nature

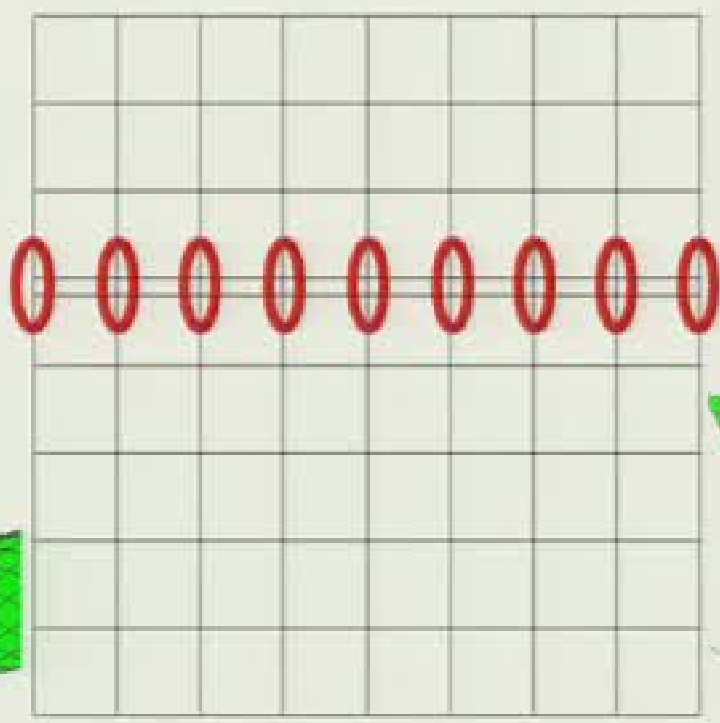




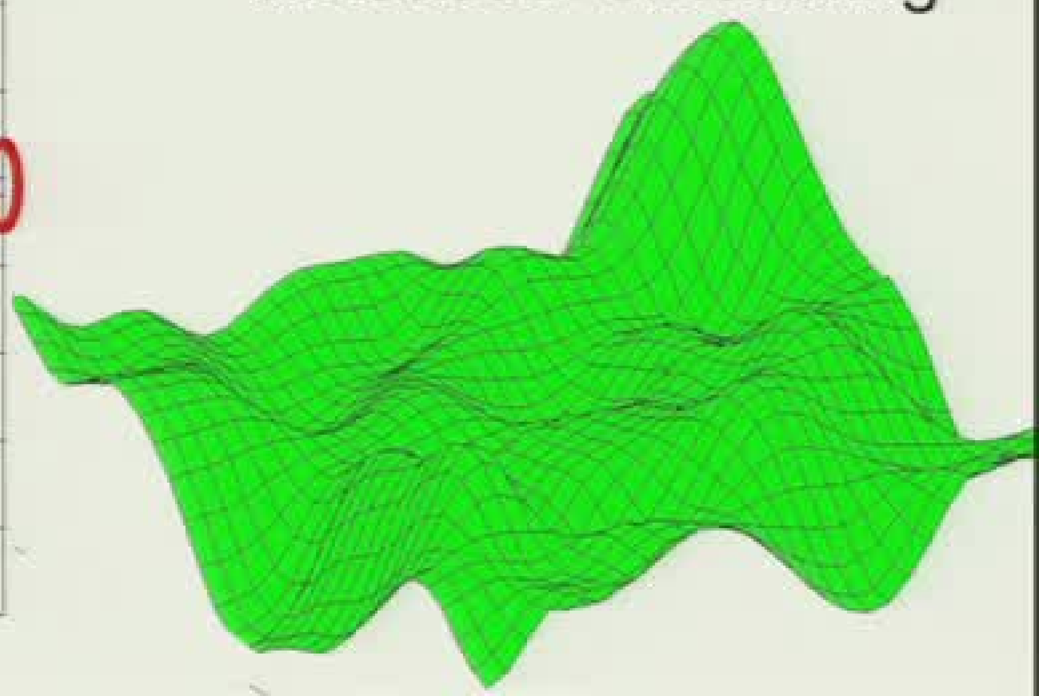
- rectify locally (e.g., mini-block smoothers)

pt Jacobi smoothing





blk Jacobi smoothing



CDFEM & MG coarse corrections

Effects of bad CDFEM elements <u>disappear</u> on coarse grids if coarse grid points not too close

Let $\mathcal{G}$ be a background mesh (without CDFEM modifications)

Let $\breve{\mathcal{G}}$ be modified mesh ($\mathcal{G}$ with newly introduced points along an interface)

Let $\mathcal{G}_c$ be a coarse mesh (subset of $\mathcal{G}$'s vertices)

Then

$$P^T A P \equiv \breve{P}^T \breve{A} \breve{P}$$

where $A\,(\breve{A})$ are discretization matrices on $\mathcal{G}$ ($\breve{\mathcal{G}}$) mesh
$P\,(\breve{P})$ are linear interpolation operators from $\mathcal{G}_c$ to $\mathcal{G}$ ($\breve{\mathcal{G}}$)

‡ some additional assumptions needed

Incompressible Navier-Stokes & AMG

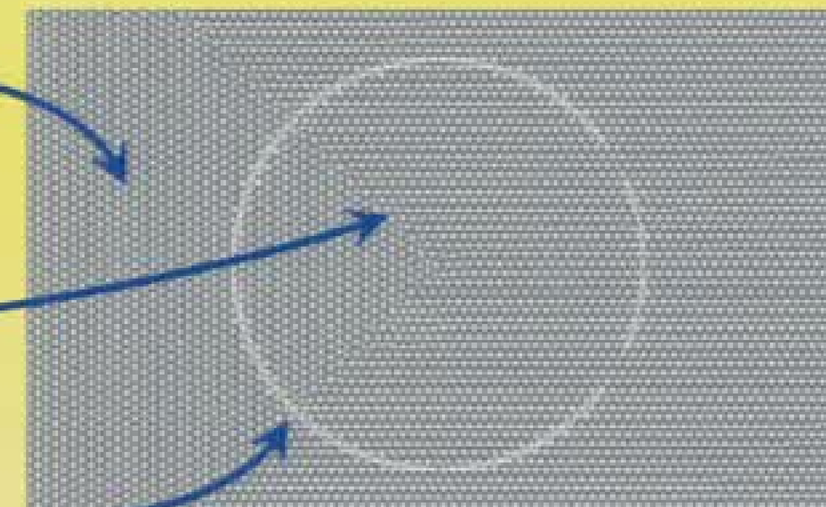
$$-\nu \nabla^2 u + (u \cdot grad)u + grad\ p = f$$
$$div\ u = 0$$

$$\begin{pmatrix} A & G \\ G^T & C \end{pmatrix}$$

Equal order/co-located FE with interfaces

Air bubble in water

- **3 dofs/node (velocities, water pressure)**
- **3 dofs/node (velocities, air pressure)**
- **4 dofs/node (velocities, air & water pressure)**



uu	uv	up
vu	vv	vp
pu	pv	pp

ithin nodes $[u_1\ v_1\ p_1\ \cdots\ u_n\ v_n\ p_n]$

- Graph algorithms on nodal system
- Grid transfer coefs on full dof system

AMG for PDE systems

- Graph algorithms on nodal system
  - \+ graph algorithms easily applied
  - \+ consistent coarsening mimics fine grid discretization
- Grid transfer coefs on full dof system
  - \+ grid transfer algorithms “utilize” coupling between fields
  - \- grid transfer software complicated for variable blocks
  - \- incompressibility condition problematics for standard AMG approaches of defining grid transfer coefficients

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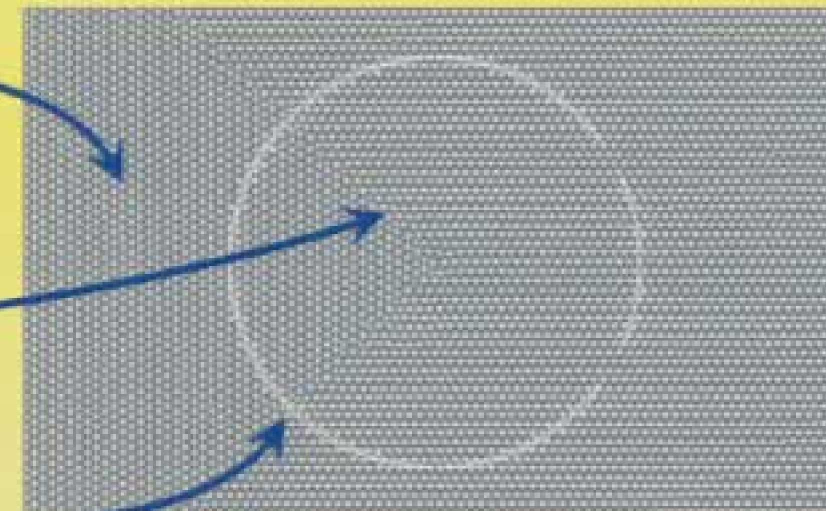
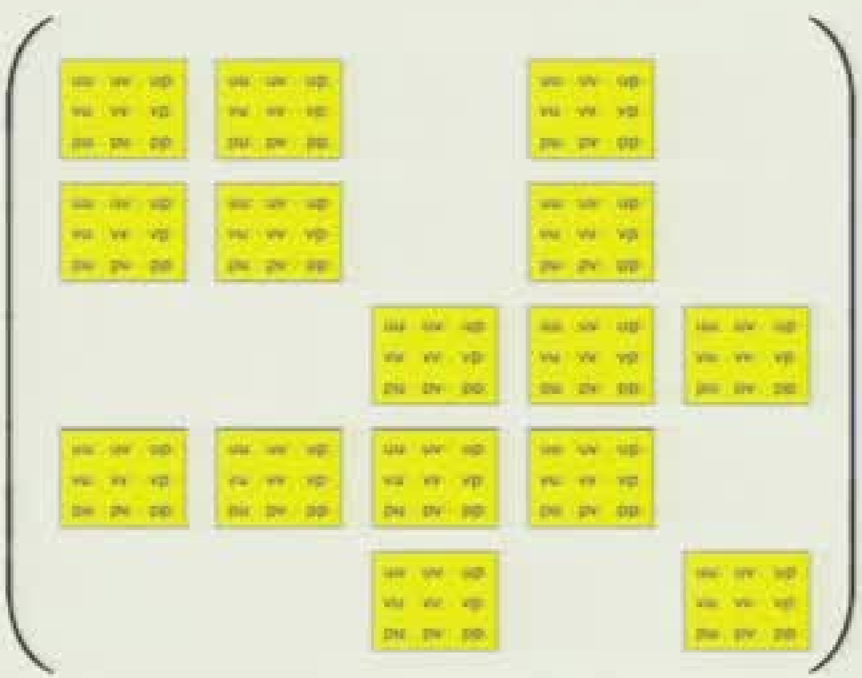


- consecutive dofs within nodes $[u_1\ v_1\ p_1 \ \cdots \ u_n\ v_n\ p_n]$



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to avoid – 's

- Separate grid transfers for each field with same underlying interpolation op.
  - \+ simplifies software
  - \- "ignores" PDE
  - \- no inter-field coupling in P

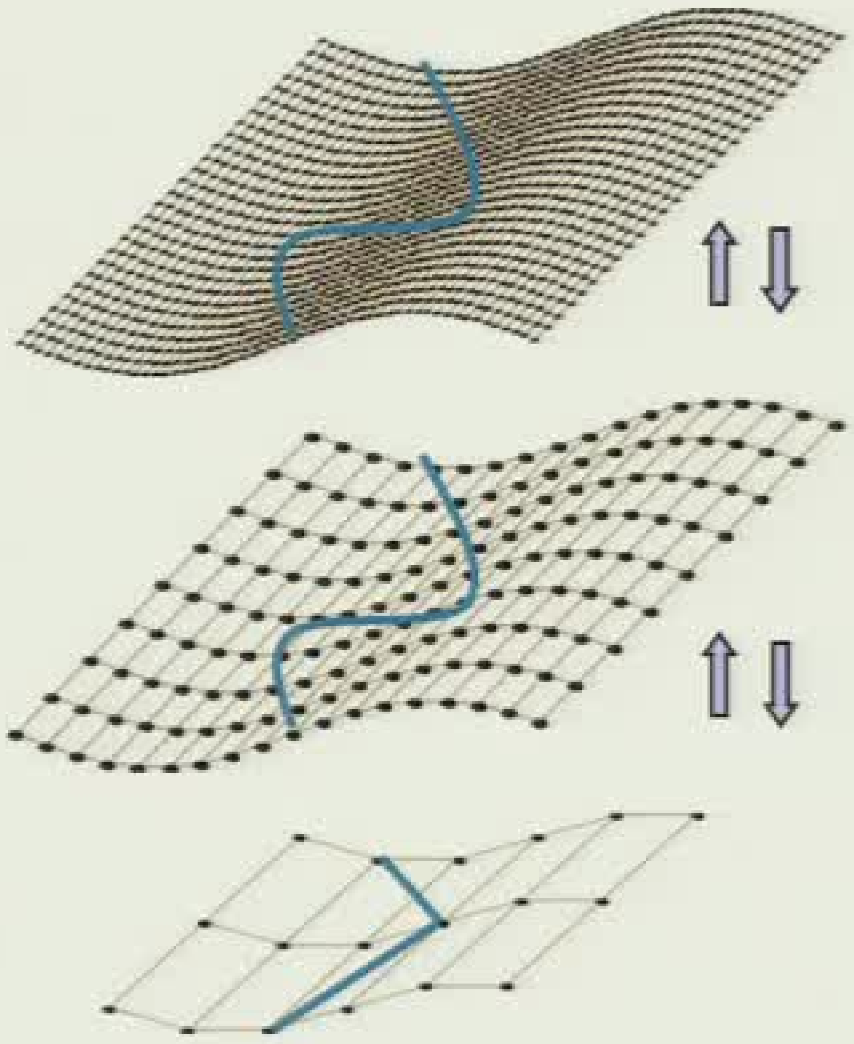
similar to geometric interpolation

$$P = \begin{pmatrix} P_u & & & \\ & P_v & & \\ & & P_{wp} & \\ & & & P_{ap} \end{pmatrix}$$

Mimic geometric MG via AMG

But … still want grid transfers to "capture" interfaces or material jumps & adapt to mesh stretching

… typically accomplished by dropping "small" terms in discretization matrix when constructing grid transfers



Drop, Distance Laplacian, Drop, AMG

Consider scalar (1 dof/mesh node) matrix operator, *L*, with off-diags defined‡ by

$$L_{ij} = \begin{cases} dist(i,j)^{-1} & \begin{array}{c} i,j \in air \ or \ i,j \in water \ or \ i,j \in surface \\ i \neq j \ and \ \hat{A}_{ij} \neq 0 \end{array} \\ 0 & otherwise \end{cases}$$

where

dist(i,j) is the distance between mesh vertices *i* & *j*

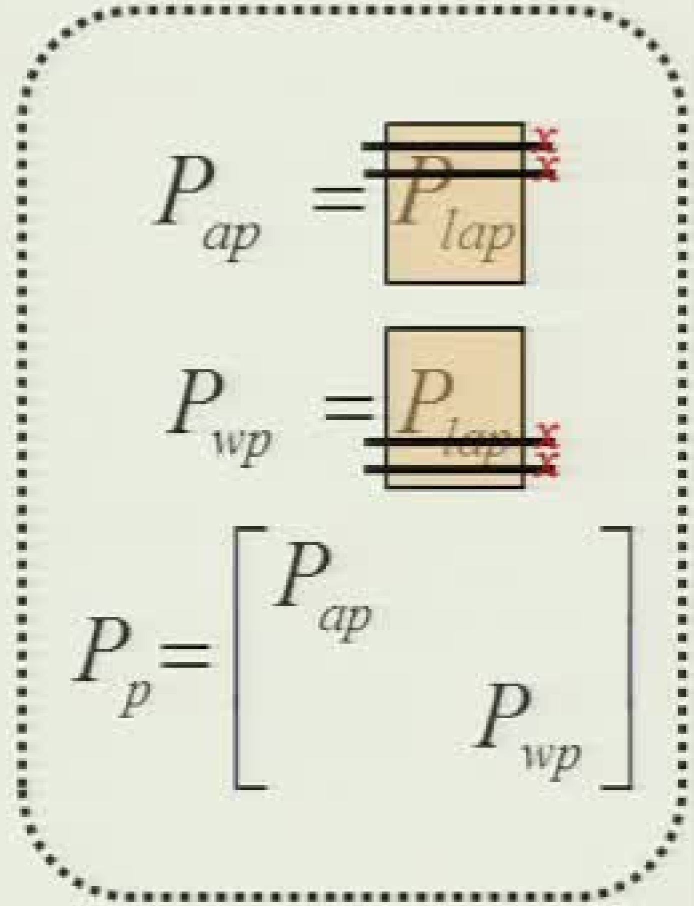
and

$\hat{A}_{ij} \neq 0$ *iff* submatrix associated with dofs at nodes i & j has at least one "large" nonzero and edge (i,j) doesn't cross regions ("large" defined in an AMG way)

‡ Can further drop small entries in *L*

Practical AMG for variable dof/node

- Construct scalar distance Laplacian matrix
- $P_{lap} \leftarrow$ **AMG(** L **)**
- Un-smoosh resulting operators for PDE system
- Pad on coarse grids



un-smoosh

- Requires coordinates & bool array indicating "active" dofs per node

u	v	p_w	p_a	
t	t	t		
t	t		t	
t	t	t	t	← interface
t	t	t	t	← interface
t	t		t	
t	t	t		
t	t	t		
t	t	t		
t	t		t	
t	t		t	

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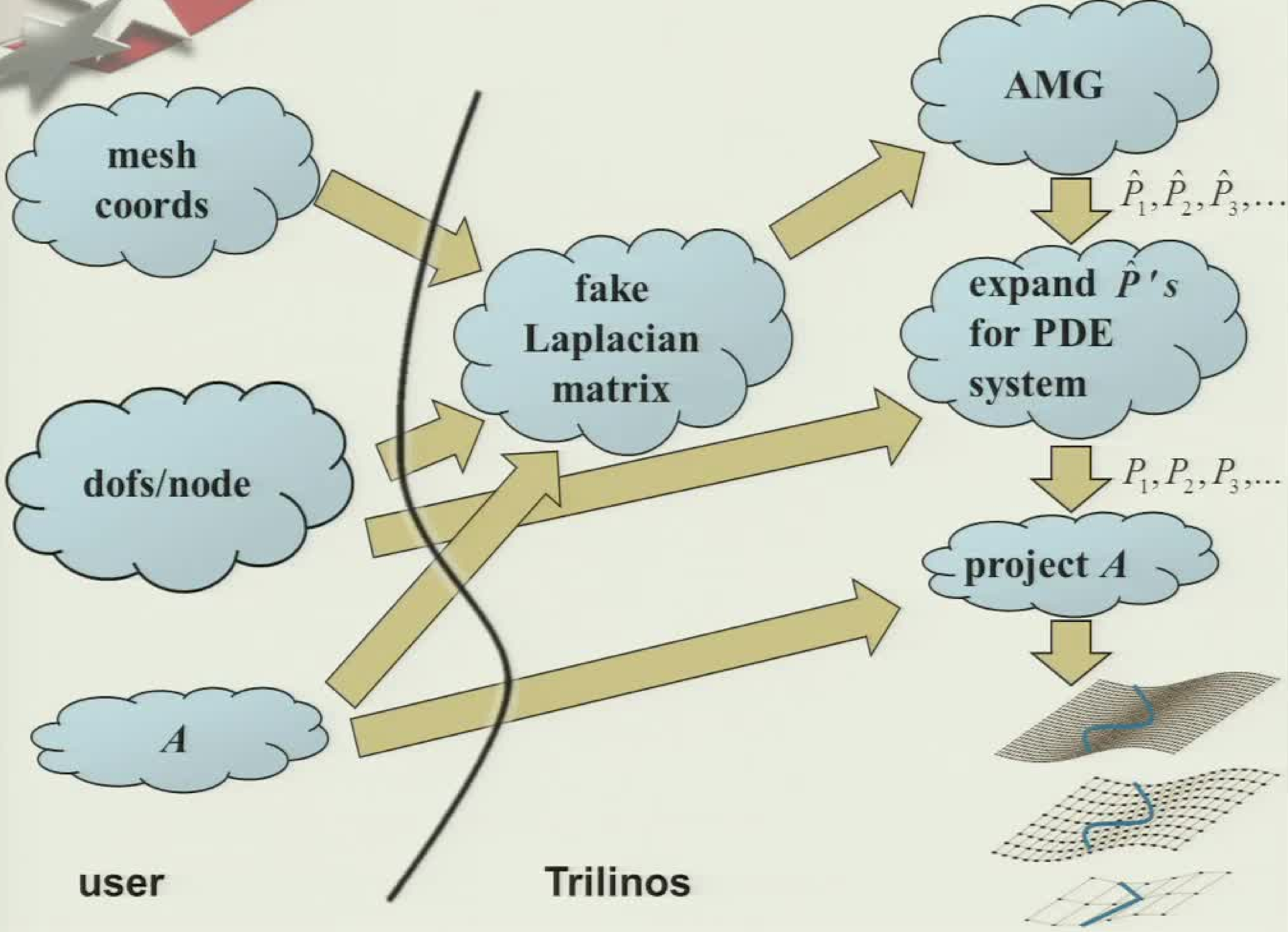
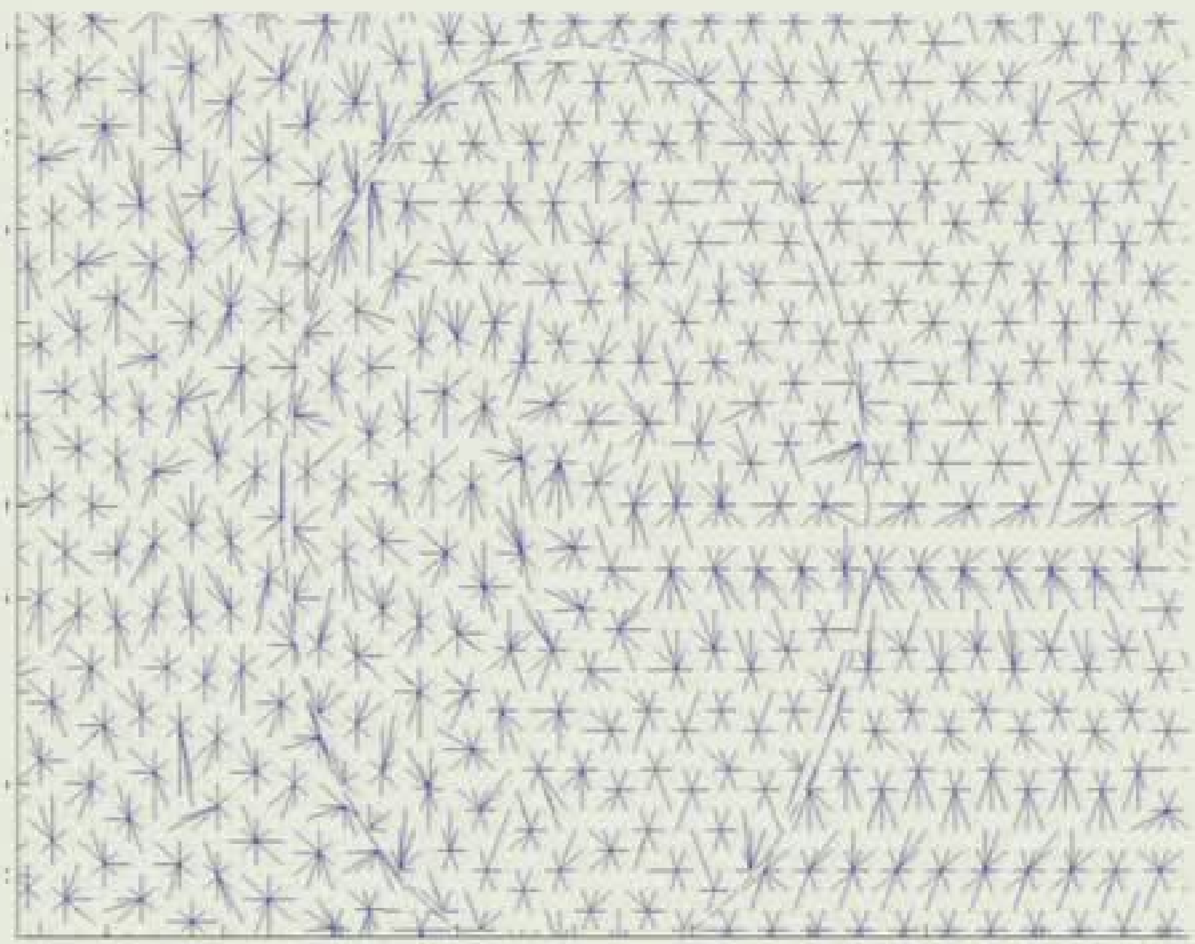
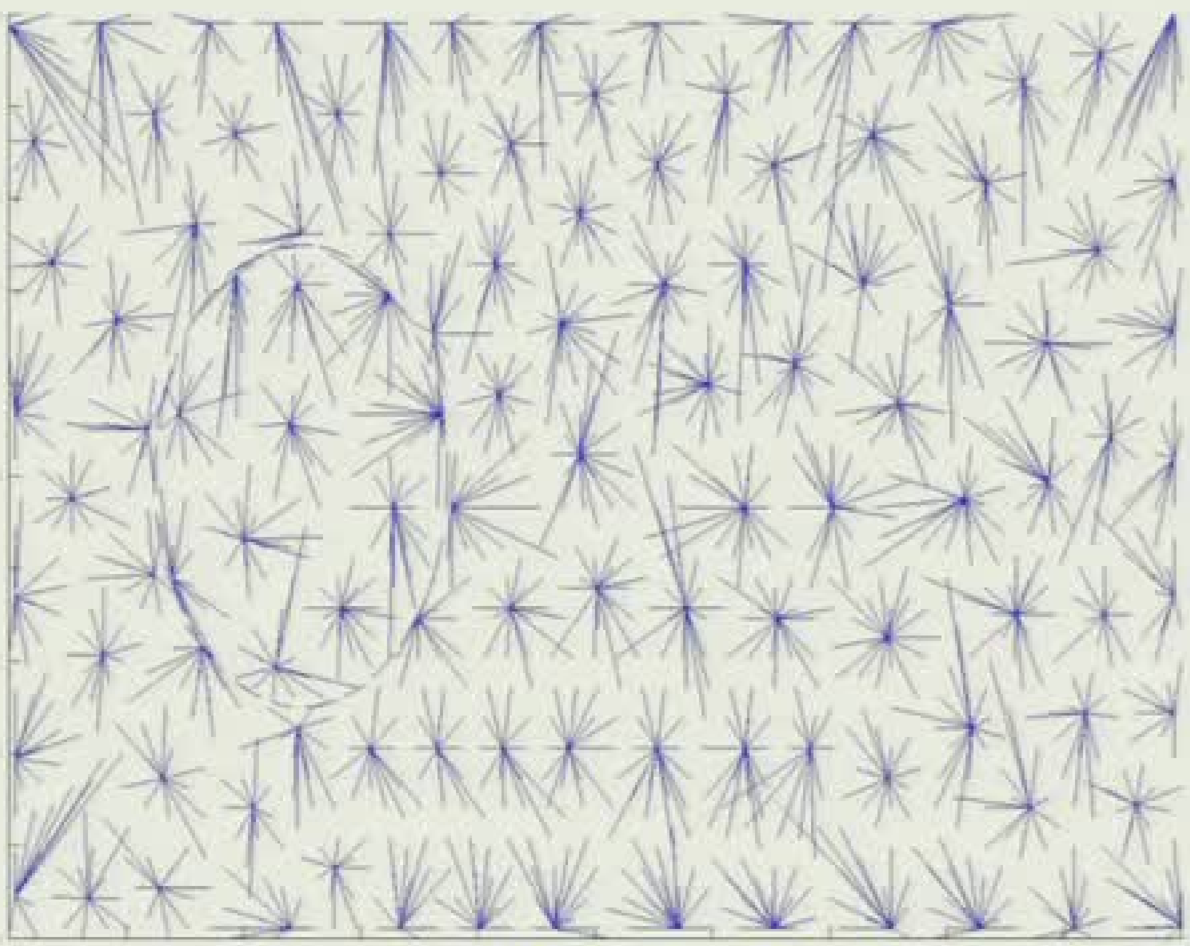


mesh coords
dofs/node
A
fake Laplacian matrix
AMG
$\hat{P}_1, \hat{P}_2, \hat{P}_3, \ldots$
expand $\hat{P}$'s for PDE system
$P_1, P_2, P_3, \ldots$
project A
user
Trilinos

air/water interface & aggregation



1st level aggregates



2nd level aggregates

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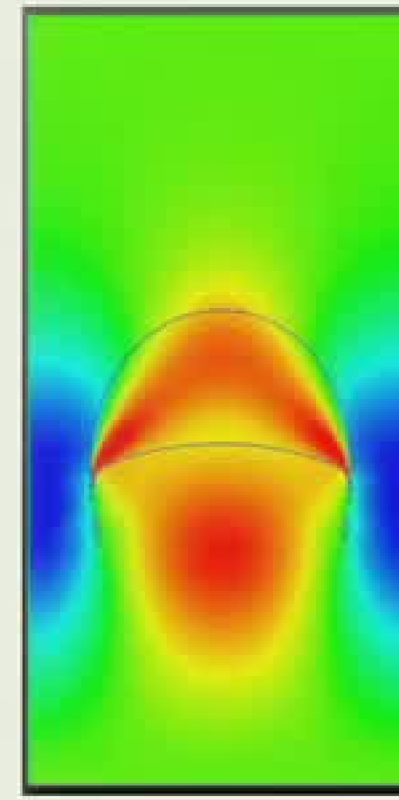
limited results

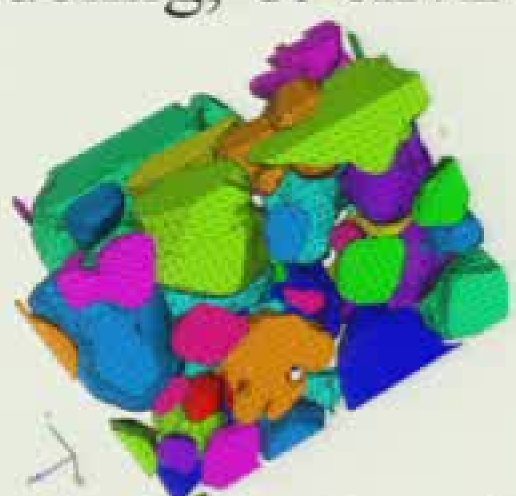
≈ # nodes	ILU precond		ML precond	
	avg its	lin. sys. time	avg its	lin. sys. time
15K	90.1	20.0	11.5	10.0
60K	218.3	473.5	21.8	44.0
238K	318.2	3198.4	21.0	256.4
948K	580*	> 10 hrs	27.2	997.2



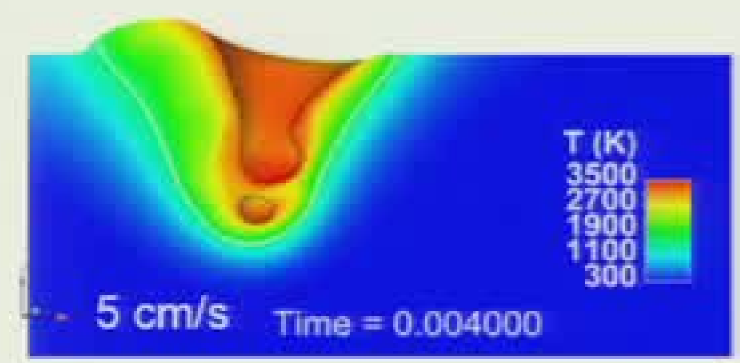
ILU relaxation seems to address smoothing concerns

- incompressibility constraint & tiny mesh spacing @ interface

Utilized by ARIA team for Navy railgun & NW (laser welding, thermal battery modeling, & environmental sensing devices) applications.



Pore Scale Battery Modeling



Laser Welding