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Toward Flexible Scalable Algebraic Multigrid Solvers

Ray Tuminaro, Sandia National Labs

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Research Spotlights: New Opportunities for SIAM Review Authors

March 18, 2012

As of January 31, 2012, *SIAM Review* has a new section that represents a new direction for the journal. Research Spotlights, which replaces Expository Research Papers, has a greatly expanded mission and welcomes interesting ideas from the SIAM community.

Articles for the new section should discuss applied and computational mathematics of particularly wide interest or importance. Contributions must be accessible to the broad and diverse *SIAM Review* readership, which includes every one of the 14,000+ SIAM members.

A principal feature of the new section is the flexibility it offers to authors, especially with respect to contribution styles. Shorter articles are particularly welcome, and an article can take a non-traditional form---such as a mini-survey, a timely communication, a description of software, or a new mathematical perspective within an application area. We hope that the expanded format will promote creativity and stimulate interesting articles for *SIAM Review*'s readers.

Prospective authors are encouraged to consult with the section editor, Ray Tuminaro, about potential contributions, especially those that lie outside the scope of traditional SIAM articles. Non-standard suggestions are welcome and will be given serious consideration; ideas that do not fit easily into the specialized journals may find a home in Research Spotlights. Though ... more relaxed, articles accepted for the section must be of broad interest ... SIAM's technical review standards.---

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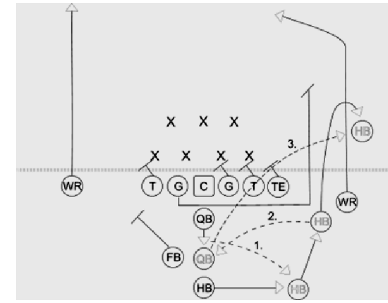
Gameplan



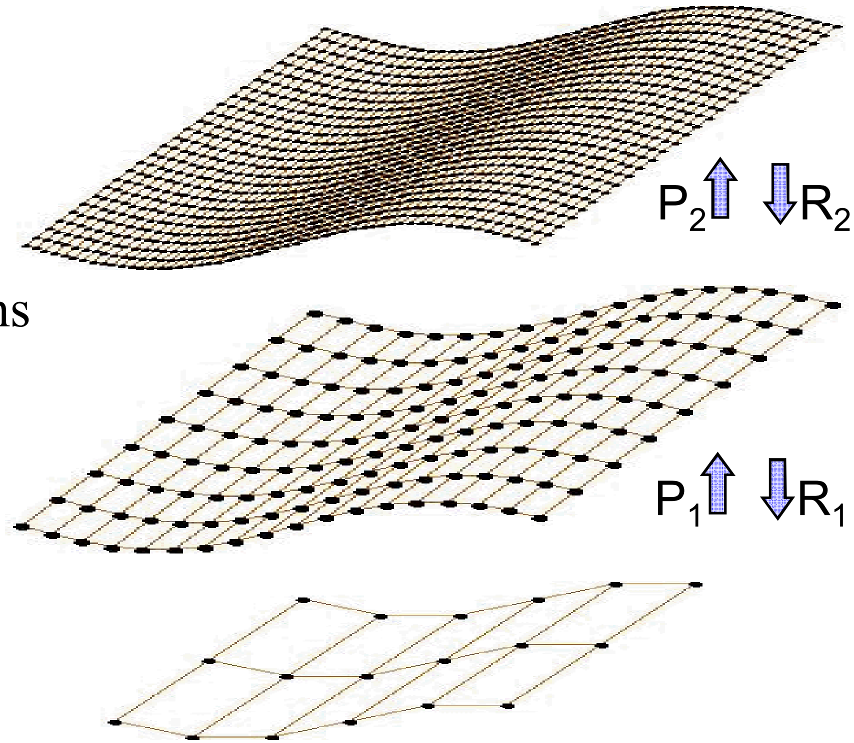
- AMG background
- Energy minimization AMG
  - arbitrary coarsening,
  - flexible coarse basis function support,
  - accurate interpolation of assorted important modes
  - varied choice of norm for minimization & search space
- Krylov methods & energy minimization
- Leveraging flexibility
  - extended finite elements, mixed finite elements, anisotropic PDEs

What is Multigrid ?

Solve $A_3 u_3 = f_3$

Basic idea:

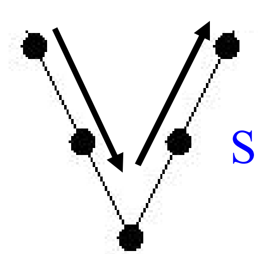
- Develop coarse approximations
- Accelerate convergence via coarse iterations to efficiently propagate information



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

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

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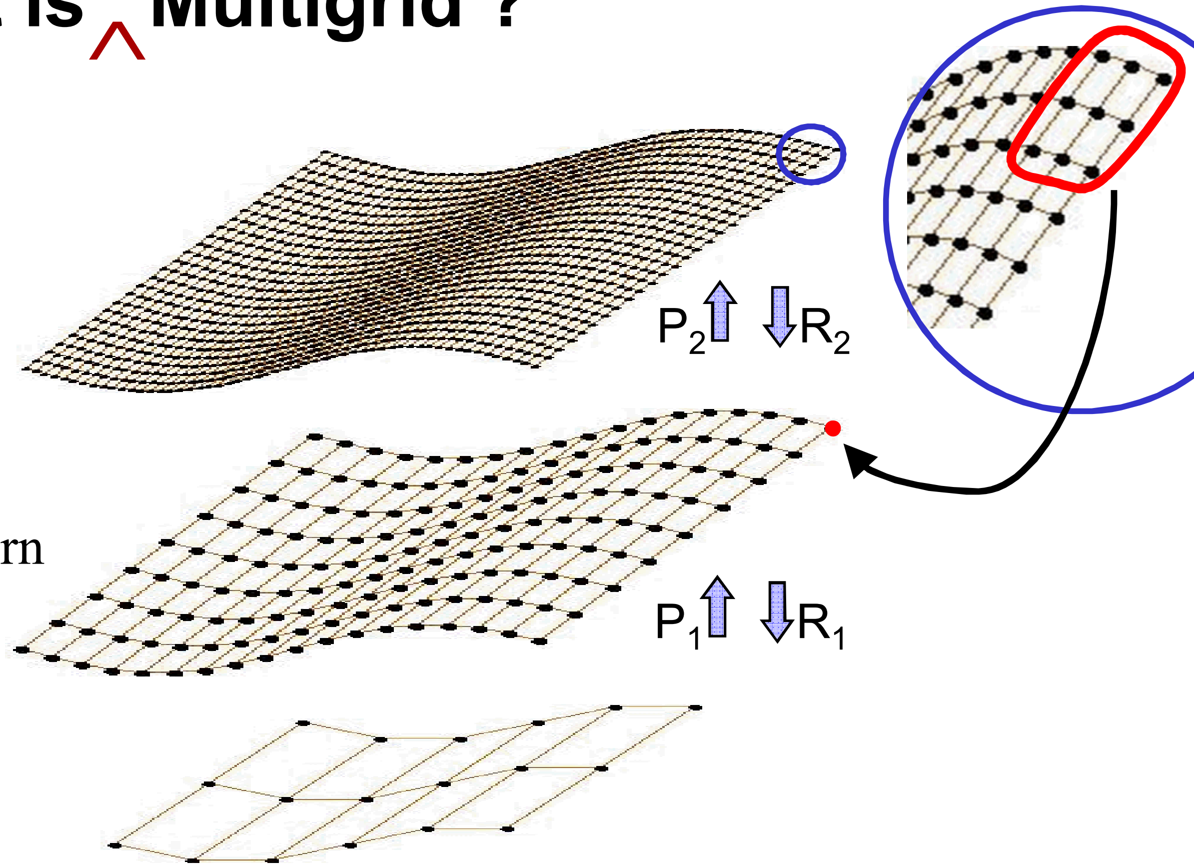
What is *Algebraic* Multigrid ?

Solve $A_3 u_3 = f_3$

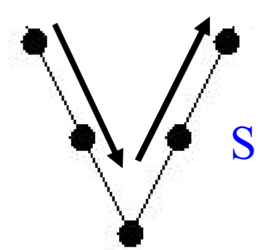


- Construct Graph & Coarsen
- Determine P_i & R_i sparsity pattern
- Determine P_i & R_i's coefs
- Project: $A_i = R_i A_{i+1} P_i$

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 $u_2 = u_2 + P_1 \mathrm{u}_1$. Smooth $A_2 u_2 = f_2$.

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AMG limitations …

Best understood theoretically for
scalar elliptic PDEs with *standard* discretizations
(e.g. linear nodal FE & finite differences),
but often works on broader range of systems.

Deficiency: **Classical AMG & smoothed aggregation are rigid & not easily adapted to *advanced* situations.**

- coarsening rules: diameter 3 aggregates or
  - (C1) for each $i \in F$, each point $j \in S_i$ should either be in C, or should be strongly connected to at least one point in $C \cap S_i$
  - (C2) C should be a maximal subset of all points with the property that no two C-points are strongly connected to each other
- coarsening, P sparsity pattern, p_{ij} choices are often tied together
- strong/weak decisions influence multiple phases of algorithm
- accurate interpolation of constants automatically addressed, but considering other important modes can be problematic

AMG & Energy Minimization

grid transfer

A_k
P_k sparsity pattern
mode constraints

→

minimize energy
while
satisfying constraints

→

P_k's
coefficients

Tradeoffs:

+ flexibility
  - any coarsening
  - any sparsity pattern
  - constraints
    - important modes requiring accurate interpolation

+ robustness

$$\min_P \; p_1^T A p_1 + p_2^T A p_2 + p_3^T A p_3 + \ldots$$

$$P = [p_1 \;\; p_2 \;\; p_3 \;\; \ldots]$$

Brandt, Brannick, Brezina, Chan, Gee, Kahl, Kolev, Livshits, Mandel, Olson, Schroder, Smith, T, Vanek, Vassilevski, Wagner, Wall, Wan, Wiesner, Xu, Zikatanov

Energy-Minimization

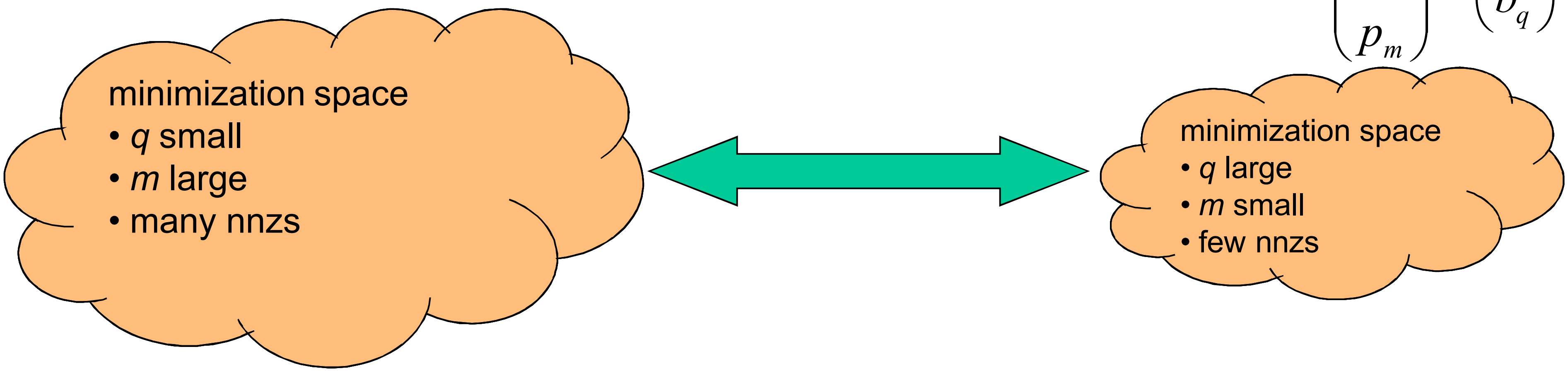
Find $P = [p_1 \; p_2 \cdots p_m] \in \mathcal{N}$ minimizing $\sum_i \|p_i\|_e^2$ in some space so that $P\,B_c = B$ $(=[b_1\, b_2\, \ldots b_q\,])$ or equivalently subject to $X \begin{pmatrix} p_1 \\ p_2 \\ \vdots \\ p_m \end{pmatrix} = \begin{pmatrix} b_1 \\ \vdots \\ b_q \end{pmatrix}$

- Expensive & unnecessary to solve exactly (need to bound energy)!
- Can consider improving an initial guess with a few iterations

Energy-Minimization

Find $P = [p_1\ p_2 \cdots p_m] \in \mathcal{N}$ minimizing $\sum_i \|p_i\|_e^2$ in some space

so that $P\,B_c = B\ \ (=[b_1\, b_2\, \ldots b_q])$ or equivalently subject to $X \begin{pmatrix} p_1 \\ p_2 \\ \vdots \\ p_m \end{pmatrix} = \begin{pmatrix} b_1 \\ \vdots \\ b_q \end{pmatrix}$



"Solve" $\hat{A}$ »P« = 0

1) with minimization algorithm

2) in space satisfying constraints

$A\ (P_0 - \Delta P) = 0$ with X»P_0« = »B«

X»ΔP« $= 0$

QZ»P_0«, QZ^2»P_0«, QZ^3»P_0«, ...

$Q = (\,I - X^T (X\,X^T)^{-1}\,X\,)$

Solve AP = 0
1) with minimization algorithm
2) in space satisfying constraints

Minimization candidates include

- CG & Chebyshev when $A = A^T$
- GMRES & CGNR when $A \neq A^T$

Constraints

- X »P_0« $= g \quad \Rightarrow \quad P_0 \ B_c = B$
- X »ΔP« $= 0 \quad \Rightarrow \quad (\Delta P)\ B_c = 0$

via »ΔP« $= Q$ »ΔP_i« *with* $Q = (\,I - X^T (X\,X^T)^{-1} X\,)$ *as* $XQ = 0$

Constraint Satisfying Space *might* be

$$QAP_0,\ (QA)^2 P_0,\ (QA)^3 P_0,\ (QA)^4 P_0,\ \ldots$$

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CG minimization

Lemma: *Let A be SPD and apply CG to*

$$Q\,\hat{A}\,Q \;\gg\!\Delta P\!\ll \;= Q\,\hat{A}\,Q \gg\!P_0\!\ll$$

with 0 initial guess, then CG computes

$$\gg\!\Delta \mathrm{P}_{\mathrm{i}}\!\ll \;= \underset{\gg \Delta \mathrm{P}_{\mathrm{i}} \ll \in \mathcal{K}_i}{\arg\min} \left\| \gg\!\mathrm{P}_{\mathrm{i}}\!\ll \right\|_{\hat{A}} \quad \textit{where} \quad P_i = P_0 - \Delta P_i$$

Proof.

$$Z = Q\,\hat{A}$$

$$\gg\!\Delta \mathrm{P}_{\mathrm{i}}\!\ll \;= \underset{\gg \Delta \mathrm{P}_{\mathrm{i}} \ll \in \mathcal{K}_i}{\arg\min} \left\| \gg\!(\Delta \mathrm{P})_{*}\!\ll - \gg\!\Delta \mathrm{P}_{\mathrm{i}}\!\ll \right\|^2_{Q\hat{A}Q}$$

$$= \underset{\gg \Delta \mathrm{P}_{\mathrm{i}} \ll \in \mathcal{K}_i}{\arg\min} \left\| \gg\!(\Delta \mathrm{P})_{*}\!\ll \right\|^2_{Q\hat{A}Q} + \left\| \gg\!\Delta \mathrm{P}_{\mathrm{i}}\!\ll \right\|^2_{Q\hat{A}Q} - 2\left\langle \gg\!\Delta \mathrm{P}_{\mathrm{i}}\!\ll, \gg\!\mathrm{P}_0\!\ll \right\rangle_{\hat{A}}$$

$$= \underset{\gg \Delta \mathrm{P}_{\mathrm{i}} \ll \in \mathcal{K}_i}{\arg\min} \left\| \gg\!\mathrm{P}_0\!\ll \right\|^2_{Q\hat{A}Q} + \left\| \gg\!\Delta \mathrm{P}_{\mathrm{i}}\!\ll \right\|^2_{Q\hat{A}Q} - 2\left\langle \gg\!\Delta \mathrm{P}_{\mathrm{i}}\!\ll, \gg\!\mathrm{P}_0\!\ll \right\rangle_{\hat{A}}$$

$$= \underset{\gg \Delta \mathrm{P}_{\mathrm{i}} \ll \in \mathcal{K}_i}{\arg\min} \left\| \gg\!\mathrm{P}_0\!\ll - \gg\!\Delta \mathrm{P}_{\mathrm{i}}\!\ll \right\|^2_{\hat{A}}$$

Corollary: CG solution is unique

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GMRES minimization

Lemma: *Let A be nonsingular and apply GMRES to*

$$Q\hat{A}\ »\Delta P« = Q\hat{A}\ »P_0« \qquad (*)$$

with 0 initial guess, then GMRES computes

$$»\Delta P_i« = \underset{»\Delta P_i« \in \mathcal{K}_i}{\arg\min} \left\| »P_i« \right\|_{\hat{A}^T Q \hat{A}} \text{ where } P_i = P_0 - \Delta P_i$$

which is unique.

$Z = Q\hat{A}$

$\| »AP_i« \|_Q$

Proof.

Define S and $\mathrm{S}_\perp$ *such that*

$$QS = 0, \quad \mathrm{S}_\perp S_\perp^T = Q, \quad S_\perp^T \mathrm{S}_\perp = I, \quad S^T \mathrm{S} = I, \quad S^T \mathrm{S}_\perp = I$$

Use properties of GMRES applied to nonsingular system

$$S_\perp^T \hat{A} \mathrm{S}_\perp y = S_\perp^T \hat{A}\, »P_0« \qquad (**)$$

Pre-multiplication of (**) & associated Kyrlov space by $\mathrm{S}_\perp$ *reveal equivalence with (*).*

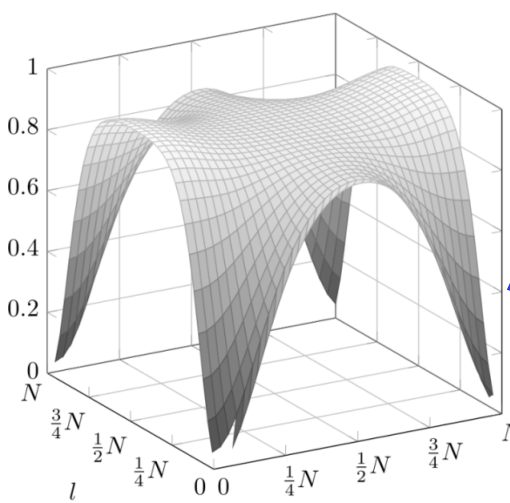
Alternative perspective Galerkin/Schur

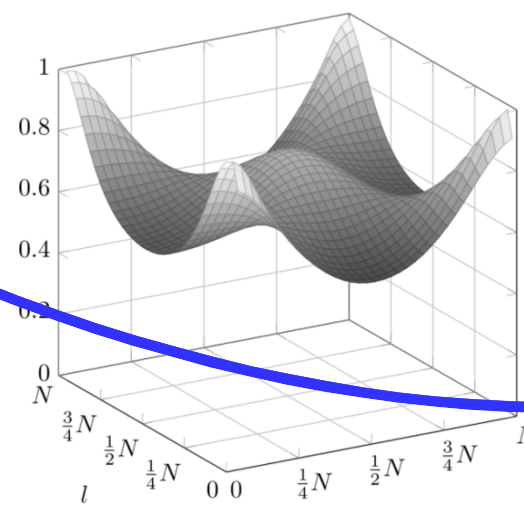
$AP = 0$, $\qquad AP \perp \mathcal{Z}$ with $P \in \mathcal{Z}_0$

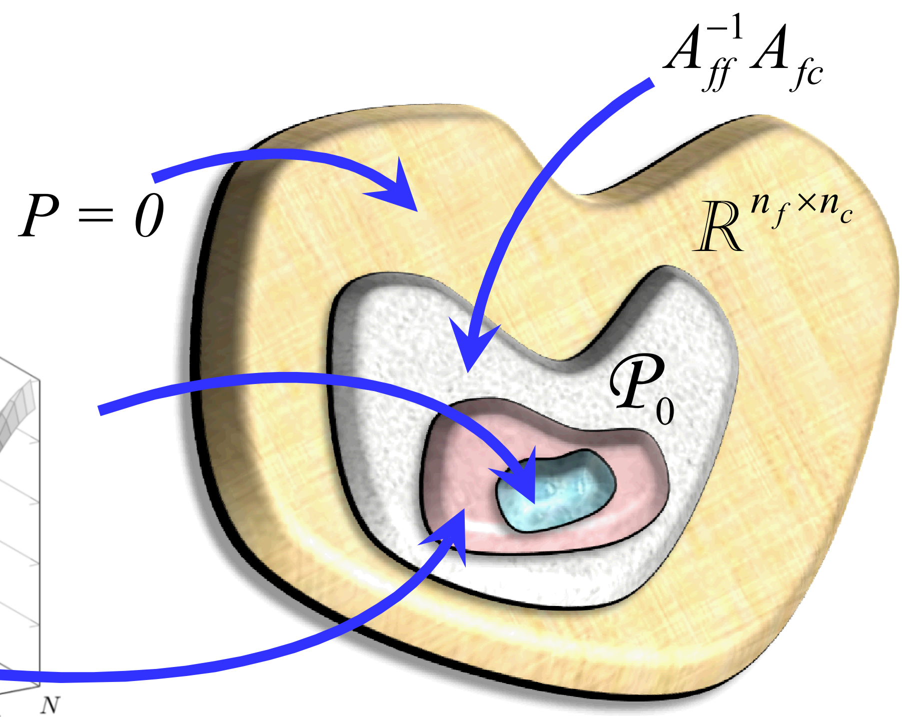
$$\mathcal{Z}_0 = \left\{ P \in \mathcal{P}_0 : N_{ij} = 0 \Rightarrow P_{ij} = 0 \right\}$$

$$M^{-1} = \begin{pmatrix} I & P_f \\ & I \end{pmatrix} \begin{pmatrix} A_{ff}^{-1} & \\ & A_{l+1}^{-1} \end{pmatrix} \begin{pmatrix} I & \\ R_f & I \end{pmatrix}$$

$$\sigma(M^{-1}A) = \left\{ 1, 1 \pm \sqrt{1 - \sigma(A_{l+1}^{-1} S)} \right\}$$

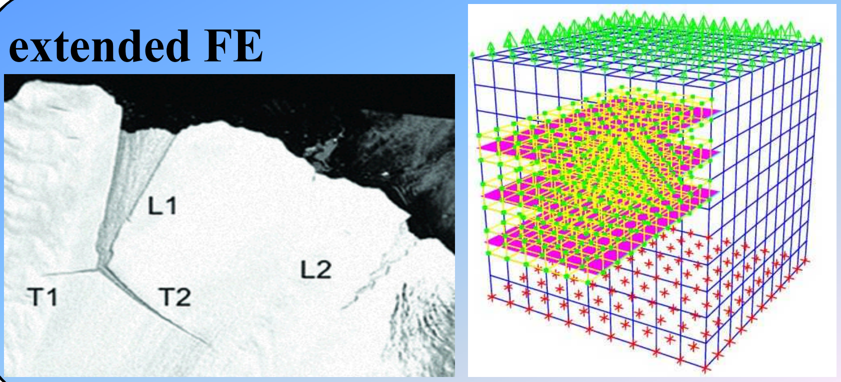


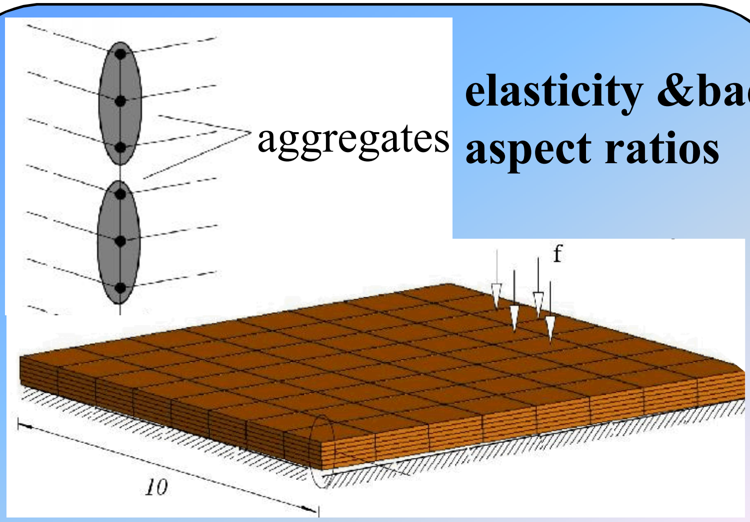




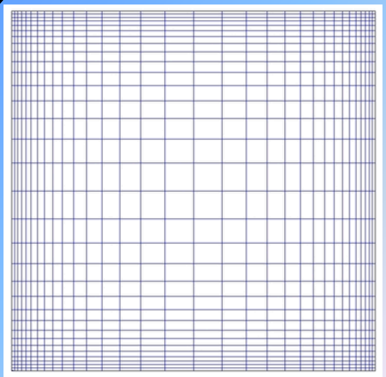
Exploiting Energy Minimization's Flexibility

extended FE

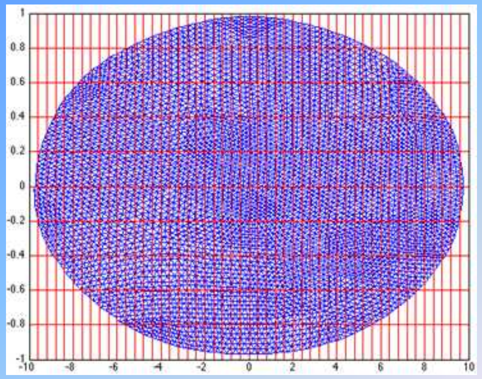




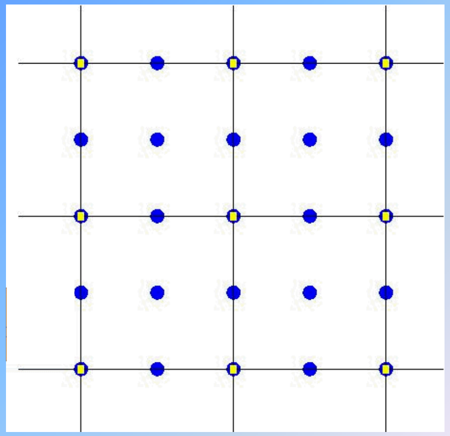
elasticity &bad aspect ratios



stretched meshes



unstructured to structured



mixed finite elements

Computational Modeling of Fracture

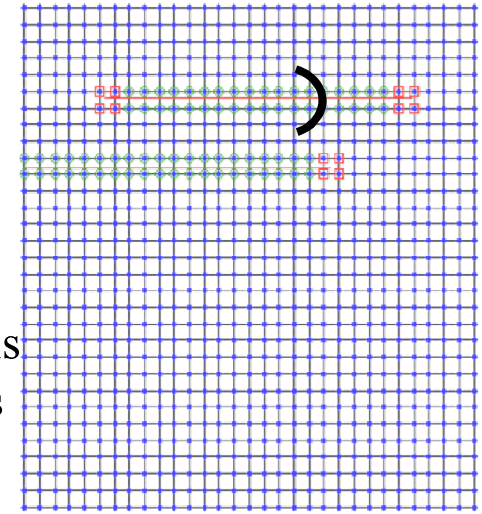
Classical FEM

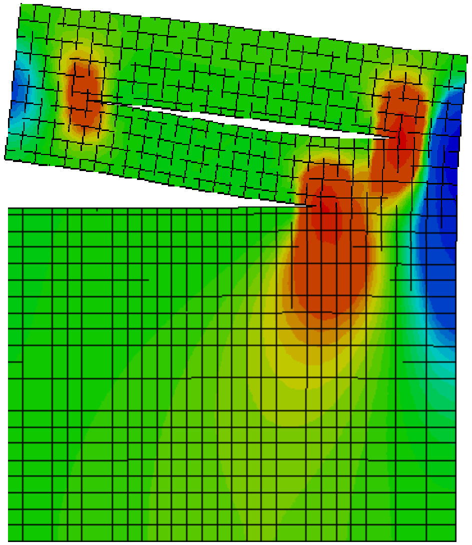
- Mesh conforms to crack boundaries

XFEM

- mesh independent of crack geometry
- Cracks → "enriched" DOF with special basis functions to handle discontinuities/singularities

XFEM mesh

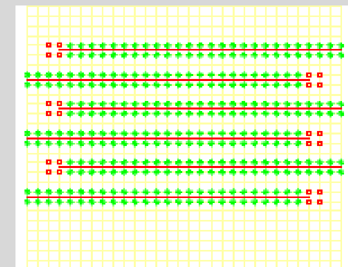


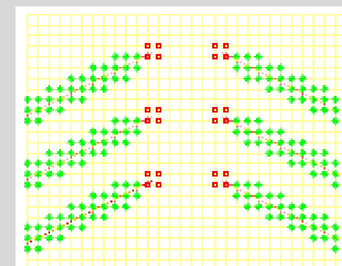


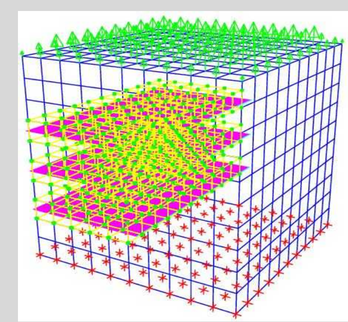
Numerical Results…

Case	VBlk AMG	Hybrid Standard AMG	Quasi AMG	Mesh	Case	VBlk AMG	Hybrid Standard AMG	Quasi AMG
1a	28	13	11	30^2	3a	154	-	16
	29	15	10	60^2		127	-	14
	37	17	12	90^2		-	-	25
	37	19	12	120^2		-	-	21
1b	24	22	11	30^2	3b	-	-	18
	24	29	12	60^2		-	-	21
	36	35	14	90^2		-	-	28
	35	41	13	120^2		-	-	22
1c	31	31	13	30^2	4	116	107	15
	32	43	14	60^2		102	154	21
	47	53	16	90^2		142	190	23
	45	61	15	120^2		151	-	22
2a	64	57	15	30^2	5a	80	76	12
	52	80	14	60^2		91	107	13
	87	98	20	90^2		124	131	15
	92	113	18	120^2		140	151	15
2b	73	59	16	30^2	5b	89	81	16
	72	81	17	60^2		103	116	15
	97	104	21	90^2		134	143	17
	95	122	19	120^2		151	165	16

mesh	complexity
30^2	1.673
60^2	1.815
90^2	1.65
120^2	1.699







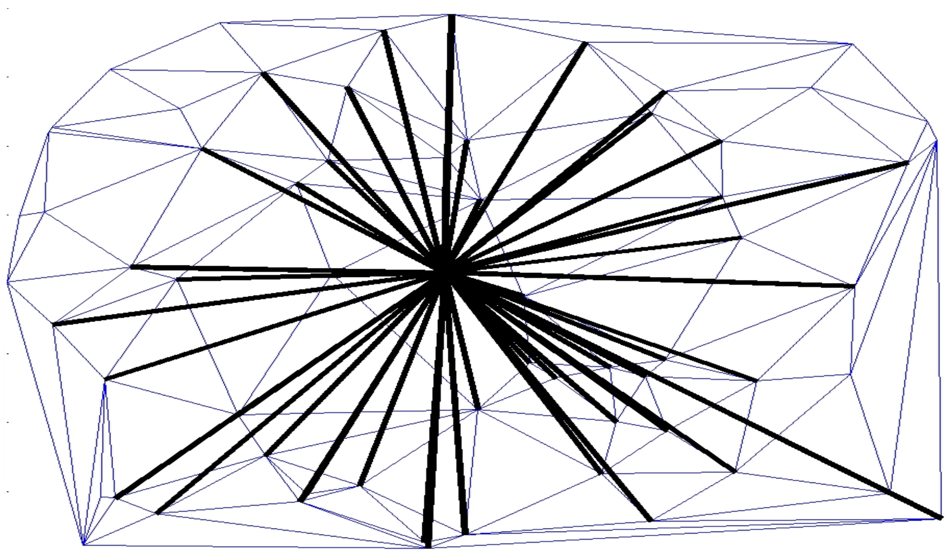
complexity: $\dfrac{\sum_i nnz(A_i)}{nnz(A)}$

# dofs	iters	complexity
33K	20	2.01
218K	25	1.81
723K	29	1.91

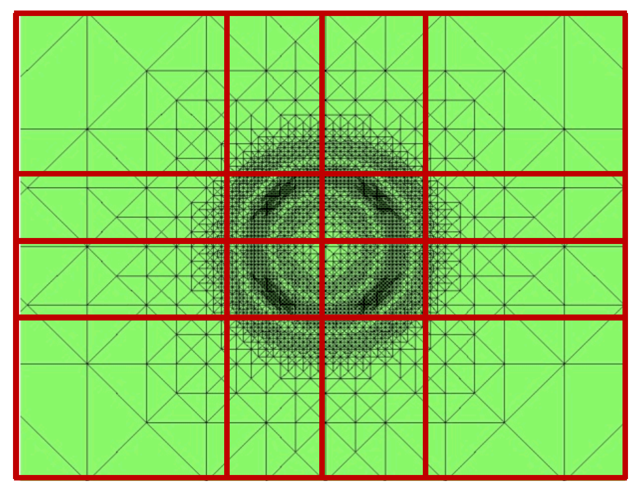
Unstructured ⇒ Structured

Why?

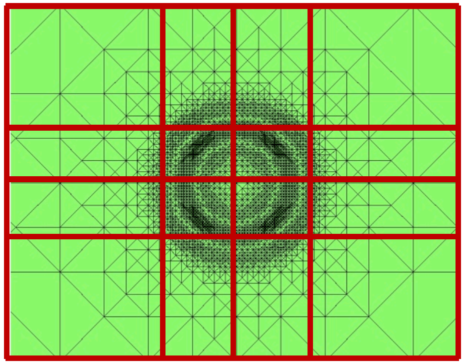
computational efficiency … on large parallel systems



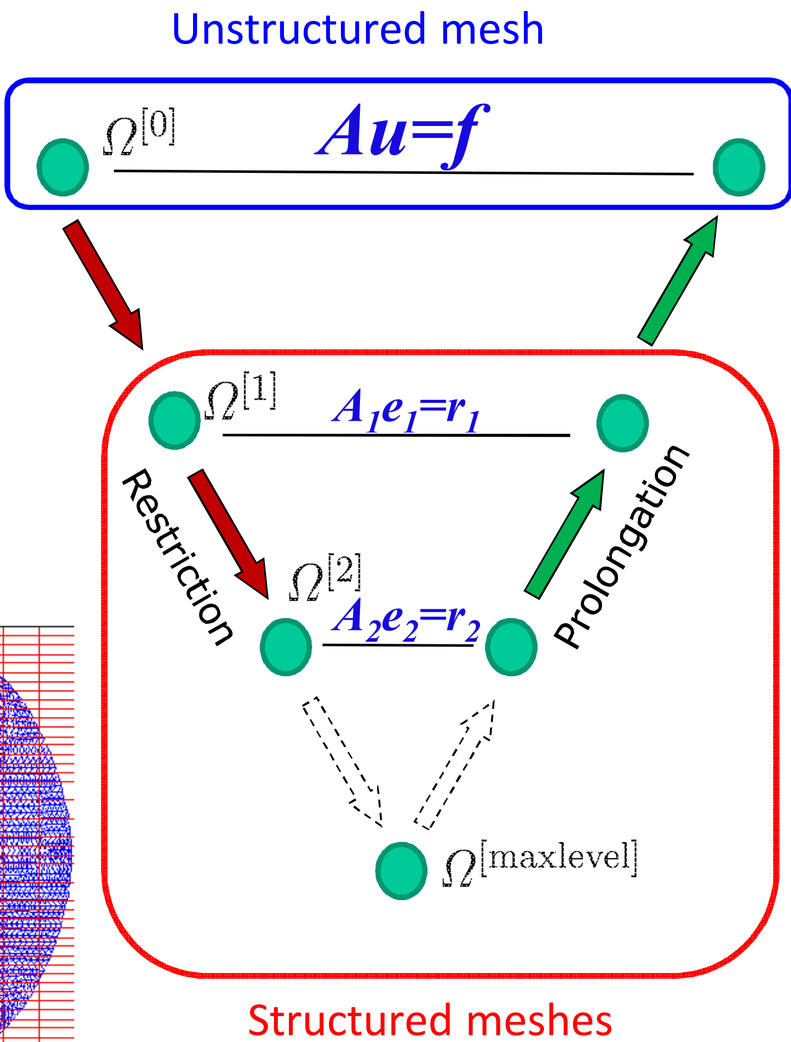
- Overlay unstructured grid with structured grid.
- Coarse DOFs on structured mesh, interpolate from fine DOFs within rectangles.
- Interpolation weights found with energy minimization.



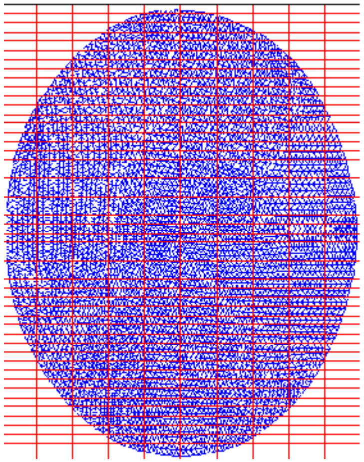
Unstructured ⇒ Structured



domains	*Emin its*
4×4	*12*
8×8	*11*
12×12	*10*
16×16	*10*



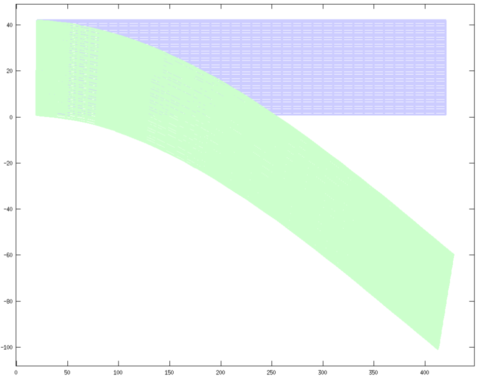
#DOFs	Unstructured AMG		Unstruct /struct AMG
	SA	Emin	Emin
69185	77 (1.95)	59 (1.95)	31 (1.59)
277633	112 (1.93)	84 (1.93)	38 (1.61)



- caveat: unstr. is 3-level, unstr. to struct. is 2-level

Energy Minimization: Plane Stress Linear Elasticity

100:1 stretching in x-direction
SA = smoothed aggregation multigrid
NSA = non-smoothed aggregation
NR = no rotational modes
EMIN = energy minimization



2D: Iterations (Complexity)

Size	SA-NR	SA-NF-NR	EMIN-NR	NSA	SA	SA-NF	EMIN
40^2	94 (1.49)	34 (2.83)	36 (1.49)	28 (2.22)	94 (2.24)	16 (5.12)	8 (2.32)
80^2	93 (1.52)	31 (3.02)	7 (1.52)	34 (2.29)	99 (2.32)	15 (5.55)	6 (2.40)
120^2	99 (1.51)	30 (2.99)	38 (1.51)	36 (2.27)	99 (2.30)	15 (5.48)	7 (2.37)
160^2	– (1.50)	50 (2.98)	54 (1.50)	37 (2.26)	99 (2.28)	15 (5.45)	8 (2.36)
200^2	97 (1.51)	29 (3.02)	36 (1.51)	38 (2.28)	– (2.31)	15 (5.56)	7 (2.38)
240^2	98 (1.51)	34 (3.01)	44 (1.51)	38 (2.27)	95 (2.30)	15 (5.52)	7 (2.37)

3D: Iterations (Complexity)

Size	SA-NR	SA-NF-NR	EMIN-NR	NSA	SA	SA-NF	EMIN
5^3	56 (1.17)	57 (1.37)	39 (1.17)	13 (1.72)	15 (1.72)	12 (2.50)	8 (1.80)
10^3	70 (1.13)	91 (1.36)	94 (1.13)	20 (1.57)	95 (1.57)	16 (2.43)	11 (1.60)
15^3	– (1.15)	98 (1.41)	88 (1.15)	25 (1.66)	81 (1.66)	18 (2.62)	12 (1.70)
20^3	98 (1.17)	96 (1.50)	79 (1.17)	28 (1.73)	91 (1.74)	18 (3.00)	9 (1.80)
25^3	87 (1.14)	99 (1.41)	96 (1.14)	30 (1.64)	91 (1.65)	19 (2.66)	11 (1.67)
30^3	92 (1.16)	97 (1.48)	83 (1.16)	33 (1.70)	96 (1.71)	18 (2.92)	9 (1.75)
35^3	99 (1.17)	94 (1.53)	82 (1.17)	35 (1.76)	89 (1.77)	18 (3.14)	9 (1.81)

- Complexity = $\sum nnz(A_i) / nnz(A_1)$
- Measures expense to apply preconditioner.
- Smaller = less expensive.

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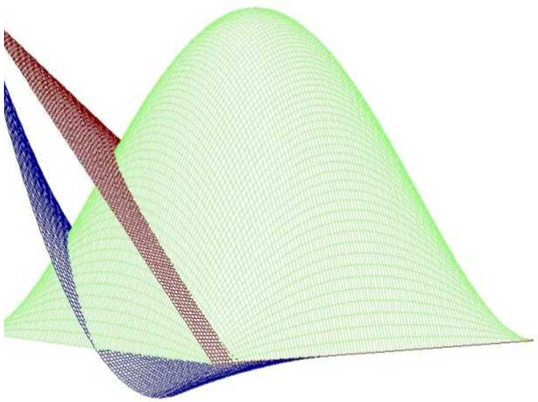
Mixed Finite Elements

Stokes flow $\begin{pmatrix} \mu\Delta & \nabla \\ \nabla\bullet & \end{pmatrix}\begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}$

Q2-Q1 elements due to Inf-Sup conditions



Mesh	Iters	complexity
9 x 9	20	2.01
17 x 17	25	1.81
65 x 65	Xx	Xx
257 x 257	29	1.91

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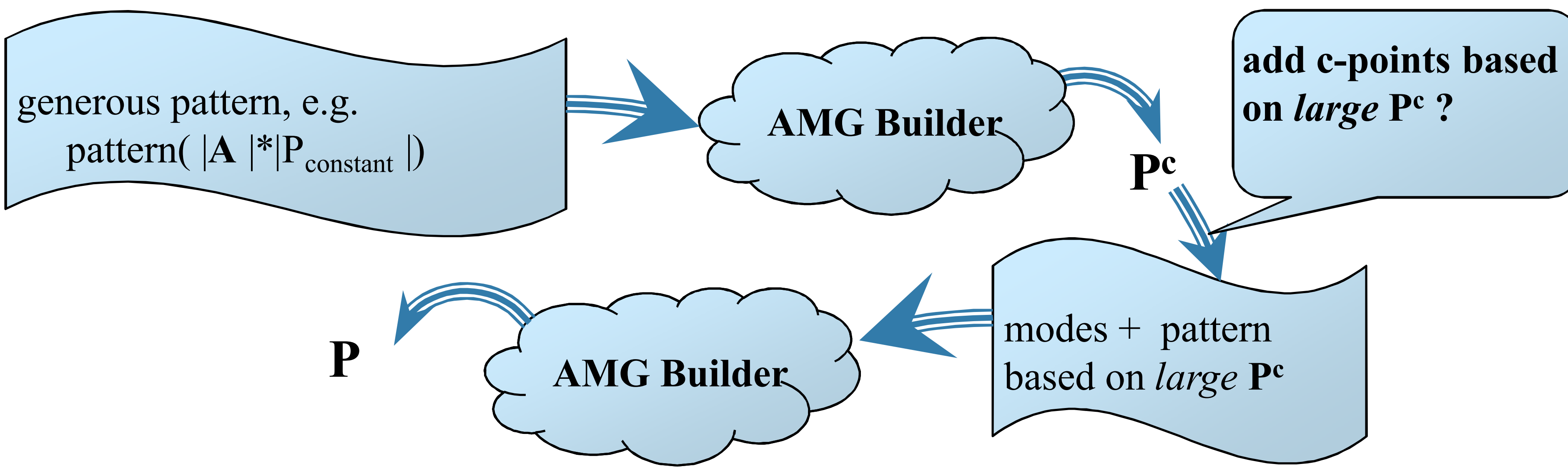
Sparsity Patterns

Strength of Connection

Remove *small* A_{ij}'s : $A \rightarrow \hat{\mathbf{A}}$ (no small entries)

Leads **indirectly** to P's pattern,

e.g. $\text{pattern}(P) \equiv \text{pattern}(|\hat{\mathbf{A}}| * |P_{constant}|)$



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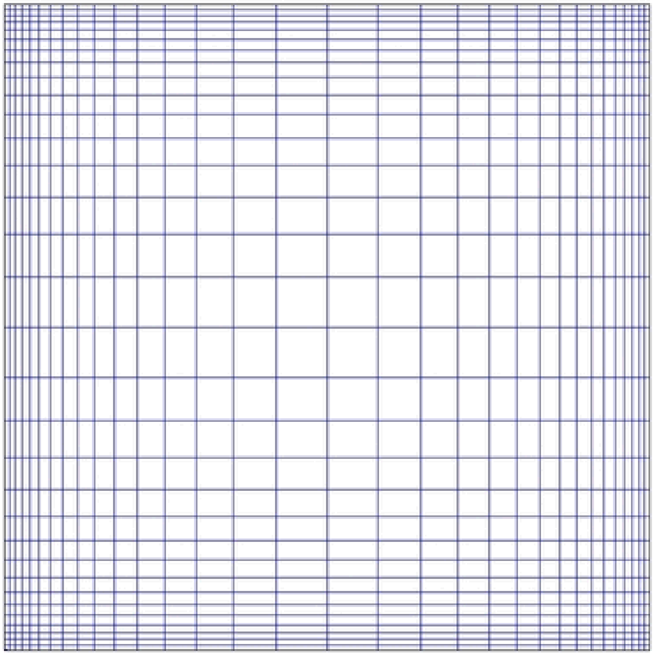
Patterns Experiments

$\Delta u = f$ **on stretched mesh**



MueMat/ MueLu

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        (__)
        (oo)   "MueMat"
  /-------\/
 / |      ||
*  ||----||
   ~~    ~~
```

sparsity pattern

constraints

→ **Solve Galerkin System via a couple of Richardson iterations** →

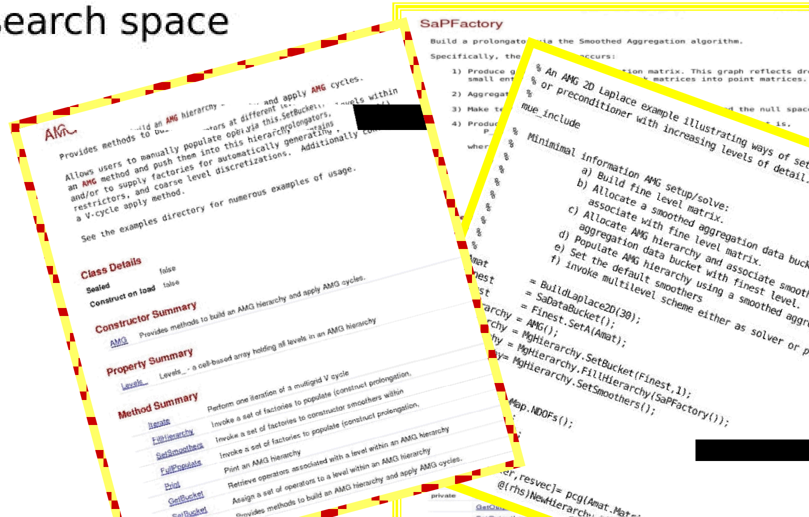
P_k's coefficients

Advantages:

- Flexibility (input):
  - arbitrary coarsening
  - accept any sparsity pattern (arbitrary basis function support)
  - enforce constraints: important modes requiring accurate interpolation
  - choice of norm for minimization and search space
- Robustness

<u>MueLu</u>

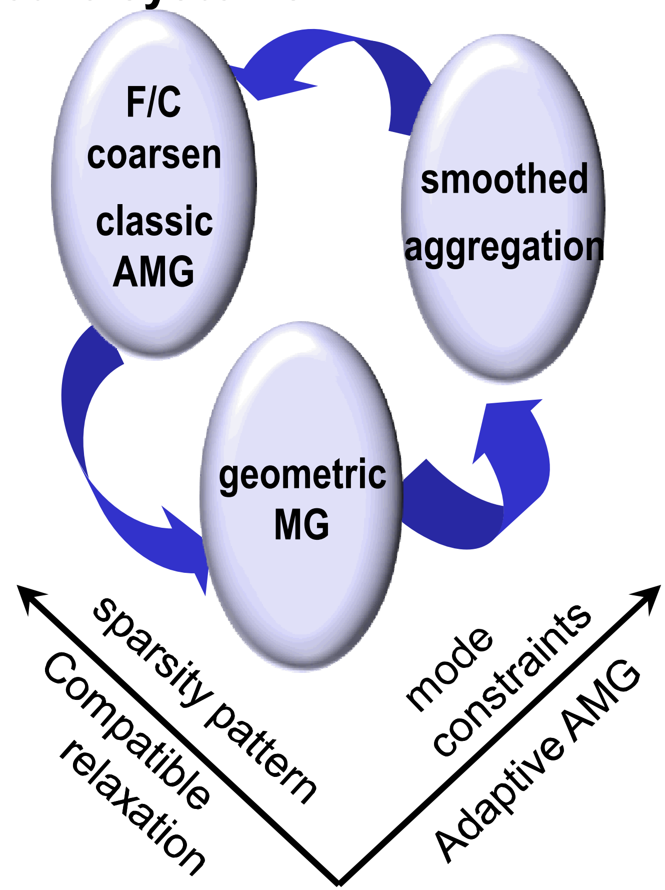
- New algorithms
- Variable block friendly
- Tpetra/Kokkos
  ⇒multicore aware, templated types



Concluding Remarks

- Krylov minimization can generate "energy" minimizing prolongators/restrictors for symmetric & non-symmetric systems
  - CG, GMRES

- Energy Minimization AMG flexibility provides leverage
  - <u>any</u> coarsening
  - <u>any</u> sparsity pattern
  - <u>any</u> definition of energy



- Fracture + XFEM ruins standard AMG, but fixed by
  - Schur complement avoiding explicit formation
  - Crack-conformal aggregates & sparsity patterns

levelsets $\Rightarrow$ sparsity pattern

$\Rightarrow$ maintain discontinuities on coarse levels