SAND2009-1534P

# Energy Minimizing Algebraic Multigrid for Systems of Partial Differential Equations

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Sandia National Labs

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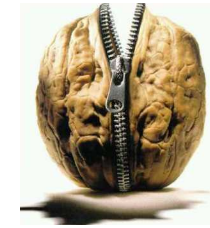
# Project in a Nutshell



PDE systems

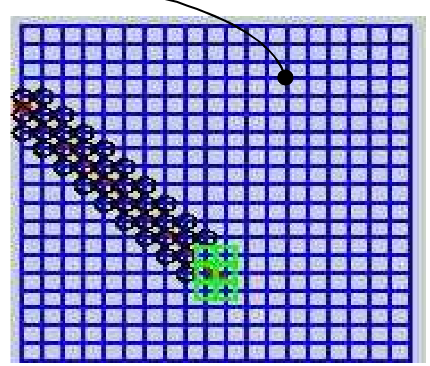
$$\begin{pmatrix} -\Delta & \nabla \\ \nabla\cdot & \end{pmatrix}\begin{pmatrix} u \\ p \end{pmatrix} = f$$

$$u = \sum_k u_k(x)\Psi_k(\omega)$$

$$\begin{pmatrix} \blacksquare & \blacksquare & & \blacksquare & & \\ \blacksquare & \blacksquare & \blacksquare & & \blacksquare & \\ & \blacksquare & \blacksquare & \blacksquare & & \blacksquare \\ \blacksquare & & \blacksquare & \blacksquare & \blacksquare & \\ & \blacksquare & & \blacksquare & \blacksquare & \blacksquare \\ & & \blacksquare & & \blacksquare & \blacksquare \end{pmatrix} u = f$$

A x = b

$$\begin{pmatrix} * & * & & \\ * & * & * & * \\ & * & * & \\ & * & & * \end{pmatrix}\begin{pmatrix} \rho \\ u \\ T \\ B \end{pmatrix} = f$$



Algebraic Multigrid

Energy Minimizing prolongators

KKT: $\begin{pmatrix} G & B^T \\ B & \end{pmatrix}$

goals: flexibility & robustness

Constraints:
- sparsity pattern
- accurate modes

Smoothers

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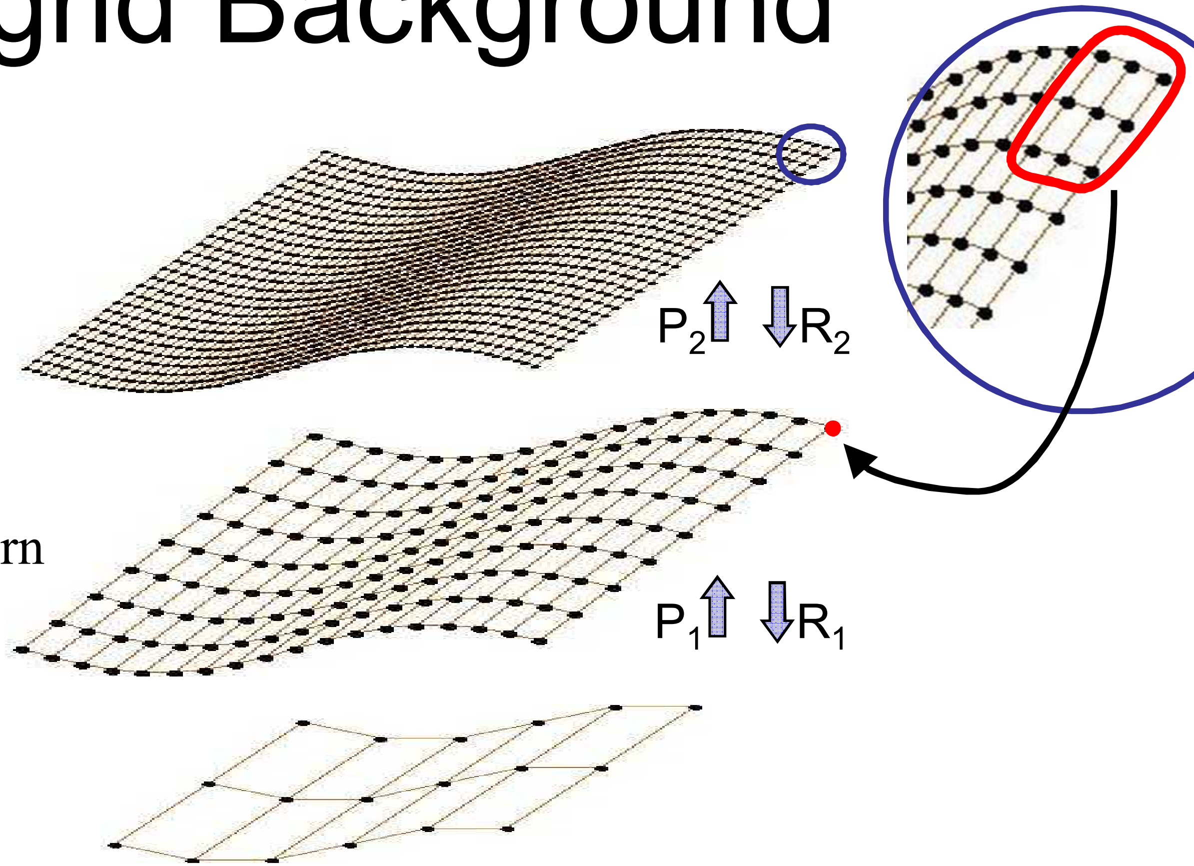
# *Algebraic* Multigrid Background

Solve $A_3 u_3 = f_3$

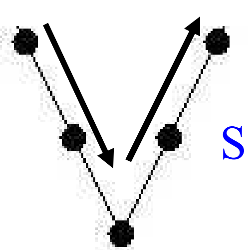
- Construct graph & coarsen
- Determine $P_i$ & $R_i$ sparsity pattern
- Determine $P_i$ & $R_i$'s coefs
- Project: $A_i = R_i A_{i+1} P_i$




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 $u_3 = u_3 + P_2 u_2$.

Set $u_2 = u_2 + P_1 u_1$.

Brandt, McCormick, Ruge, Stubën

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# Prior Accomplishments: Incompressible flow

$$A = \begin{bmatrix} F & \nabla \\ \nabla\cdot & 0 \end{bmatrix}, \quad M = \begin{bmatrix} F & \nabla \\ & -\hat{S} \end{bmatrix} \quad \& \quad S = \nabla\cdot F^{-1}\nabla$$

Murphy, Golub, Wathen

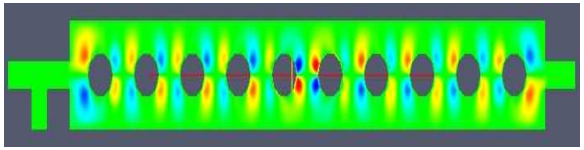
**AMG**

$$S \approx (\nabla\cdot\nabla)F_p^{-1} \Rightarrow \hat{S}^{-1} = F_p\Delta^{-1}$$

Elman ,Loghin, Kay, Silvester, Wathen '01-'03

- Algebraic Ŝ
- Ŝ for stabilized A, $A_{2,2} \neq 0$
- New BC treatment in Ŝ
- Integration in Sandia application codes

$$\min_{F_p} \left\| F_p\nabla - \nabla F \right\|$$



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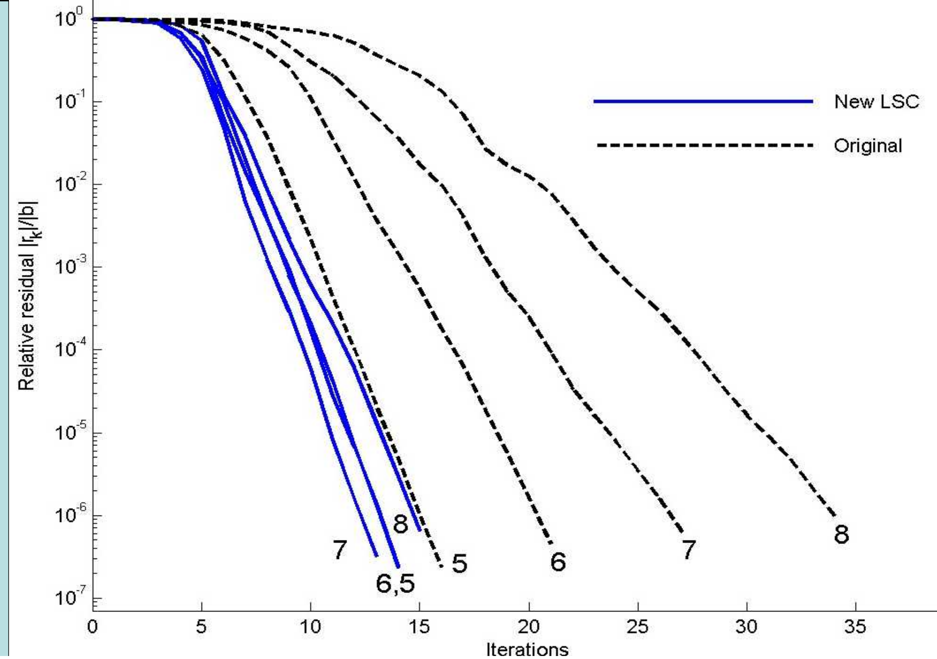
- **Smoothed Aggregation**: new AMG method for $A \neq A^T$
  - Low cost/iteration
  - Accurate interpolation of difficult modes
  - $P = (I - \Omega A)\, P_s$ $\quad$ $R = (P_s)^T(I - A\,\Theta)$
  - *Local minimization based on $A^TA$ norm*

$R$ = ? , $\omega$ = ?
Minimize what?

⇒ New algorithm fairly robust & often gives mesh independent convergence

| | | Fp | | S-LSC | |
|---|---|---|---|---|---|
| | $2^n \times 3*2^n$ | n=5 | n=6 | n=5 | n=6 |
| $Q_1$-$P_0$ | Re 10 | 35 | 37 | 16 | 22 |
| | Re 100 | 66 | 79 | 19 | 25 |
| | Re 200 | 92 | 100 | 26 | 27 |
| $Q_1$-$Q_1$ | Re 10 | 32 | 35 | 19 | 26 |
| | Re 100 | 61 | 76 | 19 | 28 |
| | Re 200 | 84 | 93 | 22 | 29 |

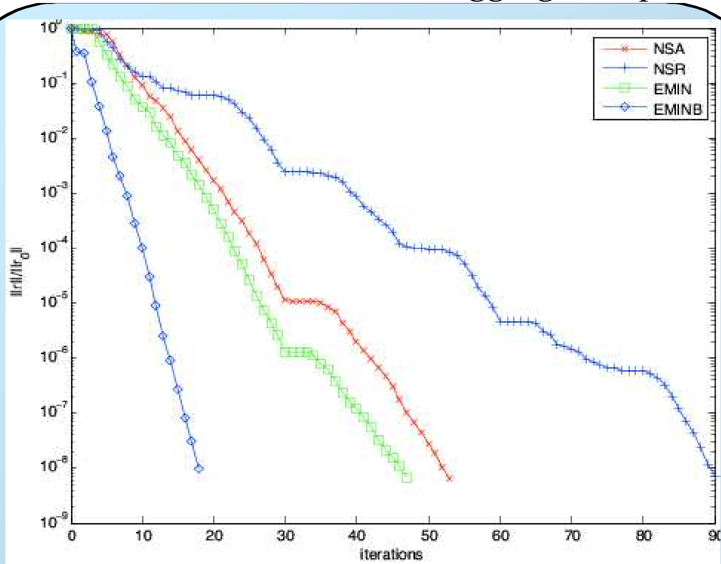



(1) *Least-squares preconditioners for stabilized … Navier-Stokes Equations, Elman,Howle, S, Silvester, T, SISC'07.*

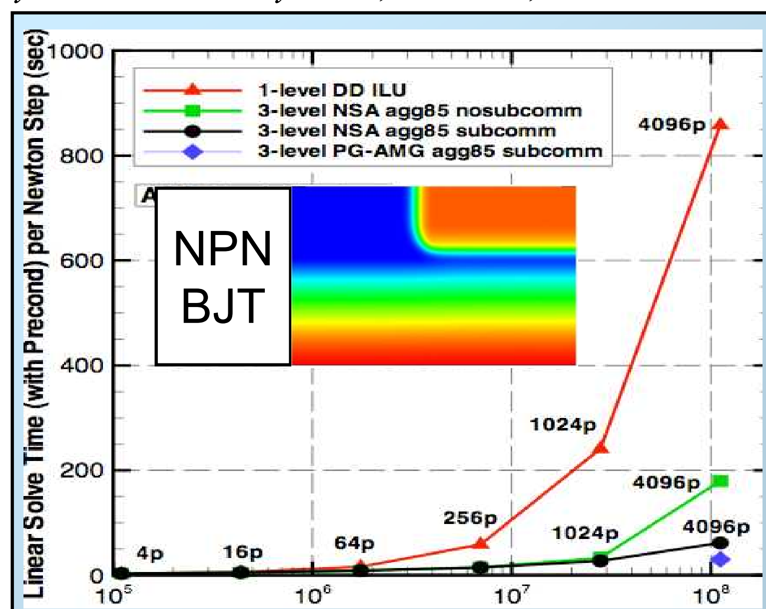
(2) *A Taxonomy … of Parallel Block Multilevel Preconditioners …, Elman, Howle, S, Shuttleworth, T, JCP'08.*

(3) *Boundary Conditions in Approximate Commutator Preconditioners …, Elman, T, submitted to ETNA.*

(4) *A new Petrov-Galerkin smoothed aggregation preconditioner for nonsymmetric linear systems*, Sala & T, SISC'08.




Euler/Jet flow, Mach .75



# Prior Accomplishments: AMG & Maxwell

$\nabla \times \nabla \times + \sigma$

Small $\sigma$

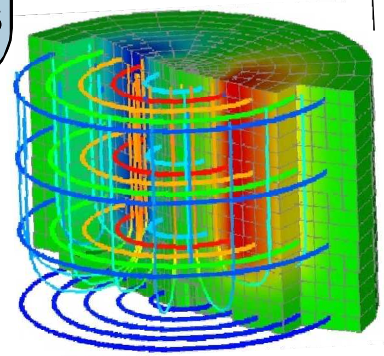
$\Rightarrow$ large near null space

$\Rightarrow$ iterative solver problems

**Exact** Discrete Reformulation

$$\begin{pmatrix} \Delta_v^{(e)} & \sigma\nabla \\ \sigma\nabla\cdot & \Delta^{(n)} \end{pmatrix}$$

$\Rightarrow$ Laplacian dominated



Ascher,Haber, Beck, Hiptmair,Xu, Kolev, Pasciak, Vassilevski, SNL

New blk diagonal preconditioner
- standard AMG on (2,2)
- 1 special prolongator + standard AMG

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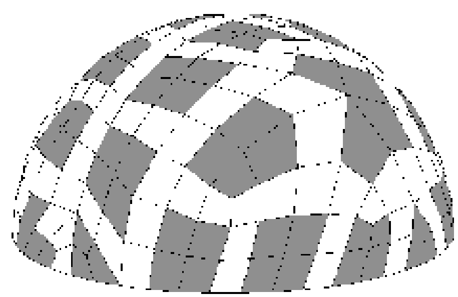
## Irregular Coarsening

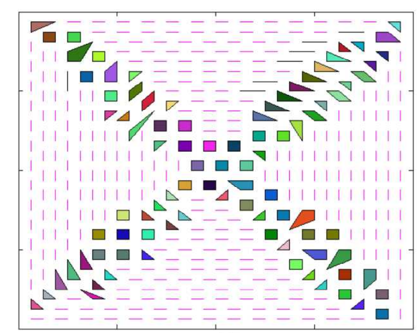
- detection

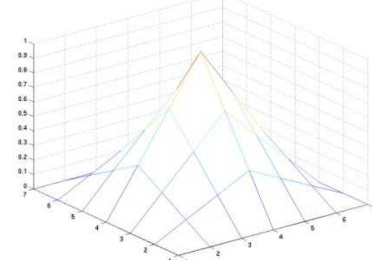
$$z_t = -Az + \delta_i \text{ with } z(0) = 0$$

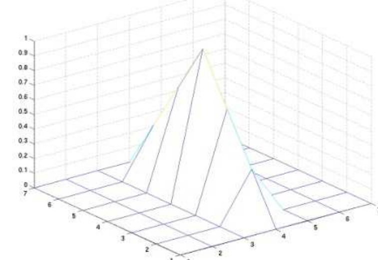
$$\Rightarrow \begin{cases} z_t(\Delta t) \approx \Delta t\, A\, \delta_i + \delta_i \\ z(\infty) = A^{-1}\, \delta_i \end{cases}$$

- prolongator basis functions





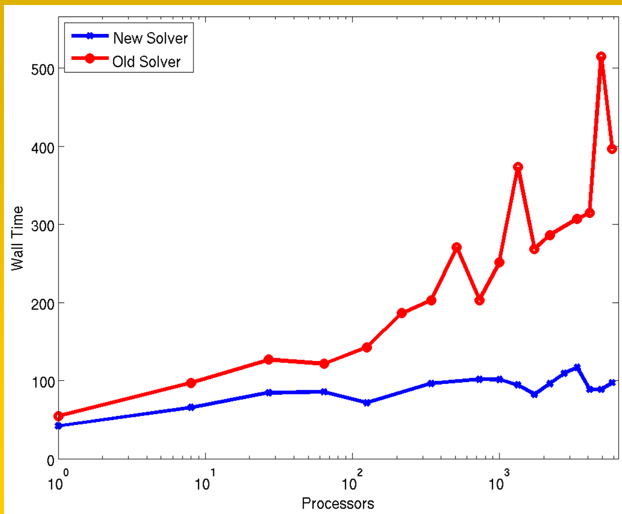




Brannick, Brezina, MacLachlan, Mantueffel, McCormick

# Pri nts: AMG & Maxwell

## Red Storm Weak Scaling




Sn

⇒

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Asc
Kole

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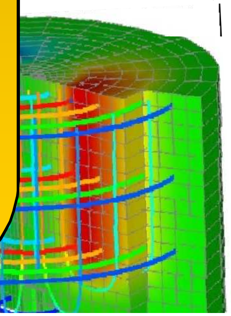
formulation

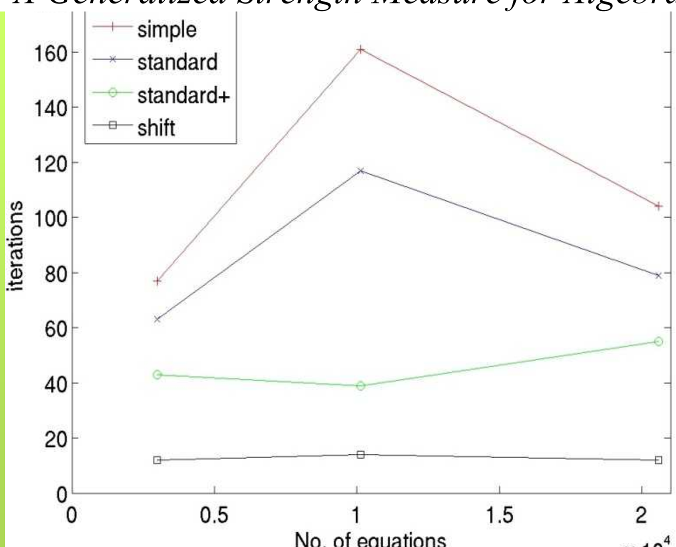


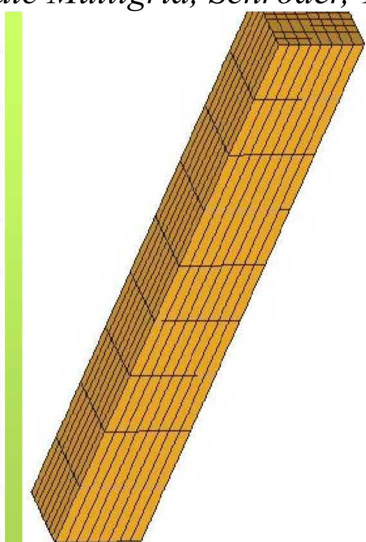
$$\begin{pmatrix} \Delta_v^{(e)} & \sigma\nabla \\ \sigma\nabla\cdot & \Delta^{(n)} \end{pmatrix}$$

⇒ Laplacian dominated

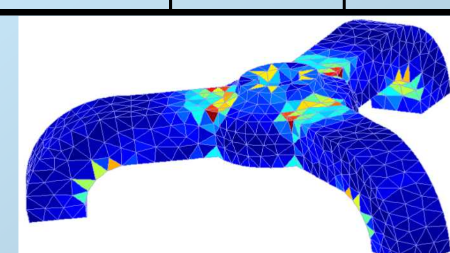
New blk diagonal preconditioner
- standard AMG on (2,2)
- 1 special prolongator + standard AMG

[(1)] *An AMG approach based on a compatible gauge reformulation of Maxwell's equations*, Bochev, H, S & T, SISC'08.
[(2)] *Auxiliary AMG preconditioners for Mixed Finite Element Methods, T., J. Xu, Y. Zhu, submitted to DD'08.*
[(3)] *A new smoothed aggregation multigrid method for anisotropic problems, Gee, H, T, NLAA, 09.*
[(4)] *A Generalized Strength Measure for Algebraic Multigrid, Schroder, T, Olson, submitted to NLAA.*

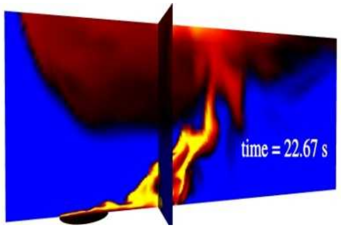


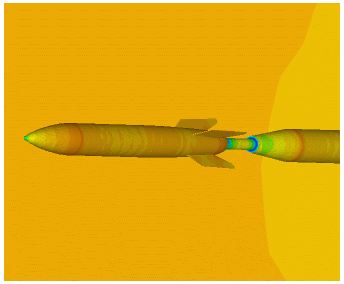



| ≈DOFs | Coefs | ODE |
|---|---|---|
| 2k | 33 | 13 |
| 14k | 67 | 13 |
| 110k | 129 | 18 |



# A Massively Parallel Algebraic Multigrid Solver



**Smoothed Aggregation Capabilities**

- Limited variable dofs/block support
- Aggregation with arbitrary coarsening, load balancing, …

**Variety of Smoothers**

**Leverages** Trilinos, PETSc, SuperLU, kLU, ParMETIS, …

**Smoothed Aggregation Advantages/Disadvantages**

**+** mesh independent convergence on many problems

**+** ability to emphasize accurate interpolation of important modes

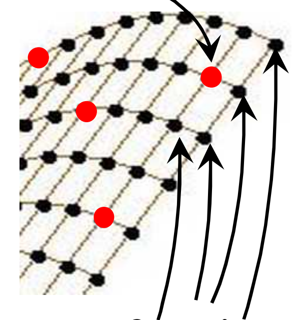
**+** relatively inexpensive cost per iteration and setup cost

-Constructing P's coefficients $\Rightarrow$ very modest control over P's sparsity pattern

$\Rightarrow$ rigid rules followed during coarsening/aggregation

-Accurate interpolation of special modes requires widening P

# Prolongation & Minimization: $\| P \|_A$




Consider

$$\begin{pmatrix} A_{ff} & A_{fc} \\ A_{cf} & A_{cc} \end{pmatrix}\begin{pmatrix} u_f \\ u_c \end{pmatrix} = \begin{pmatrix} b_f \\ b_c \end{pmatrix}$$

Then

$$\underbrace{\begin{pmatrix} I_f & 0 \\ R_f & I_c \end{pmatrix}\begin{pmatrix} A_{ff} & A_{fc} \\ A_{cf} & A_{cc} \end{pmatrix}\begin{pmatrix} I_f & P_f \\ 0 & I_c \end{pmatrix}}_{\begin{pmatrix} A_{ff} & E_{fc} \\ E_{cf} & A_H \end{pmatrix}}\begin{pmatrix} y_f \\ y_c \end{pmatrix} = \begin{pmatrix} b_f \\ Rb \end{pmatrix}$$

$$P = \begin{pmatrix} P_f \\ I_c \end{pmatrix}, \quad R = \begin{pmatrix} R_f & I_c \end{pmatrix}$$

$$A_H = RAP$$

$\Leftrightarrow$ 2 level AMG with $(A_{ff})^{-1}$ as relaxation

$\Rightarrow$ want $E_{fc} = \begin{pmatrix} A_{ff} & A_{fc} \end{pmatrix} P$ & $E_{cf} = R\begin{pmatrix} A_{ff} \\ A_{cf} \end{pmatrix}$ to be small

$\Rightarrow$ want $A_{ff}$ to be well-conditioned

Brandt, Brannick, Livne, Falgout, Zikatinov

Ideal $P_f = -A_{ff}^{-1} A_{fc}$ $\Rightarrow$ perhaps use to guide sparsity pattern of $P_f$

**Difficult to do some of these things in smoothed aggregation**

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# Energy Minimizing Prolongators

$$\min_{\bar{p}} \sum_i \|p_i\|_A^2 \quad \text{subject to} \quad B\begin{pmatrix} p_1 \\ \vdots \\ p_m \end{pmatrix} = g \quad , \quad P = [p_1 \; p_2 \cdots p_m]$$

B : accurate interpolation of important modes, e.g. P const = const

$$\Rightarrow \begin{pmatrix} A & & & & \\ & A & & & \\ & & A & & B^T \\ & & & A & \\ & B & & & \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ \lambda \end{pmatrix} = \begin{pmatrix} \\ \\ 0 \\ \\ g \end{pmatrix}$$

**Constraints improve conditioning!**

$$BB^T = \begin{pmatrix} * & * & * & & & \\ * & * & * & & & \\ * & * & * & & & \\ & & & \ddots & & \\ & & & * & * & * \\ & & & * & * & * \\ & & & * & * & * \end{pmatrix}$$

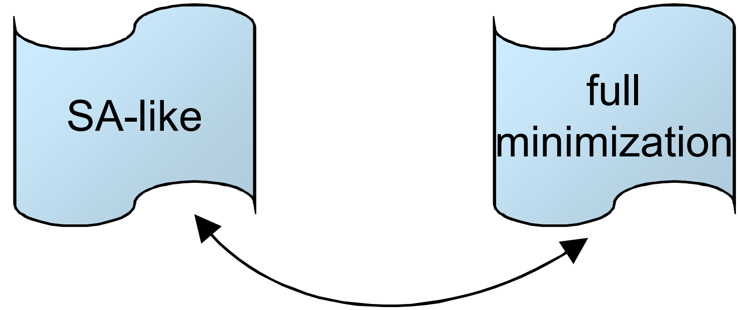
1) Solve via CG & enforce constraints each iteration:

$$Q \hat{A} Q \; p = rhs \qquad Q = I - B^T(B\,B^T)^{-1}B$$

2) Each iteration …
   a) A P
   b) Remove nonzeros that extend beyond desired sparsity pattern
   c) Apply projection

Mandel, Brezina, Vanek, Brannick, Zikatanov, Wan

# Research Issues




- Cost of P's construction
  - smoothed aggregation connection
  - selective iteration
  - Amortize multiple linear systems
  - $\Rightarrow$ Criteria for acceptable columns of P

- Prolongator sparsity patterns
  - easy to consider irregular sparsity patterns

    application driven vs. $P_f = -A_{ff}^{-1} A_{fc}$
  - widening P & linear independence

- Nonsymmetric
  - Perhaps GMRES on

    *Q Â Q »P« = 0* $\qquad$ *Q = I – $B^T(B\,B^T)^{-1}B$*

    *Q $\hat{A}^T$ Q »R« = 0*
  - Norms/scaling for minimization

- Additional constraints
  - application driven vs. adaptive AMG

Brezina, Falgout, MacLachlan, Manteuffel, McCormick, Ruge, Sanders

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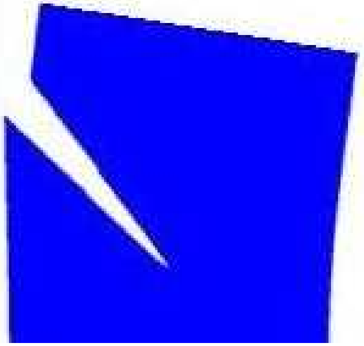
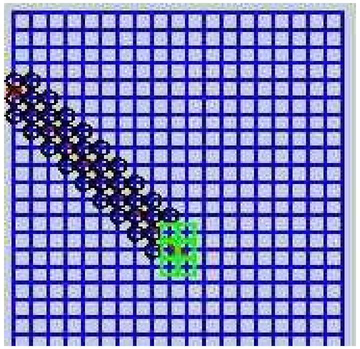


# XFEM & AMG



$$u(x)=\sum_i \phi_i(x)u_i+\sum_i \phi_i(x)H(x)z_i+\dots \quad , \quad H(x)=\begin{cases}1 & \varphi\geq 0\\ 0 & \varphi<0\end{cases}, \quad \Gamma=\{(x,y)\,|\,\varphi(x,y)=0\}$$

How to interpolate to special degrees of freedom?

XFEM philosophy would probably coarsen normally
but have coarse special functions embedded in $A_H$

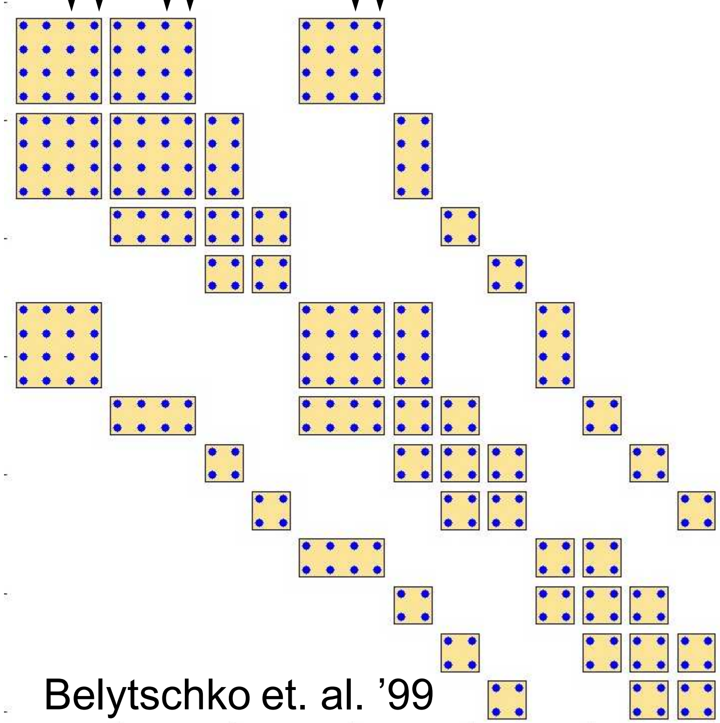
Could project level set information to coarse grids?

<u>sparsity pattern</u>

- coarse special DOFs interpolate only to fine special DOFS
- restrict basis function support to one side of discontinuity

<u>special constraints?</u>

- enforce accurate interpolation of Heaviside function?



Belytschko et. al. '99

# MHD

$$\mathbf{R_m} = \frac{\partial(\rho\mathbf{v})}{\partial t} + \nabla\cdot[\rho\mathbf{v}\otimes\mathbf{v} - \mathbf{T}] - \boxed{\mathbf{J}\times\mathbf{B}} = \mathbf{0}\,; \quad \mathbf{T} = -\left(P + \frac{2}{3}\mu(\nabla\bullet\mathbf{u})\right)\mathbf{I} + \mu[\nabla\mathbf{u} + \nabla\mathbf{u}^T]$$

$$R_p = \frac{\partial(\rho)}{\partial t} + \nabla\cdot[\rho\mathbf{v}] = 0$$

$$R_e = \frac{\partial(\rho e)}{\partial t} + \nabla\cdot[\rho\mathbf{v}e + \mathbf{q}] - \mathbf{T}:\nabla\mathbf{v}\boxed{-\eta\|\mathbf{J}\|^2} + Q^{rad} + Q = 0$$

$$\mathbf{R_B} = \frac{\partial\mathbf{B}}{\partial t} + \nabla\times\mathbf{E} = 0 \quad \mathbf{J} = \frac{1}{\mu_0}\nabla\times\mathbf{B} \quad \mathbf{E} = -\mathbf{v}\times\mathbf{B} + \eta\mathbf{J} + \underbrace{\frac{1}{en}(\mathbf{J}\times\mathbf{B} - \nabla\mathbf{P_e})}_{\text{Hall}}$$

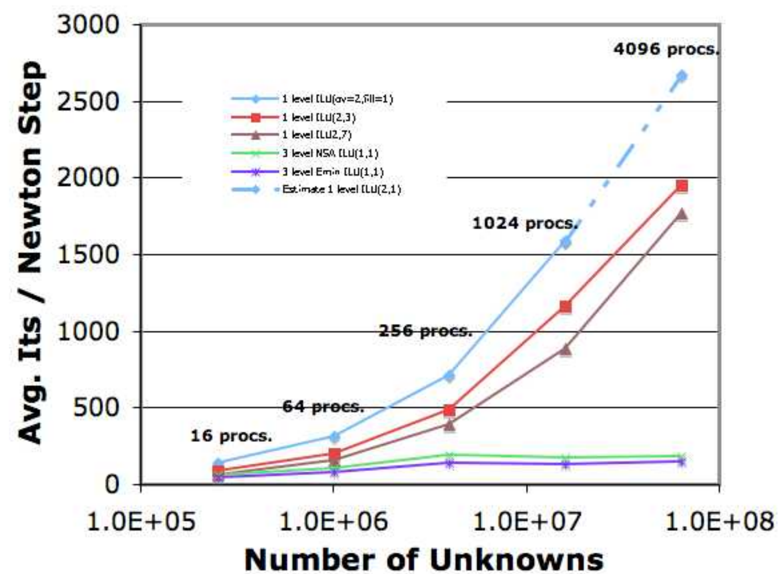
**Ion Momentum Diffusion $10^{-7} \rightarrow 10^{-3}$**
**Magnetic Flux Diffusion $10^{-7} \rightarrow 10^{-3}$**
**Ion Momentum Advection $10^{-4} \rightarrow 10^{-2}$**
**Alfven Wave $10^{-4} \rightarrow 10^{-2}$**
**Whistler Wave $10^{-7} \rightarrow 10^{-1}$**
**Magnetic Island Sloshing $10^{0}$**
**Magnetic Island Merging $10^{1}$**

$\Rightarrow$ Strongly Coupled, Multiple Time- and Length-Scale, Nonlinear, Nonsymmetric System with Parabolic and Hyperbolic Character

**Steady-state Resistive MHD**

- **$1^+$ Billion unknowns**
- **6000 cores Cray XT3/4**
- **Newton-GMRES/ML 4 level**
- **18 Newton steps**
- **223 Avg. Linear Its./ Newton step**
- **84 min. for solution**

**Weak Scaling Study: Resisitve MHD VP Formulation (2D MHD Pump)**



# MHD & AMG

- Explore better *minimization* prolongators
- Possibly new constraints based on analysis

$$\begin{pmatrix} * & * & & \\ * & * & * & * \\ & * & * & \\ & * & & * \end{pmatrix}\begin{pmatrix} \rho \\ u \\ T \\ B \end{pmatrix} = f$$

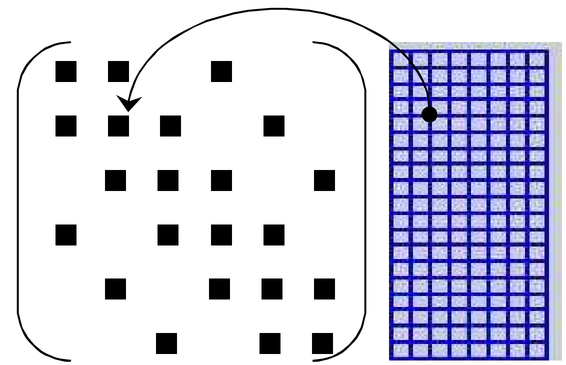
Use

$$\begin{pmatrix} F & \\ & \hat{S} \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} F & B^T \\ B & \hat{S} \end{pmatrix}$$

$\Rightarrow$ generate hierarchy

$\Rightarrow$ generate prolongators

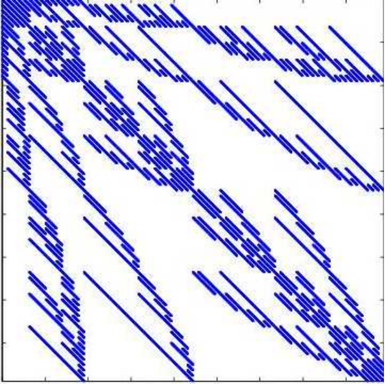
- Grid/spatially based block smoothers



- F/C choice via compatible relaxation-like
- Sparsity pattern choice via $A_{ff}$ iteration
- Schur complement-based smoothers

$$\begin{pmatrix} u \\ p \end{pmatrix} \leftarrow \begin{pmatrix} u \\ p \end{pmatrix} + \omega \begin{pmatrix} F & B^T \\ & \hat{S} \end{pmatrix}^{-1} r$$

Pernice, Tocci, Chacon, Knoll

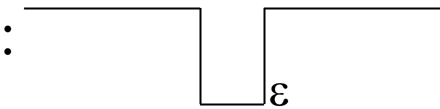


# Stochastic PDEs

$$u = \sum_k u_k(x)\Psi_k(\omega)$$
$$\lambda = \sum_k \lambda_k(x)\Psi_k(\omega)$$
$$M_{ijk} = \int \Psi_i \Psi_j \Psi_k \, d\mu$$

$$\boxed{-\sum_j \left[\sum_k M_{ijk}\lambda_k(x)\,[u_j(x)]_x\right]_x = f_i}$$

Different diffusion coefficients $\Rightarrow$ different features, e.g. $\sum_k M_{ijk}\lambda_k$ :




Gaussian variables $\Rightarrow$ potential loss of SPD

spatial coarsening

$$M = \begin{pmatrix} M_{11} & & \\ & M_{22} & \\ & & M_{33} \end{pmatrix} \qquad P = \begin{pmatrix} P_1 & & \\ & P_2 & \\ & & P_3 \end{pmatrix} \qquad P = \begin{pmatrix} P_1 & \iddots & \vdots \\ \iddots & P_2 & \ddots \\ \vdots & \ddots & P_3 \end{pmatrix}$$

Nonintrusive $\longrightarrow$ Intrusive

$[A_H]_{ij} = P_i \; A_{ij} \; P_j \quad , \quad P_i \leftarrow AMG(A_{ii})$

Elman, Furnival, Powell, LeMaire, Knio, Debusschere, Najm, Ghanem

- Stochastic coarsening (or spectral coarsening)
  - Interplay with spatial coarsening
  - Special constraints when nearly non-spd?
- *Drop* higher order terms or leave choice to energy minimization

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# Summary

- Energy minimizing framework **(Tuminaro,Hu)**
  - Sparsity patterns
  - Family of methods with varying costs
  - Nonsymmetric
  - Multiple constraints
- XFEM with Waisman(Columbia) & within SNL applications **(Tuminaro)**
  - Broaden variable block capability
  - Coarse level sets & additional constraints
  - Sparsity patterns
- MHD with Shadid(SNL)/Chacon(Oakridge) **(Tuminaro,Cyr,Hu)**
  - Schur complements & smoothers
  - Special constraints to address difficult modes
- Stochastic PDEs with Phipps/Najm(SNL), Elman(Maryland) **(Tuminaro)**
  - Stochastic coarsening
  - Special constaints as system approaches non-SPD

**Application areas are important … but research is applicable to a broader class of difficult problems**

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