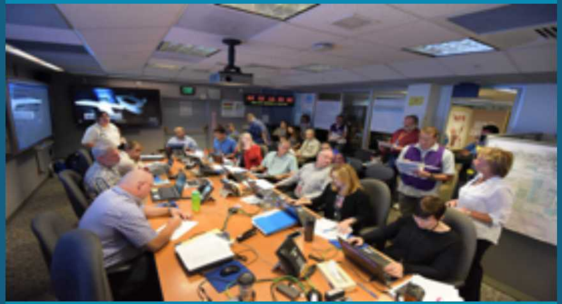
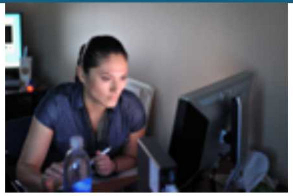
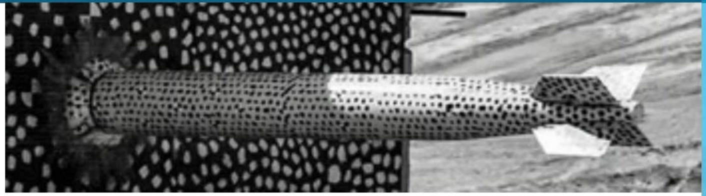
SAND2019-9886PE

Scalable Preconditioners to Improve Time to Solution for Magnetohydrodynamics Applications







PRESENTED BY

Ray Tuminaro

Sandia : J. Shadid, E. Cyr, P. Lin, R. Pawlowski, E. Phillips, T. Wiesner (Leicia)
Non-Sandia: J. Adler (Tufts), T. Benson (LLNL), L. Chacon (LANL), P. Farrell (Oxford), A. Rappaport (UNM), S. Maclachlan (Mem U N)

MueLu team: J. Hu, L. Berger-Vergiat, C. Glusa, C. Siefert

CIS External Review, August 26-29, 2019
SAND 2019XXX-XX

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Project/Mission Scope

≈1995-1999

Past

Original driver:
- Chem. react. flow via MPSalsa (ASCR)

incompressible Navier-Stokes solvers

curl x curl AMG solvers

Original driver:
- Z-pinch via ALEGRA (ASC/ATDM)

≈2008

Present

Recent driver:
- multiphase flow via ARIA (ASC)

AMG ASCR base math ≈500K/yr,%25

MHD ASCR base math SNL≈500K/yr, %25

FastMath SciDAC ≈75K/yr, 2 yrs

ASCR/OFES SciDAC Tok. Disrupt. ≈75K, 1 yr

Recent driver:
- E&M re-entry via EMPIRE (ATDM)

Current MHD Driver:
- multifluid EM Plasmas via Drekar
  - tokamak equilibrium & disruption/mitigation

Presentation focuses on recent developments (3-5 years).

Future

non-MHD Applications:
- hypersonic fluid flow via SPARC (ASC/ATDM)
- wind energy NREL project (ASCR/ECP)
- ice sheet flow Prospect project (SciDAC)
- ocean system E3SM project (BER Cimate)

MHD Potential Impact:
- Drekar for MHD turbulence & multifluid E & M plasmas for tokamak & Z-pinch type fusion (ASCR)
- EMPIRE for plasma in radiation environments (ASC/ATDM)
- ALEGRA for improved fidelity Z machine (NNSA)

Staffing/Mentorship (focusing on early career)

K. Devine, A. Salinger, S. Hutchinson, P. Lin, R. Pawlowski, M. Sala

incompressible Navier-Stokes solvers

curl x curl AMG solvers

J. Hu & C. Siefert

AMG ASCR base math ≈500K/yr,%25

MHD ASCR base math SNL≈575K/yr, %25

FastMath SciDAC ≈75K/yr, 2 yrs

ASCR/OFES SciDAC Tok. Disrupt. ≈75K, 1 yr

L. Berger-Vergiat, T. Wiesner (-'18), M. Mayr (-'18), P. Ohm, A. Rappaport,

P. Lin, E. Cyr, J. Banks, E. Phillips, S. Conde, M. Crockatt

J. Hu & L. Berger-Vergiat work on ExaWind (ECP)

J. Hu, C. Siefert, E. Phillips, C. Glusa work on Empire (ASC/ATDM)

Besides R. Tuminaro & J. Shadid many others associated with these projects: H. Waisman, V. Howle, R. Shuttleworth, P. Tsuji, M. Lupo Pasini, Y. Zhu, T. Benson, M. Gee, A. Prokopenko, J. Gaidamour,

MHD: Magnetohydrodynamics Background

- Plasma systems are multiscale & multiphysics, encompassing a range of phenomena
  fast waves: Whistler, Magneto-sonic, Alfven; slow: material transport;
  diffusion: anisotropic heat transport; complex multifluid models: speed of light, collisions, plasma/cyclotron frequencies, ionization/recombination, …

- Hierarchy of formulations: Ideal MHD, resistive MHD, Hall physics, extended MHD

- Couples fluids and electro-magnetics (Navier-Stokes + Maxwell)

An example,

⇨

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} - \nabla\cdot\nu\nabla\boldsymbol{u} + \nabla p + \nabla\cdot\left(-\frac{1}{\mu_0}\boldsymbol{B}\otimes\boldsymbol{B} + \frac{1}{2\mu_0}\|\boldsymbol{B}\|^2\boldsymbol{I}\right) = \boldsymbol{0}$$

$$\nabla\cdot\boldsymbol{u} = 0$$

$$\frac{\partial \boldsymbol{B}}{\partial t} + \nabla\times(\boldsymbol{u}\times\boldsymbol{B}) - \nabla\times\frac{\eta}{\mu_0}\nabla\times\boldsymbol{B} + \nabla r = 0$$

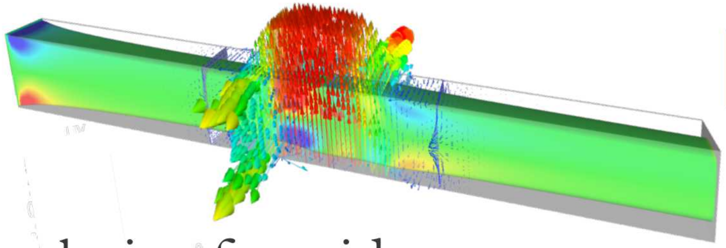
$$\nabla\cdot\boldsymbol{B} = 0$$

$\boldsymbol{u}$: velocity, p: pressure,
μ: viscosity
$\boldsymbol{B}$: magnetic induction,
η: resistivity,
μ_0: magnetic permeability of free space

- Numerical challenges of fluids, of electro-magnetics (E & M) and of their inter-coupling
- Flexible linear solvers needed to address range of formulations & physical effects

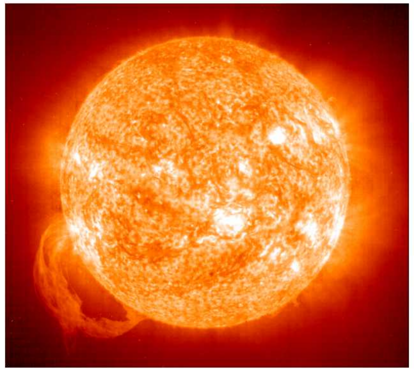
⇨ **it's all about solver speed, robustness, scalability & adaptability !**

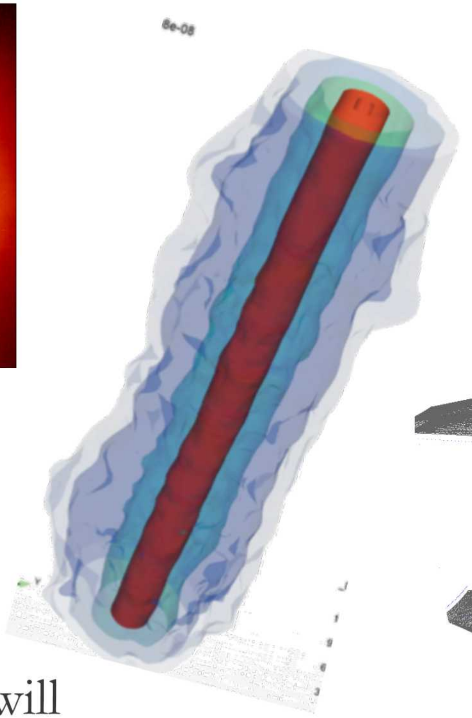
MHD Motivating Applications

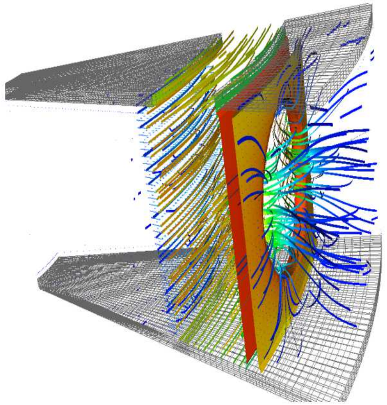


- Significant DOE/Sandia science & weapons applications require analysis of a wide-range of electro-magnetically (EM) driven experiments producing complex multi-physics plasmas

- Programs include:
  - Radiation effects
  - Dynamic materials
  - Magneto-inertial fusion
  - High energy density physics







Numerical simulation needed to understand fundamental physical properties, investigate current devices, design future devices & formulate future experiments

- Advanced multilevel methods have impacted ALEGRA, Drekar, EMPIRE and will impact next generation pulsed-power applications.

Boyd et.al. (Cambridge Press'03), Seyler et.al. (Phys. Plasma'11), Gourdain et.al. ((Phys. Plasma'14), Harned et.al. (JCP'89), Schnack et.al. (JCP'87), Jardin et.al. (Phys. Plasma'05), Sovinec et.al. (JCP'04), Hujeirat (Mon. Not. R Astron. Soc.'98), Robinson et.al. (AIAA'08), Chacon (Phys. Plasma'08), Shadid et.al. (CNMAME'16), Shumlak et.al. (JCP'03), Srinivasan et.al. (Phs. Plasma'11), Takanobu (JCP'15).

Linear Solver Challenges

$$u = A^{-1} f$$

- PDE applications → wide range of matrix inverses (PDE + discretization)
- $O(N)$ algorithms for N x N matrices is hard ⇨ assumptions made based on character of PDEs

Algebraic Multigrid (AMG) Challenges

- special saddle point $\begin{bmatrix} F & B^T \\ B & 0 \end{bmatrix}$ smoothers
  - no diagonal dominance, complex field interactions

smoothers

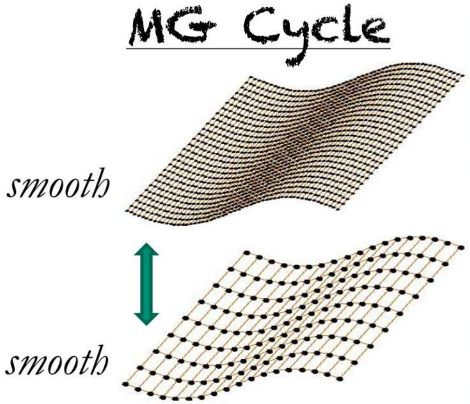
- projection issues for PDE systems
  - akin to algebraic re-discretization with similar concerns (e.g., preservation of key properties)

grid transfers

projection

finite elements: $A_0 = \mathcal{R}\mathcal{A}\mathcal{P}$

algebraic: $A_1 = R \quad A_0 \quad P$



AMG: Brandt et. al. (Spars. & Appl.'84), Ruge et. al. (Front. App. Math'87), Henson & Yang (App. Num. Math.'02), Falgout et. al. (Num. Sol. PDEs), Notay et. al. (SISC'12), Vassilevski (Springer'08), Bochev et. al. (SISC'08), Dendy (App. Math Com.'83), Mandel et. al. (Comput.'99), Brannick et. al. (NLAA '06), Trottenberg et al. (Aca. Press'01), Adams et. al. (JCP'03)

Significant LLNL contribution via Hypre/BoomerAMG

Leveraging PDE properties to improve scalability & robustness (with J. Shadid & …)

Previously, we applied somewhat generic algorithms (e.g., ILU + simple AMG) to multiphysics systems

Our research leads to **state-of-the-art** new algorithms that take account of the nature of PDEs

Two paths:

Physics-Based or Approx. Block-Factorizaiton (ABF)

- Inexact Block Factorization + Schur
- comp. approximations
- AMG only used to invert sub-blocks
- Avoids some AMG challenges including mixed FEs

$$\approx \begin{bmatrix} F & & Z \\ & I & \\ Y & & D \end{bmatrix} \begin{bmatrix} F^{-1} & & \\ & I & \\ & & I \end{bmatrix} \begin{bmatrix} F & B^T & \\ B & C & \\ & & I \end{bmatrix}$$

- Builds on incompressible Navier-Stokes solvers & electromagnics solver (e.g., $\nabla\times\nabla\times$)

Monolithic Multigrid

- Apply AMG directly to entire system
- Smoothing for PDE systems
- Projection of entire system
- Avoid Schur comp. approximations

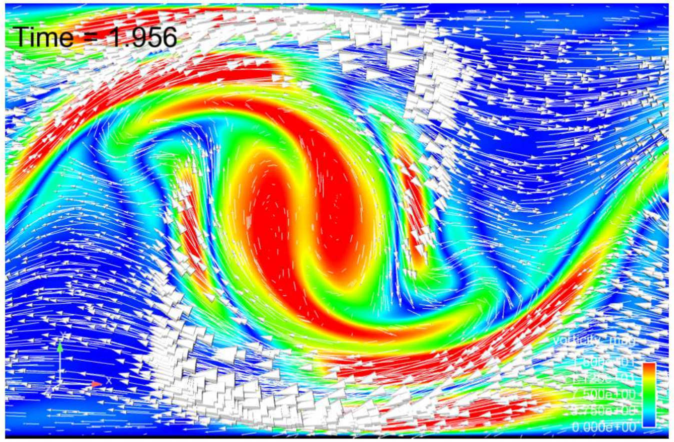
$$\begin{bmatrix} R_v & & \\ & R_p & \\ & & R_b \end{bmatrix} \begin{bmatrix} F & B^T & Z \\ B & C & \\ Y & & D \end{bmatrix} \begin{bmatrix} P_v & & \\ & P_p & \\ & & P_b \end{bmatrix}$$

- Builds on incompressible Navier-Stokes solvers & electromagnics solver (e.g., $\nabla\times\nabla\times$)

ABF: Elman, Silvester, Wathen (Oxford Press'14), Benzi et.al. (Acta Num..'05), Knoll et. al. (SISC '05), Chacon (J of Phys. '08), Phillips et. al. (SISC'16) Wathen et. al. (SISC'18), Ma et. al. (JCP'16), Mardal et. Al. (NLAA'11), Greif et. al. (NLAA'07), Wu et. al. (J. Comp. App. Math'13)
Mono. MG: Fullenbach et. al. (Ell. & Para. Probl.'02), Richter (IJNME'15), Gee et. al. (IJNME'10), Turkel et. Al. (Fluid Str. Inter. '10), Mavriplis (JCP'98)

ABF methods lead to scalable MHD solvers

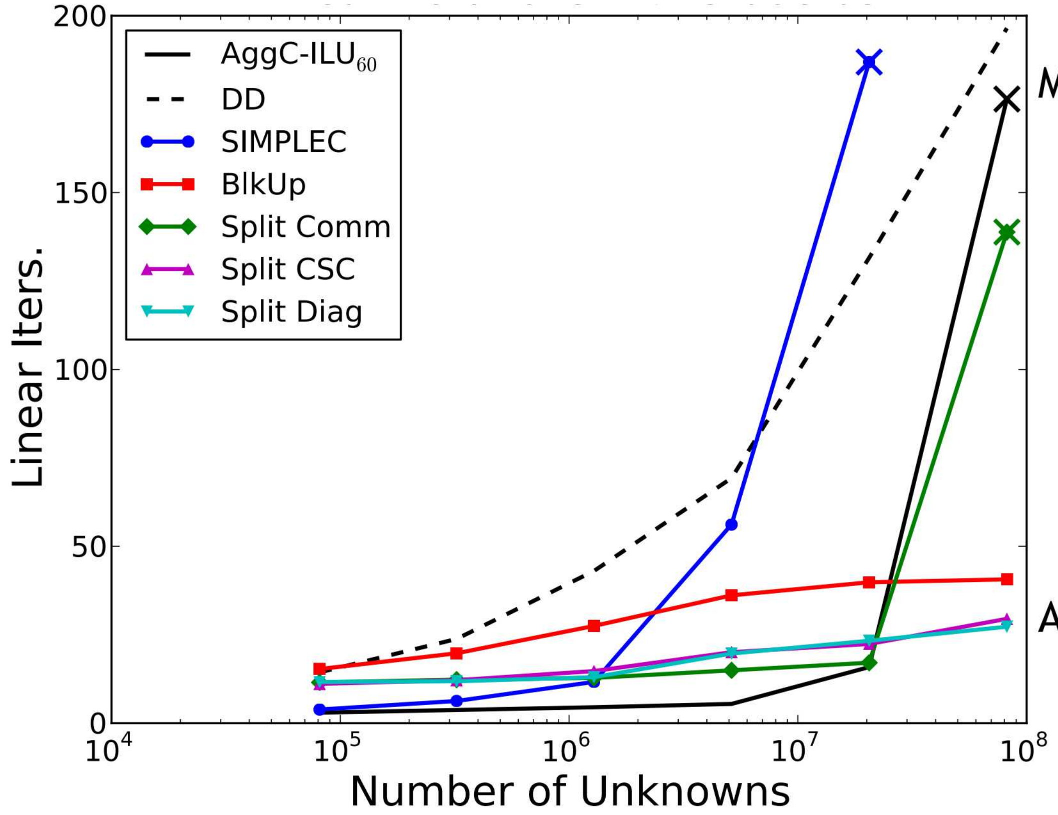
(with E. Cyr, J. Shadid, R. Pawlowski, L. Chacon)



- New approximate factorization preconditioners

$$\begin{bmatrix} F & B^T & Z \\ B & C & \\ Y & & D \end{bmatrix} \approx \begin{bmatrix} F & & Z \\ & I & \\ Y & & D \end{bmatrix} \begin{bmatrix} F^{-1} & & \\ & I & \\ & & I \end{bmatrix} \begin{bmatrix} F & B^T & \\ B & C & \\ & & I \end{bmatrix}$$

- New Schur complement approx. based on analysis of idealized MHD system
- Flexible general purpose software, Teko, allows custom ABF preconditioners to employ multigrid solvers.



Monolithic

ABF

> 5x

- ABF provides robust alternatives to monolithic AMG
- ABF addresses mixed finite element discretization
- TRILINOS **Teko** for multiphysics formulations

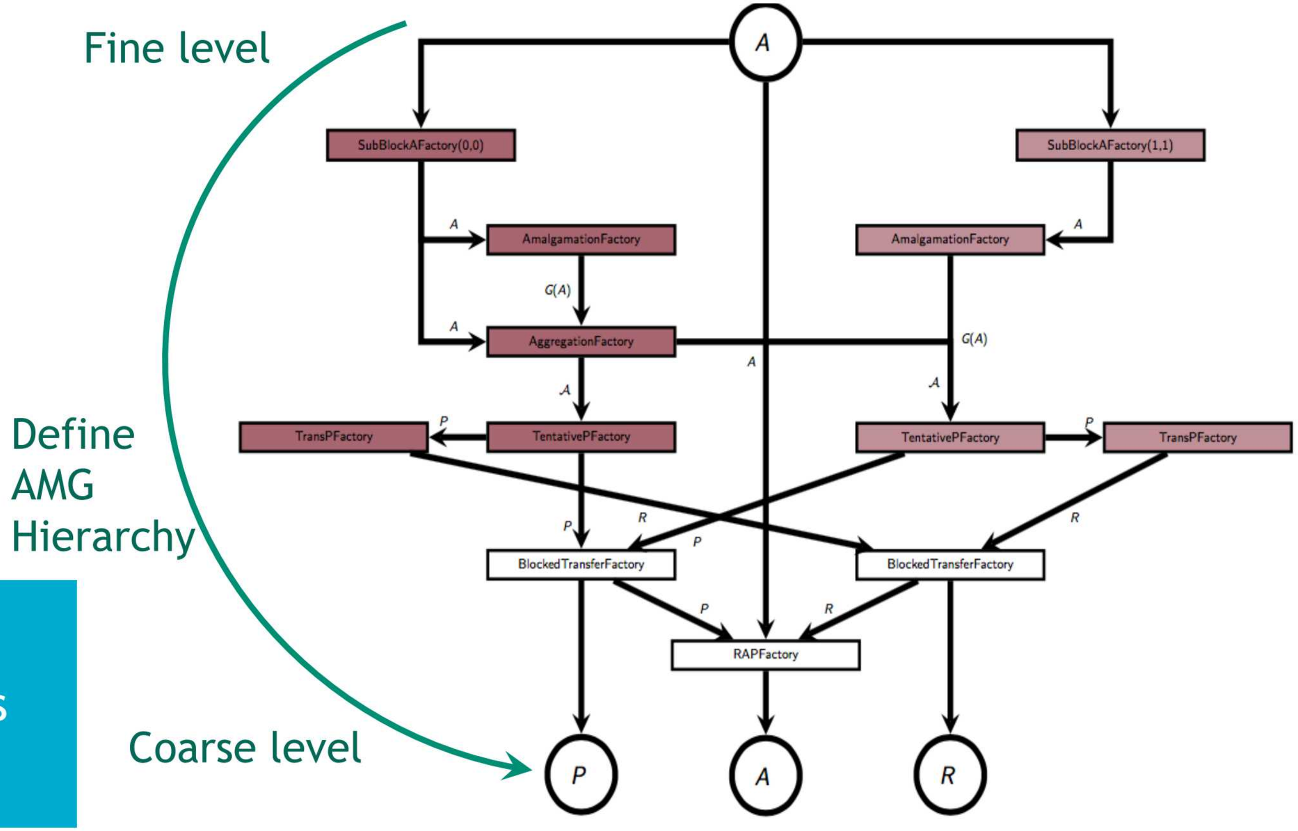
Builds on our earlier incompress. Navier-Stokes ABF methods (e.g., LSC: least squares commutator)

A customizable approach to monolithic AMG (with E. Cyr, J. Shadid, T. Wiesner)

Previously, somewhat rigid monolithic AMG scheme

- Same grid transfer & same smoother algorithm needed applied to entire system, which doesn't always make sense, e.g., character of divergence constraint vs. momentum equations is very different
- Preservation of discretization structure problematic

- Designed & implemented a new monolithic AMG framework for multiphysics
  - Allows different algorithms for individual components to be combined (like  's), e.g., apply a symmetric AMG method to construct pressure interpolation & a nonsymmetric scheme for velocity interpolation

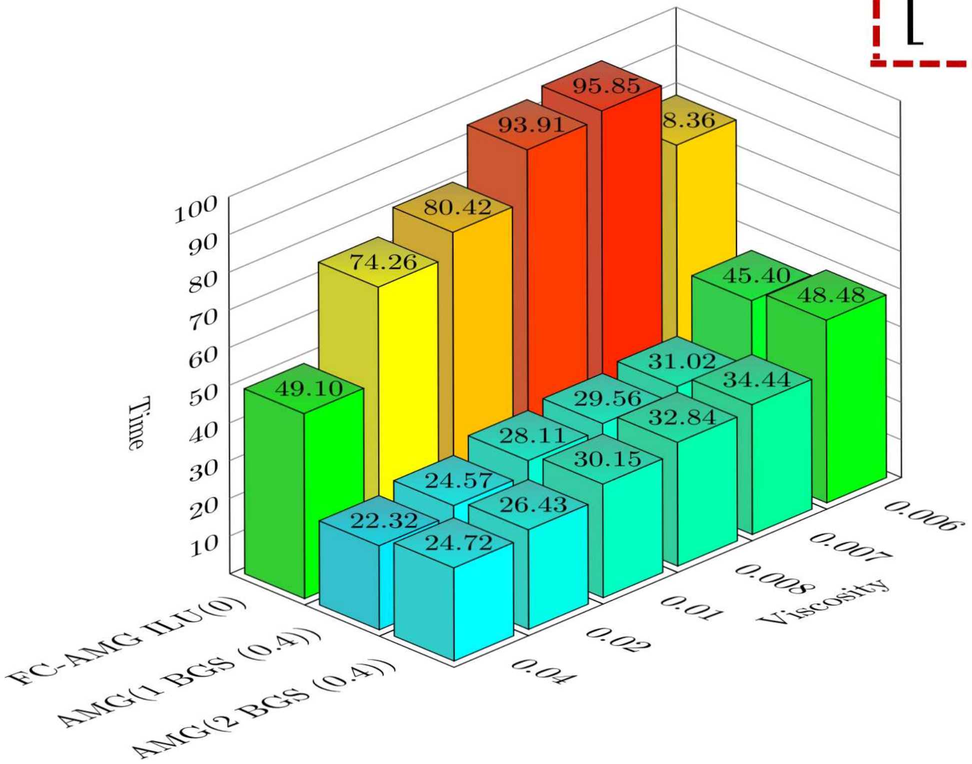


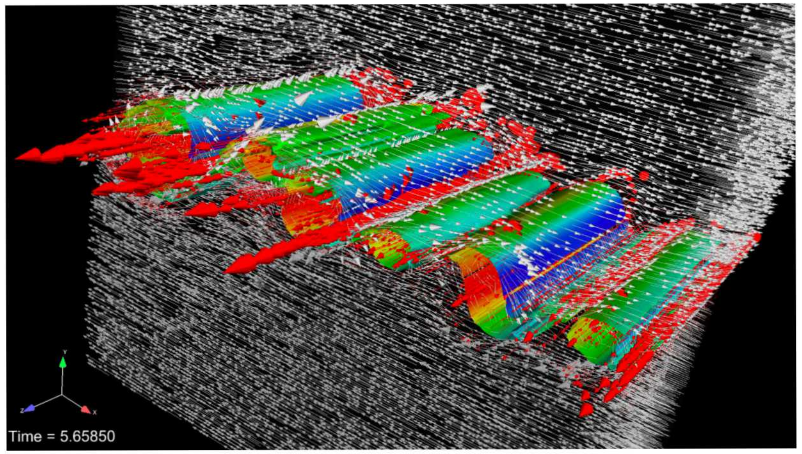
- Monolithic MG schemes often fastest
- Flexibility essential for efficient multiphysics solutions
- Framework facilitates new algorithm exploration

Faster Solution times via smoother customization

Different blocking choices & combinations of damped block Gauss-Seidel & ILU as an AMG smoother

$$\begin{bmatrix} F & B^T & Z & \\ \bar{B} & L_p & & \\ Y & & D & C^T \\ & & \bar{C} & L_r \end{bmatrix} \quad \begin{bmatrix} F & B^T & Z & \\ \bar{B} & L_p & & \\ Y & & D & C^T \\ & & \bar{C} & L_r \end{bmatrix} \quad \begin{bmatrix} F & B^T & Z & \\ \bar{B} & L_p & & \\ Y & & D & C^T \\ & & \bar{C} & L_r \end{bmatrix}$$





2x – 3x run time gain by applying a multiphysics-based smoother

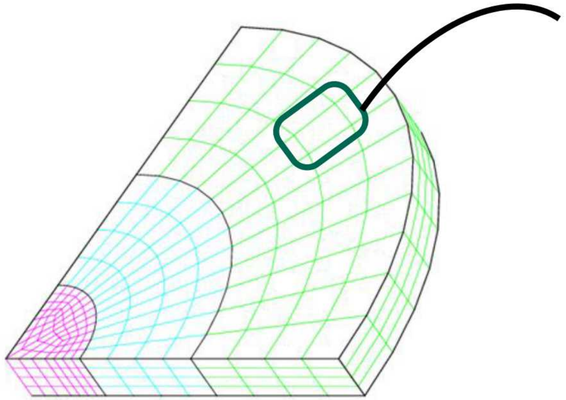
Have investigated many smoother combinations with different Schur complement approximations

Specialized AMG smoothers to further improve scalability

(with J. Adler, T. Benson, P. Farrell, S. Maclachlan)

Two styles : overlapping Schwarz & block factorization with Schur complement approximation
we essentially generalize older ideas for incompressible Navier Stokes and E&M to MHD.

Vanka or Overlapping Schwarz



Prescribe a set of small overlapping patches to define a set of small blocks for use in a block Gauss-Seidel or Jacobi style smoother

- choices for blocks & Navier Stokes / E&M coupling & details matter
- Generalization of Vanka (JCP'86), Arnold, Falk, Winter (Numer. Math., '00)
- Fourier analysis in Maclachlan et. al.
- Cost/robustness tradeoffs

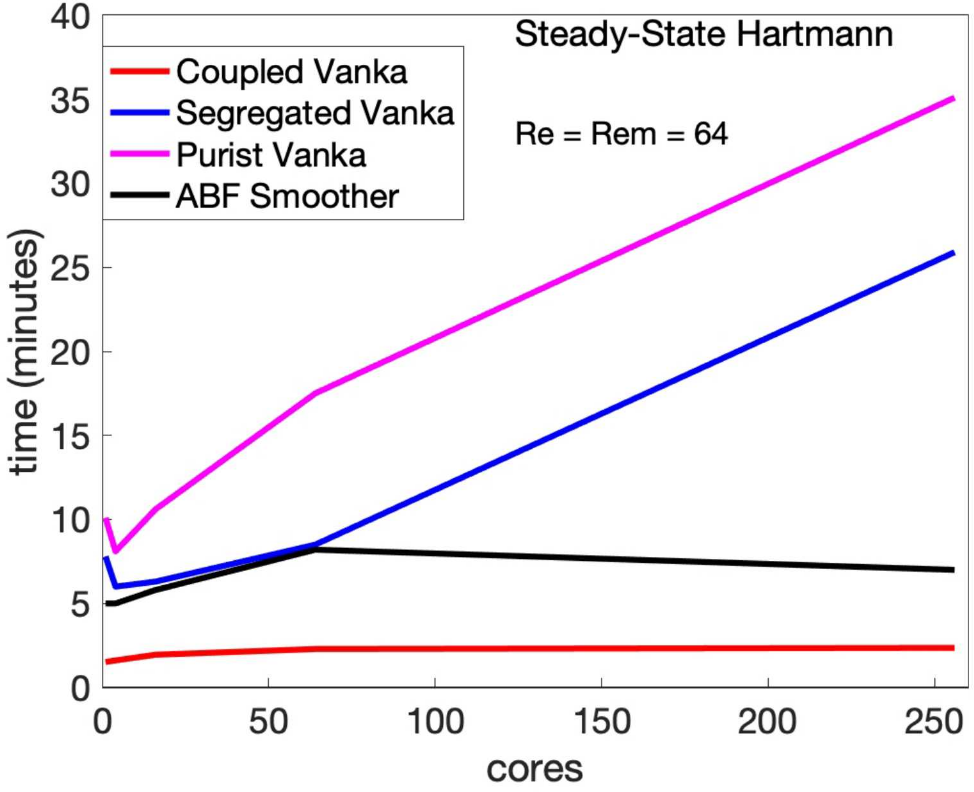
Almost fully algebraic

$$\begin{bmatrix} F & Z & B^T & \\ Y & D & & C^T \\ B & & & \\ & C & & \end{bmatrix}$$

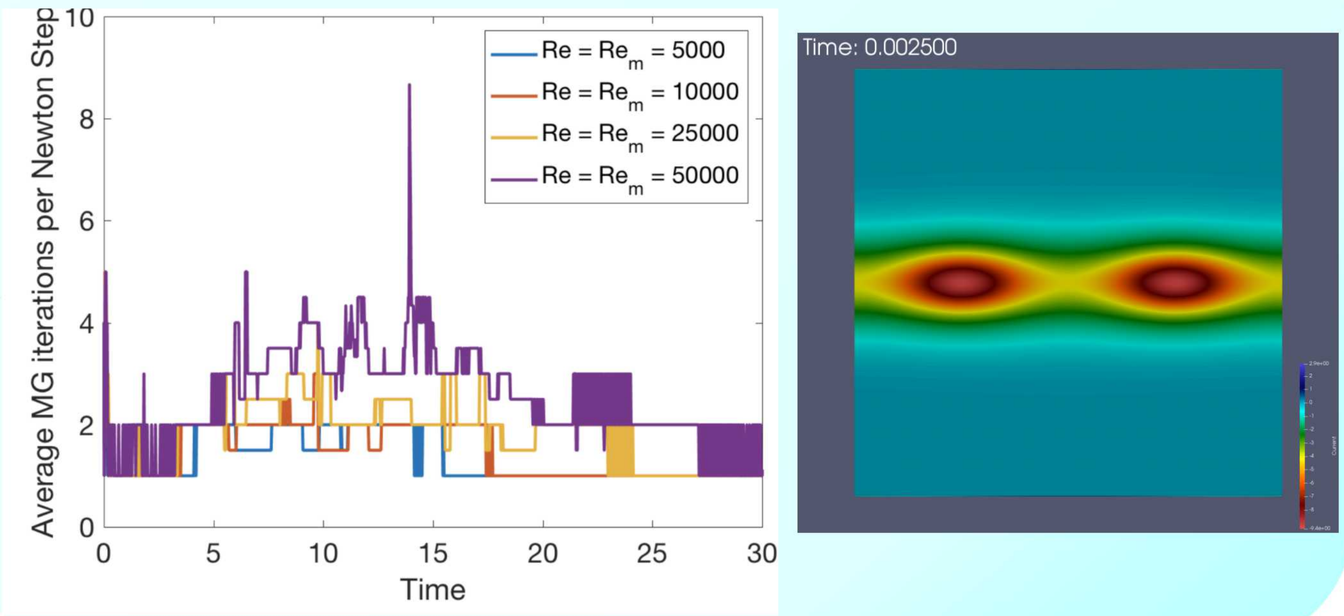
Requires an understanding of operator properties, e.g. capture null space of $\nabla\times\nabla\times$, address potential singular with augmented Lagrange mass term.

* 2016 paper for a vector potential formulation
* 2019 paper in progress for B-field/Lagrange multiplier divergence formulation

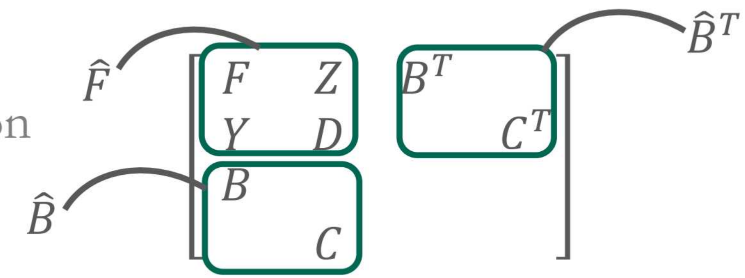
Nearly perfect scalability



Island Coalescence



ABF Smoother uses Jacobi-style relaxation for inverses & approximates $\hat{B}\hat{F}^{-1}\hat{B}^T$



Significant time saving/more robust using coupled Vanka, though not needed for lower Re/Rem numbers

Different code base & geometric grid transfers !!

Braess & Sarazin, “An efficient smoother …”, Appl. Num. Math’97

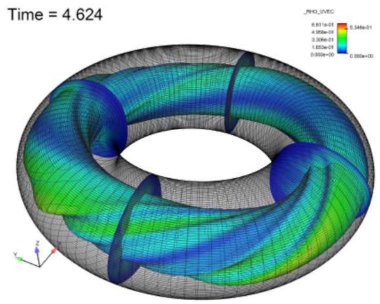
Hiptmair, “Multigrid Method for Maxwell” (SIAM Num. Anal’98)

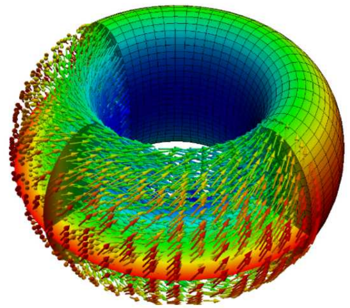
Impact: Enabling Scalable Plasma Physics Simulations

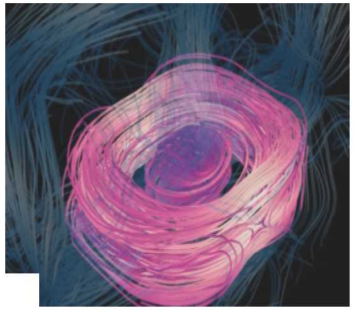
Scalable solvers for a hierarchy of MHD models employing sophisticated time integration & advanced discretizations

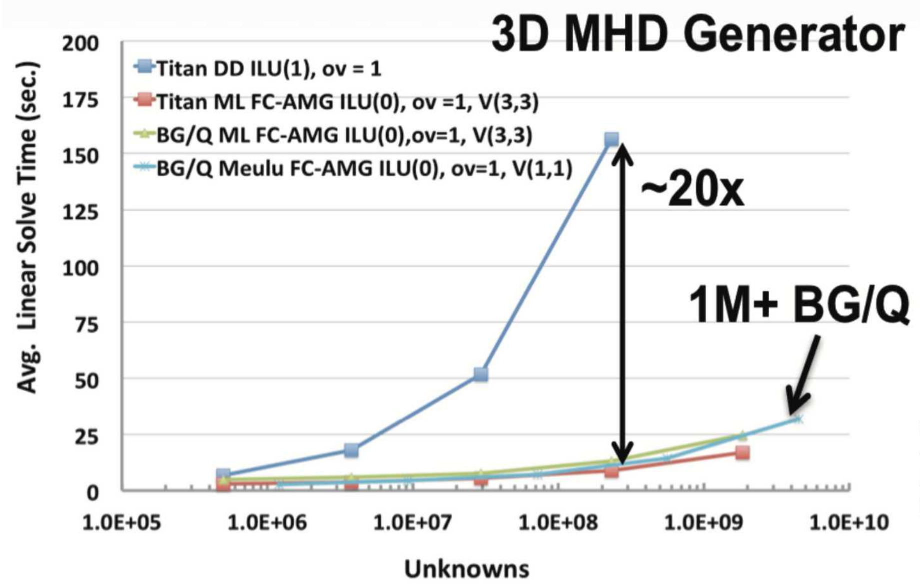
⇒ essential for multiple-time-scale plasma systems

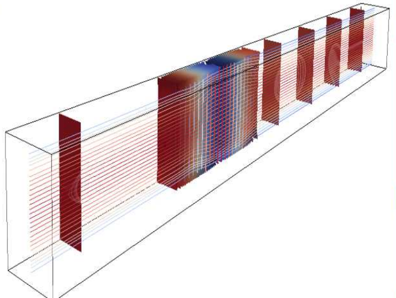
- Improved time to solution & robustness
  - ➢ predictive computational plasma simulations
  - ➢ accurate and efficient longer time-scale simulations
  - ➢ beyond forward simulation: design/optimization/UQ
  - ➢ physics / mathematical model validation, experimental data interpretation & inference
- Increased flexibility to adapt to different scenarios with more coupled physics









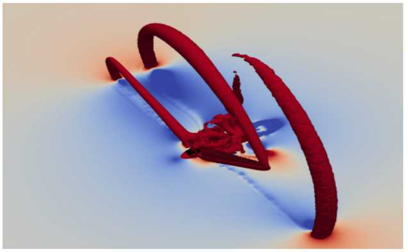


Has enabled scalable MHD calculations with up to 30 billion unknowns & weak scaling to 1M cores & AMG calculations @ 1.6M cores

Impact: Many Other Exascale Simulations Benefit

Linear solutions often bottleneck in numerical simulations

MHD-driven algorithms & software enable others projects



ExaWind

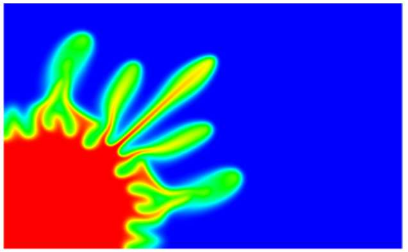
EXASCALE COMPUTING PROJECT

- Our solvers enable a range of simulations,

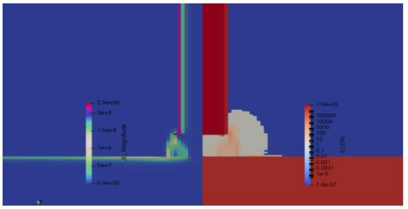
  plasma physics, ice sheets, multi-phase flow, porous media flow + fracture, shock hydro-dynamics, wind energy, additive manufacturing, blood flow & weapons.

- New capabilities to address applications, e.g.

  H(Curl) AMG, H(Grad) AMG, interfaces, thin domains, advanced discretizations (high order adaptive, compatible, DG)



Porous Media Flow (CRADA)



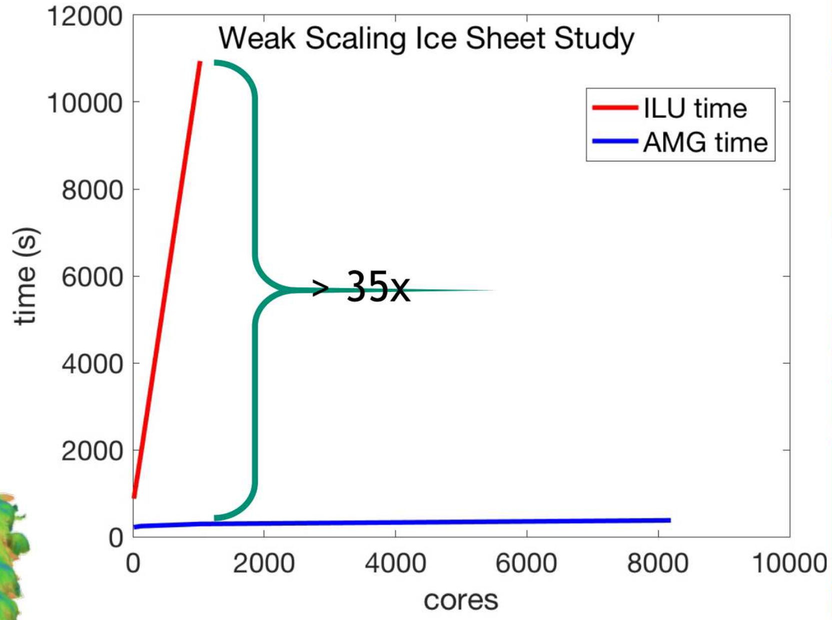
Electrified Taylor Anvil (ARL)

Our Open Source Software

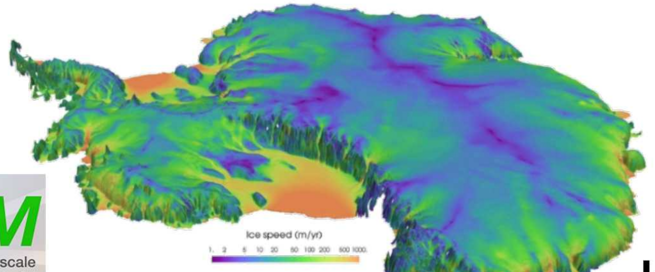
TRILINOS

ML

MueLu Multigrid Framework



E3SM Energy Exascale Earth System Model



Ice Flow (SciDAC)

Key Points

Our research is unique in developing advanced AMG-based linear solvers for advanced MHD applications

- Driven by DOE need for high-fidelity MHD/plasma simulation advances

The MHD solver project has lead to new leading-edge AMG solvers & block preconditioners

- New smoothers & new block preconditioners (ABFs) are tailored to/leverage MHD system

  ⇒ enables the use of AMG technique in some cases where not previously possible

  ⇒ improved robustness and time to solution in MHD applications

- Suitably-designed AMG-based solvers are significant faster (e.g., 20x or more) than non-multilevel methods
- We have solved MHD problems with 30 billion unknowns on 1M core systems in a scalable fashion

Our project has lead to software associated with modeling, discretization and solvers benefiting others

Future AMG+MHD Work: Robustness & Enhanced Scalability

- Extend recent monolithic **smoothers** to Drekar relevant MHD
- **grid transfer** improvements
  - Auxiliary distance Laplacian AMG for MHD systems
    - Developed for SIERRA multiphase interface flow applications
  - Geometric or structured AMG
    - Fundamental research on semi-structured multigrid
  - AMG for convection dominated flows
- AMG Performance (GPUs)
- New MHD formulations/discretizations
  - High order continuous Galerkin, discontinuous Galerkin, hybridized discontinuous Galerkin

- improve robustness
- broaden applicability
- extend scalability
- increase NGP Performance
- fundamental solver research

Dendy & Moulton, "Black Box Multigrid …", NLAA'10
Prokopenko & T., "A Algebraic …", NLAA'16
Kuzman & Moller, "Algebraic Flux …", Springer'08.
Kalchev, Lee, Vill, Efendiev, Vassilevski, "Upscaling …", SISC'16
Gmeiner, Kostler, Sturmer, Ruede, "Parallel Multigrid …", Concur & Comp.'12

More information

J. H. Adler, T. R. Benson, E. C. Cyr, S. P. MacLachlan, and R. S. Tuminaro. Monolithic Multigrid Methods for Two-Dimensional Resistive Magnetohydrodynamics. *SIAM J. Sci. Comput. (SISC)*, **38**(1):B1-B24, 2016.

E.C. Cyr, J.N. Shadid, and R.S. Tuminaro, Teko: A Block Preconditioning Capability with Concrete Example Applications in Navier-Stokes and MHD, SISC, Vol. 38 (5), 2016.

J. N. Shadid, R. P. Pawlowski, E. C. Cyr, R. S. Tuminaro, L. Chacon, and P. D. Weber, Scalable Implicit Incompressible Resistive MHD with Stabilized FE and Fully-coupled Newton-Krylov-AMG, CMAME, 304, 1-25, 2016.

E.C. Cyr, J.N. Shadid, R.S. Tuminaro, R.P. Pawlowski, and L. Chac´on, A New Ap- proximate Block Factorization Preconditioner for Two Dimensional Incompressible (Re- duced) Resistive MHD, SIAM Journal on Scientific Computing, 35:B701-B730, 2013.

A. Prokopenko, R.S. Tuminaro, An algebraic multigrid method for Q 2-Q1 mixed discretizations of the Navier-Stokes equations,

L. Chacón, An optimal, parallel, fully implicit Newton-Krylov solver for three-dimensional visco-resistive magnetohydrodynamics, Phys. Plasmas 15 (2008)

Jardin, Stephen C. "Review of implicit methods for the magnetohydrodynamic description of magnetically confined plasmas." *Journal of Computational Physics* 231.3 (2012): 822-838.

Bergen, Wellein, Hulsemann, U. Ruede, "Hierarchical Hybrid Grids …", Int. J. Par. Emerg. Dist. Syst.'07

Xu, "The Auxiliary Space Method and Optimal Multigrid …", Computing '95

Dendy & Moulton, "Black Box Multigrid …", NLAA'10

Contact: Ray Tuminaro, rstumin@sandia.gov

Extra Slide: Better grid transfers (geometric-*like*) to improve convergence

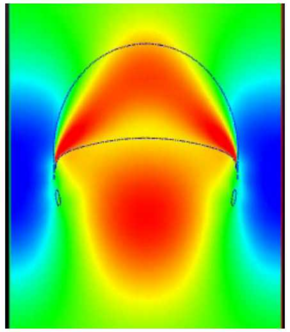
(with D. Noble)

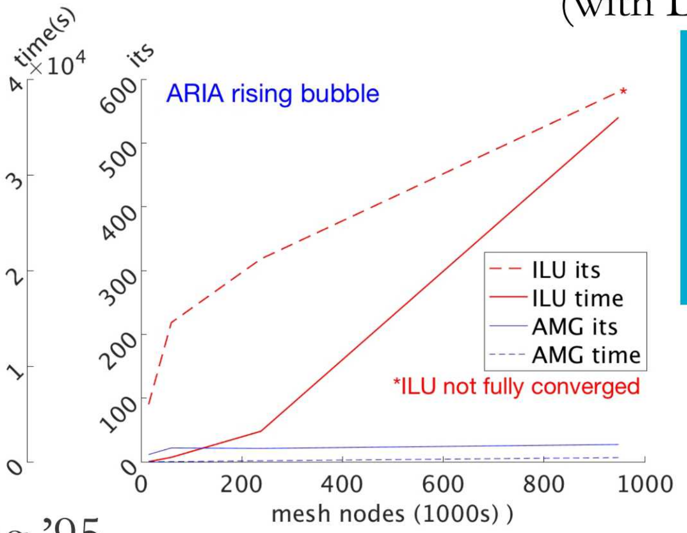
0 in $\begin{bmatrix} F & B^T \\ B & 0 \end{bmatrix}$ problematic for AMG $\Longrightarrow$ simple grid transfers

Idea*: Apply AMG to distance Laplacian to generate grid transfers. Then, use these to project MHD matrix

$\Rightarrow$ *mimics* geometric grid transfers

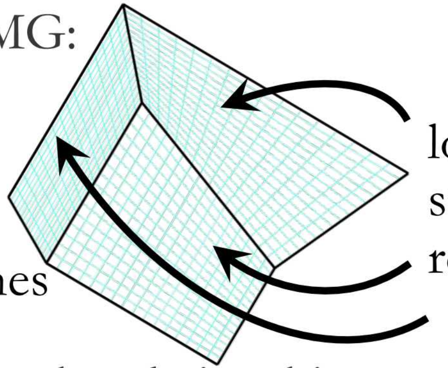
*Xu, "The Auxiliary Space Method and Optimal Multigrid …", Computing '95





Significant savings in SIERRA (not MHD)

Semi-structured MG:



logically structured regions

uniformly refined unstructured meshes

$\Rightarrow$ formalized math. relationship to standard MG, abstracted idea for adaptation, MueLu code

*Bergen, Wellein, Hulsemann, Ruede, "Hierarchical Hybrid Grids …", I. J. Par. Emerg. Dist. Syst.'07

Idea*: Apply geometric MG within structured regions

$\Rightarrow$ much faster kernels in addition to better transfers

(with L. Berger-Vergiat)

Lemma $R\,\psi = \psi_c\,\widehat{R}$

Lemma $\psi^T\,P = \widehat{P}\,\psi_c^T$

Thm: $\psi_c\,\widehat{R}\,\breve{A}\,\widehat{P}\,\psi_c^T = RAP$

regional

standard

ψ's are transformations

LLNL hypre has capability for semi-structured

LBL's Chombo has geo. AMR+MG