Finite Element Methods for High Order PDEs and Relevant Algebraic Solvers

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Outline

1. Introduction
2. Algebraic solvers
   - The method of subspace corrections
   - Practical and optimal solvers for H(curl) and H(div) systems
   - Indefinite systems: Stokes equations
3. Higher order PDEs
   - Conforming and nonconforming finite element methods
   - On the reduction of higher order to lower order systems
   - Two families of new nonconforming elements
4. Electron Magneto Hydrodynamics
   - A (curl curl curl curl)-formulation
   - A new nonconforming element for $(\nabla\times)^4$ systems
5. Solver-friendly discretization for incompressible MHD
   - A family of non-Newtonian models
   - Mathematical similarity between MHD and non-Newtonian models
   - A possible new "solver-friendly" discretization approach
6. Concluding remarks

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Some aspects of numerical methods for partial differential equations (PDEs):

- Modeling
- Qualitative analysis
- Discretization
- Grid adaptation
- Algebraic solver
- Parallelization
- Model validation

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integrated study

Discretization, Adaptivity and Algebraic Solver

- Integrated study: (The interplay between discretization, adaptivity and algebraic solution method)
  - Design of algebraic solvers should take advantages of special properties of underlying PDEs and discretization (discretization-friendly solvers).
  - Design of discretization should take into account how the discretized system is solved (solver-friendly discretizations)
  - Adaptivity is critically important for the efficiency of both discretization and solver

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- Problem-oriented approach
  - optimized design and integrated appliation of discretization, adaptivity, solvers (multigrid) and parallelization

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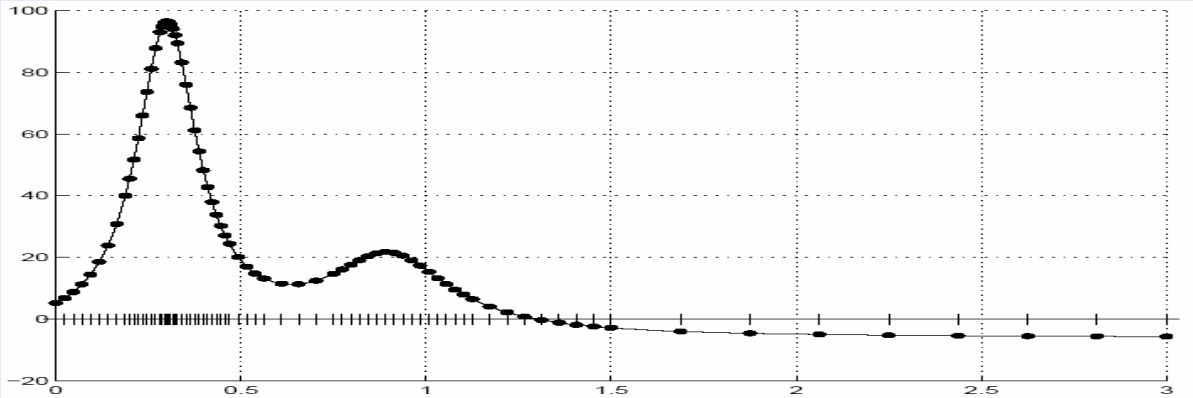
- Problem-oriented approach
  - optimized design and integrated appliation of discretization, adaptivity, solvers (multigrid) and parallelization
- Algorithm-oriented approach
  - less problem-dependent, more user friendly
  - black-box: algebraic multigrid method
  - grey box: use whatever information available such as grid ...

Robustness with respect to various physical parameters

- Accuracy: discretization with grid adaptation



- Stability: discretization with grid adaptation
  - Example: convection dominated problems $(-\epsilon\Delta u + v \cdot \nabla u = f)$
    - special discretization: upwinding scheme
    - standard discretization: OK on adaptive grid (Chen and Xu 2006)
- Efficiency (discretization and solver)
  - Robust solvers

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Basic problem:

Given $A \in R^{N \times N}, b \in R^N$, *how to solve* $Ax = b$?

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- Gaussian elimination
  - most commonly used method in practice
  - black-box
  - expensive: $\mathcal{O}(N^3), \mathcal{O}(N^2), \ldots$ ($N^3 = 10^{18}$ if $N = 10^6$!)

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- Optimal solvers: multigrid methods
  - $\mathcal{O}(N|\log N|^\sigma)$ operations
  - difficult to use, problem-dependent, robust?

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This talk: how multigrid methods can be made

- practical and user-friendly
- applicable to complicated PDEs
- robust w.r.t. various discretization and physical parameters

Linear iterative methods

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consisting of the following three steps:

1. Form the residual: $r = f - Au^{k-1}$
2. Solve the residual equation $Ae = r$ approximately $\hat{e} = Br$ with $B \approx A^{-1}$
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Example. Assume $A = (a_{ij}) \in R^{n \times n}$ and $A = D - L - U$. We may take

$$B = D^{-1}(\text{Jacobi}) \ \ \& \ \ or \quad B = (D - L)^{-1}(\text{Gauss-Seidel}).$$

Preconditioned Krylov space methods

- The PCG for symmetric, positive and definite (SPD) system

$$\frac{\|u-u^k\|_A}{\|u-u^0\|_A} \le 2\left(\frac{\sqrt{\kappa(BA)}-1}{\sqrt{\kappa(BA)}+1}\right)^k (k \ge 1), \quad \left(\kappa(BA) = \frac{\lambda_{\max}(BA)}{\lambda_{\min}(BA)}\right)$$

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- non-SPD systems: MINRes, GMRes (usually not as efficient or robust as CG for SPD systems)

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  where $e_i \in V_i$ solves $a_i(e_i, v_i) = f(v_i) - a(u, v_i) \quad \forall v_i \in V_i$.
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  - (e.g. Gauss-Seidel: $u \leftarrow u + (D - L)^{-1}(b - Au)$)
- Parallel subspace correction (BPX preconditioner):

$$u \leftarrow u + B(f - Au), \qquad B = \sum_{i=1}^{J} I_i A_i^{-1} I_i^T.$$

  - (e.g. Jacobi: $u \leftarrow u + D^{-1}(b - Au)$)

A sharp convergence identity

(SPD case)

Theorem (Xu and Zikatanov (2002, J. AMS))

The MSC is convergent if each subspace solver is convergent.

A sharp convergence identity

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Theorem (Xu and Zikatanov (2002, J. AMS))

The MSC is convergent if each subspace solver is convergent. Furthermore

$$\|\prod_{i=1}^{J}(I-T_i)\|^2 = 1-\frac{1}{K}, \quad K = \sup_{\|v\|=1}\inf_{\sum_i v_i = v}\sum_{i=1}^{J}\|v_i + T_i^*\sum_{j=i+1}^{J} v_j\|^2_{\bar{R}_i^{-1}}$$

Special case:

$$\|\prod_{i=1}^{J}(I-P_i)\|^2 = 1-\left(\sup_{\|v\|=1}\inf_{\sum_i v_i = v}\sum_{i=1}^{J}\|P_i\sum_{j=i}^{J} v_i\|^2\right)^{-1} \qquad \text{if } T_i = P_i$$

Applications: Multigrid and domain decomposition methods

Singular and nearly singular SPD systems

A simple example:

$$A_0 = \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}, \quad b = \begin{pmatrix} -1 \\ -1 \\ 2 \end{pmatrix} \in R(A_0)$$

The Gauss-Seidel method for $(A_0 + \varepsilon I)x = b$ (with $x_0 = b$ and stopping criterion: $\|Ax^k - b\| \le 10^{-8}$):

ε	# of iterations

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10^{-2}	852

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More general nearly singular systems

Given A_0 (semi-definite) and D (SPD), consider

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Questions:

- Why?
- How to fix the problems?

MSC still efficient for singular systems:

(Another sharp convergence identity for semi-definite case system)

Theorem (Y. Lee, J. Wu, J. Xu and L. Zikatanov, Math. Comp.)

The MSC is (semi-)convergent if each subspace solver is (semi-)convergent and

$$|E_J|_a^2 = 1 - \frac{1}{K}$$

where

$$K = \sup_{|v|_a=1, v\in N^\perp} \inf_{c\in N} \inf_{\sum v_i = v+c} \sum_{i=1}^{J} \|v_i + T_i^* \sum_{j=i+1}^{J} v_j\|_{\tilde{R}^\dagger}^2 .$$

References: Keller 1965, Berman and Plemmons 1994, Marek and Szyld 2000, Cao 2001

A general critierion for designing robust iterative solvers for nearly singular systems

$(A_0 + \varepsilon D)u = f$

Theorem (Lee, Wu, Xu and Zikatanov M3AS (2007))

The MSC method converges uniformly w.r.t. ε as long as the decomposition $V = \sum_{j=1}^{J} V_j$ satisfies the near-null space recovery condition:

$$N(A_0) = \sum_{j=1}^{J} [V_j \cap N(A_0)].$$

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Important note: The exact information on the near-null space $N(A_0)$ is not needed as long as it is fully (perhaps over) represented by its components in all subspaces.

Related methods: *augmented or bordered matrix method: Keller 1977, . . .*

Application to previous example: MSC (modified Gauss-Seidel) converges uniformly w.r.t ε by introducing additional subspace $N(A_0)$:

$$R^3 = \sum_{i=1}^{3}\{e_i\} + \{e\}, \quad e = (1,1,1)^T, \quad (N(A_0) = \sum_{j=1}^{J}[V_j \cap N(A_0)]).$$

The resulting algorithm is:

$$x \leftarrow x_{GS} + \alpha(b - Ax_{GS}), \quad \alpha = \frac{e^T(b - Ax_{GS})}{\varepsilon\|e\|^2}$$

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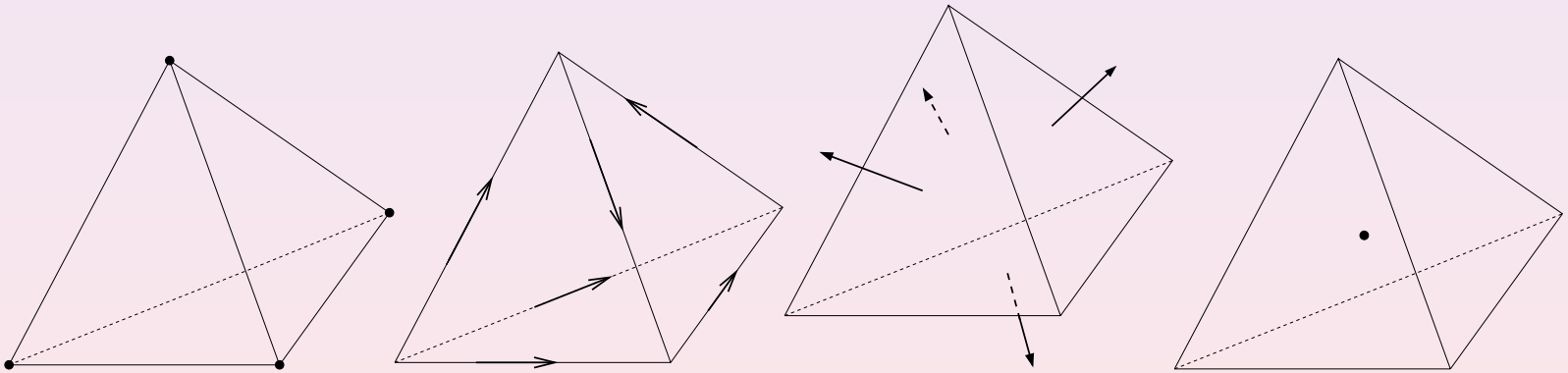
ε	iterations	modified algorithm
1.	18	12
10^{-1}	100	10
10^{-2}	852	6
10^{-3}	6982	6
10^{-4}	54470	4
0. [singular case]	2	2

More examples: H(curl) and H(div) systems

$$
\begin{tikzcd}
R \arrow[r] & C^\infty \arrow[r, "\mathrm{grad}"] \arrow[d, "\Pi_h^{\mathrm{grad}}"] & C^\infty \arrow[r, "\mathrm{curl}"] \arrow[d, "\Pi_h^{\mathrm{curl}}"] & C^\infty \arrow[r, "\mathrm{div}"] \arrow[d, "\Pi_h^{\mathrm{div}}"] & C^\infty \arrow[r] \arrow[d, "\Pi_h^{0}"] & 0 \\
R \arrow[r] & H_h(\mathrm{grad}\ ) \arrow[r, "\mathrm{grad}"] & H_h(\mathrm{curl}\ ) \arrow[r, "\mathrm{curl}"] & H_h(\mathrm{div}\ ) \arrow[r, "\mathrm{div}"] & L_h^2 \arrow[r] & 0
\end{tikzcd}
$$



- N(grad)=R, N(curl)=R(grad), N(div)=R(curl).
- Related minisymposium: 11:15am, Room K02 F180

H(curl) and H(div) systems

Let $D =$grad, curl or div, and $V = H(D;\Omega)$ or $V = H_0(D;\Omega)$, consider

$$\text{Find } u \in V : a(u,v) \equiv (Du, Dv) + (u,v) = (f,v), \quad v \in V$$

<u>Relevant applications:</u> Poisson equations ($D =$grad), Maxwell equations ($D =$curl) and Darcy's law (with mixed FE) ($D =$div).

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Finite element discretization:

$$\text{Find } u_h \in V_h : a(u_h, v_h) = (f, v_h), \quad v \in V_h.$$

Or equivalently, with $(A_h u_h, v_h) = a(u_h, v_h)$ and $f_h = Q_h f$,

$$A_h u_h = f_h, \qquad (A_h \approx D_h^* D_h + h^2 I)$$

A_h, for $D = \mathrm{curl}$ or div , is nearly singular with a huge near-null subspace.

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$$H_h(\mathrm{curl}\,) = \{\phi_i^{\mathrm{curl}}\} + \sum_j \{\mathrm{grad}\ \phi_j^{\mathrm{grad}}\}.$$

or more generally:

$$H_h(\mathrm{curl}\,) = \sum_k V_k : \qquad \{\mathrm{grad}\ \phi_j^{\mathrm{grad}}\} \subset V_{k(j)} \text{ for each } j.$$

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Examples of relevant references:

- H(curl) and H(div) systems
  - Ewing and Wang (1991)
  - Hiptmair (1997)
  - Arnold, Falk and Winther (1997)
- Stokes and nearly incompressible elasticity:
  - Schöberl (1999)
  - Lee, Wu, Xu and Zikatanov (2006)
- Divergence dominated systems
  - Austin, Manteuffel and McCormick (2000)

From geometric to algebraic multigrid (AMG) methods

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AMG for H(curl) and H(div) systems:

- Large (near-)null spaces, not easily recoverable algebraically

From geometric to algebraic multigrid (AMG) methods

Facts: Geometric MG are optimal ($\mathcal{O}(N)$), but difficult to apply.

AMG: More algebraic/user-friendly, but less efficient?

AMG for H(grad) system:

- Simple (near-)null space easily recoverable algebraically
- Various robust and efficient AMG solvers have been developed.

AMG for H(curl) and H(div) systems:

- Large (near-)null spaces, not easily recoverable algebraically
- Few robust methods have been developed
  - R. Beck, Tech Report, ZIB, 1999
  - Reitzinger and Schöberl, 2002, NLAA
  - Bochev, Garasi, Hu, Robinson and Tuminaro, SISC, 2003
  - Bochev, Hu, Siefert and Tuminaro, SISC (submitted) 2007

An "auxiliary space preconditioner" for H(curl)/H(div)

(Hiptmair and Xu 2005, 2007)

Given $v_h \in H_h(\mathrm{curl}\,)$, $\exists\, \tilde{v}_h \in H_h(\mathrm{curl}\,), \Phi_h \in [H_h^1(\Omega)]^3, p_h \in H_h^1(\Omega)$ s.t.

$$v_h = \tilde{v}_h + \Pi_h^{\mathrm{curl}} \Psi_h + \mathrm{grad}\; p_h$$

and $\|h^{-1}\tilde{v}_h\|_{L^2} + \|\Psi_h\|_{H^1} + \|p_h\|_{H^1} \lesssim \|v_h\|_{H(\mathrm{curl})}$.

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Using Xu (Computing'1996), and Hiptmair and Xu (SINUM, to appear),

$$B_h^{\mathrm{curl}} = S_h^{\mathrm{curl}} + \Pi_h^{\mathrm{curl}} \begin{pmatrix} B_h^{\mathrm{grad}} & 0 & 0 \\ 0 & B_h^{\mathrm{grad}} & 0 \\ 0 & 0 & B_h^{\mathrm{grad}} \end{pmatrix} (\Pi_h^{\mathrm{curl}})^T + \mathrm{grad}\;\; B_h^{\mathrm{grad}}\; (\mathrm{gra}$$

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Features:

- consisting of 4 Poisson solvers such as AMG (B_h^{grad}) and 1 simple relaxation method such as point Jacobi (S_h^{curl});
- optimal and efficient for problems on unstructured grids
- very little programming effort

Similarly

$$B_h^{\mathrm{div}} = S_h^{\mathrm{div}} + \Pi_h^{\mathrm{div}} \mathbf{B}_h^{\mathrm{grad}} (\Pi_h^{\mathrm{div}})^T + \mathrm{curl}\ B_h^{\mathrm{curl}} (\mathrm{curl}\ )^T$$

Similarly

$$
\begin{aligned}
B_h^{\mathrm{div}} &= S_h^{\mathrm{div}} + \Pi_h^{\mathrm{div}} \mathbf{B}_h^{\mathrm{grad}} (\Pi_h^{\mathrm{div}})^T + \mathrm{curl}\ B_h^{\mathrm{curl}} (\mathrm{curl}\ )^T \\
&= S_h^{\mathrm{div}} + \Pi_h^{\mathrm{div}} \mathbf{B}_h^{\mathrm{grad}} (\Pi_h^{\mathrm{div}})^T \\
&+ \mathrm{curl}\ S_h^{\mathrm{curl}} (\mathrm{curl}\ )^T + (\Pi_h^{\mathrm{div}} \mathrm{curl}\ ) \mathbf{B}_h^{\mathrm{grad}} (\Pi_h^{\mathrm{div}} \mathrm{curl}\ )^T
\end{aligned}
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&= S_h^{\mathrm{div}} + \Pi_h^{\mathrm{div}} \mathbf{B}_h^{\mathrm{grad}} (\Pi_h^{\mathrm{div}})^T \\
&+ \mathrm{curl}\ S_h^{\mathrm{curl}} (\mathrm{curl}\ )^T + (\Pi_h^{\mathrm{div}} \mathrm{curl}\ ) \mathbf{B}_h^{\mathrm{grad}} (\Pi_h^{\mathrm{div}} \mathrm{curl}\ )^T
\end{aligned}
$$

Features:

- consisting of 6 Poisson solvers (B_h^{grad}) and 2 simple relaxation (S_h^{curl} and S_h^{div});
- optimally efficient for unstructured grids

Numerical Experiment I: uniform grid

- B_h^{grad} : one iteration of a symmetric AMG solver for the Poisson equation

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$\mathcal{T}_h$	# iter (with S_h^{curl})	# iter (without S_h^{curl})
8^3	14	28
16^3	14	53
32^3	14	107

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Recall:

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Experiment II: unstructured grids on unit ball

$sphere$	$elem$	$iter$	$CPUtimes(s)$
8	8865	11	
9	17260	12	
10	35849	13	
11	46543	12	
12	66402	13	
13	95593	13	26.76
14	148554	13	45.30
15	242588	14	83.48

More general equations

Consider:

$$\mathrm{curl}\,(\mu(x)\mathrm{curl}\,u) + \sigma(x)u = f$$

μ and σ may be discontinuous, degenerating, and large variations

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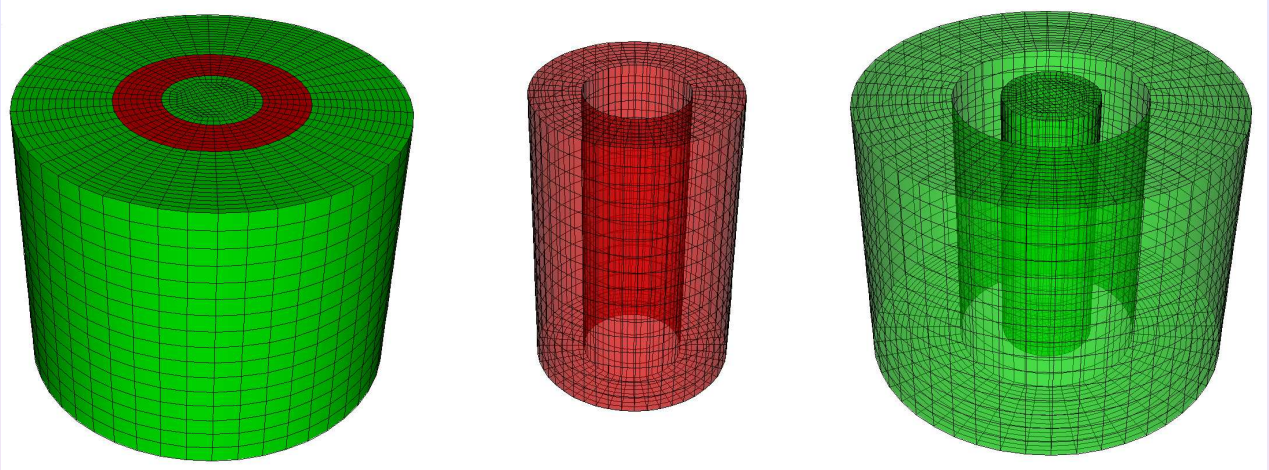
2. Numerical experiments show that our preconditioners are very robust and efficient in both two [Hiptmair and Xu] and three [Kolev and Vassilevski, LLNL] dimensions
3. The preconditioners have been included and tested in LLNL's *hypre* package.

Applications: (LLNL)

Auxiliary space Maxwell solver (AMS)

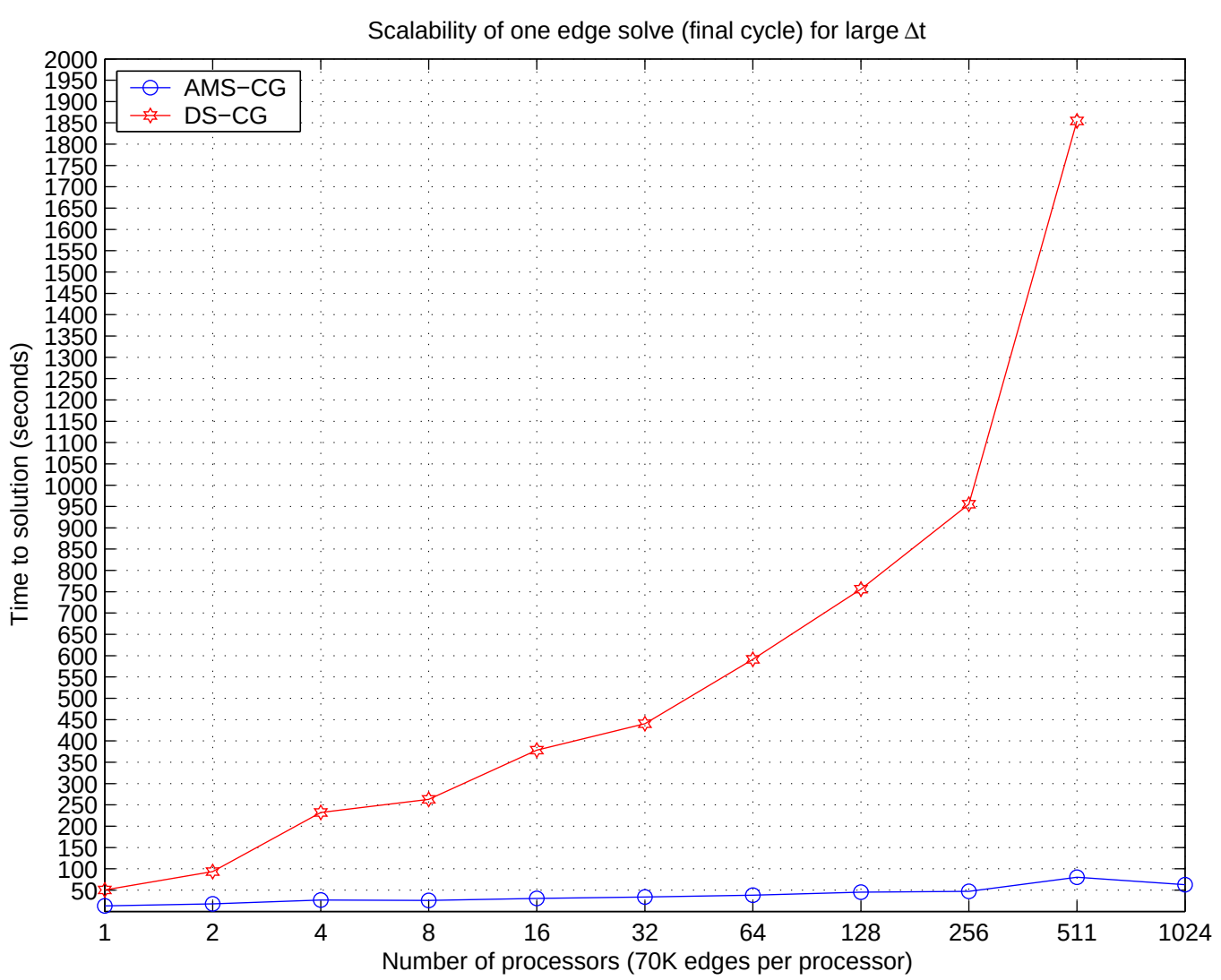
- *AMS*: a massively parallel implementation in .
- "Black-box": requires only discrete gradient matrix + vertex coordinates.
- Can handle complicated geometries and coefficient jumps.
- Scales with the problem size and on large parallel machines.
- Supports simplified magnetostatics mode.
- Can utilize Poisson matrices, when available.
- Based on *hypre*'s parallel algebraic multigrid solver BoomerAMG.
- Freely available (under LGPL).

Copper wire in a cylinder

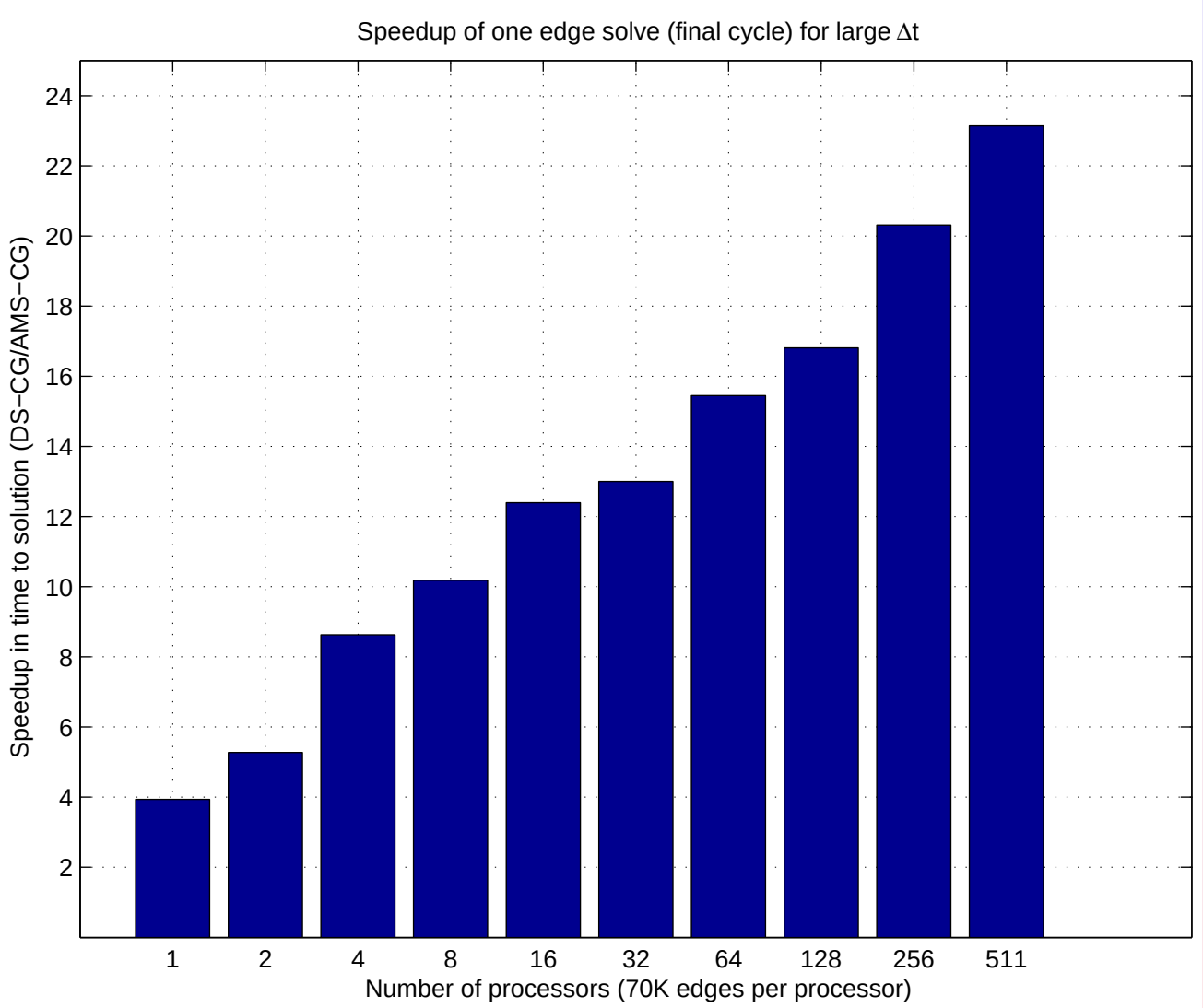


- Simulation of the electromagnetic diffusion of a copper wire (red region) in air (green region) using the AMS solver in *hypre*.
- This is a test problem for one of the MHD packages in LLNL with large jumps in the material coefficients (6 orders of magnitude).
- Weak parallel scalability of one representative definite Maxwell solve (more processors are used, while the problem size per processor remains constant).
- Comparison of AMS-CG and DS-PCG with PCG tolerance 10^{-9}.
- Courtesy of Tzanio Kolev (LLNL).

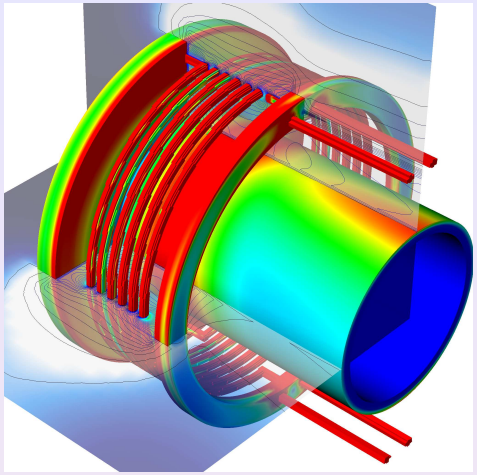
Scalability (70K edge unknowns per processor)



Speedup (compared to previous solver)



Bifilar helical coil



- Results from a simulation of the electromagnetic diffusion in a bifilar helical coil using the AMS solver in *hypre*.
- This is a real application (a model of an actual device) having complicated geometry and large jumps in the material coefficients.
- On a coarser model, AMS-CG is 4 times faster than DS-CG, while producing 2 orders of magnitude more accurate residual error.
- Courtesy of Robert Rieben (LLNL).

Indefinite problems

(reduction to nearly singular symmetric positive definite (SPD) system)

$$\left\{ \begin{array}{rcl} Au + B^*p & = & f \\ Bu & = & g \end{array} \right. \qquad \underline{\text{Stokes:}} \left\{ \begin{array}{rcl} -\Delta u - \nabla p & = & f \\ \operatorname{div} u & = & g \end{array} \right. \tag{2.1}$$

Decoupling: Given $\varepsilon > 0$, let $\tilde{p} = \varepsilon^{-1}(B\tilde{u} - g)$ and $\tilde{u}$ solves

$$(\varepsilon A + B^*B)\tilde{u} = \varepsilon f + B^*g \qquad \underline{\text{Elasticity:}} \quad (-\varepsilon\Delta - \nabla\operatorname{div})\tilde{u} = \varepsilon f - \nabla g. \tag{2.2}$$

Then, we have $\|u - \tilde{u}\|_A = \mathcal{O}(\varepsilon^{1.5})$ and $\|p - \tilde{p}\| = \mathcal{O}(\varepsilon)$.

Consequently

Indefinite (2.1) $\Longrightarrow$ (nearly singular) SPD

- 1 Stokes equation: $\Rightarrow$ 1 linear elasticity (div free space has a locally supported basis?)

which can be efficiently solved by (robust) method of subspace corrections!

Related methods: Augmented Lagrangian: Fortin and Glowinski 1983, ...

Outline

1. Introduction
2. Algebraic solvers
   - The method of subspace corrections
   - Practical and optimal solvers for H(curl) and H(div) systems
   - Indefinite systems: Stokes equations
3. Higher order PDEs
   - Conforming and nonconforming finite element methods
   - On the reduction of higher order to lower order systems
   - Two families of new nonconforming elements
4. Electron Magneto Hydrodynamics
   - A (curl curl curl curl)-formulation
   - A new nonconforming element for $(\nabla\times)^4$ systems
5. Solver-friendly discretization for incompressible MHD
   - A family of non-Newtonian models
   - Mathematical similarity between MHD and non-Newtonian models
   - A possible new "solver-friendly" discretization approach
6. Concluding remarks

Higher order partial differential equations

Examples

- Kirchhoff thin plate bending problem and tream function formulation of Stokes equation (2D):

$$\Delta^2 u = f$$

Higher order partial differential equations

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- Kirchhoff thin plate bending problem and tream function formulation of Stokes equation (2D):

$$\Delta^2 u = f$$

- A Cahn-Hilliard equation modeling the spinodal decomposition and coarsening phenomena in binary alloys.

$$\begin{cases} \frac{\partial u}{\partial t} = \nabla \cdot (b(u)\nabla(-\gamma\Delta u + \Psi'(u))), & \text{in } \Omega_T := \Omega \times (0,T) \\ u(x,0) = u_0(x), & \forall\, x \in \Omega, \\ \frac{\partial u}{\partial \mathbf{n}} = b(u)\frac{\partial}{\partial \mathbf{n}}(-\gamma\Delta u + \Psi'(u)) = 0, & \text{on } \partial\Omega \times (0,T) \end{cases}$$

- A 6th order phase field simulation of the morphological evolution of a strained epitaxial thin film on a compliant substrate

$$\frac{\partial c}{\partial t} = \frac{1}{\varepsilon_0^2}\nabla \cdot (M(c)\nabla\mu) + S(c)$$
$$\mu = F(c) - \varepsilon_0^2\nabla^2 c + \chi_0^2\nabla^4 c$$

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- A 6th equation on the oxidation of silicon in superconductor devices

$$\begin{cases} \frac{\partial u}{\partial t} = \nabla(b(u)\nabla\Delta^2 u), & \text{in } \Omega_T := \Omega \times (0,T) \\ u(x,0) = u_0(x), & \forall\, x \in \Omega, \\ \frac{\partial u}{\partial \mathbf{n}} = \frac{\partial \Delta u}{\partial \mathbf{n}} = b(u)\frac{\partial \Delta^2 u}{\partial \mathbf{n}} = 0, & \text{on } \partial\Omega \times (0,T) \end{cases}$$

Internal approximation and conforming finite element

The approximation space is a subspace of H^m (for 2m-th oder PDE)

$$V_h \subset H^m(\Omega) \quad \text{(globally } C^{m-1}\text{)}$$

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$n > 1$ and general (polyhedral) domain with simplicial partition

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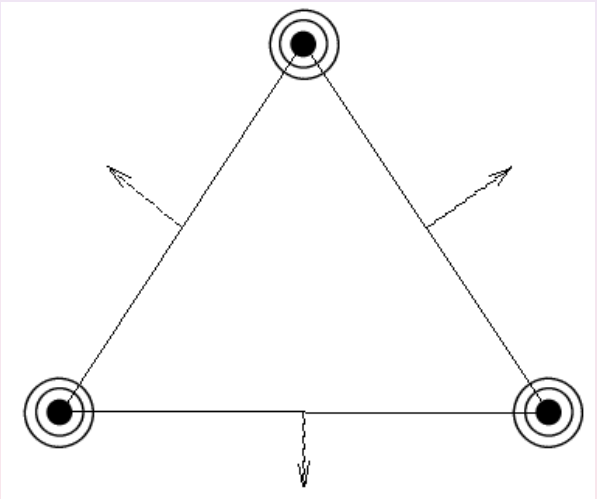
$n > 1$ and general (polyhedral) domain with simplicial partition

1. $m = 0, 1$: easy
2. $m \geq 2$: complicated and require very high degree of polynomials.

Difficulty for constructing conforming elements for high order PDEs

$n = 2$ and $m = 2$ (for 4-th order PDEs)

- minimal order: 5-th order polynomial (with 21 degrees of freedom) in each triangle (Argyris elements)



Bell element (dof=18): application to MHD (2D) (Jardin 2004, Jardin and Breslau 2005, Jardin, Breslau and Ferraro 2007)

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Minimal (?) degree (for FE):

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$$(m-1)2^n+1=\begin{cases} 1 & m=1, n\geq 1 \quad (\text{dof}=n+1) \\ 5 & m=2, n=2 \quad (\text{dof}=21) \\ 9 & m=3, n=2 \quad (\text{dof}=55) \\ 9 & m=2, n=3 \quad (\text{dof}=220) \\ 17 & m=3, n=3 \quad (\text{dof}=1180) \end{cases}$$

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- lower orders are possible but complicated: super-splines (difficult to get locally supported basiss), composite elements
- references: Alfeld, Boor, Cui, Lai, Davydov, Schumake, Sirvent, Zenisek, ...

A commonly used methods: reduction to 2nd order systems

For 4th order, introduce an intermediate variable:

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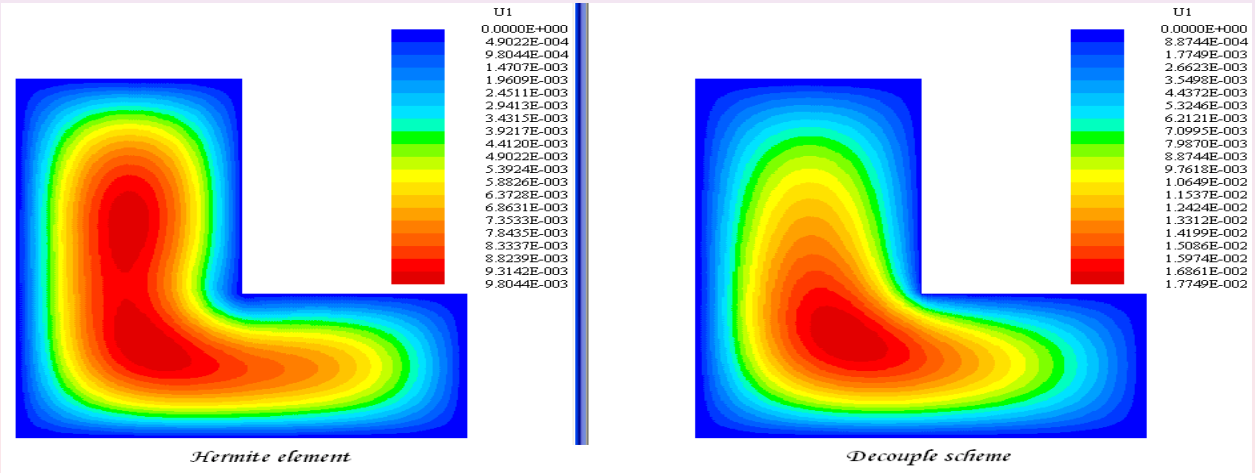
As a result, 4th or 6th order equations are reduced to a system of Poisson (like) equations!

Example: a simply supported polygonal plate

$$\begin{cases} \Delta^2 u = f, & \text{in } \Omega, \\ u = \Delta u = 0, & \text{on } \partial\Omega. \end{cases}$$

With $v = -\Delta u$, we obtain two decoupled Poisson equations:

$$\begin{cases} -\Delta v &= f, & \text{in } \Omega, \\ v &= 0, & \text{on } \partial\Omega. \end{cases} \qquad \begin{cases} -\Delta u &= v, & \text{in } \Omega, \\ u &= 0, & \text{on } \partial\Omega. \end{cases}$$



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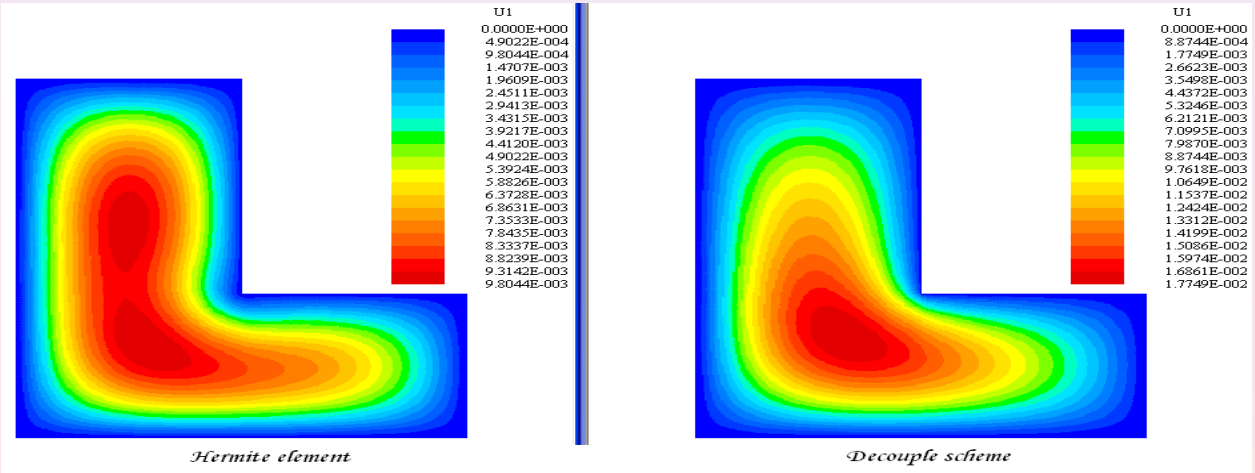

Observation ($f = 1$): Two solutions are different!

External approximation: nonconforming FE

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Completely discontinuous approximation space:

- Trivial to construct spaces
- DG methods: using many penalty terms to enforce "smoothness" approximately (G. Baker 1977 and others)

Nonconforming finite elements and advantages

- minimal smoothness [to assure the right amount consistency] are imposed in the spaces so that lower order elements can be constructed:

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Variational: Let $a(u,v) = \sum_{|\alpha|\le m}(\partial^\alpha u, \partial^\alpha v)$, $f \in W^*$

$$\text{Find } u \in W\colon\ a(u,v) = \langle f, v\rangle \equiv \sum_{|\alpha|\le m} (f_\alpha, \partial^\alpha v), \quad \forall v \in W \quad (f_\alpha \in L^2).$$

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Variational: Let $a(u,v) = \sum_{|\alpha|\le m}(\partial^\alpha u, \partial^\alpha v)$, $f \in W^*$

$$\text{Find } u \in W\colon\ a(u,v) = \langle f, v\rangle \equiv \sum_{|\alpha|\le m}(f_\alpha, \partial^\alpha v), \quad \forall v \in W \quad (f_\alpha \in L^2).$$

PDE: With some Neumann boundary conditions and

$$\sum_{|\alpha|\le m}(-1)^{|\alpha|}\partial^\alpha(\partial^\alpha u) = f \quad \text{in } \Omega.$$

FEM: $a_h(u,v) = \sum_\alpha(\partial_h^\alpha u\, \partial_h^\alpha v)$, $\langle f, v_h\rangle_h = \sum_\alpha(f_\alpha, \partial_h^\alpha v)$

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Convergence:

$$\lim_{h\to 0}\|u - u_h\|_{m,h} = 0.$$

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Let $n \geq m \geq 1$. Define (T, P_T, D_T^m) by

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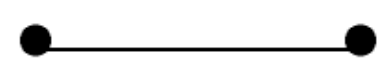
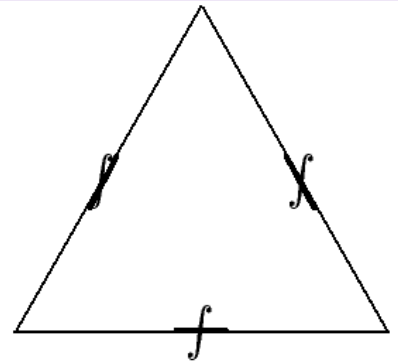
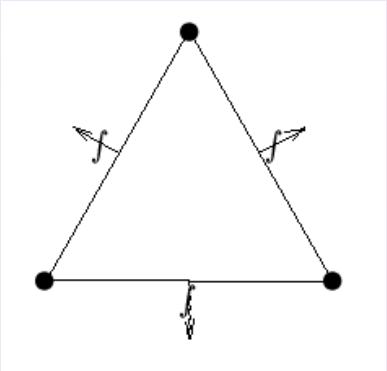
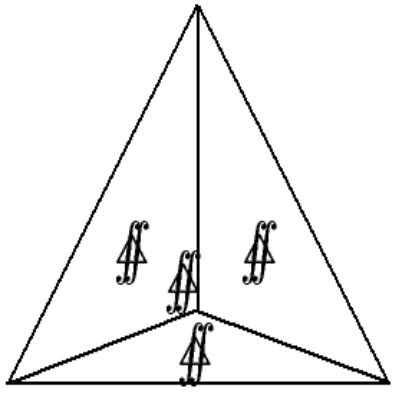
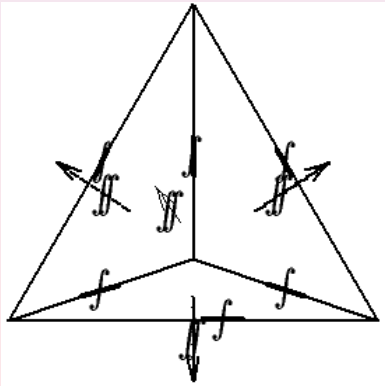
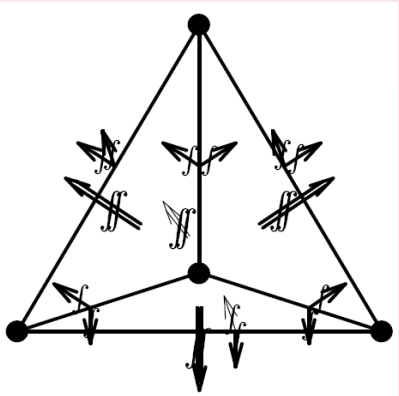
Global FE space W_h: piecewise P_m that is continuous on all d.o.f. (w.r.t. simplicial partition $\mathcal{T}_h$).

Table: Some examples (degrees of freedom)

	$m = 1$	$m = 2$	$m = 3$
$n = 1$			
$n = 2$			
$n = 3$			

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- For $m = 3$ and $n = 3$, we obtain a new cubic element on a simplex that has 20 degrees of freedom.

Nonconforming FE for $2m$-th order elliptic problems

FEM: $a_h(u,v) = \sum_\alpha (\partial_h^\alpha u\, \partial_h^\alpha v)$, $\langle f, v_h\rangle_h = \sum_\alpha (f_\alpha, \partial_h^\alpha v)$

$$\text{Find } u_h \in W_h\text{: } a_h(u_h, v_h) = \langle f, v_h\rangle_h \quad \forall v_h \in W_h. \tag{3.3}$$

Error estimates:

$$\|u - u_h\|_{m,h} = \mathcal{O}(h)$$

Inclusion property: $\partial_h M_h^{m+1} = M_h^m$

- Given any $n > m \geq 1$ and a simplex T, the set of subsimplexes of T that are used to define for D_T^m is a subset of that for D_T^{m+1}.
- More precisely, the degrees of freedom for D_T^{m+1} can be obtained by taking the integral of one order higher normal derivatives of functions on the same subsimplexes used for D_T^m, plus the integral average of function over all the additional $(n-m-1)$ dimensional subsimplexes.
- Furthermore,

$$M_h^m = \mathrm{span}\{\partial^{e_1} M_h^{m+1}, \partial^{e_2} M_h^{m+1}, \cdots, \partial^{e_n} M_h^{m+1}\},$$

Nodal basis function

It is both theoretically and (apparently) practically interesting to see if a set of nodal basis functions can be explicitly constructed for our new finite element spaces. We are indeed able to do so. In particular, we have given all the details for $m = 1, 2$ and 3.

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- Theory: are nonconforming more natural (better) than conforming? Example($n = 2, m = 1$): nonconforming P_1
  - With a slight local modification, it provides a local conservation property like the one by the finite volume method
  - Together with piecewise constant, it provides a stable element for Stokes equation (whereas the conforming P_1 does not)
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- Practical use?

A modified Zienkiewicz element for 4th order PDEs in n-D

(Wang, Shi and Xu 2007)

Given an n-simplex T, let $q_0 = \lambda_1\lambda_2\ldots\lambda_{n+1}$, and, for $1 \leqslant i < j \leqslant n+1$

$$q_{ij} = \lambda_i^2\lambda_j - \lambda_i\lambda_j^2 + \frac{(2n-1)!}{n!}\Big(\frac{(n-1)n}{n+1}(\lambda_i - \lambda_j) + \sum_{1\leqslant k\leqslant n+1, k\neq i,j} \frac{(\nabla\lambda_i - \nabla\lambda_j)^\top \nabla\lambda_k}{\|\nabla\lambda_k\|}(n\lambda_k - 1)\Big)q_0.$$

A Z-type nonconforming element is defined by (T, P_T, Φ_T) with

1. T is an $n-$simplex, with $a_1, \ldots, a_{n+1}$ the vertices;
2. $P_T = P_2(T) + span\{q_{ij}, 1 \leqslant i \neq j \leqslant n+1\}$;
3. The components of Φ_T are

$$v(a_j), \quad 1 \leqslant j \leqslant n+1, \quad (a_j - a_i)^\top \nabla v(a_i), 1 \leqslant i \neq j \leqslant n+1.$$

Nodal basis functions

For $1 \le i \ne j \le n+1$, the nodal basis functions can be given explicitly:

$$\begin{aligned} p_{ij} &= \frac{1}{2}\lambda_i\lambda_j(1+\lambda_i-\lambda_j) + \frac{(2n-1)!}{2n!}\left(\frac{(n-1)n}{n+1}(\lambda_i-\lambda_j)\right. \\ &\quad \left. + \sum_{1\le k\le n+1, k\ne i,j} \frac{(\nabla\lambda_i-\nabla\lambda_j)^T\nabla\lambda_k}{\|\nabla\lambda_k\|^2}(n\lambda_k-1)q_0\right) \\ p_i &= \lambda_i^2 + 2\sum_{1\le j\le n+1, j\ne i} p_{ij} \end{aligned}$$

It can be verified that for $1 \le i \ne j \le n+1$ and $1 \le k \ne l \le n+1$

$$p_i(a_k) = \delta_{ik}, (a_l - a_k)^T\nabla p_i(a_k) = 0, p_{ij}(a_k) = \delta_{ik}, (a_l - a_k)^T\nabla p_{ij}(a_k) = \delta_{ik}\delta_{jl}.$$

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Electron Magnetohydrodynamics

- A single electron fluid description of plasma behaviors at
  - fast time scale: $t \ll \omega_{ci}^{-1}/2\pi$
  - small spatial scale: $L \ll c/\omega_{pi}$
  - ions are stationary, electron flow determines electric current
  - $\mathbf{B}$: magnetic field
  - $\mathbf{v} = -\frac{1}{en}\mathbf{j} = -\frac{c}{4\pi en}\nabla \times \mathbf{B}$, $\mathbf{j}$ is plasma current density
  - $d_e = c/\omega_{pe}L$: electron inertial skin depth
- Governing equations for magnetic field $\mathbf{B}$:

$$\partial_t(\mathbf{B} - d_e^2\nabla^2\mathbf{B}) + \nabla \times [\mathbf{v} \times (\mathbf{B} - d_e^2\nabla^2\mathbf{B})] = \eta_1\nabla^2\mathbf{B} - \eta_2(\nabla^2)^2\mathbf{B}$$

When $d_e \approx 0$, we have

$$\partial_t\mathbf{B} + \nabla \times (\mathbf{v} \times \mathbf{B}) = \eta_1(\nabla\times)^2\mathbf{B} - \eta_2(\nabla\times)^4\mathbf{B}$$

A new formulation of in terms of curl operators

The Electron MHD equation can be reformulated as

$$\partial_t \mathbf{B} - \nabla \times (\mathbf{v} \times \mathbf{B}) = \eta_1 (\nabla \times)^2 \mathbf{B} - \eta_2 (\nabla \times)^4 \mathbf{B}$$

Since $\nabla \cdot \mathbf{B} = 0$, we have

$$-\Delta \mathbf{B} = \nabla \times (\nabla \times \mathbf{B}) - \nabla(\nabla \cdot \mathbf{B}) = \nabla \times \nabla \times \mathbf{B}$$

and

$$\Delta^2 \mathbf{B} = \nabla \times \nabla \times \nabla \times \nabla \times \mathbf{B}$$

Advantage:

- $\nabla \cdot \mathbf{B} = 0$ is built-in: $\partial_t (\nabla \cdot \mathbf{B}) = 0$ (from the equation in curl form)
- finite element approximation (properly constructed) with fewer d.o.f!

A new finite element for 4th order curl equations in 3D

(Zheng 2008 (thesis), Hu, Xu and Zheng 2008)

1. finite element: a tetrahedron K
2. f.e. space $\mathcal{P}_K = R_2(K)$, incomplete quadratic polynomial space.
3. (20) Degrees of freedom (d.o.f):

$$M_e(u) = \left\{ \int_e u \cdot \tau \; q \; ds \mid \forall \, q \in P_1(e), \right\}, \quad \forall \text{ edge } e \subset K$$

$$M_f(u) = \left\{ \frac{1}{|f|^2} \int_f (\nabla \times u) \times \mathbf{n} \cdot \mathbf{q} \; dA \mid \forall \, \mathbf{q} \in (P_0(f))^2 \right\}. \quad \forall \text{ face } f \subset K$$

- Number of d.o.f. $= 20$.

Nodal basis functions

Explicit expression of basis functions (tricky and lucky!)

- Two basis functions on each face k $(1 \le k \le 4)$:

$$\psi_k^m = \lambda_k((-1)^m L_{k+m,k+2} - L_{k+1,k+2}) \quad (m = 1, 2)$$

  where $L_{ij} = \lambda_i \nabla \lambda_j - \lambda_j \nabla \lambda_i$.

- Two basis functions on each edge ij $(1 \le i < j \le 4)$:

$$\psi_{ij}^1 = \lambda_i \nabla \lambda_j + \lambda_j \nabla \lambda_i,$$

$$\psi_{ij}^2 = L_{ij} + \sum_{l=1}^{4} \sum_{m=1}^{2} M_l^m(L_{ij}) \psi_l^m.$$

Error estimates

First order convergence:

$$\|\mathbf{B} - \mathbf{B}_h\| + \|\nabla \times (\mathbf{B} - \mathbf{B}_h)\| + \|(\nabla\times)^2(\mathbf{B} - \mathbf{B}_h)\| = \mathcal{O}(h).$$

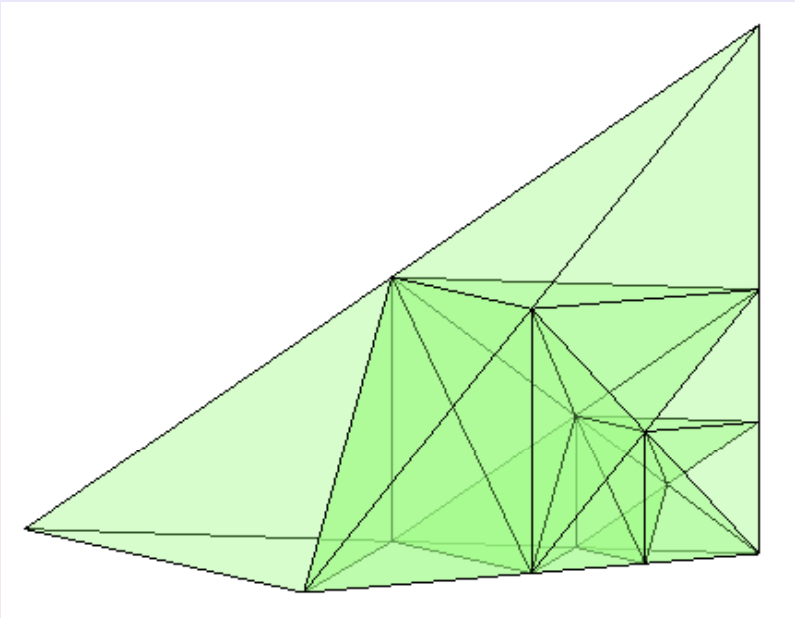
Discrete divergence free:

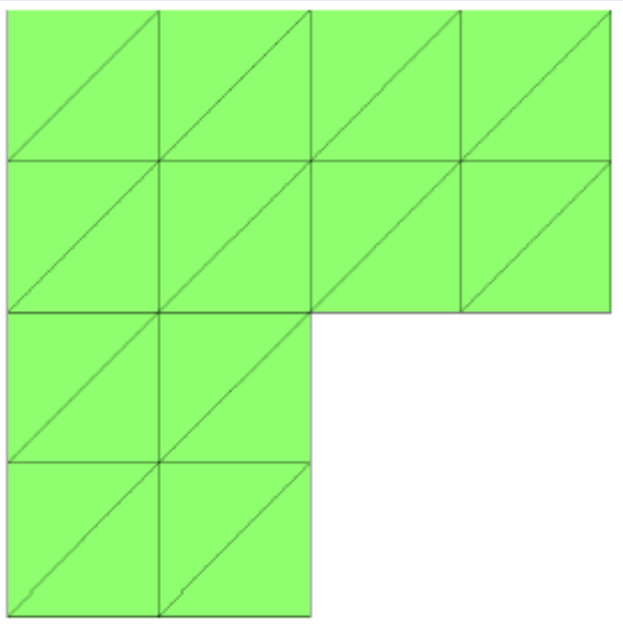
$$(\mathbf{B}_h, \nabla p_h) = 0, \text{ for any continuous piecewise quadratic } p_h$$

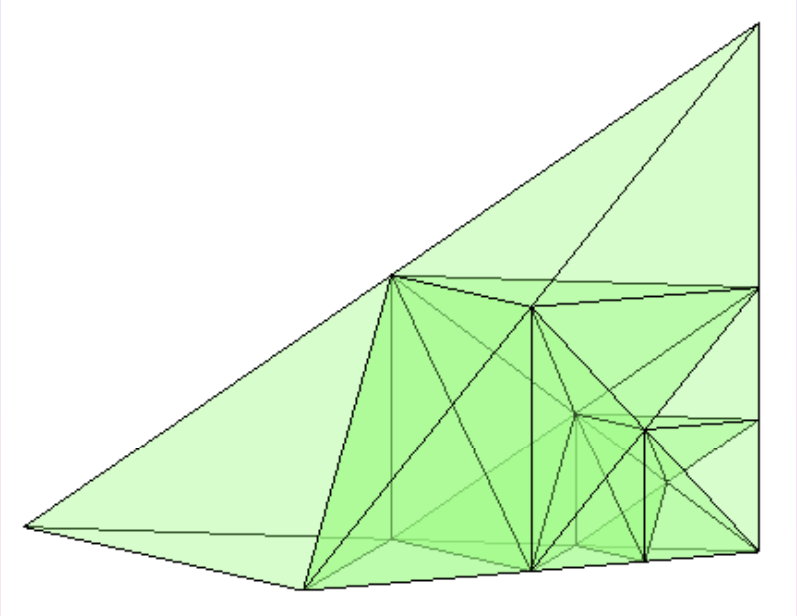
Ongoing work

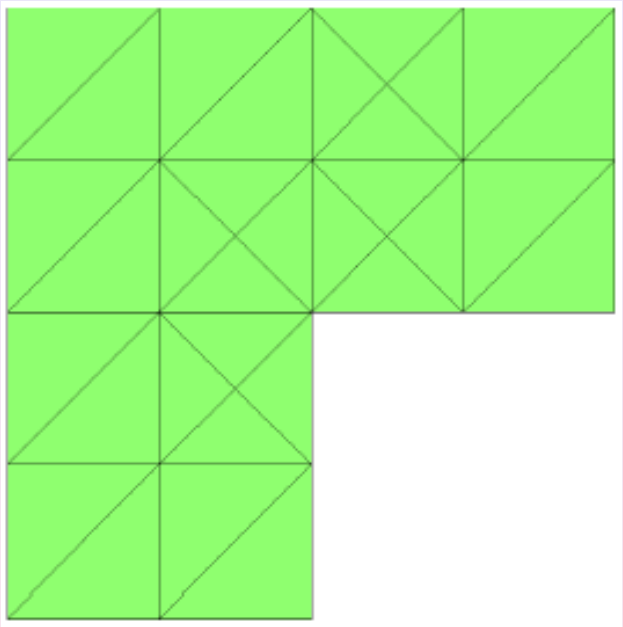
(Zheng)

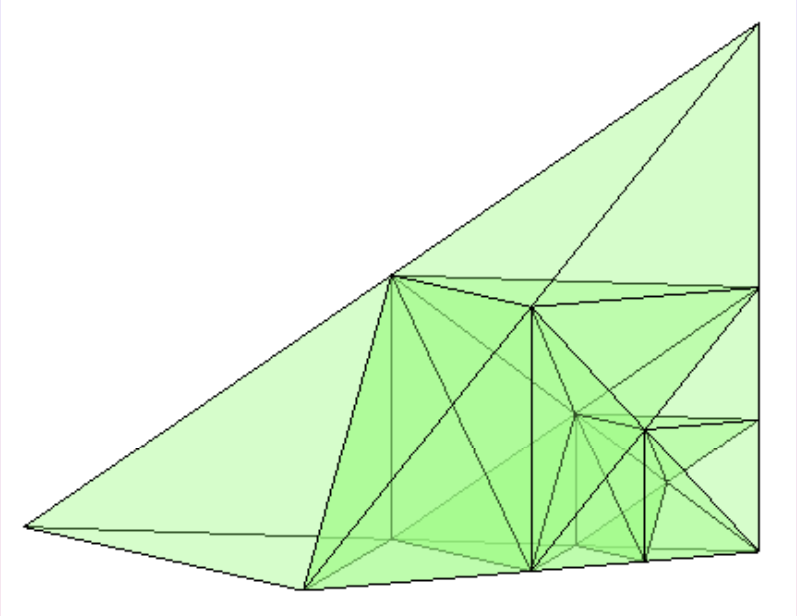
- implementation (3D)
  - Morley element
  - Modified Zienkiewicz element (with Zhang)
  - New 4th order curl element
- solvers
  - geometric multigrid methods
  - Navier-Stokes equations
- a posterior error estimates
  - problem-independent: Bank, Xu and Zheng (2006)
  - problem-specific
  - 3D bisection refinement (with Chen)

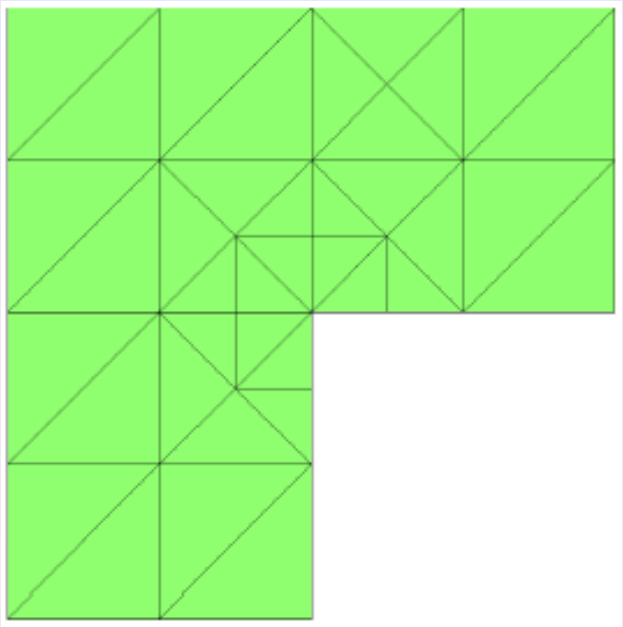


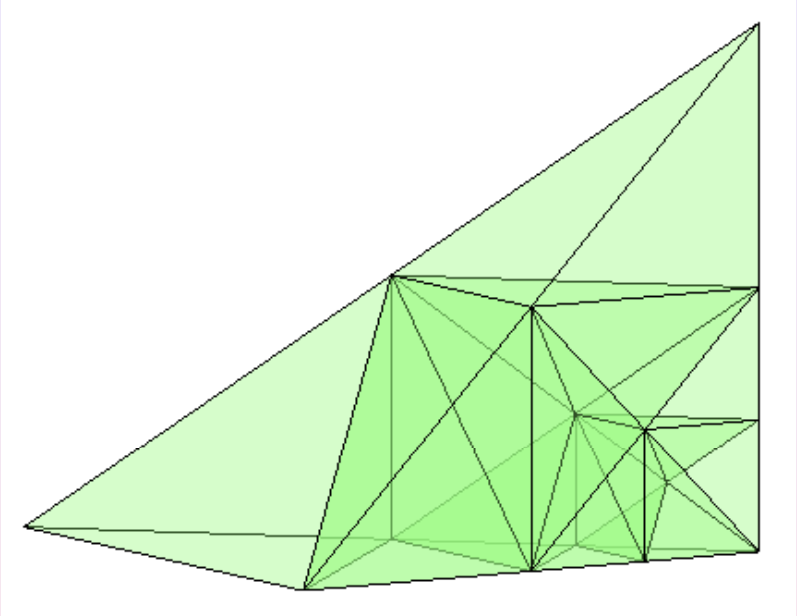


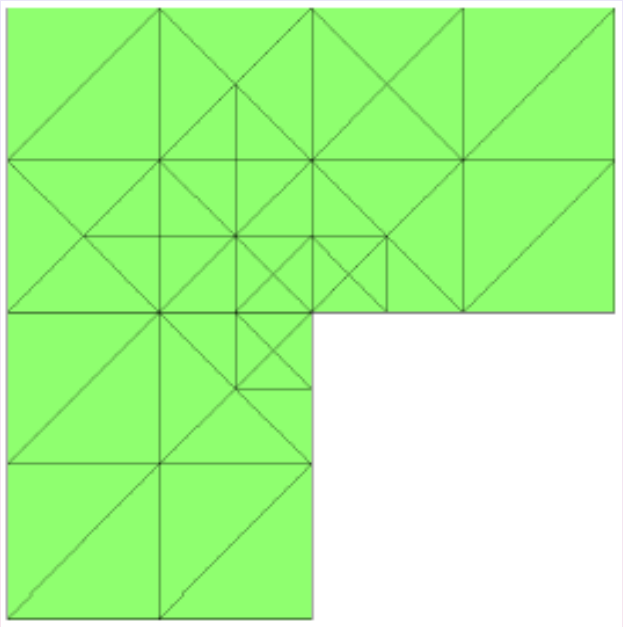


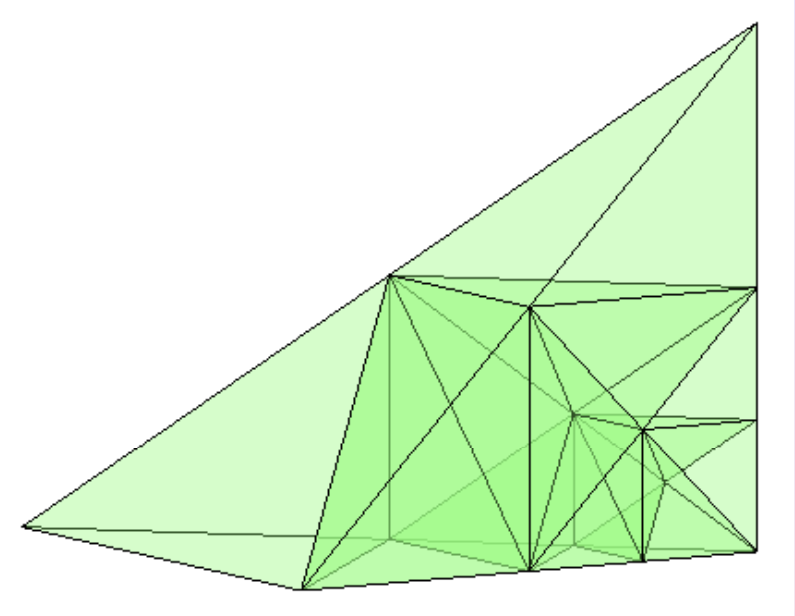


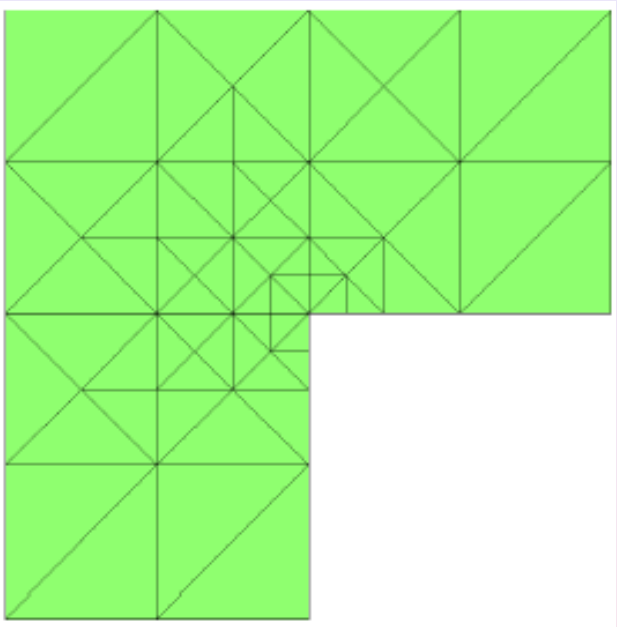












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A nonlinear example: non-Newtonian fluid models

(development of "solver-friendly" discretization!)

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Complex fluids: blood, milk, petroleum, drugs, cosmetics, slurries, and wastewater ....

The Johnson-Segalman model: ($\Rightarrow$ Navier-Stokes if $\mathrm{We} = 0$)

$$\begin{cases} \mathrm{Re}\frac{Du}{Dt} = \mathrm{div}\,[\tau + \mu_s \mathcal{D}(u)] - \nabla p \\ \mathrm{div}\, u = 0 \\ \tau + \mathrm{We}[\frac{D\tau}{Dt} - \mathcal{R}(u)\tau - \tau\mathcal{R}(u)^T] = 2\mu_p \mathcal{D}(u), \end{cases}$$

where

$\frac{Du}{Dt} = \frac{\partial u}{\partial t} + (u \cdot \nabla)u,$

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A nonlinear example: non-Newtonian fluid models

(development of "solver-friendly" discretization!)

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- More difficult than Navier-Stokes equations
- The high Weissenberg number problem:
  Most (all?) existing discretizations start to diverge at critical values of the Weissenberg number (We).

First key step: reformulation of constitutive equation

(Lee and Xu 2006)

Johnson-Segalman derivative:

$$\frac{\delta_E \tau}{\delta t} \equiv \frac{D\tau}{Dt} - \mathcal{R}(u)\tau - \tau\mathcal{R}(u)^T = \lim_{s\to t} \frac{D(E(s,t)\tau(t,s)E(s,t)^T)}{Ds}$$

where

$$\frac{DE(s,t)}{Dt} = R(t)E(s,t), \quad E(s,s) = I. \tag{5.4}$$

Note that

$$\frac{\delta_L I}{\delta t} = \frac{DI}{Dt} - \mathcal{R}(u)I - I\mathcal{R}(u)^T = -\mathcal{R}(u) - \mathcal{R}(u)^T = -2a\mathcal{D}(u).$$

Thus $\tau + \mathrm{We}[\frac{D\tau}{Dt} - \mathcal{R}(u)\tau - \tau\mathcal{R}(u)^T] = 2\mu_p\mathcal{D}(u)$ can be written as

$$\frac{\delta_E \tau_A}{\delta t} + \frac{1}{\mathrm{We}}\tau_A = \frac{\mu_p}{a\mathrm{We}^2} I.$$

A "clean" first order "linear" ODE (along particle trajectory)!

A new discretization

[Lee (2004, Ph.D. thesis), Lee and Xu 2006]

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5. Volume preserving schemes for characteristic feet [Feng and Shang (1995)]

An example of full discretization schemes

$$\frac{x-y^n}{k} = \frac{1}{2}\left(u(\frac{x+y^n}{2}, t^{n+1}) + u(\frac{x+y^n}{2}, t^n)\right) \quad (d=2)$$

$$\mathrm{Re}\frac{u_h^{n+1} - \Pi_h^v\left(u_h^n \circ y^n\right)}{k} + \nabla_h p_h^{n+1} + \eta_s A_h u_h^{n+1} = \mathrm{div}_h \tau_{A,h}^{n+1}$$

$$\mathbf{div} u_h^{n+1} = 0$$

$$\frac{E_h(t^n, t^{n+1}) - I}{k} = R_h(t^{n+1}) E_h(t^n, t^{n+1})$$

$$\frac{\tau_{A,h}^{n+1} - \Pi_h^S\left(E_h(t^n, t^{n+1})(\tau_{A,h}(t^n) \circ y^n) E_h(t^n, t^{n+1})^T\right)}{k} = -\alpha^{n+1}\tau_{A,h}^{n+1} + \beta^{n+1} I,$$

Two important properties

Theorem (Positivity preserving property)

If $\Pi_h^S \geq 0$ *and* $\tau_{A,h}^0 \geq 0$, *then* $\tau_{A,h}^n \geq 0, \quad n \geq 0.$

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Theorem (Discree energy estimates)

$$E_n \equiv \mathrm{Re}\|u_h^n\|_0^2 + \frac{1}{2a}\|\tau_{A,h}^n\|_{L^1} : \qquad E_n \leq c_0 e^{-c_1 t^n} E_0 + c_2 \frac{\mu_p}{(a\mathrm{We})^2}$$

where c_0, c_1 *and* c_2 *are generic constants.*

The energy of the discrete solution E_n *remains bounded for any number of time steps with any sizes of Weissenberg number.*

Other features of the new scheme

- **Solver-friendly:** At each time step in the new discretization, the following Stokes like system needs to be solved:

$$\begin{pmatrix} \frac{Re}{k} I - \eta_s \Delta_h & \nabla_h \\ -\mathbf{div} & 0 \end{pmatrix} \begin{pmatrix} u_h \\ p_h \end{pmatrix} = \begin{pmatrix} f_h \\ 0 \end{pmatrix},$$

  together with a number of independent [parallel] nonlinear ODEs.
- **Generality:** It works for a whoel range of models including Oldrolyd-B ($a = 1$), FENE-PM, Phan-Thien and Tanner ....

Incompressible Magneto Hydrodynamics

$$\rho(u_t + u \cdot \nabla u) + \nabla p = \mu \triangle u + \frac{1}{c} J \times B,$$

$$\nabla \cdot u = 0,$$

$$\frac{1}{c} B_t + \nabla \times E = 0,$$

$$\nabla \times B = \frac{4\pi}{c} J,$$

$$\sigma(E + \frac{1}{c} u \times B) = J.$$

- ρ is the fluid density, u the fluid velocity
- B, J, E: the magnetic field, the electric current density, the electric field
- μ, σ, c: the viscosity, the electric conductivity, the speed of light
- Lorentz's force (induced stress): $J \times B$

MHD: a reformulation similar to the non-Newtonian model

$$\rho \frac{Du}{Dt} - \mu \Delta u + \nabla p = \frac{1}{c} \nabla \cdot (B \times B),$$

$$\nabla \cdot u = 0,$$

$$\frac{\delta_F B}{\delta t} + \frac{\sigma c^2}{4\pi} \nabla \times \nabla \times B = 0.$$

where

$$\frac{Du}{Dt} = u_t + u \cdot \nabla u \text{ and } \frac{\delta_F B}{\delta t} = B_t + u \cdot \nabla B - B \cdot \nabla u.$$

With similar numerical techniques applied to this system (but using edge elements to discretize B), at each time-step, we mainly need to solve one (or few)

Stokes system + H(curl) system!

which can be both solved using optimal multilevel methods!

Outline

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2. Algebraic solvers
   - The method of subspace corrections
   - Practical and optimal solvers for H(curl) and H(div) systems
   - Indefinite systems: Stokes equations
3. Higher order PDEs
   - Conforming and nonconforming finite element methods
   - On the reduction of higher order to lower order systems
   - Two families of new nonconforming elements
4. Electron Magneto Hydrodynamics
   - A (curl curl curl curl)-formulation
   - A new nonconforming element for $(\nabla\times)^4$ systems
5. Solver-friendly discretization for incompressible MHD
   - A family of non-Newtonian models
   - Mathematical similarity between MHD and non-Newtonian models
   - A possible new "solver-friendly" discretization approach
6. Concluding remarks

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