Performance of a Parallel Algebraic Multilevel Preconditioner for Coupled Nonlinear PDE Systems: Transport/Reaction, Semiconductor Device, and MHD Applications

John N. Shadid

Computational Sciences R&D Group
Sandia National Laboratories

Collaborators

Paul T. Lin, Ray S. Tuminaro, Roger P. Pawlowski

Sandia National Laboratories
Outline

• Motivation: Scalable Solvers for Couple Nonlinear PDEs -
  • Scientific/Technology Applications
  • Multiphysics and Multiple-time Scale Systems

• Brief Overview of Governing PDEs

• Brief Description of Block Aggressive Coarsening AMG Preconditioner

• Examples of Performance on
  • CFD
  • Transport / Reaction
  • Drift-Diffusion
  • Resistive MHD

• Concluding Remarks
Scientific / Technology Motivation

- Resistive and extended MHD models a variety of important plasma physics
  - Astrophysics: Solar flares, sunspots, reconnection
  - Geophysics: Earth’s magnetospheric sub-storms, geo-dynamo
  - Fusion: Magnetic confinement (ITER - Tokamak), Inertial conf. (NIF, Z-pinch)
  - Technology/Engineering: Plasma Reactors, MHD Pumps, ...
  - ...

- Transport / Reaction Systems model a very broad range of scientific & energy/technology systems
  - Conventional / Alternate Energy: Combustion, Fuel Cells, bio-fuels, ...
  - Chemical Processing: CVD (Poly-Si, GaAs, GaN) for semiconductors, Photo-voltaic materials, ...
  - Partial Catalytic Reactors e.g. methane (g) ➔ methanol (l), ...
  - Semiconductor devices: Performance and radiation damage
  - Biological cells: Heart / ER simulations
  - ....
Mathematical / Computational Motivation: Achieving Scalable Predictive Simulations of Complex Highly Nonlinear Multi-physics PDE Systems

What are multi-physics systems? (A multiple-time-scale perspective)

These systems are characterized by a myriad of complex, interacting, nonlinear multiple time- and length-scale physical mechanisms.

These mechanisms can balance to produce:

• steady-state behavior,

• nearly balance to evolve a solution on a dynamical time scale that is long relative to the component time scales,

• or can be dominated by one, or a few processes, that drive a short dynamical time scale consistent with these dominating modes.

e.g. Nuclear Fusion / Fission Reactors; Astrophysics; Conventional /Alternate Energy Systems

Our approach - pursue new applied math/algorithms to develop robust, accurate, scalable, and efficient implicit formulations and fully-coupled Newton-Krylov methods with integrated optimization/UQ tools for predictive simulation technologies for complex coupled multi-physics systems.
Transport / Reaction and Resistive MHD Models

**Navier Stokes**

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} - \mathbf{T}) = 0
\]

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

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

\[
- \rho \mathbf{g} = 0, \quad \mathbf{T} = - \left( P + \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \right) \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)
\]

**Galerkin FE (Mixed interpolation FEM):**

\[
\begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ \dot{P} \end{bmatrix} + \begin{bmatrix} A & -B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} v \\ P \end{bmatrix}
\]

Stokes Flow: \( A - \) SPD

Navier-Stokes: \( A - \) Nonsymm.

**Stabilized FE (Hughes et. al)**

Q1/Q1 V-P elements, SUPG like terms and Discontinuity Capturing type operators

\[
\begin{bmatrix} M & 0 \\ N & 0 \end{bmatrix} \begin{bmatrix} \dot{v} \\ \dot{P} \end{bmatrix} + \begin{bmatrix} A & -B^T \\ BR & K \end{bmatrix} \begin{bmatrix} v \\ P \end{bmatrix}
\]

\[
K = \sum_e \int_{\Omega_e} \rho \tau_m \nabla \Phi \cdot \nabla \Phi d\Omega
\]

General Case a Strongly Coupled, Multiple Time- and Length-Scale, Nonlinear, Nonsymmetric System with Parabolic and Hyperbolic Character
Transport / Reaction and Resistive MHD Models

Navier Stokes + Transport / Reaction Physics

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot [\rho \mathbf{v} \otimes \mathbf{v} - \mathbf{T}] - \rho \mathbf{g} = 0; \quad \mathbf{T} = - \left( P + \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \right) \mathbf{I} + \mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T];
\]

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

\[
\frac{\partial (\rho e)}{\partial t} + \nabla \cdot [\rho \mathbf{v} + \mathbf{q}] + \sum_{k=1}^{N} \mathbf{j}_k \cdot \hat{C}_{p,k} \nabla T - \sum_{k=1}^{N} h_k W_k \omega_k = 0
\]

Species Transport / Reaction Equation

\[
\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\mathbf{u} Y_k + \mathbf{j}_k) - W_k \dot{\omega}_k; \quad k = 1, 2, ..., N - 1; \quad \sum_{k=1}^{N} Y_k = 1
\]

General Case a Strongly Coupled, Multiple Time- and Length-Scale, Nonlinear, Nonsymmetric System with Parabolic and Hyperbolic Character
Summary of Stabilized FE Weak form of Equations for Transport / Reaction Systems; Seek $x^h \approx x$; where $x^h \subseteq F^h(x^h) = 0$

<table>
<thead>
<tr>
<th>Governing Equation</th>
<th>Stabilized FE Residual</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Momentum</strong></td>
<td>$F_{m,i} = \int_{\Omega} \Phi R_{m,i} , d\Omega + \sum_{e} \int_{\Omega^e} \rho \tau_m \left( \mathbf{u} \cdot \nabla \Phi \right) R_{m,i} , d\Omega + \sum_{e} \int_{\Omega^e} \nabla \Phi \cdot G^c \nabla u_i , d\Omega$</td>
</tr>
<tr>
<td><strong>Total Mass</strong></td>
<td>$F_p = \int_{\Omega} \Phi R_p , d\Omega + \sum_{e} \int_{\Omega^e} \rho \tau_m \nabla \Phi \cdot R_m , d\Omega$</td>
</tr>
<tr>
<td></td>
<td>$\sum_{e} \int_{\Omega^e} \rho \tau_m \nabla \Phi \cdot \left[ \rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla \mathbf{u}) + \nabla P - \nabla \cdot \mathbf{Y} - \rho g \right] , d\Omega$</td>
</tr>
<tr>
<td><strong>Thermal Energy</strong></td>
<td>$F_T = \int_{\Omega} \Phi R_T , d\Omega + \sum_{e} \int_{\Omega^e} \rho \hat{C}<em>p \tau_T \left( \mathbf{u} \cdot \nabla \Phi \right) R_T , d\Omega + \sum</em>{e} \int_{\Omega^e} \nabla_T \nabla \Phi \cdot G^c \nabla T , d\Omega$</td>
</tr>
<tr>
<td><strong>Species Mass</strong></td>
<td>$F_{Y_k} = \int_{\Omega} \Phi R_{Y_k} , d\Omega + \sum_{e} \int_{\Omega^e} \rho \tau_{Y_k} \left( \mathbf{u} \cdot \nabla \Phi \right) R_{Y_k} , d\Omega + \sum_{e} \int_{\Omega^e} \nabla_{Y_k} \nabla \Phi \cdot G^c \nabla Y_k , d\Omega$</td>
</tr>
</tbody>
</table>
Why Newton-Krylov Methods?

Newton-Krylov

Direct-to-steady-state

Convergence Properties
Design Optimization

Characterization
Complex Soln. Spaces.
Bifurcation, Stability

Fully-implicit transient

Stability
Accuracy
Efficiency

Very Large Problems -> Parallel Iterative Solution of Sub-problems

Krylov Methods - Robust, Scalable and Efficient Parallel Preconditioners

• Approximate Block Factorizations
• Physics-based Preconditioners
• Multi-level solvers for systems and scalar equations
ML library: Multilevel Preconditioners
(R. Tuminaro, M. Sala (BMW-Sauber), J. Hu, C. Siefert, M. Gee (UT Munich)]

2-level and N-level Aggressive Coarsening Graph-based Block AMG

1. Aggregation is used to produce a coarse operator
   • Create graph where vertices are block nonzeros in matrix $A_k$
   • Edge between vertices i and j included if block $B_k(i,j)$ contains nonzeros
   • Decompose graph into aggregates (subgraphs) [Metis/ParMetis]

2. Construction of simple restriction/interpolation operators (e.g. piecewise constants on agg.)

3. Smoothing of Tentative Prolongator

4. Construction of $A_{k-1}$ as $A_{k-1} = R_k A_k P_k$

Aggregation based Multigrid:
• Vanek, Mandel, Brezina, 1996
• Vanek, Brezina, Mandel, 2001

Aggregation used in DD:
• Paglieri, Scheinine, Formaggia, Quateroni, 1997
• Jenkins, Kelley, Miller, Kees, 2000
• Toselli, Lasser, 2000
• Sala, Formaggia, 2001
Choice of Prolongation/Restriction

♦ Non-smoothed aggregation and a Galerkin Projection (simple choice, good stability, more optimal for hyperbolic operators)

\[ \hat{P}(i, \alpha) = \begin{cases} 
1 & \text{if } i \in \text{agg}(\alpha) \\
0 & \text{otherwise} 
\end{cases}; \quad R = \hat{P}^T \]

♦ Smoothed aggregation and a Galerkin projection. Damped Jacobi a typical choice for smoothing prolongator in smoothed aggregation (optimal smoothing parameters for Laplace, etc.)

\[
\begin{align*}
P_i &= (I - \omega_i D^{-1} A) \hat{P}_i \\
R &= P^T 
\end{align*}
\]

\[ \hat{P}_i: \text{ tentative prolongator} \]
\[ D = \text{diag}(A) \]
\[ \omega_i: \text{ damping parameter} \]

♦ Petrov-Galerkin type smoothed aggregation preconditioner for nonsymmetric linear systems [Sala and Tuminaro, SISC 2008]

\[
\begin{align*}
P_i &= (I - \omega_i D^{-1} A) \hat{P}_i \\
R_i &= \hat{P}_i^T (I - AD^{-1} \omega_i^{(r)}) 
\end{align*}
\]

+ Perform restriction smoothing
+ Restriction operator does not correspond to transpose of prolongator for nonsymmetric problems
+ Rather than use a single damping parameter, calculate values to minimize \( P_i \) and \( R_i \)

- Sub-domain decomposition smoothers (sub-domain GS and ILUT, ILU(k), LU)
- Coarse grid solver can use fewer processors than for fine mesh solve (sparse direct (KLU, SuperLU) / approximate (ILUT) / iterative
Multilevel Preconditioner Scaling Study: 3D Thermal Buoyancy Driven Convection
### Comparison of 1-level with 2-level geometric & algebraic 2D & 3D Thermal Convection Problem

<table>
<thead>
<tr>
<th>proc</th>
<th>fine grid unknowns</th>
<th>1 - level Method Ilu DD</th>
<th>coarse unknowns</th>
<th>2-level: ilu-superlu</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>avg its per Newt step</td>
<td>time (sec)</td>
<td>geometric</td>
</tr>
<tr>
<td>1</td>
<td>4356</td>
<td>41</td>
<td>23</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>16,900</td>
<td>98</td>
<td>62</td>
<td>324</td>
</tr>
<tr>
<td>16</td>
<td>66,564</td>
<td>251</td>
<td>275</td>
<td>1156</td>
</tr>
<tr>
<td>64</td>
<td>264,196</td>
<td>603</td>
<td>1,399</td>
<td>4356</td>
</tr>
<tr>
<td>256</td>
<td>1,052,676</td>
<td>1,478</td>
<td>8,085</td>
<td>16,900</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>proc</th>
<th>fine grid unknowns</th>
<th>1 - level Method Ilu DD</th>
<th>coarse unknowns</th>
<th>2-level: gs2-superlu</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>avg its per Newt step</td>
<td>time (sec)</td>
<td>geometric</td>
</tr>
</tbody>
</table>

Sala, S, Tuminaro; accepted in SIMAX
Numerical Exp:
Lin, Sala, S, Tuminaro; IJNME, 2006

- Coarse mesh: SuperLU direct solver
- Run on Sandia ASCI Red machine
3D Thermal Convection CFD Problem
1- and 3-level Preconditioners
CFD: Steady-State Thermal Convection
3-level Preconditioner Scaling Study

- Steady-state 3D thermal convection problem
- Run on Sandia Red Storm machine

<table>
<thead>
<tr>
<th>proc size (elem)</th>
<th>fine grid size unknown</th>
<th>1-level Aztec ILUT</th>
<th>3-level (GS/ILU/KLU) agg125</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>iter/Newt</td>
<td>prec time/N</td>
</tr>
<tr>
<td>4</td>
<td>36^3</td>
<td>253264</td>
<td>109</td>
</tr>
<tr>
<td>32</td>
<td>72^3</td>
<td>1.95M</td>
<td>286</td>
</tr>
<tr>
<td>256</td>
<td>144^3</td>
<td>15.2M</td>
<td>691</td>
</tr>
<tr>
<td>2048</td>
<td>288^3</td>
<td>120.7M</td>
<td><strong>est 1675</strong></td>
</tr>
</tbody>
</table>

- “prec time/N”=time to construct preconditioner per Newton step (sec)
- “prec+lin sol time/N”=time to construct preconditioner and perform linear solve per Newton step (sec)
- Ave (matrix fill)/(Newt step) time approximately 3 sec
- Simulation typically required 5 Newton steps
• Transient LES-k (dt=0.01) simulation in building

<table>
<thead>
<tr>
<th>proc</th>
<th>fine grid unknown</th>
<th>1-level Aztec ILUT</th>
<th>3-level (GS/ILU/KLU) agg85</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>iter/prec time/N</td>
<td>medium coarse iter/prec time/N</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Newt prec+lin sol t/N</td>
<td>unk unk Newt prec+lin sol t/N</td>
</tr>
<tr>
<td>4</td>
<td>284360</td>
<td>108</td>
<td>3335</td>
</tr>
<tr>
<td></td>
<td></td>
<td>13</td>
<td>35</td>
</tr>
<tr>
<td></td>
<td></td>
<td>34</td>
<td>62</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>4</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>31</td>
</tr>
<tr>
<td>32</td>
<td>2.13M</td>
<td>161</td>
<td>24930</td>
</tr>
<tr>
<td></td>
<td></td>
<td>43</td>
<td>290</td>
</tr>
<tr>
<td></td>
<td></td>
<td>70</td>
<td>89</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>4</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>47</td>
</tr>
<tr>
<td>256</td>
<td>16.4M</td>
<td>320</td>
<td>192585</td>
</tr>
<tr>
<td></td>
<td></td>
<td>44</td>
<td>2265</td>
</tr>
<tr>
<td></td>
<td></td>
<td>167</td>
<td>101</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>55</td>
</tr>
<tr>
<td>2048</td>
<td>129.1M</td>
<td>552</td>
<td>15.1M</td>
</tr>
<tr>
<td></td>
<td></td>
<td>49</td>
<td>17805</td>
</tr>
<tr>
<td></td>
<td></td>
<td>450</td>
<td>113</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>27</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>105</td>
</tr>
</tbody>
</table>

3D Transient turbulent flow (LES-ksgs)
CFL ~ 0.3

• “prec time/N”=time to construct preconditioner per Newton step (sec)
• “prec+lin sol time/N”=time to construct preconditioner and perform linear solve per Newton step (sec)
• Ave (matrix fill)/(Newt step) time 45-58 sec
• Data from third time step of simulation (took 3 Newton steps)
**Aggressive Coarsening Graph based Block AMG 3-level MPSalsa/ML Preconditioner Scaling Study**

3D Steady-state (Laminar flow)

<table>
<thead>
<tr>
<th>proc</th>
<th>fine mesh unknowns</th>
<th>hexahedral</th>
<th>tetrahedral</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>3-level</td>
<td>1-level</td>
</tr>
<tr>
<td></td>
<td>avg its per Newt step</td>
<td>time (sec)</td>
<td>avg its per Newt step</td>
</tr>
<tr>
<td>1024</td>
<td>103M</td>
<td>136 [5]</td>
<td>2924</td>
</tr>
</tbody>
</table>

- Laminar steady-state (artificially low Re to get direct to steady-state) and transient LES-k in building
- Smoothers/solvers: Gauss-Seidel, ILU, SuperLU
- Nodes per aggregate: 100, 100
- Run on CPlant
Preliminary Scaling with Reactions: Poly-Silicon CVD

- Deposition of poly-Silicon
  - 3 species (8 unknowns per node)
- Steady-state calculation restarted from steady-state solution at lower pressure (one solution in continuation run)
- Run on Cplant

<table>
<thead>
<tr>
<th>proc</th>
<th>fine unknowns</th>
<th>coarser unknowns</th>
<th>1-level (ILU)</th>
<th>5-level (GS/ILU/ILU/ILU/KLU) damp 0.67</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>no auxiliary matrix</td>
<td>aux. matrix</td>
<td>no auxiliary matrix</td>
</tr>
<tr>
<td>2</td>
<td>87,400</td>
<td>3560/296/24</td>
<td>17K/1240/120/16</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>636K</td>
<td>22K/1816/224/72</td>
<td>120K/9096/880/136</td>
<td></td>
</tr>
<tr>
<td>128</td>
<td>4.85M</td>
<td>161K/12K/1440/368</td>
<td>967K/75K/6744/1296</td>
<td></td>
</tr>
</tbody>
</table>

- Aspect Ratio Effect; Even with auxiliary matrix, still does not scale; more work necessary
Drift-Diffusion / Radiation Damage for Modeling Semiconductor Devices

Electric potential
\[ \chi^2 \nabla \cdot (\varepsilon_r \mathbf{E}) = p - n + C + \sum_{i=1}^{N_s} q_i X_i q \]

\[ E = -\nabla \psi \]

Electron/Hole current conservation
\[ \nabla \cdot J_n = \frac{\partial n}{\partial t} + R \]
\[ -\nabla \cdot J_p = \frac{\partial p}{\partial t} + R \]

\[ |\Delta C| = 10^{19} \]

Radiation Damage Model:
\( N_s \) - Charge Species
Transport / Reaction Equations
\[ \nabla \cdot (\mu_i X_i \nabla \psi + D_i \nabla X_i) = \frac{\partial X_i}{\partial t} + R X_i, \quad \mu_i = \frac{q_i D_i}{kT} \]

Modified Equation for Electric Potential
- \( X_i \): species concentration
- \( q \): charge of electron
- \( q_i \): integer charge for species

W / Hennigan, Hoekstra, Castro
Weak Scaling Study: 1-level and 3-level (NSA and PG-SA)

- 3-level ML-AMG: NSA and Petrov-Galerkin SA
- Red Storm
• 3-level ML-AMG: NSA and Petrov-Galerkin SA
• Red Storm - Quad core nodes

<table>
<thead>
<tr>
<th>configuration</th>
<th>Newton Step</th>
</tr>
</thead>
<tbody>
<tr>
<td>(quad core)</td>
<td>time(s)</td>
</tr>
<tr>
<td>4096n 1ppn</td>
<td>28.7</td>
</tr>
<tr>
<td>2048n 2ppn</td>
<td>31.2</td>
</tr>
<tr>
<td>1366n 3ppn</td>
<td>35.4</td>
</tr>
<tr>
<td>1024n 4ppn</td>
<td>39.3</td>
</tr>
</tbody>
</table>

Our Largest Simulations to Date:

Steady-state: [Drift-Diffusion: \((\psi, n, p)\)]

1+ Billion unknowns
24,000 cores Cray XT3/4

110+ Million unknowns
38,360 cores Cray XT3/4

Implicit Transient: [D-D + Radiation Damage: \((\psi, n, p, X_i)\) - 36 species]

250 Million unknowns
8,192 cores IBM eServer
Transport / Reaction and Resistive MHD Models

**Navier Stokes + Electro-magnetics**

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

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

\[
\frac{\partial (\rho e)}{\partial t} + \nabla \cdot [\rho \mathbf{v} + \mathbf{q}] - \eta ||\mathbf{J}||^2 = 0
\]

**Reduced form of Maxwell’s Equations**

\[
\frac{\partial \mathbf{B}}{\partial t} - \nabla \times [\mathbf{v} \times \mathbf{B}] + \nabla \times (\eta \mathbf{J}) = 0 ; \quad \mathbf{J} = \frac{1}{\mu_0} \nabla \times \mathbf{B}
\]
Scaling Performance for Fully-coupled Resistive MHD/ Block AMG - Cray XT3/4

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

- 4096 procs.
- 1024 procs.
- 256 procs.
- 64 procs.
- 16 procs.

Avg. Its / Newton Step vs Number of Unknowns

Avg. CPU Time / Newton Step (sec.) vs Number of Unknowns

~20x improvement in scaling performance.
Multicore Performance of Fully-coupled Resistive MHD Simulations - Cray XT3/4

Our Largest Steady-state Simulation to Date:

1+ Billion unknowns
250 Million Quad elements
24,000 cores Cray XT3/4

Newton-GMRES / ML: PG-AMG 4 level
18 Newton steps
86 Avg. No. Linear Its. / Newton step
33 min. for solution

<table>
<thead>
<tr>
<th>Nodes</th>
<th>Cores</th>
<th>Compute Jac+Prec</th>
<th>Linear Solve</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Time (sec)</td>
<td>η (%)</td>
<td>Time (sec)</td>
</tr>
<tr>
<td>4096</td>
<td>1</td>
<td>16.9</td>
<td>---</td>
<td>4.3</td>
</tr>
<tr>
<td>2048</td>
<td>2</td>
<td>18.2</td>
<td>93</td>
<td>4.5</td>
</tr>
<tr>
<td>1024</td>
<td>4</td>
<td>17.7</td>
<td>95</td>
<td>4.9</td>
</tr>
</tbody>
</table>

By
Velocity
MHD Pump
Hydromagnetic Rayleigh-Bernard Linear Stability Problem

\[ g \]

\[ T_C \]

\[ T_H \]

\[ B_y = B_0 \]

\[ x \]

\[ y \]

\[ z \]

\[ Ra = \frac{g \beta}{\nu \alpha} \Delta T d^3 \]: Rayleigh Number

\[ Q = \frac{B_0^2 d^2}{\mu_0 \rho \nu \eta} \]: Chandrasekhar Number

\[ Pr = \frac{\nu}{\alpha} \]: Prandtl Number

\[ Pr_m = \frac{\nu}{\eta} \]: Magnetic Prandtl Number
Hydro-Magnetic Rayleigh-Bernard Stability

Stable Fields/Flow at Ra = 4000, Q = 81

Unstable Flow at Ra = 4000, Q = 144

\[ Ra = \frac{g\beta \Delta T d^3}{\nu \alpha} \quad \text{and} \quad Q = \frac{B_0^2 d^2}{\mu_0 \rho \nu \eta} \]
Hydro-Magnetic Rayleigh-Bernard Stability: Direct Determination of Nonlinear Equilibrium Solutions (Steady State Solves, \( Ra = 2500 \))
Hydro-Magnetic Rayleigh-Bernard Stability: Direct Determination of Nonlinear Equilibrium Solutions (Steady State Solves, $Ra = 2500$)

### Robustness and Efficiency of DD and Multilevel Preconditioners

<table>
<thead>
<tr>
<th>proc size</th>
<th>fine grid size</th>
<th>fine grid unknowns</th>
<th>1-level ILU avg its/ Newt step</th>
<th>time (sec)</th>
<th>3-level V(1,1) ILU-ILU-KLU medium unkns size</th>
<th>coarse unkns size</th>
<th>avg its/ Newt step</th>
<th>time (sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2048</td>
<td>500x5000</td>
<td>12.5M</td>
<td>1910[40] &gt; 7200*</td>
<td>412450</td>
<td>13745</td>
<td>115[17]</td>
<td>226</td>
<td></td>
</tr>
</tbody>
</table>
Driven Magnetic Reconnection: Magnetic Island Coalescence
Unstructured Mesh Resistive MHD with Algebraic Multilevel Preconditioners

Approx. Computational Time Scales:
- Ion Momentum Diffusion: $10^{-7}$ to $10^{-3}$
- Magnetic Flux Diffusion: $10^{-7}$ to $10^{-3}$
- Alfven Wave: $10^{-4}$ to $10^{-2}$
- Whistler Wave: $10^{-7}$ to $10^{-1}$
- Magnetic Island Sloshing: $10^0$
- Magnetic Island Merging: $10^1$

W/ Luis Chacon - ORNL
Preliminary Weak Scaling Results on Island Coalescence Problem (@resistivity $\eta=1.0\times10^{-3}$)

Charon_xmhd, FE

<table>
<thead>
<tr>
<th>Procs</th>
<th>Mesh</th>
<th># Unk</th>
<th>Newton / $\Delta\tau$</th>
<th>Gmres / Newton</th>
<th>Time / Newton</th>
<th>Gmres / $\Delta\tau$</th>
<th>Time / $\Delta\tau$</th>
<th>Est. Serial Time</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>64x64</td>
<td>16K</td>
<td>3.9</td>
<td>4.4</td>
<td>2.1</td>
<td>17.2</td>
<td>8.1</td>
<td>810</td>
<td>3.6486</td>
</tr>
<tr>
<td>4</td>
<td>128x128</td>
<td>64K</td>
<td>4.6</td>
<td>5.8</td>
<td>2.6</td>
<td>26.7</td>
<td>11.9</td>
<td>4760</td>
<td>4.379</td>
</tr>
<tr>
<td>16</td>
<td>256x256</td>
<td>.25M</td>
<td>4.9</td>
<td>6.3</td>
<td>2.9</td>
<td>30.9</td>
<td>14.2</td>
<td>22720</td>
<td>3.8944</td>
</tr>
<tr>
<td>64</td>
<td>512x512</td>
<td>1M</td>
<td>6.2</td>
<td>8.8</td>
<td>4</td>
<td>54.6</td>
<td>24.6</td>
<td>157440</td>
<td>5.7502</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Grid</th>
<th>Newton</th>
<th>GMRES/dt</th>
<th>CPU(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>64x64</td>
<td>3.3</td>
<td>3.3</td>
<td>222</td>
</tr>
<tr>
<td>128x128</td>
<td>4</td>
<td>4.5</td>
<td>1087</td>
</tr>
<tr>
<td>256x256</td>
<td>4.5</td>
<td>6.2</td>
<td>5834</td>
</tr>
<tr>
<td>512x512</td>
<td>4.7</td>
<td>8.3</td>
<td>27380</td>
</tr>
</tbody>
</table>

L. Chacon, FV Physics-based Prec.

Surprising comparison: Only ~4 times slower, considering...

- Research code – no investment in efficiency (coming soon)
- Unstructured FE vs Structured FV solver: no leveraging of mesh structure.
- No physics based preconditioning (Block - AMG)
- Need faster and lower memory physics based approach for transients and lower resistivity.
Conclusions

• Newton-Krylov /block AMG methods can provide a very effective, robust and flexible solution technology for analysis and characterization of complex nonlinear solution spaces. For steady state, time dependent and optimization type solutions.

• Parallel multilevel preconditioners have shown promising results for algorithmic scalability and CPU time performance of transport solutions.

  (Issues: Strong convection effects, reaction and FE aspect ratios for multilevel methods)

• For transient simulations combination of approximate block factorizations, physics based preconditioners are required for fast solutions. Use block AMG as sub-system solvers.

• Need to study coarse operator solvers based on threads/shared memory for multicore node architectures.
The End