Solution Techniques for Large-scale Fully-Implicit Multi-Physics Systems Using Trilinos

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Mathematical Motivation
Achieving Scalable Predictive Simulations of Complex Highly Nonlinear Multi-physics PDE Systems

• Multiphysics systems are characterized by a myriad of complex, interacting, nonlinear multiple time- and length-scale physical mechanisms:

  – Dominated by **short dynamical time-scales**
  – Widely separated time-scales (**stiff system**)
  – Evolve a solution on a **long time scale relative to component time scales**
  – Balance to produce **steady-state** behavior.

  Explicit Methods

Typically requires some form of Implicit Methods

  e.g. Nuclear Fission / Fusion Reactors; Conventional /Alternate Energy Systems; High Energy Density Physics; Astrophysics; etc .

• Our approach:

  – Stable and higher-order accurate implicit formulations and discretizations
  – Robust, scalable and efficient prec. for fully-coupled Newton-Krylov methods
  – Integrate sensitivity and error-estimation to enable UQ capabilities.
Tools for Multiphysics Simulation
(Spanning Individual Applications and Coupled Systems)

• Domain Model (SAND2011-2195)

• Abstraction Layer ANAs
  – Thyra::ModelEvaluator: Application Interface
  – Thyra: Operator, Vector

• Implicit Nonlinear Solution Algorithms
  – NOX: Globalized Newton-Krylov and JFNK
  – LIME/PIKE: Multiphysics coupling driver. Picard iteration and tools to assemble block aggregate systems to call with NOX

• Linear Algebra and Linear Solution Algorithms
  – Epetra, Tpetra: Concrete Linear Algebra
  – Stratimikos, Belos, AztecOO, Amesos: Linear Solvers
  – ML, MueLE, Ifpack, Teko: Preconditioners

• Examples
Implicit Climate Simulators can be Built on Trilinos Solvers and Software

- HOMME Atmospheric Model
- POP Ocean Model
- THCM Ocean Model
- Glimmer Ice Sheet Model
- FELIX Ice Sheet Model
- + IBECS, Sea Ice

Software Quality
- Version Control
- Regression Testing
- Build System
- Verification Tests
- Bug Tracking
- Web Documentation
- Release Process

Parallelization Tools
- Data Structures
- Partitioning
- Load Balancing
- Architecture-Dependent Kernels

Linear Solvers
- Iterative Solvers
- Direct Solvers
- Eigen Solver
- Preconditioners
- Multi-Level Algs

Analysis Tools
- Nonlinear Solver
- Time Integration
- Stability Analysis
- Optimization
- UQ Algorithms
A Domain Model

\[ f(\dot{x}, x, \{p_l\}, t) = 0 \]

- **Input Arguments:** state time derivative, state, parameters, time
- **Output Arguments:** Residual, Jacobian, response functions, etc...

\[ \dot{x} = \frac{\partial x}{\partial t} \]

- Residual
- State (DOF)
- Time
- Set of parameters

**Response Function**

\[ g_j(\dot{x}, x, \{p_l\}, t) = 0, \text{ for } j = 0, \ldots, N_g - 1 \]

\[ g_j(\dot{x}, x, \{p_l\}, t) : \mathbb{R}^{2n_x + (\sum_{i=0}^{N_p-1} n_{p_i})+1} \rightarrow \mathbb{R}^{n_{g_j}} \text{ is the } j^{\text{th}} \text{ response function.} \]

- **Input Arguments:** state time derivative, state, parameters, time
- **Output Arguments:** Residual, Jacobian, response functions, etc...
Extension to Multiphysics

Split parameters into “coupling” and truly independent.

\[ f_i(\dot{x}_i, x_i, \{z_{i,k}\}, \{p_{i,l}\}, t) = 0 \]

 Require transfer functions:
• Can be complex nonlinear functions themselves

\[ z_{i,k} = r_{i,k}(\{x_m\}, \{p_{m,n}\}) \]

Transfer Function

Response functions now dependent on \( z \)
• Can be used as coupling parameters \((z)\) for other codes

\[ g_{i,j}(\dot{x}_i, x_i, \{z_{i,k}\}, \{p_{i,l}\}, t) \]

Response Function
Abstract Interfaces
What is an abstract numerical algorithm (ANA)?

An ANA is a numerical algorithm that can be expressed abstractly solely in terms of vectors, vector spaces, linear operators, and other abstractions built on top of these without general direct data access or any general assumptions about data locality.

Introducing Abstract Numerical Algorithms

Block composition operators and vectors:

\[
\begin{bmatrix}
J_{TT} & J_{TW} \\
J_{WT} & J_{WW}
\end{bmatrix}
\begin{bmatrix}
\Delta T \\
\Delta W
\end{bmatrix}
= -
\begin{bmatrix}
F_T \\ F_W
\end{bmatrix}
\]

Block Factorization Preconditioners:

\[
\begin{bmatrix}
I & 0 \\
\hat{B}H_1 & I
\end{bmatrix}
\begin{bmatrix}
F \\
0
\end{bmatrix}
\begin{bmatrix}
I & H_2B^T
\end{bmatrix}
= -
\begin{bmatrix}
\hat{S} \\
0
\end{bmatrix}
\begin{bmatrix}
I \\
0
\end{bmatrix}
\]

\[
S = c + \hat{B}F^{-1}B^T
\]
Fundamental Thyra ANA Operator/Vector Interfaces

A Few Quick Facts about Thyra Interfaces
- All interfaces are expressed as abstract C++ base classes (i.e. object-oriented)
- All interfaces are templated on a Scalar data type (i.e. generic)

The Key to success!
Reduction/Transformation Operators
- Supports all needed element-wise vector operations
- Data/parallel independence
- Optimal performance

Matrix/Vector operations are handled in app’s native data structures!

Application Interface: Model Evaluator

Nonlinear ANA

Thyra::ModelEvaluator

```
createInArgs() : InArgs
createOutArgs() : OutArgs
create_W() : LinearOpWithSolveBase
create_W_op() LinearOpBase
...
evalModel( in InArgs, out OutArgs )
```

- Set your inputs in an **InArgs** container: \( \dot{x}, x, p, t \)
- Set your outputs in an **OutArgs** container: \( f, W, M, g, \frac{\partial f}{\partial p}, \frac{\partial g}{\partial x}, \frac{\partial g}{\partial p} \)
- `model_evaluator->evalModel(in_args, out_args)`

- Common interface for ANAs: Nonlinear, Optimization, Bifurcation, …
- Inputs and outputs are extensible without requiring changes to apps
- Efficient shared calculations (e.g. automatic differentiation)
- Self describing: query what inputs and outputs it supports
Application Classification

Inputs and outputs are **optionally** supported by physics model → restricts allowed solution procedures

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Required Inputs</th>
<th>Required Outputs</th>
<th>Optional Outputs</th>
<th>Time Integration Control</th>
</tr>
</thead>
<tbody>
<tr>
<td>Response Only Model</td>
<td>$p \rightarrow g(p)$</td>
<td>$p$</td>
<td>$g$</td>
<td></td>
<td>Internal</td>
</tr>
<tr>
<td>(Coupling Elimination)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>State Elimination Model</td>
<td>$p \rightarrow x(p)$</td>
<td>$p$</td>
<td>$x, g$</td>
<td></td>
<td>Internal</td>
</tr>
<tr>
<td>Fully Implicit Time Step Model</td>
<td>$f(x, p) = 0$</td>
<td>$x, p$</td>
<td>$f$</td>
<td>$W, M, g$</td>
<td>Internal</td>
</tr>
<tr>
<td>Transient Explicitly Defined ODE Model</td>
<td>$\dot{x} = f(x, p, t)$</td>
<td>$x, p, t$</td>
<td>$f$</td>
<td>$W, M, g$</td>
<td>External</td>
</tr>
<tr>
<td>Transient Fully Implicit DAE Model</td>
<td>$f(\dot{x}, x, p, t) = 0$</td>
<td>$\dot{x}, x, p, t$</td>
<td>$f$</td>
<td>$W, M, g$</td>
<td>External or Internal</td>
</tr>
</tbody>
</table>

\[
W = \alpha \frac{\partial f}{\partial \dot{x}} + \beta \frac{\partial f}{\partial x} \quad M = \text{preconditioner}
\]
An Assortment of Coupling Algorithms

- **Picard-based (Black-Box)**
  - Block Nonlinear Jacobi
  - Block Nonlinear Gauss-Seidel
  - Anderson Acceleration
- **Newton Based (Block Implicit)**
  - Jacobian-free Newton-Krylov
  - Newton-Krylov (Explicit Jacobian)
  - Nonlinear Elimination (Schur complement formulation)

Example: Two Component system

\[
\begin{align*}
    f_0(x_0, z_{0,0}) &= 0 \\
    f_1(x_1, z_{1,0}) &= 0 \\
    z_{0,0} &= r_{0,0}(x_1) \\
    z_{1,0} &= r_{1,0}(x_0)
\end{align*}
\]

**Picard Iteration: Nonlinear Block Gauss-Seidel**

Require: Initial guesses \(x_0^{(0)}\) and \(x_1^{(0)}\) for \(x_0\) and \(x_1\):

\[
k = 0
\]

while not converged do

\[
k = k+1
\]

Solve \(f_0(x_0^{(k)}, r_{0,0}(x_1^{(k-1)})) = 0\) for \(x_0^{(k)}\)

Solve \(f_1(x_1^{(k)}, r_{1,0}(x_0^{(k)})) = 0\) for \(x_1^{(k)}\)

end while

\[
\begin{bmatrix}
    \frac{\partial f_0}{\partial x_0} & \frac{\partial f_0}{\partial r_{0,0}} & \frac{\partial f_0}{\partial z_{0,0}} & \frac{\partial f_0}{\partial x_1} \\
    \frac{\partial f_1}{\partial z_{1,0}} & \frac{\partial r_{1,0}}{\partial x_0} & \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_0}
\end{bmatrix}
\begin{bmatrix}
    \Delta x_0^{(k)} \\
    \Delta x_1^{(k)}
\end{bmatrix}
= -
\begin{bmatrix}
    f_0(x_0^{(k-1)}, r_{0,0}(x_1^{(k-1)})) \\
    f_1(x_1^{(k-1)}, r_{1,0}(x_0^{(k-1)}))
\end{bmatrix}
\]

- Off-block diagonals may be hard to compute
- Can avoid computing Jacobian by using JFNK,
- BUT you still need to precondition \((M \approx W^{-1})\)
Implicit Solvers
NOX and LOCA: Nonlinear Solution and Homotopy

- Efficient: Quadratic convergence rates, no CFL limit
- Robust: globalization techniques

**Model**
- Tensor Method
  \[ MT = F(x_c) + J_c d + 1/2T_c dd \]
- Newton’s Method
  \[ M_N = F(x_c) + J_c d \]
- Broyden’s Method
  \[ M_N = F(x_c) + B_c d \]

**Globalizations**
- Line Search
- Backtracking
- Quadratic
- Cubic
- More’-Thuente
- Trust Region
- Dogleg
- Inexact Dogleg

**Homotopy (LOCA)**
- Artificial Parameter Continuation
- Natural Parameter Continuation

**Difficulties (Missing or Inaccurate J/M)**
- Jacobian-Free Newton-Krylov (JFNK)
- Finite Difference
- Colored Finite Difference
- Broyden (rank-1 updates)
Simple Nonlinear Solve

Main()

NOX::Solver

Application
Thyra::ModelEvaluator

Physics Application: Drekar

Globalized Newton-Krylov

\[ x^k = x^{k-1} - \alpha J^{-1} f \]

\[ f_{Drekar} \]
Block Composite Model

• The entire coupled system can be cast as a monolithic system:

\[
\hat{f}(\hat{x}, \hat{x}, \hat{p}, t) = 0
\]

\[
\hat{x} = \begin{bmatrix} \dot{x}_0, \ldots, \dot{x}_i, \ldots, \dot{x}_{N_f-1} \end{bmatrix},
\]

\[
\hat{x} = \begin{bmatrix} x_0, \ldots, x_i, \ldots, x_{N_f-1} \end{bmatrix},
\]

\[
\hat{p} = \begin{bmatrix} p_{0,0}, \ldots, p_{0,N_{p0}-1}, \ldots, p_{i,0}, \ldots, p_{i,N_{pi}-1}, \ldots, p_{N_f-1,0}, \ldots, p_{N_f-1,N_{pN_f-1}} \end{bmatrix},
\]

\[
\hat{f} = \begin{bmatrix}
\begin{bmatrix}
\end{bmatrix}^{f_0}(\hat{x}_0, x_0, \{r_{0,k}(\{x_m\}, \{p_{m,n}\})\}, \{p_{0,l}\}, t)) \\
\vdots \\
\begin{bmatrix}
\end{bmatrix}^{f_i}(\hat{x}_i, x_i, \{r_{i,k}(\{x_m\}, \{p_{m,n}\})\}, \{p_{i,l}\}, t)) \\
\vdots \\
\begin{bmatrix}
\end{bmatrix}^{f_{N_f-1}}(\hat{x}_{N_f-1}, x_{N_f-1}, \{r_{N_f-1,k}(\{x_m\}, \{p_{m,n}\})\}, \{p_{N_f-1,l}\}, t))
\end{bmatrix}.
\]
The Power of Decorators

- Use inheritance and composition to wrap analysis tools as model evaluators to build a hierarchical chain.

- Example ANA decorator subclasses
  - BlockCompositeModelEvaluator: Aggregate physics into blocked objects
  - FiniteDifferenceModelEvaluator: Global finite differences w.r.t. inputs
  - JacobianFreeNewtonKrylovModelEvaluator: Wraps a “residual-only” model evaluator to provide a Jacobian operator
  - StateEliminationModelEvaluator: Eliminates steady state equations/variables using a NonlinearSolverBase object
  - DiagonalScalingModelEvaluator: Apply a user defined diagonal scaling operator for outArgs
  - DefaultEvaluationLoggerModelEvaluator: Log evaluations vs. time and print out summary table
Uses **Decorator** to better condition a poorly scaled system of equations

\[ f(x + \delta v) - f(x) \approx J v = \frac{f(x + \delta v) - f(x)}{\delta} \]

\[ f = \begin{bmatrix} f_{Drekar} \\ f_{Exnihilo} \end{bmatrix} \]

\[ f_{Exnihilo} \leftarrow \text{Application} \rightarrow f_{Drekar} \]

\[ \text{Physics set: Exnihilo} \]

\[ \text{Physics set: Drekar} \]

\[ x^k = x^{k-1} - \alpha J^{-1} f \]

Globalized Newton-Krylov

\[ f \rightarrow D_f f \]

\[ J \rightarrow D_f J \]

Applies Scaling Matrix, \( D \), to Evaluated Quantities

\[ \text{Main()} \rightarrow \text{NOX::Solver} \rightarrow \text{NOX::JFNK Model Evaluator} \rightarrow \text{Thyra::Scaled Model Evaluator} \rightarrow \text{Thyra::Block Composite ME} \rightarrow \text{NOX::JFNK Model Evaluator} \rightarrow \text{NOX::Solver} \rightarrow \text{Main()} \]
Linear Solvers and Preconditioners
Nonlinear Algorithms and Applications: Thyra & Model Evaluator!

Nonlinear ANA Solvers in Trilinos

Key Points

- Provide single interface from nonlinear ANAs to applications
- Provide single interface for applications to implement to access nonlinear ANAs
- Provides shared, uniform access to linear solver capabilities
- Once an application implements support for one ANA, support for other ANAs can quickly follow

Stratimikos!

Sandia Applications

Xyce | Charon | Tramonto | Aria | Panzer

Trilinos and non-Trilinos Preconditioner and Linear Solver Capability
All Linear Solvers in Trilinos can be selected at run time from an XML File

```
<ParameterList name="Stratimikos">
  <ParameterList name="AztecOO">
    <Parameter name="Aztec Preconditioner" type="string" value="ilu"/>
    <Parameter name="Aztec Solver" type="string" value="GMRES"/>
    <Parameter name="Maximum Iterations" type="int" value="100"/>
    ...
  </ParameterList>
  <ParameterList name="Belos">
    <ParameterList name="Solver Types">
      <ParameterList name="Block GMRES">
        <Parameter name="Convergence Tolerance" type="double" value="1e-5"/>
        <Parameter name="Maximum Iterations" type="int" value="100"/>
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        <Parameter name="Orthogonalization" type="string" value="DGKS"/>
      </ParameterList>
      <ParameterList name="Block CG">
        ...
      </ParameterList>
    </ParameterList>
    ...
  </ParameterList>
  <ParameterList name="Preconditioner Types">
    <ParameterList name="Ifpack">
      <Parameter name="Prec Type" type="string" value="ILU"/>
      <Parameter name="Overlap" type="int" value="0"/>
      <Parameter name="Fill Factor" type="int" value="1"/>
      ...
    </ParameterList>
    <ParameterList name="ML">
      <Parameter name="nodes per aggregate" type="int" value="27"/>
      <Parameter name="coarse: max size" type="int" value="512"/>
      ...
    </ParameterList>
  </ParameterList>
</ParameterList>
```
Three Types of Preconditioning

1. Domain Decomposition (Trilinos/IFPack)
   - 1-level Additive Schwarz DD
   - ILU(k) Factorization on each processor (variable levels of overlap)
   - High parallel efficiency, non-optimal algorithmic scalability

2. Multilevel Methods for Systems: (Trilinos/ML/MueLu)
   - Fully-coupled Algebraic Multilevel methods
   - Consistent set of DOF at each node (e.g. stabilized FE)
   - Uses block non-zero structure of Jacobian
   - Aggregation techniques and coarsening rates can be set
     - Smoothed aggregation (SA)
     - Aggressive Coarsening (AggC)
   - Jacobi, GS, ILU(k) as smoothers
   - Can provide optimal algorithmic scalability

3. Approximate Block Factorization / Physics-based (Trilinos/Teko)
   - Applies to mixed interpolation (FE), staggered (FV), using segregated unknown blocking
   - Applied to systems where coupled AMG is difficult or might fail
   - Can provide optimal algorithmic scalability
TFQMR: used to look at time/iteration of multilevel preconditioners.

W-cyc time/iteration not doing well due to significant increase in work on coarse levels (not shown)

Good scaled efficiency for large-scale problems on larger core counts for 31K Unknowns / core
Scalability
(MHD Pump, Cray XT3)

Preconditioners
- 1-level \( ILU(2,1) \)
- 1-level \( ILU(2,3) \)
- 1-level \( ILU(2,7) \)
- 3-level ML(\text{NSA,Gal})
- 3-level ML(\text{EMIN, PG})

ML: Tuminaro, Hu
Ifpack: Heroux
Block preconditioning: CFD example

Consider discretized Navier-Stokes equations

\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \nabla^2 \mathbf{u} + \nabla p = f \\
\nabla \cdot \mathbf{u} = 0
\]

\[
\iff \begin{bmatrix} F & B^T \\ B & C \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}
\]

Properties of block factorization
1. Important coupling in Schur-complement
2. Better targets for AMG → leveraging scalability

Properties of approximate Schur-complement
1. “Nearly” replicates physical coupling
2. Invertible operators → good for AMG

Fully Coupled Jacobian
\[ \mathbf{A} = \begin{bmatrix} F & B^T \\ B & C \end{bmatrix} \]

Block Factorization
\[ \mathbf{A} = \begin{bmatrix} I & F \\ BF^{-1} & I \\ B & C - BF^{-1}B^T \end{bmatrix} \begin{bmatrix} F & B^T \\ S \end{bmatrix} \]

- Coupling in Schur-complement

Preconditioner
\[ \mathbf{A}^{-1} \approx \mathbf{M}^{-1} = \begin{bmatrix} \hat{F} & B^T \\ \hat{S} \end{bmatrix}^{-1} \]

Required operators:
- \( F^{-1} \approx \hat{F}^{-1} \rightarrow \text{Multigrid} \)
- \( S^{-1} \approx \hat{S}^{-1} \rightarrow \text{PCD, LSC, SIMPLEC} \)
Brief Overview of Block Preconditioning Methods for Navier-Stokes:
(A Taxonomy based on Approximate Block Factorizations, JCP – 2008)

<table>
<thead>
<tr>
<th>Discrete N-S</th>
<th>Exact LDU Factorization</th>
<th>Approx. LDU</th>
</tr>
</thead>
<tbody>
<tr>
<td>((F \ B^T \ -C) (\Delta u_k = (g_{u_k}^k \ g_{p_k}^k)))</td>
<td>((I \ 0 \ (F \ 0 \ (I \ F^{-1}B^T)) \ (I \ F^{-1}B^T)))</td>
<td>([I \ 0] [F \ 0] [I \ H_2B^T] )</td>
</tr>
<tr>
<td>(S = C + \hat{B}F^{-1}B^T)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Precond. Type</th>
<th>(H_1)</th>
<th>(H_2)</th>
<th>(\hat{S})</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pres. Proj; 1(^{st})Term Nuemann Series</td>
<td>(F^{-1})</td>
<td>((\Delta tI)^{-1})</td>
<td>(C + \Delta t\hat{BB}^T)</td>
<td>Chorin(1967); Temam (1969); Perot (1993): Quateroni et. al. (2000) as solvers</td>
</tr>
<tr>
<td>SIMPLEC</td>
<td>(F^{-1})</td>
<td>((\text{diag}(\sum</td>
<td>F</td>
<td>))^{-1})</td>
</tr>
<tr>
<td>Pressure Convection / Diffusion</td>
<td>(0)</td>
<td>(F^{-1})</td>
<td>(A_pF_p^{-1})</td>
<td>Kay, Loghin, Wathan, Silvester, Elman (1999 - 2006); Elman, Howle, S., Shuttleworth, Tuminaro (2003,2008)</td>
</tr>
</tbody>
</table>

Now use AMG type methods on sub-problems.

Momentum transient convection-diffusion:
\[ F\Delta u = \mathbf{r_u} \]

Pressure – Poisson type:
\[ -\hat{S}\Delta p = \mathbf{r_p} \]
Transient Kelvin-Helmholtz

Kelvin Helmholtz: Re=5000, Weak scaling at CFL=2.5
- Run on 1 to 256 cores
- Pressure - PSPG, Velocity - SUPG (residual and Jacobian)

1. SIMPLEC strongly dependent on CFL
2. Block methods scale as well as AggC and do not require non-zero C matrix
Incompressible MHD
2D Vector Potential Formulation

Magnetohydrodynamics (MHD) equations couple fluid flow to Maxwell’s equations

\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \nabla^2 \mathbf{u} + \nabla p + \nabla \cdot \left( -\frac{1}{\mu_0} \mathbf{B} \otimes \mathbf{B} + \frac{1}{2\mu_0} \|\mathbf{B}\|^2 \mathbf{I} \right) = \mathbf{f}
\]

\[\nabla \cdot \mathbf{u} = 0\]

\[
\frac{\partial A_z}{\partial t} + \mathbf{u} \cdot \nabla A_z - \frac{\eta}{\mu_0} \nabla^2 A_z = -E_z^0
\]

where \( \mathbf{B} = \nabla \times \mathbf{A}, \mathbf{A} = (0, 0, A_z) \)

Discretized using a stabilized finite element formulation

Structure of discretized Incompressible MHD system is

\[
\mathbf{J} \mathbf{x} = \begin{bmatrix} F & B^T & Z \\ B & C & 0 \\ Y & 0 & D \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{p} \\ \mathbf{A} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ 0 \\ \mathbf{e} \end{bmatrix}
\]

Matrices \( F \) and \( D \) are transient convection operators, \( C \) is stabilization matrix
Teko Block Preconditioners

Nested Schur Complements:

\[
\mathcal{J} = \begin{bmatrix}
F & B^T & Z \\
B & C & 0 \\
Y & 0 & D
\end{bmatrix} = \begin{bmatrix}
I \\
BF^{-1} \\
YF^{-1}
\end{bmatrix} \begin{bmatrix}
I \\
I \\
-YF^{-1}B^TS^{-1}
\end{bmatrix} \begin{bmatrix}
F & B^T & Z \\
S & -BF^{-1}Z \\
P
\end{bmatrix}
\]

\[
S = C - BF^{-1}B^T \\
P = D - YF^{-1}(I + B^TS^{-1}BF^{-1})Z
\]

\[
\mathcal{M} = \begin{bmatrix}
F & B^T & Z \\
S_{Neu} & -BF^{-1}Z \\

\end{bmatrix}
\]

Physics Based: Operator Splitting:

\[
\hat{x} = SplitPrec-NS(\mathcal{J}, b):
\]

\[
x^* = \begin{bmatrix}
F & Z \\
I \\
Y & D
\end{bmatrix}^{-1} b,
\]

\[
r^* = b - \mathcal{J}x^*,
\]

\[
e = \begin{bmatrix}
F & B^T \\
B & C \\
I
\end{bmatrix}^{-1} r^*,
\]

\[
\hat{x} = x^* + e
\]

- Eliminates nested Schur Complements
- Requires two 2x2 solves
- Navier-Stokes operator well studied
- Magnetics-Velocity operator is difficult
Physics-based/ABF Preconditioning

\[ \frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u \otimes u + p \mathbb{I} + \Pi) - \frac{1}{\mu_0} \nabla \times B \times B = 0 \]

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

\[ \frac{\partial B}{\partial t} - \nabla \times (u \times B) + \nabla \times \left( \frac{\eta}{\mu_0} \nabla \times B \right) = 0 \]

\[
\begin{bmatrix}
F & B^T & Z \\
B & C & 0 \\
Y & 0 & D
\end{bmatrix}
\begin{bmatrix}
Z \\
0 \\
D
\end{bmatrix}
\begin{bmatrix}
u \\
p \\
b
\end{bmatrix}
= 
\begin{bmatrix}
f \\
g \\
h
\end{bmatrix}
\]

JFNK + Block Scattering for Preconditioning

\[ S_M^J \quad S_L^J \quad f_k^i \]

\[ \widetilde{R}_{uk} \]

\[ \nabla \phi^i_u \]

\[ \phi^i_u \]

\[ u^i \]

\[ \nabla u \]

\[ |j| \]

\[ q \]

\[ s \]

\[ w_q \]
Hydromagnetic Kelvin-Helmholtz

- Velocity shear flow
- Magnetic field in x-direction
- Reynolds number = $10^3$
- Lundquist number = $10^4$
MHD Weak Scaling: Hydromagnetic Kelvin-Helmholtz
(Fixed time step)

Take home: Split preconditioner scales algorithmically, more relevant for mixed discretizations, multiphysics
Hydromagnetic Rayleigh-Bernard

\[ v_x = 0 \quad v_y = 0 \quad T = -0.5 \quad \frac{\partial A}{\partial y} = 0 \]

\[ v_x = 0 \quad A = C\sqrt{Q} \]

Parameters:
- \( Q \sim B_0^2 \) (Chandresekhar number)
- \( \text{Ra} \) (Rayleigh number)

No flow \[ \rightarrow \] Recirculations

\[ Q = \frac{B_0^2 d^2}{\mu_0 \rho \nu \eta} \]
\[ \text{Ra} = \frac{g \beta \Delta T d^3}{\nu \alpha} \]
\[ Pr = \frac{\nu}{\alpha} \quad Pr_m = \frac{\nu}{\eta} \]

- Buoyancy driven instability initiates flow at high Ra numbers.
- Increased values of Q delay the onset of flow.
- Domain: 1x20
Hydro-Magnetic Rayleigh-Bernard Stability: Direct Determination of Nonlinear Equilibrium Solutions (Steady State Solves, Ra=2500, Q=4)

Temp

Vx

Vy

Jz

Bx

By

Nonlinear Solver Convergence; Ra = 2500

Linear Solver Convergence; Ra = 2500, Q = 4
Hydro-Magnetic Rayleigh-Bernard Stability: Direct Determination of Linear Stability and Nonlinear Equilibrium Solutions (Steady State Solves)

Leading Eigenvector at Bifurcation Point,
Ra = 1945.78, Q=10

- 2 Direct-to-steady-state solves at a given Q
- Arnoldi method using Cayley transform to determine approximation to 2 eigenvalues with largest real part
- Simple linear interpolation to estimate Critical Ra*

<table>
<thead>
<tr>
<th>Q</th>
<th>Ra*</th>
<th>Racr [Chandrasekhar[]]</th>
<th>% error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1707.77</td>
<td>1707.8</td>
<td>0.002</td>
</tr>
<tr>
<td>10^1</td>
<td>1945.78</td>
<td>1945.9</td>
<td>0.006</td>
</tr>
<tr>
<td>10^2</td>
<td>3756.68</td>
<td>3757.4</td>
<td>0.02</td>
</tr>
</tbody>
</table>
Arc-length Continuation: Identification of Pitchfork Bifurcation, $Q=10$

Nonlinear system:

\[ f(x(s), p(s)) = 0 \]
\[ g(x(s), p(s), s) = 0 \]

Newton System:

\[
\begin{bmatrix}
J & f_p \\
\partial x & \partial p
\end{bmatrix}
\begin{bmatrix}
\Delta x \\
\Delta p
\end{bmatrix}
= -
\begin{bmatrix}
f \\
g
\end{bmatrix}
\]

Bordered Solver:

\[ Ja = -f \quad \Delta p = -(g + \frac{\partial x}{\partial s} \cdot a)/(\frac{\partial p}{\partial s} + \frac{\partial x}{\partial s} \cdot b) \]
\[ Jb = -f_p \quad \Delta x = a + \Delta pb \]
• “No flow” does not equal “no-structure” – pressure and magnetic fields must adjust/balance to maintain equilibrium.
• LOCA can perform multi-parameter continuation
Bifurcation Tracking
(Govaerts 2000)

Moore-Spence

- Turning point formulation:
  \[
  f(x, p) = 0 \\
  Jn = 0 \\
  \phi \cdot n - 1 = 0
  \]

- Newton’s method (2N+1):
  \[
  \begin{bmatrix}
  J & 0 & f_p \\
  (Jn)_x & J & Jpn \\
  0 & \phi^T & 0
  \end{bmatrix}
  \begin{bmatrix}
  \Delta x \\
  \Delta n \\
  \Delta p
  \end{bmatrix}
  =
  \begin{bmatrix}
  -f \\
  -Jn \\
  1 - \phi^T \cdot n
  \end{bmatrix}
  \]

- 4 linear solves per Newton iteration:
  \[
  Ja = -f \\
  Jb = -fp \\
  Jc = -(Jn)_xa - Jn \\
  Jd = -(Jn)_xb - Jpn
  \]

- \[\Delta p = (1 - \phi \cdot n - \phi \cdot c) / (\phi \cdot d)\]

- \[\Delta n = c + \Delta pd\]

- \[\Delta x = a + \Delta pb\]

Minimally Augmented

- Widely used algorithm for small systems:
  \[
  \begin{bmatrix}
  J & a \\
  b^T & 0
  \end{bmatrix}
  \begin{bmatrix}
  v \\
  s
  \end{bmatrix}
  =
  \begin{bmatrix}
  0 \\
  1
  \end{bmatrix},
  \begin{bmatrix}
  J^T & b \\
  a^T & 0
  \end{bmatrix}
  \begin{bmatrix}
  u \\
  t
  \end{bmatrix}
  =
  \begin{bmatrix}
  0 \\
  1
  \end{bmatrix}
  
  \implies s = t = -u^T Jv
  \]

- J is singular if and only if s = 0

- Turning point formulation (N+1):
  \[
  f(x, p) = 0 \\
  s(x, p) = 0
  \]

- Newton’s method:
  \[
  \begin{bmatrix}
  J & f_p \\
  s_x & s_p
  \end{bmatrix}
  \begin{bmatrix}
  \Delta x \\
  \Delta p
  \end{bmatrix}
  =
  \begin{bmatrix}
  f \\
  s
  \end{bmatrix},
  s_x = -(u^T Jv)_x = -(u^T J)_x v.
  \]

- 3 linear solves per Newton iteration

Extension to large-scale iterative solvers
Leading Mode is different for various Q values

- Analytic solution is on an infinite domain with two bounding surfaces (top and bottom).
- Multiple modes exist, mostly differentiated by number of cells/wavelength.
- Therefore tracking the same eigenmode does not give the stability curve!!!
- Periodic BCs will not fix this issue.

Mode: 20 Cells: Q=100, Ra=4017
Mode: 26 Cells: Q=100, Ra=3757
SEACISM: Parallel Glimmer-CISM2

Evans, Worley, Nichols, Norman (ORNL)  
Price, Lipscomb, Hoffman (LANL)  
Salinger, Kalashnikova, Tuminaro (SNL)  
Lemieux (NYU), Sachs (NCAR)

Glimmer Code ~2009:  
• First-Order Approx to Stokes: 3D for [U,V]  
• Structured Grid  
• Finite Difference  
• Serial  
• Picard Solver  
• Autoconf

Glimmer Code ~2013:  
• Parallel Assembly  
• Parallel Solve  
• Newton Solver  
• Cmake  
• Built in CESM development branch
Convergence is not adequately robust reliable for Greenland problems

Why the poor robustness?
• Real, noisy data
• Nonlinear viscosity model
• Structured grid Finite Diff
• Finite Diff for Stress BCs
• Jacobian-Free perturbations
• Picard matrices
New FELIX Codes address many of these issues (PISCEES SciDAC-BER)

FELIX Codes\textsuperscript{1,2}:

- Real, noisy data
- Nonlinear viscosity model
  - Included in Jacobian
- Unstructured Grid
- Finite Element Stress BCs
- Newton, Analytic Jacobian
- Rigorous Verification
- Hooks to UQ Algorithms
- Numerous Trilinos Libraries
  - Discretization
  - Load Balancing

1. Perego, Gunzberger, Ju (LifeV, Trilinos, MPAS)
2. Salinger, Kalashnikova, Perego, Tuminaro (Albany, Trilinos, MPAS)
Full Newton with Analytic Jacobian fixes some causes of robustness issues

Perego, FSU
Conclusions

• Trilinos contains a diverse set of algorithms
  – Abstract Interfaces
  – Linear Algebra
  – Linear solvers
  – Preconditioners
  – Nonlinear solvers and Analysis
  – Discretization libraries

• The toolkit approach is critical
  – Flexibility is key
  – Each physics is unique and requires its own strategy

• Coupled codes must leverage large body of knowledge from stand-alone applications
  – Directly use app solver: Picard it
  – Use app solver in a physics-based preconditioner