SAND2013-1798C

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

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European Trilinos User Group Meeting 2015
Tuesday March 3, 2015

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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** → **Explicit Methods**
  - 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.

  (Last three items) → **Typically requires some form of Implicit Methods**

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

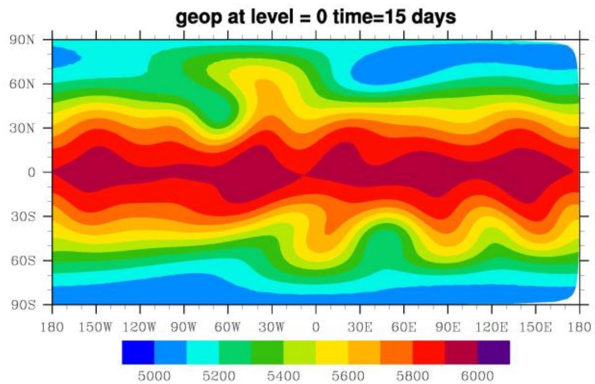
- Our approach:
  - Stable and higher-order accurate implicit formulations and discretizations
  - Robust, scalable and efficient prec. for fully-coupled Newton-Krylov methods
  - Integrate sensitivity and error-estimation to enable UQ capabilities.

Tools for Multiphysics Simulation
(Spanning Individual Applications and Coupled Systems)

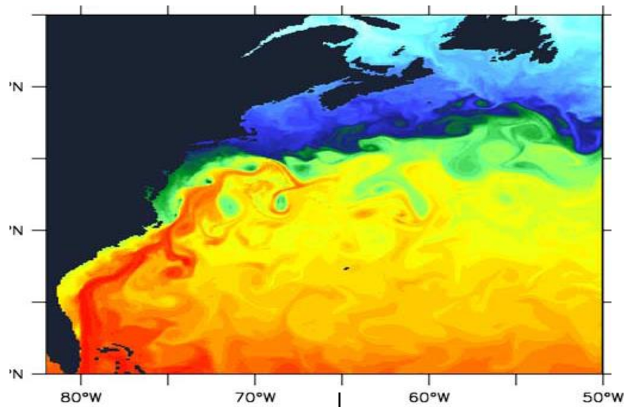
- **Domain Model (SAND2011-2195)**
- **Abstraction Layer ANAs**
  - Thyra::ModelEvaluator: Application Interface
  - Thyra: Operator, Vector
- **Implicit Nonlinear Solution Algorithms**
  - **NOX**: Globalized Newton-Krylov and JFNK
  - **LIME/PIKE**: Multiphysics coupling driver. Picard iteration and 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

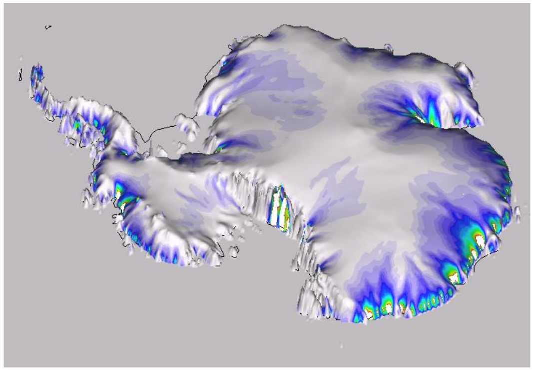
HOMME Atmospheric Model



POP Ocean Model
THCM Ocean Model



Glimmer Ice Sheet Model
FELIX Ice Sheet Model



+ IBECS, Sea Ice

Trilinos

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

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

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A Domain Model

<u>A Theory Manual for Multiphysics Code Coupling in LIME</u>, R. Pawlowski, R. Bartlett, R. Schmidt, R. Hooper, and N. Belcourt, SAND2011-2195

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

Residual — f

$$\dot{x} = \frac{\partial x}{\partial t}$$

State (DOF) — x

Set of parameters — $\{p_l\}$

Time — t

$x \in \mathbb{R}^{n_x}$ is the vector of state variables (unknowns being solved for),
$\dot{x} = \partial x / \partial t \in \mathbb{R}^{n_x}$ is the vector of derivatives of the state variables with respect to time,
$\{p_l\} = \{p_0, p_1, \ldots, p_{N_p-1}\}$ is the set of N_p independent parameter sub-vectors,
$t \in [t_0, t_f] \in \mathbb{R}^1$ is the time ranging from initial time t_0 to final time t_f,

$$f(\dot{x}, x, \{p_l\}, t) : \mathbb{R}^{\left(2n_x + \left(\sum_{l=0}^{N_p-1} n_{p_l}\right) + 1\right)} \rightarrow \mathbb{R}^{n_x}$$

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

Response Function — g_j

$g_j(\dot{x}, x, \{p_l\}, t) : \mathbb{R}^{\left(2n_x + \left(\sum_{l=0}^{N_p-1} n_{p_l}\right) + 1\right)} \rightarrow \mathbb{R}^{n_{g_j}}$ is the j^{th} response function.

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

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Extension to Multiphysics

Split parameters into “coupling” and truly independent.

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

Set of *coupling* parameters

Set of *independent* parameters

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

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

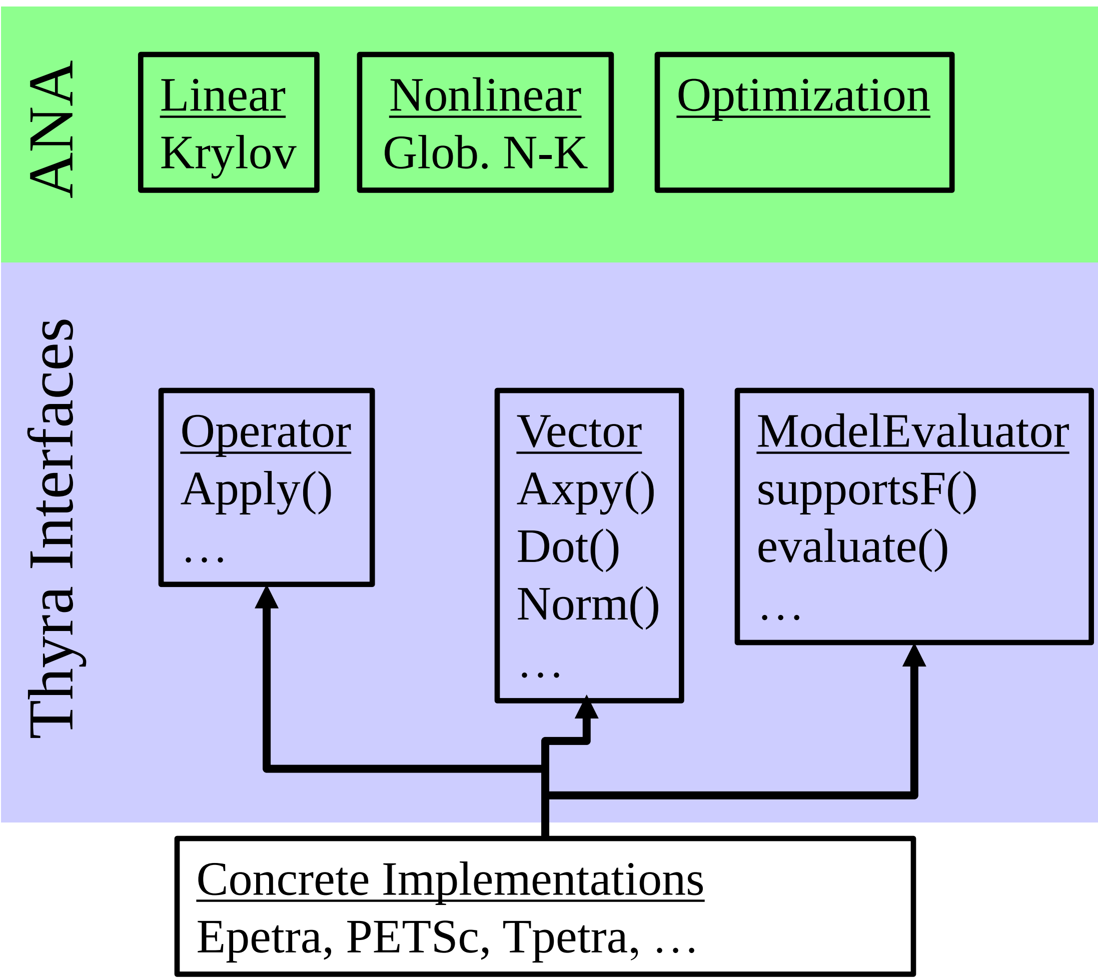
Response Function

Abstract Interfaces

Introducing Abstract Numerical Algorithms

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***



Block composition operators and vectors:

$$\begin{bmatrix} \mathbf{J}_{TT} & \mathbf{J}_{T\mathbf{W}} \\ \mathbf{J}_{\mathbf{W}T} & \mathbf{J}_{\mathbf{WW}} \end{bmatrix} \begin{bmatrix} \Delta T \\ \Delta \mathbf{W} \end{bmatrix} = - \begin{bmatrix} \mathbf{F}_T \\ \mathbf{F}_{\mathbf{W}} \end{bmatrix}$$

Block Factorization Preconditioners:

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

$$S = c + \hat{B}F^{-1}B^T$$

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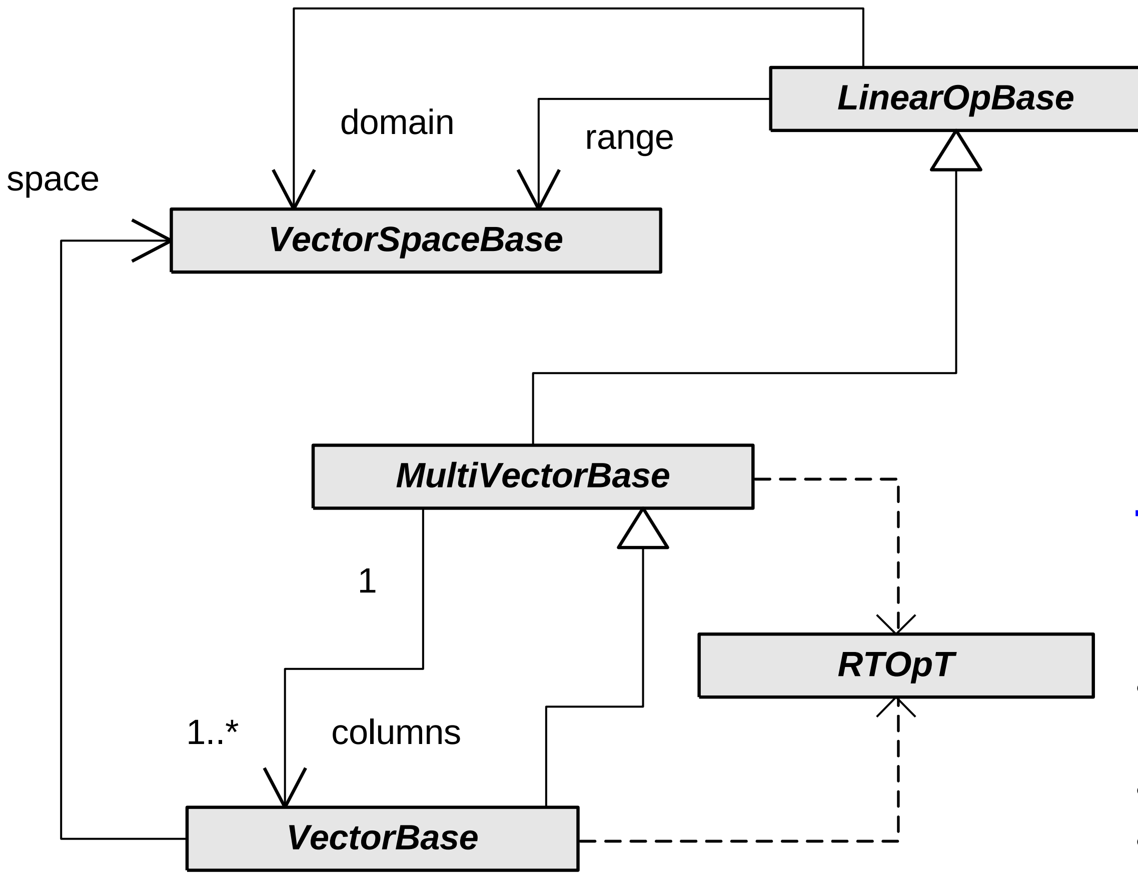
Fundamental Thyra ANA Operator/Vector Interfaces



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!

R. A. Bartlett, B. G. van Bloemen Waanders and M. A. Heroux. *Vector Reduction/Transformation Operators*, ACM TOMS, March 2004

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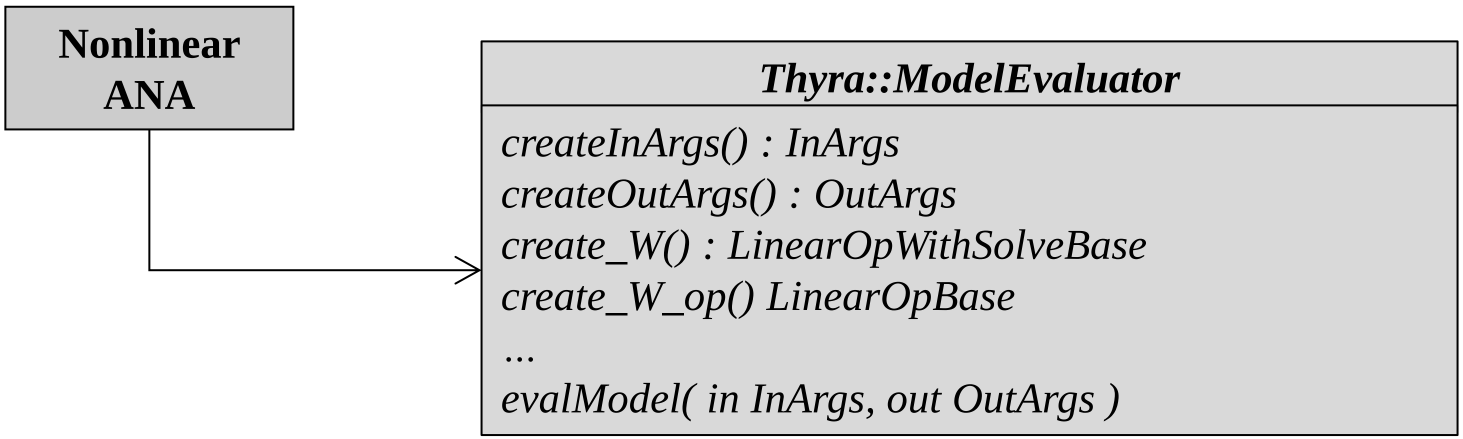
Application Interface: Model Evaluator



- **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

Name	Definition	Required Inputs	Required Outputs	Optional Outputs	Time Integration Control
Response Only Model **(Coupling Elimination)**	$p \to g(p)$	p	g		**Internal**
State Elimination Model	$p \to x(p)$	p	x	g	**Internal**
Fully Implicit Time Step Model	$f(x,p) = 0$	x, p	f	$W,\ M,\ g$	**Internal**
Transient Explicitly Defined ODE Model	$\dot{x} = f(x,p,t)$	x, p, t	f	$W,\ M,\ g$	**External**
Transient Fully Implicit DAE Model	$f(\dot{x},x,p,t) = 0$	$\dot{x}, x, p, t$	f	$W,\ M,\ g$	**External or Internal**

$$W = \alpha \frac{\partial f}{\partial \dot{x}} + \beta \frac{\partial f}{\partial x} \qquad M = \text{preconditioner}$$

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

$$f_0(x_0, z_{0,0}) = 0$$
$$f_1(x_1, z_{1,0}) = 0$$
$$z_{0,0} = r_{0,0}(x_1)$$
$$z_{1,0} = r_{1,0}(x_0)$$

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

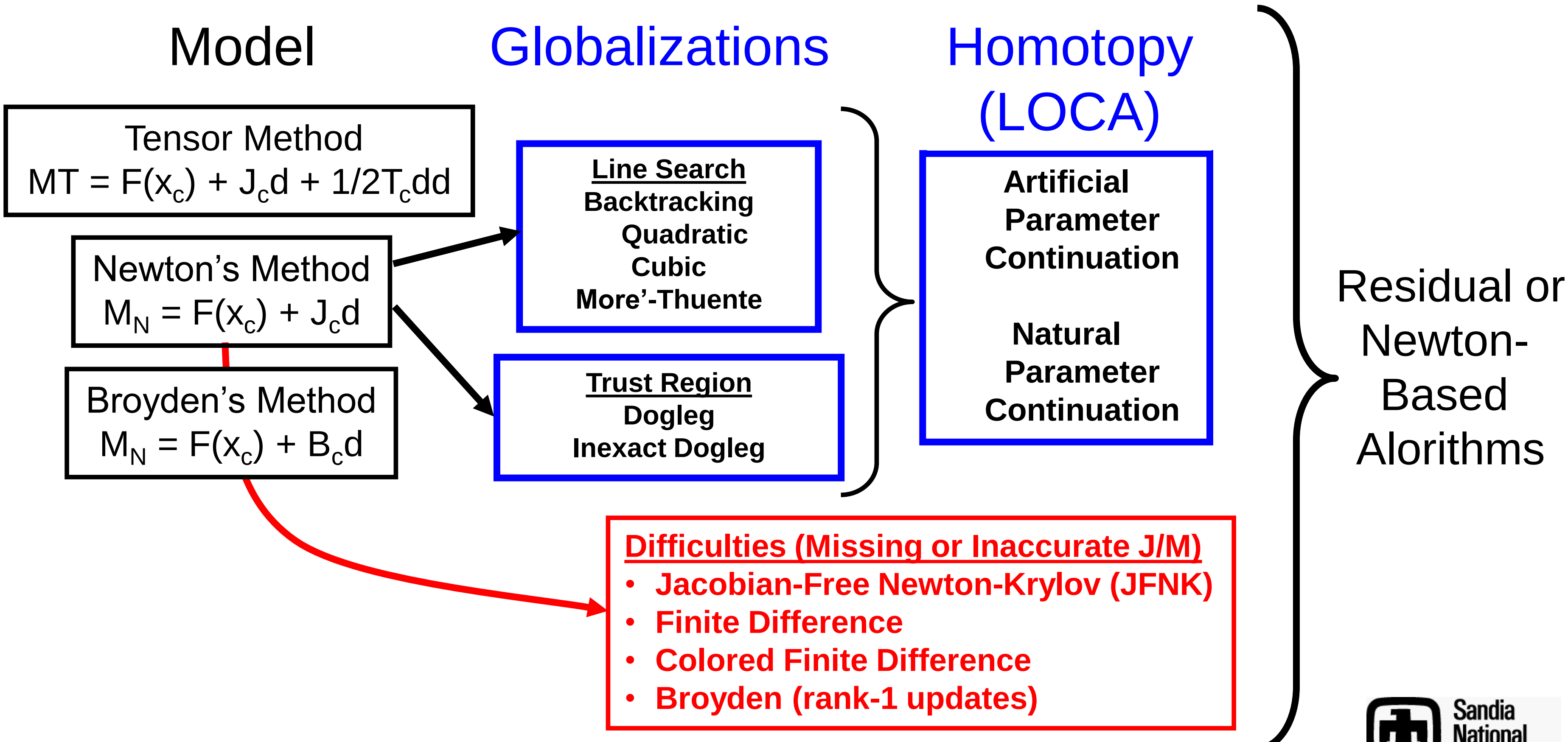
Newton-based

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

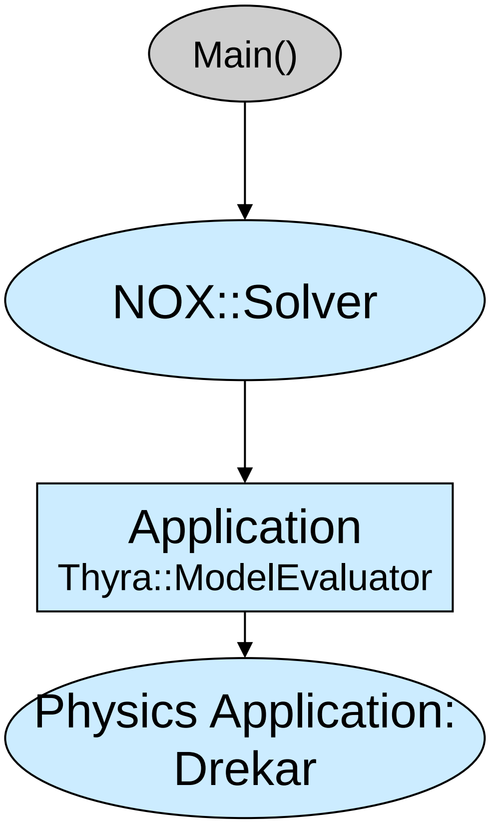
- Off-block diagonals may be hard to compute
- Can avoid computing Jacobian by using JFNK,
- BUT you still need to precondition ($M \approx W^{-1}$)

Implicit Solvers
NOX and LOCA: Nonlinear Solution and Homotopy

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



Simple Nonlinear Solve



Globalized
Newton-Krylov

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

$$f_{Drekar}$$

Block Composite Model

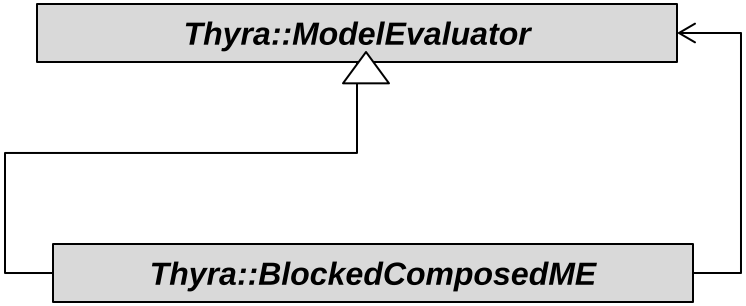
- The entire coupled system can be cast as a monolithic system:

$$\hat{f}(\dot{\hat{x}}, \hat{x}, \hat{p}, t) = 0$$

$$\begin{aligned}
\dot{\hat{x}} &= \left[\dot{x}_0, \ldots, \dot{x}_i, \ldots, \dot{x}_{N_f-1}\right], \\
\hat{x} &= \left[x_0, \ldots, x_i, \ldots, x_{N_f-1}\right], \\
\hat{p} &= \left[p_{0,0}, \ldots, p_{0,N_{p0}-1}, \ldots, p_{i,0}, \ldots, p_{i,N_{p_i}-1}, \ldots, p_{N_f-1,0}, \ldots, p_{N_f-1,N_{p_{N_f-1}}-1}\right], \\
\hat{f} &= \begin{bmatrix} f_0(\dot{x}_0, x_0, \{r_{0,k}(\{x_m\},\{p_{m,n}\})\}, \{p_{0,l}\}, t)) \\ \vdots \\ f_i(\dot{x}_i, x_i, \{r_{i,k}(\{x_m\},\{p_{m,n}\})\}, \{p_{i,l}\}, t)) \\ \vdots \\ f_{N_f-1}(\dot{x}_{N_f-1}, x_{N_f-1}, \{r_{N_f-1,k}(\{x_m\},\{p_{m,n}\})\}, \{p_{N_f-1,l}\}, t)) \end{bmatrix}.
\end{aligned}$$

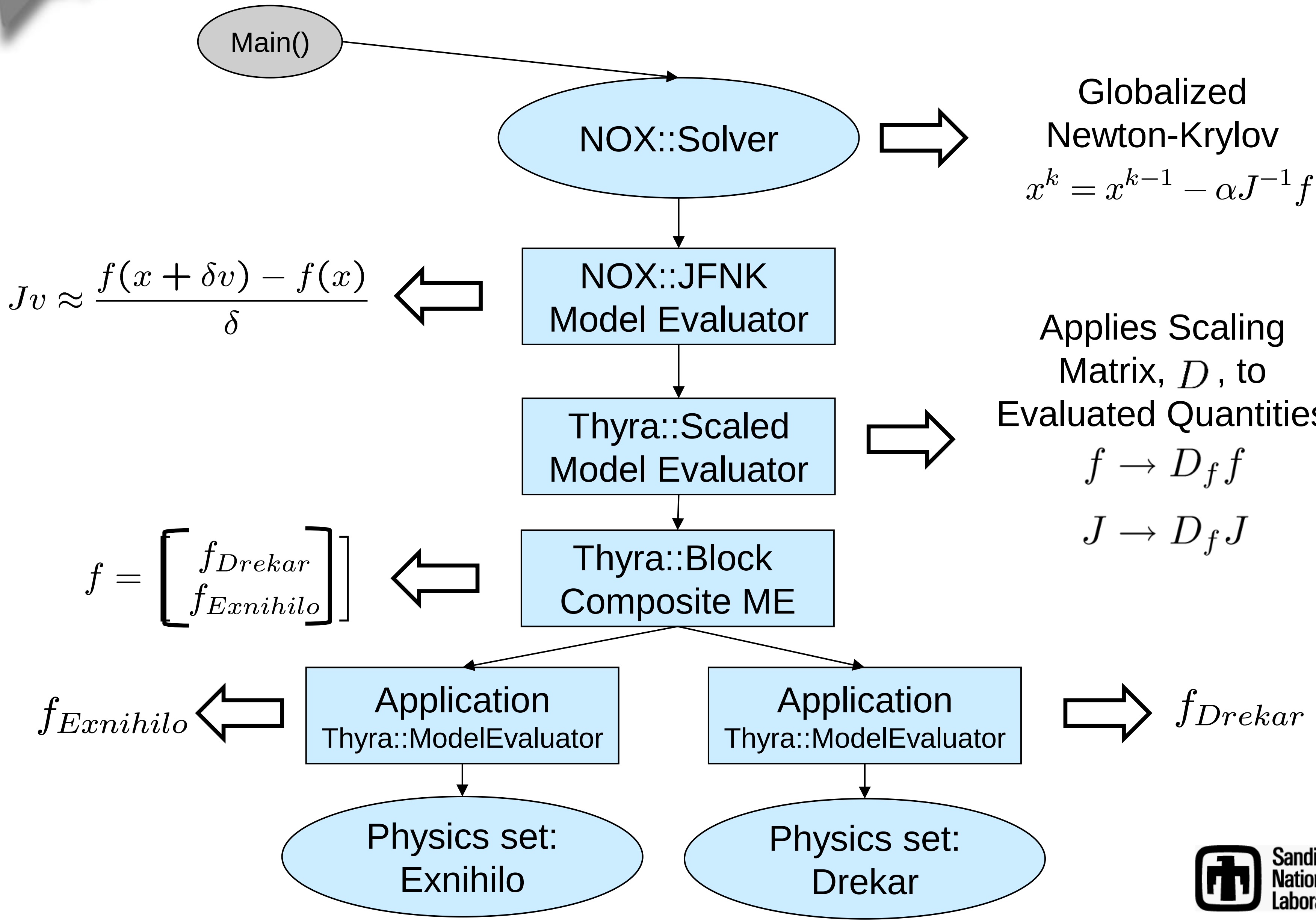
The Power of Decorators

- 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
  - DiagonalScalingModelEvalautor: 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



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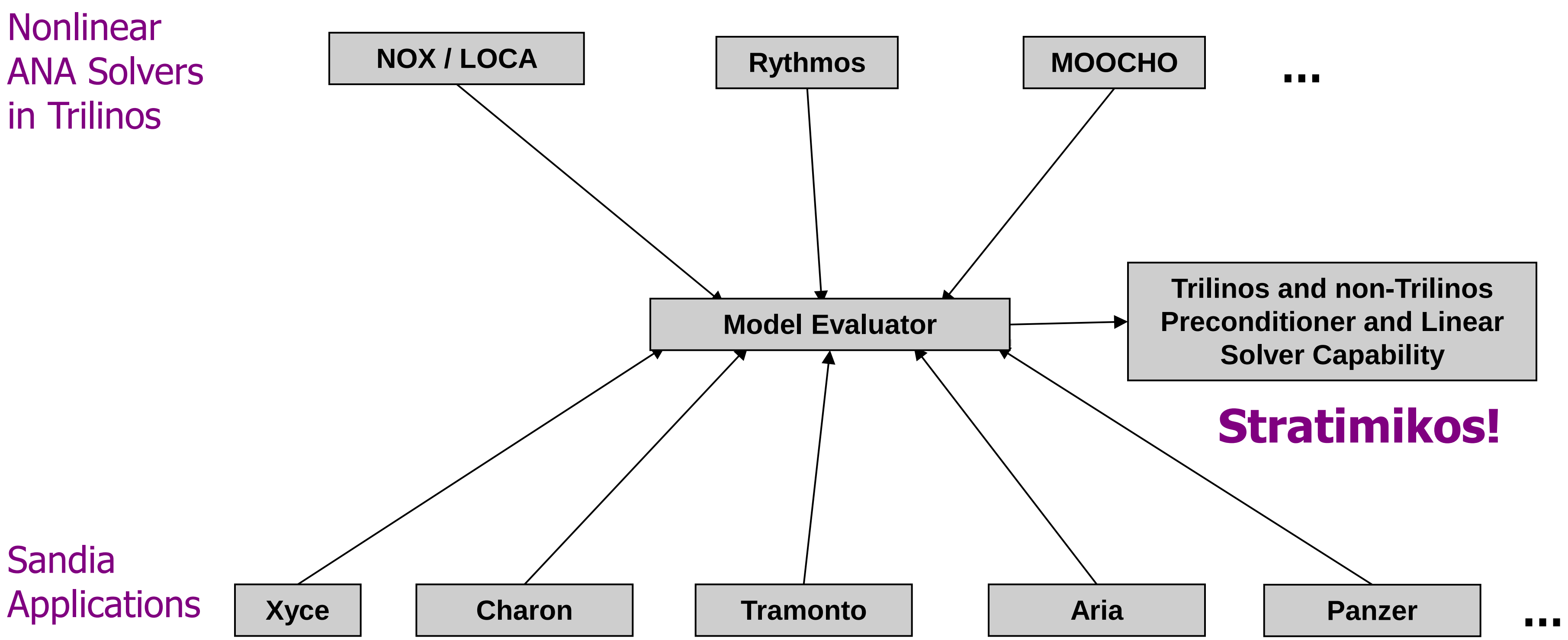
Linear Solvers
and Preconditioners

Nonlinear Algorithms and Applications : Thyra & Model Evaluator!



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

All Linear Solvers in Trilinos can be selected at run time from an XML File

```xml
<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 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"/>
            <Parameter name=”Flexible GMRES" type=”bool" value=”false"/>
            <Parameter name="Orthogonalization" type="string" value="DGKS"/>
          <ParameterList name="Block CG”>
         ...
   <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 name="ML">
        <Parameter name=”nodes per aggregate" type="int" value=“27"/>
        <Parameter name=”coarse: max size" type="int" value=“512"/>
       ...
</ParameterList>
```

Trilinos Linear Solvers: Heroux, Tuminaro, Hu, Bartlett, Thornquist, Hoemmen, Cyr,…

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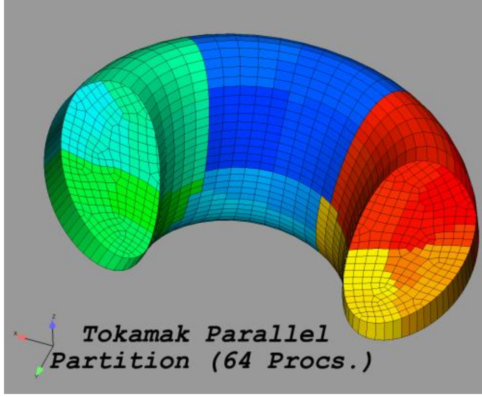
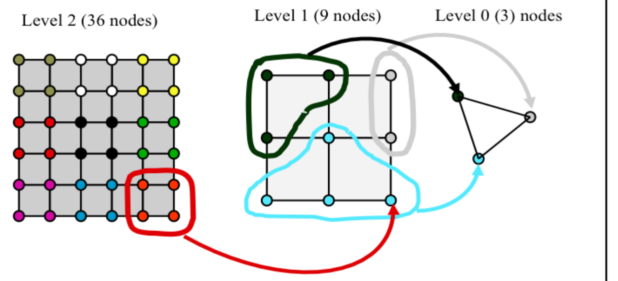
Three Types of Preconditioning



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



Visualization of effect of partition of matrix graph on mesh

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

Aggregation based Multigrid: Vanek, Mandel, Brezina, 1996; Vanek, Brezina, Mandel, 2001; Sala, Formaggia, 2001

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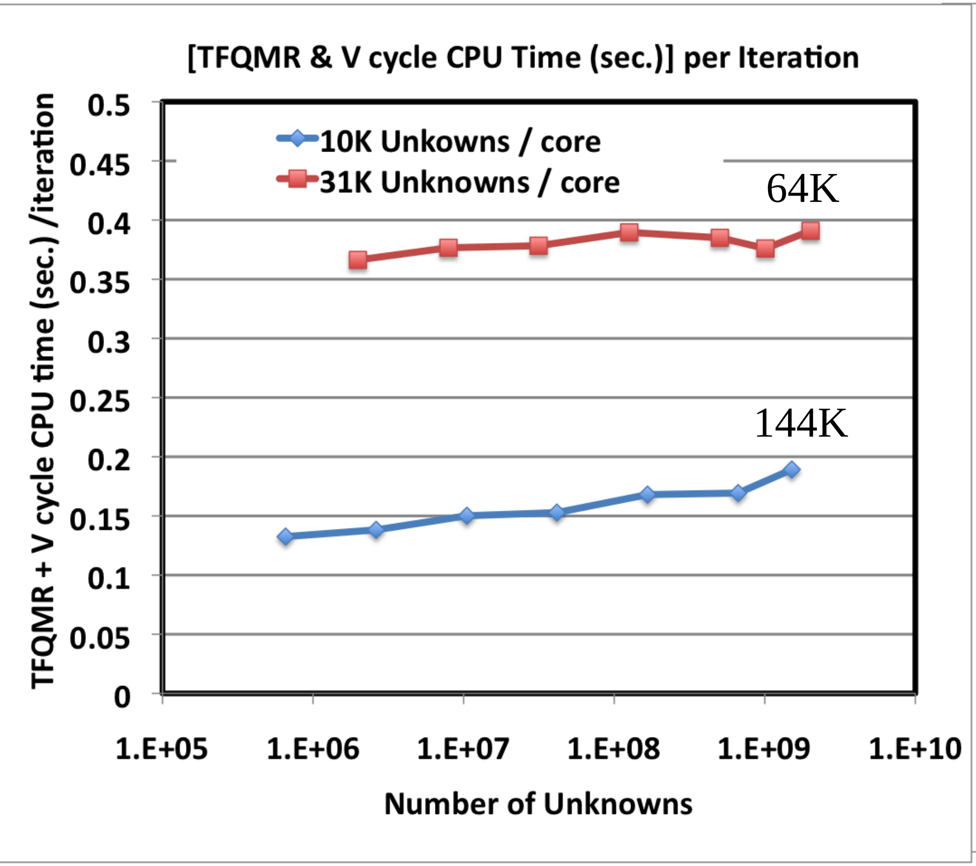
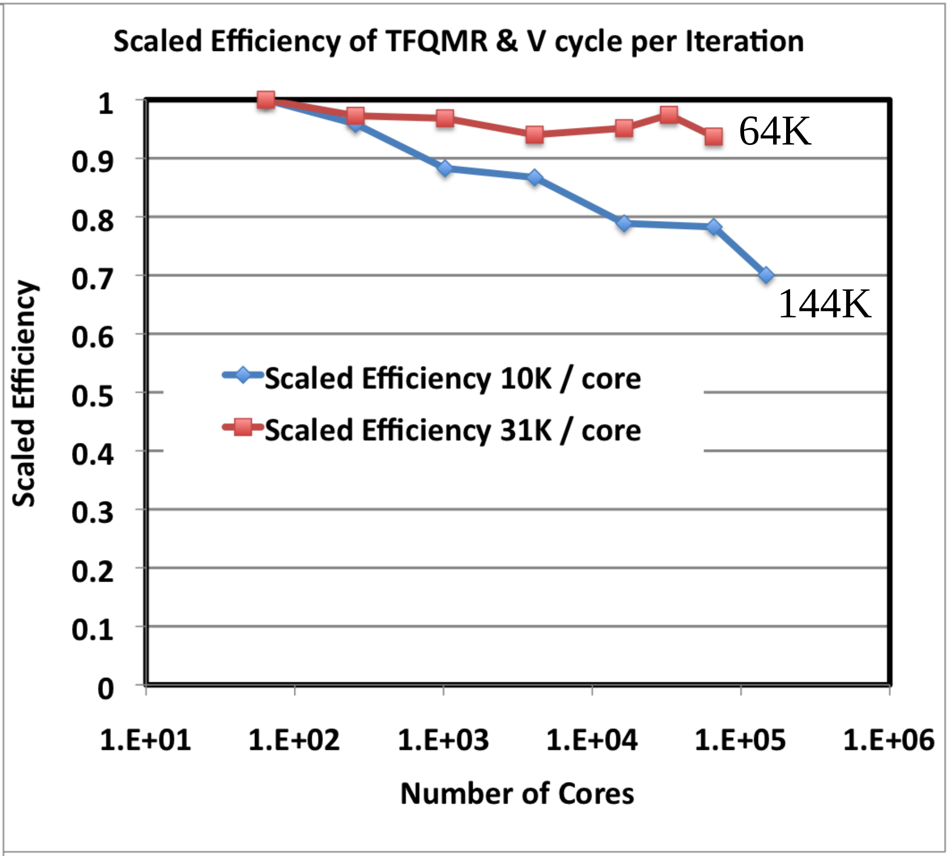
Weak Scaling Uncoupled Aggregation Scheme: Time/iteration on BlueGene/P





- 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

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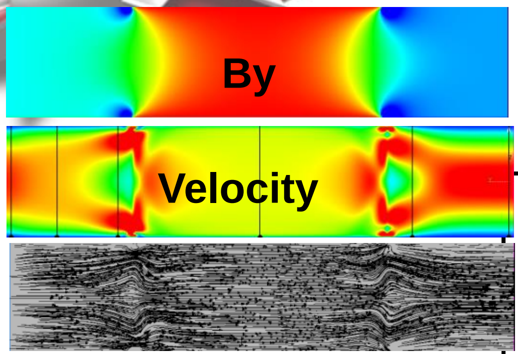
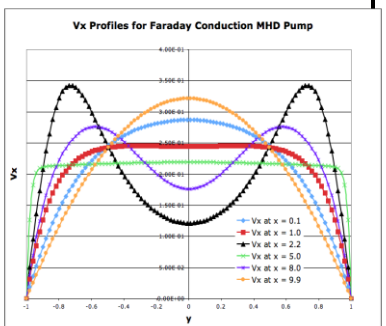
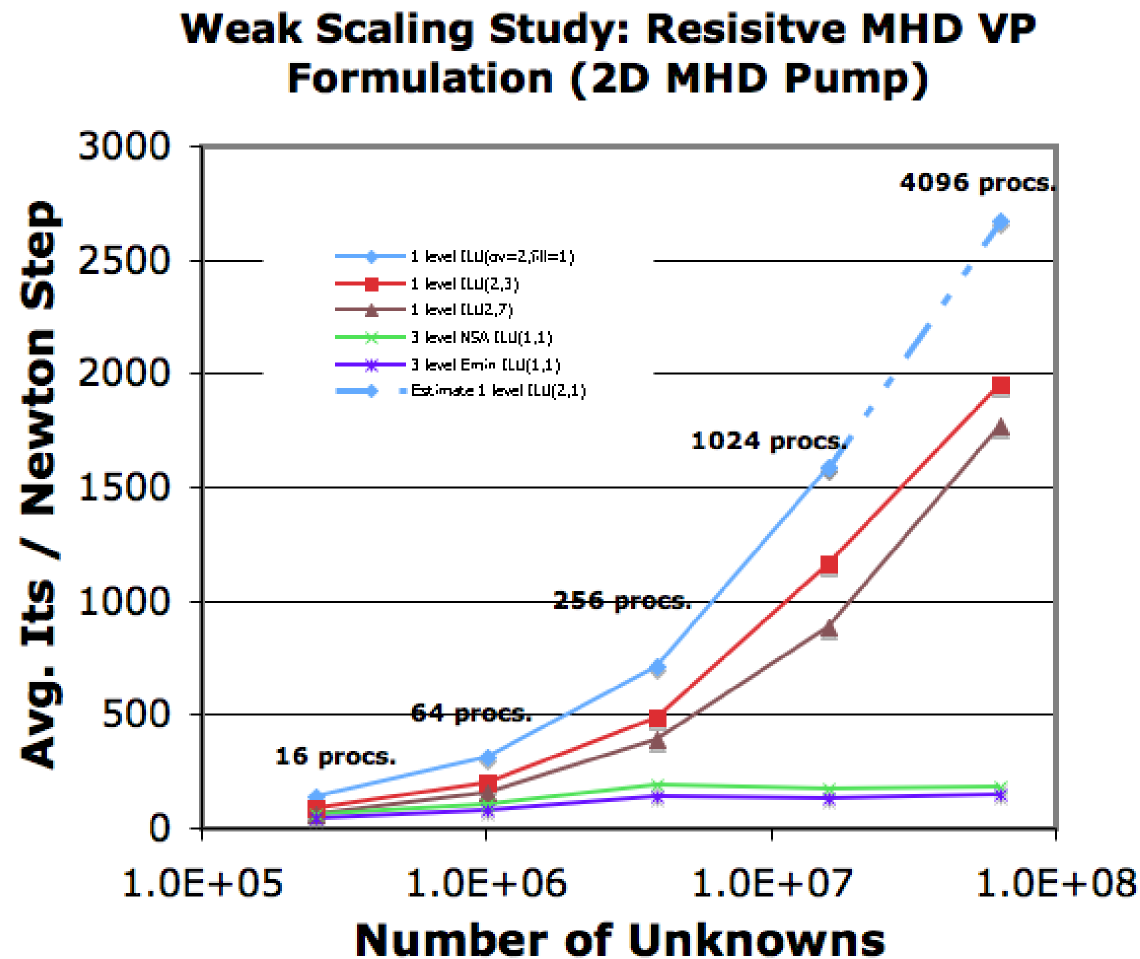
Scalability
(MHD Pump, Cray XT3)





MHD Pump



Preconditioners

- 1-level ILU(2,1)
- 1-level ILU(2,3)
- 1-level ILU(2,7)
- 3-level ML(NSA,Gal)
- 3-level ML(EMIN, PG)

ML: Tuminaro, Hu
Ifpack: Heroux

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Block preconditioning: CFD example

Consider discretized Navier-Stokes equations

$$\left.\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} - \nu\nabla^2\mathbf{u} + \nabla p = f \\ \nabla\cdot\mathbf{u} = 0 \end{aligned}\right\} \Leftrightarrow \begin{bmatrix} F & B^T \\ B & C \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}$$

Fully Coupled Jacobian

$$\mathcal{A} = \begin{bmatrix} F & B^T \\ B & C \end{bmatrix}$$

Block Factorization

$$\mathcal{A} = \begin{bmatrix} I & \\ BF^{-1} & I \end{bmatrix} \begin{bmatrix} F & B^T \\ & S \end{bmatrix}$$

$$S = C - BF^{-1}B^T$$

- Coupling in Schur-complement

Preconditioner

$$\mathcal{A}^{-1} \approx \mathcal{M}^{-1} = \begin{bmatrix} \hat{F} & B^T \\ & \hat{S} \end{bmatrix}^{-1}$$

Required operators:
- $F^{-1} \approx \hat{F}^{-1} \rightarrow$ Multigrid
- $S^{-1} \approx \hat{S}^{-1} \rightarrow$ PCD, LSC, SIMPLEC

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

Properties of approximate Schur-complement
1. "Nearly" replicates physical coupling
2. Invertible operators $\rightarrow$ good for AMG

Brief Overview of Block Preconditioning Methods for Navier-Stokes: (A Taxonomy based on Approximate Block Factorizations, JCP – 2008)

Discrete N-S	Exact LDU Factorization	Approx. LDU
$\begin{pmatrix} F & B^T \\ \hat{B} & -C \end{pmatrix} \begin{pmatrix} \Delta u_k \\ \Delta p_k \end{pmatrix} = \begin{pmatrix} g_u^k \\ g_p^k \end{pmatrix}$	$\begin{pmatrix} I & 0 \\ \hat{B}F^{-1} & I \end{pmatrix} \begin{pmatrix} F & 0 \\ 0 & -S \end{pmatrix} \begin{pmatrix} I & F^{-1}B^T \\ 0 & I \end{pmatrix}$ $S = C + \hat{B}F^{-1}B^T$	$\begin{bmatrix} I & 0 \\ \hat{B}H_1 & I \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & -\hat{S} \end{bmatrix} \begin{bmatrix} I & H_2 B^T \\ 0 & I \end{bmatrix}$

Precond. Type	H_1	H_2	$\hat{S}$	References
Pres. Proj; 1st Term Nuemann Series	$\mathbf{F}^{-1}$	$(\Delta t \mathbf{I})^{-1}$	$\mathbf{C} + \Delta t \hat{\mathbf{B}} \mathbf{B}^T$	Chorin(1967);Temam (1969); Perot (1993): Quateroni et. al. (2000) as solvers
SIMPLEC	$\mathbf{F}^{-1}$	$(\mathrm{diag}(\sum \lvert \mathbf{F} \rvert))^{-1}$	$\mathbf{C} + \hat{\mathbf{B}}(\mathrm{diag}(\sum \lvert \mathbf{F} \rvert))^{-1}\mathbf{B}^T$	Patankar et. al. (1980) as solvers; Pernice and Tocci (2001) smothers/MG
Pressure Convection / Diffusion	0	$\mathbf{F}^{-1}$	$\mathbf{A}_p \mathbf{F}_p^{-1}$	Kay, Loghin, Wathan, Silvester, Elman (1999 - 2006); Elman, Howle, S., Shuttleworth, Tuminaro (2003,2008)

Now use AMG type methods on sub-problems.

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

Pressure – Poisson type: $-\hat{S}\Delta p = \mathbf{r}_p$

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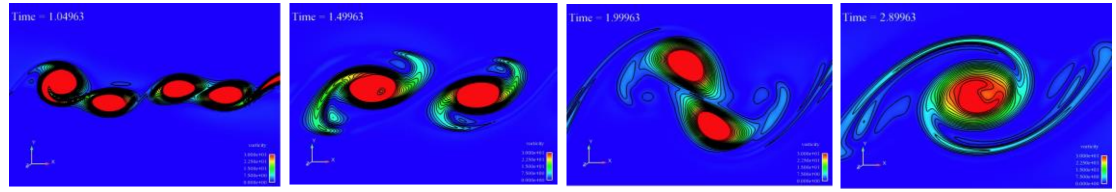
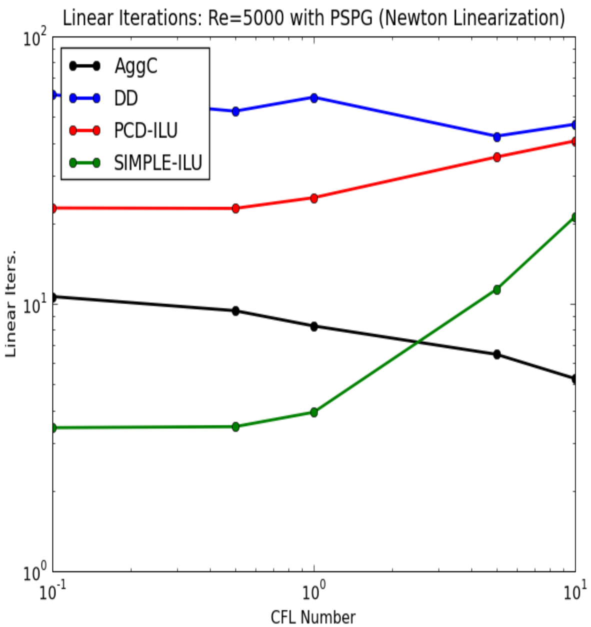
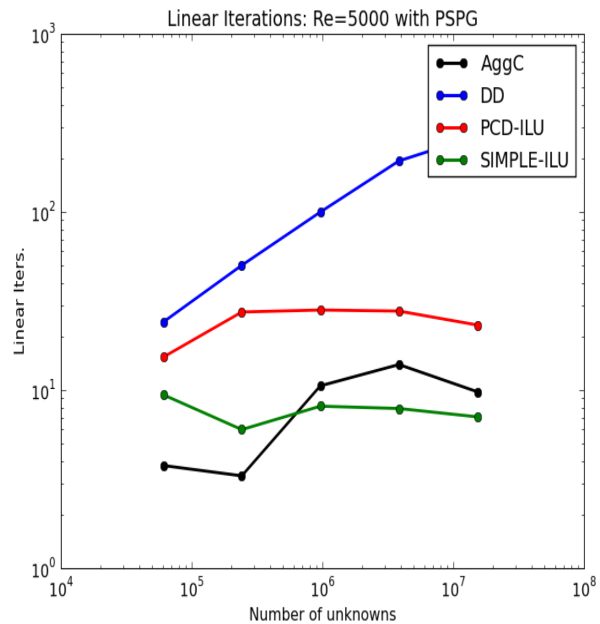
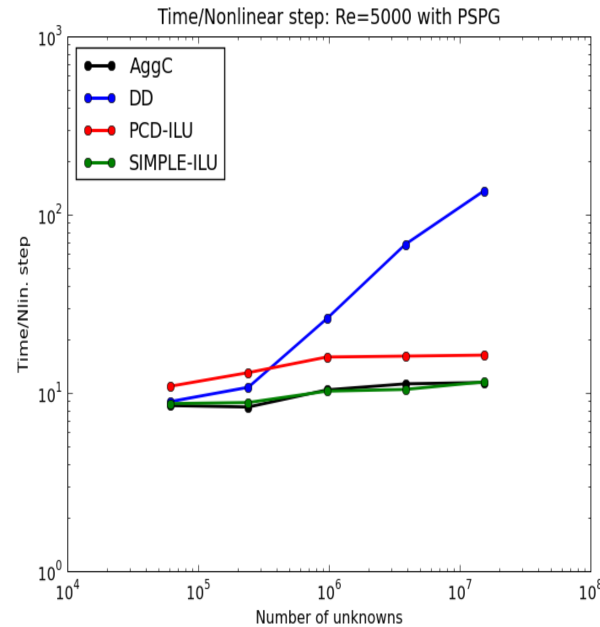
Transient Kelvin-Helmholtz









Kelvin Helmholtz: Re=5000, Weak scaling at CFL=2.5

- **Run on 1 to 256cores**
- **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**

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Incompressible MHD
2D Vector Potential Formulation

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

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

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

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

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

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

Matrices F and D are transient convection operators, C is stabilization matrix

Teko Block Preconditioners

Nested Schur Complements:

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

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

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

Physics Based: Operator Splitting:

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

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

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

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

$$\hat{x} = x^* + e$$

$$\mathcal{M}_{Split} = \begin{bmatrix} F & B^T & Z \\ B & C & \\ Y & \boxed{YF^{-1}B^T} & D \end{bmatrix} = \begin{bmatrix} F & & Z \\ & I & \\ Y & & D \end{bmatrix} \begin{bmatrix} F^{-1} & & \\ & I & \\ & & I \end{bmatrix} \begin{bmatrix} F & B^T & \\ B & C & \\ & & I \end{bmatrix}$$

- Eliminates nested Schur Complements
- Requires two 2x2 solves
- Navier-Stokes operator well studied
- Magnetics-Velocity operator is difficult

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Physics-based/ABF Preconditioning

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

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

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

⇩

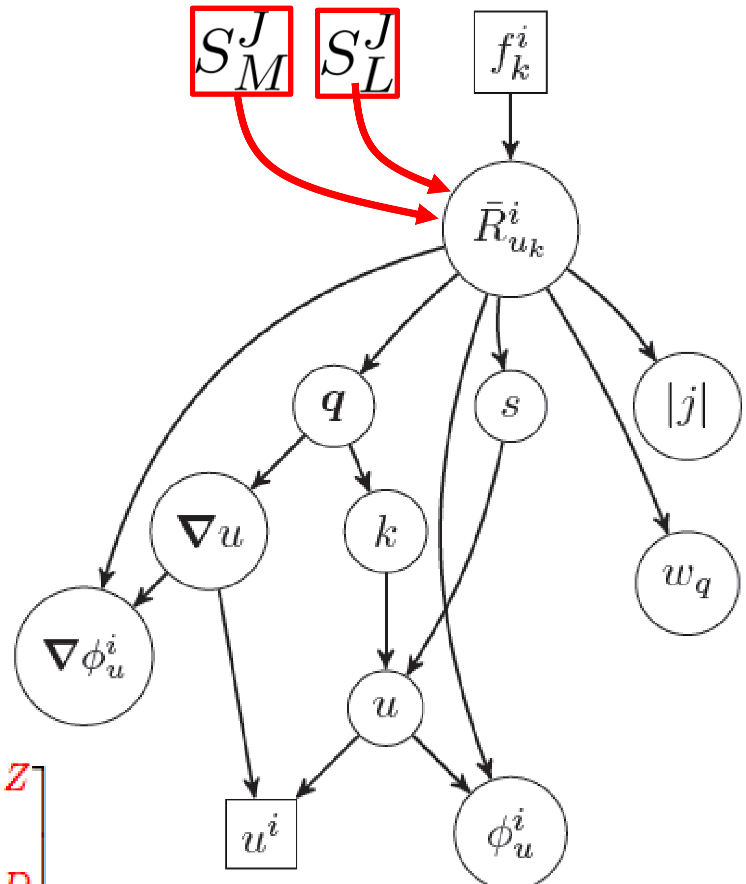
$$\begin{bmatrix} \begin{bmatrix} F & B^T \\ B & C \end{bmatrix} & \begin{bmatrix} Z \\ 0 \end{bmatrix} \\ \begin{bmatrix} Y & 0 \end{bmatrix} & D \end{bmatrix} \begin{bmatrix} u \\ p \\ b \end{bmatrix} = \begin{bmatrix} f \\ g \\ h \end{bmatrix}$$

⇩

$$\begin{bmatrix} F & B^T & Z \\ B & C & 0 \\ Y & 0 & D \end{bmatrix}$$

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

JFNK + Block Scattering for Preconditioning



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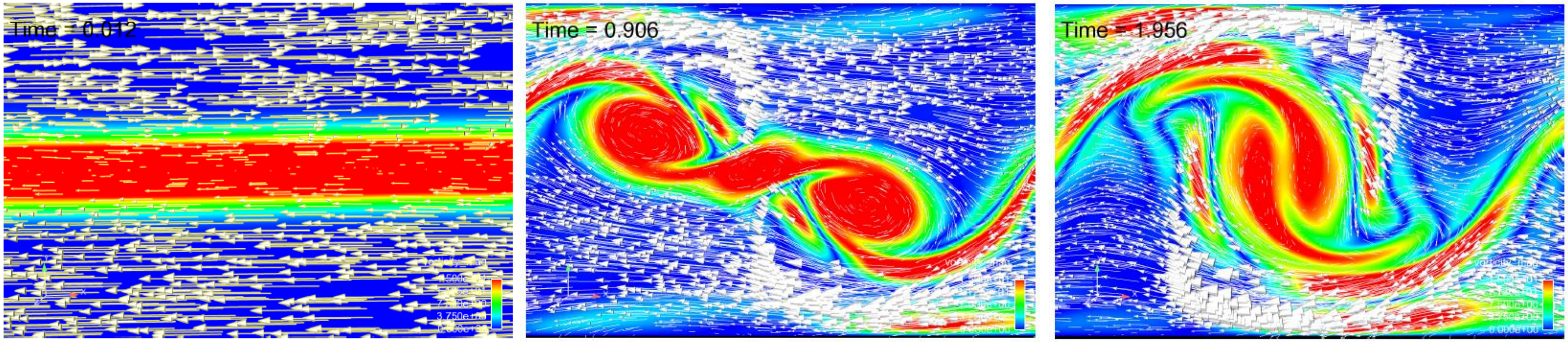
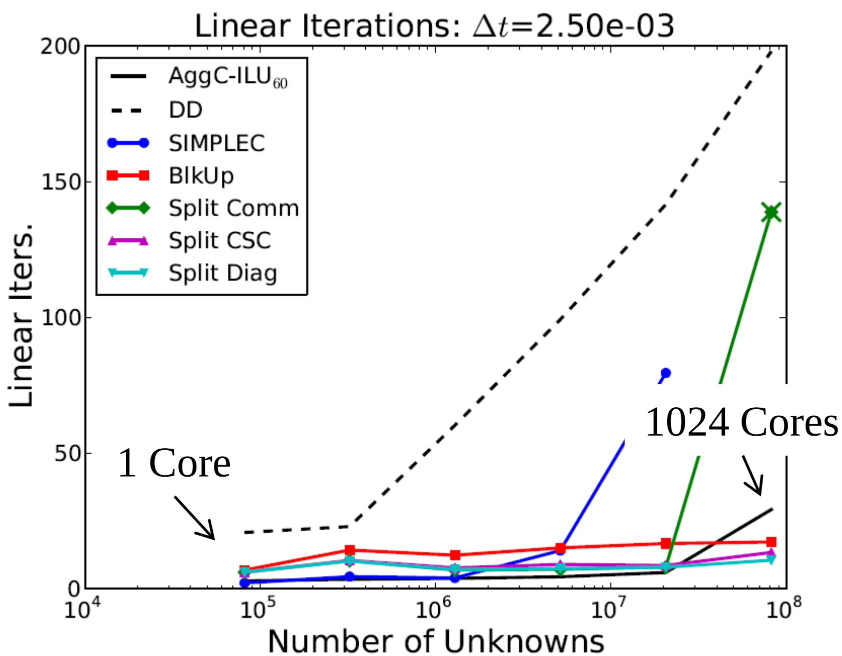
Hydromagnetic Kelvin-Helmholtz

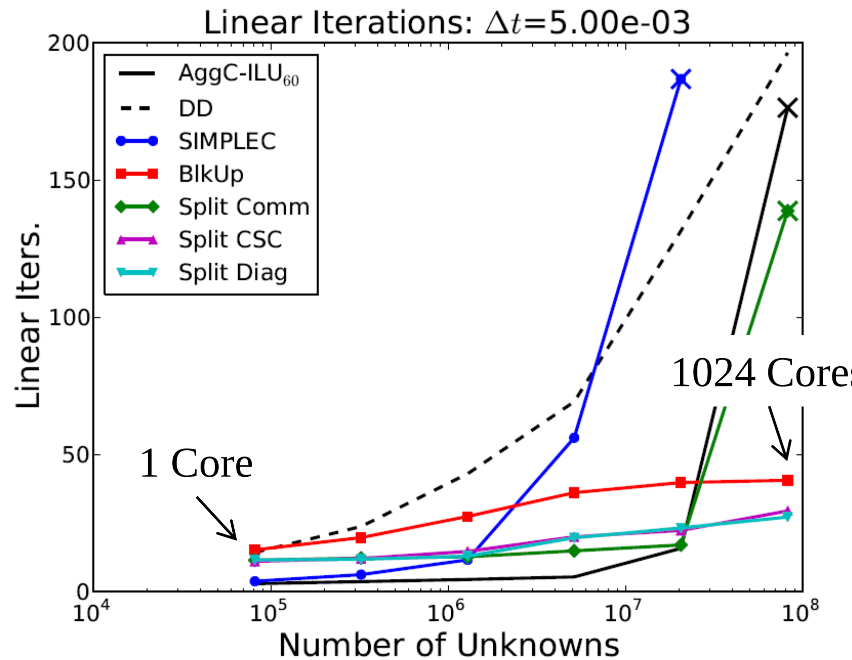


t = 0.012 t = 0.906 t = 1.956

- Velocity shear flow
- Magnetic field in x-direction
- Reynolds number = 10^3
- Lundquist number = 10^4

MHD Weak Scaling: Hydromangetic Kelvin-Helmholtz (Fixed time step)





Fully coupled Algebraic

AggC: Aggressive Coarsening Multigrid

DD: Additive Schwarz Domain Decomposition

Block Preconditioners

Split: New Operator split preconditioner

SIMPLEC: Extreme diagonal approximations

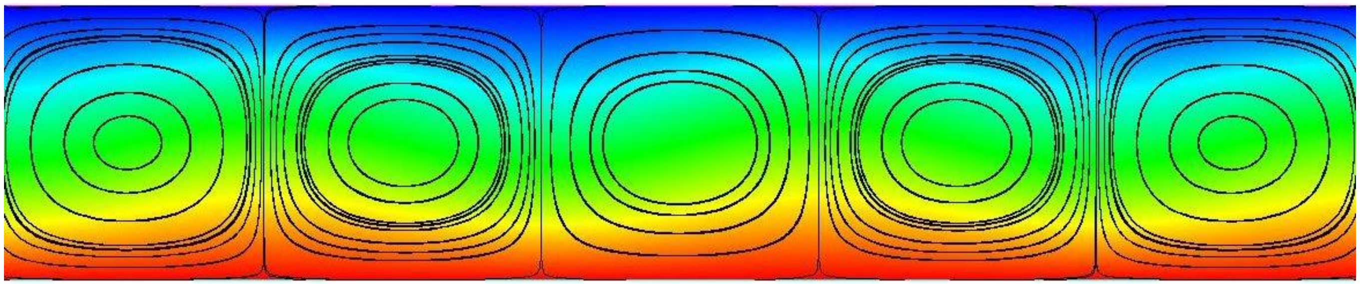
Take home: Split preconditioner scales algorithmically, more relevant for mixed discretizations, multiphysics

Hydromagnetic Rayleigh-Bernard

B_0 ↑ g ↓

$v_x = 0$, $v_y = 0$ $\quad T = -0.5 \quad \frac{\partial \mathcal{A}}{\partial y} = 0$

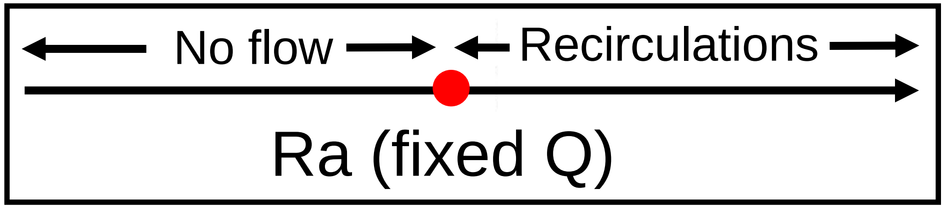
$v_x = 0$, $\mathcal{A} = C\sqrt{(Q)}$



$v_x = 0$, $\mathcal{A} = -C\sqrt{(Q)}$

$v_x = 0$, $v_y = 0$ $\quad T = 0.5 \quad \frac{\partial \mathcal{A}}{\partial y} = 0$

Parameters:
- Q ~ B_0^2 (Chandresekhar number)
- Ra (Rayleigh number)



$$Q = \frac{B_0^2 d^2}{\mu_0 \rho \nu \eta} \qquad Ra = \frac{g\beta \Delta T d^3}{\nu \alpha} \qquad Pr = \frac{\nu}{\alpha} \qquad Pr_m = \frac{\nu}{\eta}$$

- Buoyancy driven instability initiates flow at high Ra numbers.
- Increased values of Q delay the onset of flow.
- Domain: 1x20

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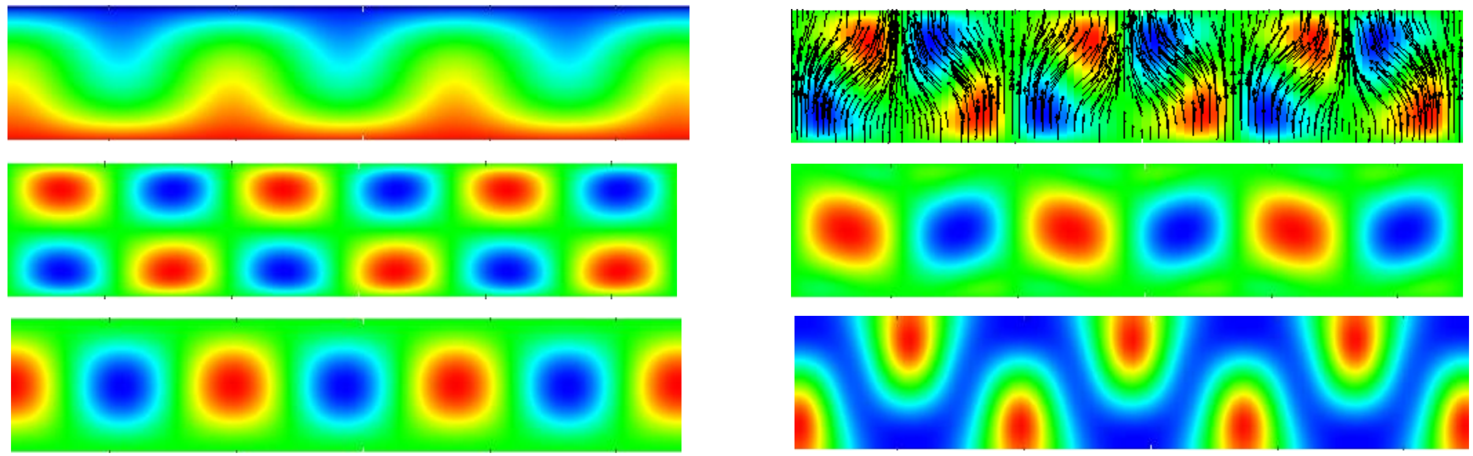
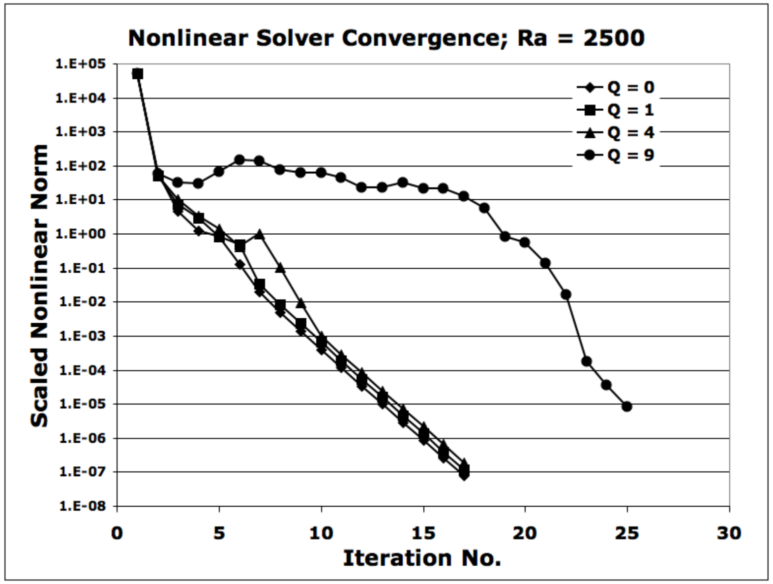
Hydro-Magnetic Rayleigh-Bernard Stability: Direct Determination of Nonlinear Equilibrium Solutions (Steady State Solves, Ra=2500, Q=4)

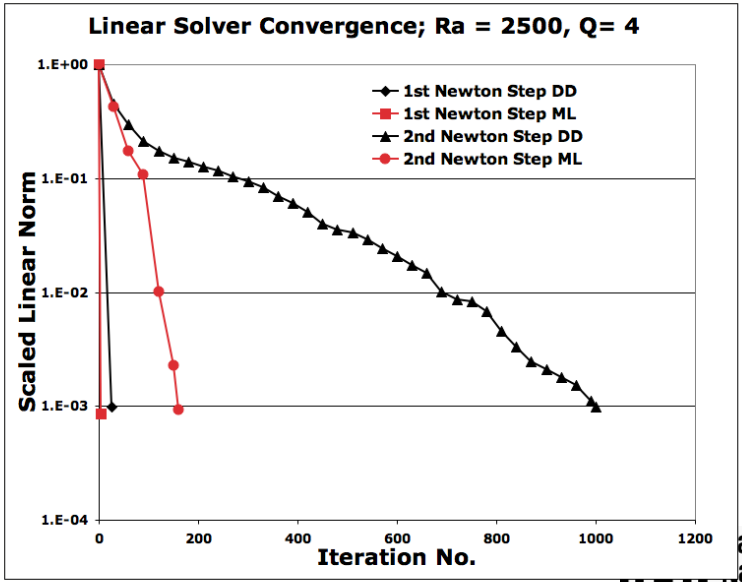


Temp Jz

Vx Bx

Vy By





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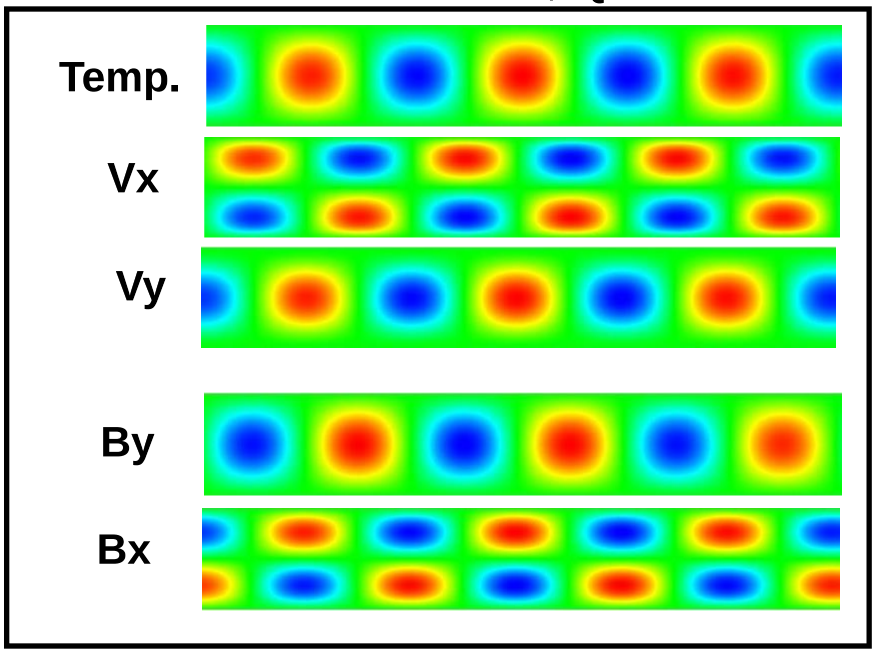
Hydro-Magnetic Rayleigh-Bernard Stability: Direct Determination of Linear Stability and Nonlinear Equilibrium Solutions (Steady State Solves)

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



Q	Ra*	Ra_{cr} [Chandrasekhar[]]	% error
0	1707.77	1707.8	0.002
10^1	1945.78	1945.9	0.006
10^2	3756.68	3757.4	0.02

- 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*

Arc-length Continuation: Identification of Pitchfork Bifurcation, Q=10

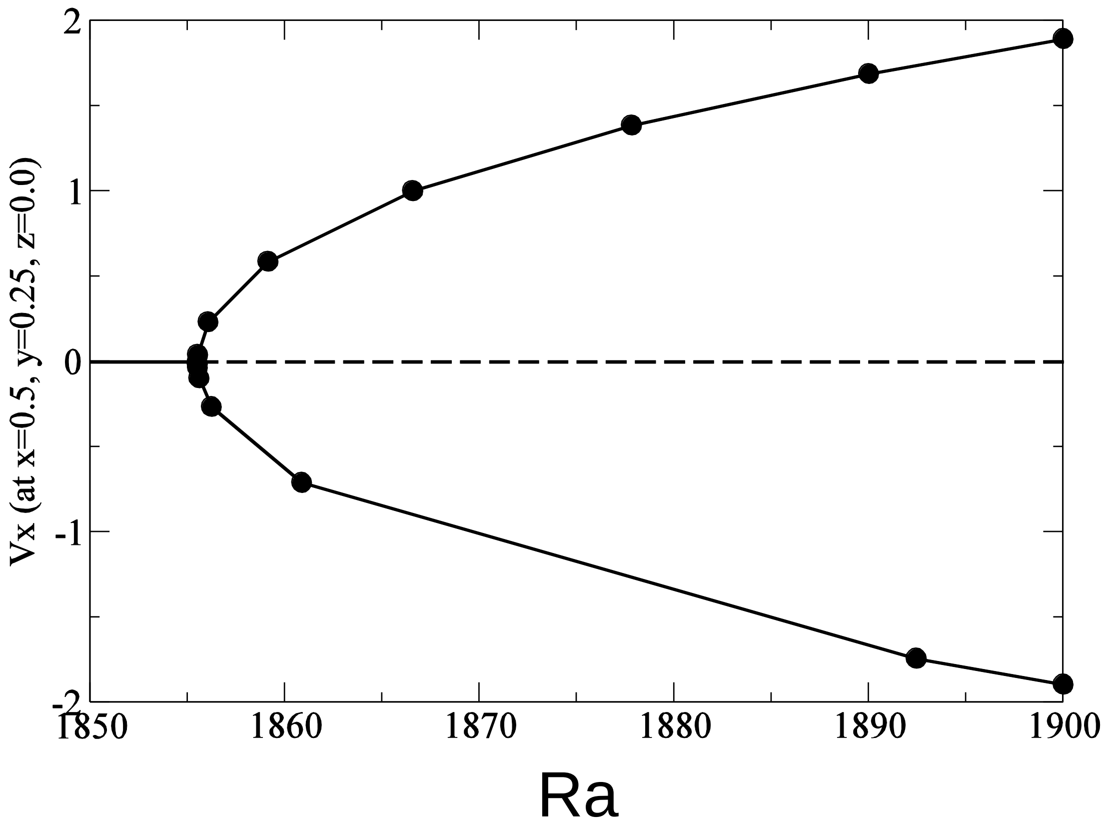
Nonlinear system:

$$f(x(s), p(s)) = 0$$

$$g(x(s), p(s), s) = 0$$

Newton System:

$$\begin{bmatrix} \boldsymbol{J} & \boldsymbol{f_p} \\ \left(\frac{\partial x}{\partial s}\right)^T & \frac{\partial p}{\partial s} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Delta x} \\ \boldsymbol{\Delta p} \end{bmatrix} = - \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{bmatrix}$$



Bordered Solver:

$$Ja = -f \qquad \Delta p = -(g + \frac{\partial x}{\partial s} \cdot a)/(\frac{\partial p}{\partial s} + \frac{\partial x}{\partial s} \cdot b)$$

$$Jb = -f_p \qquad \Delta x = a + \Delta p b$$

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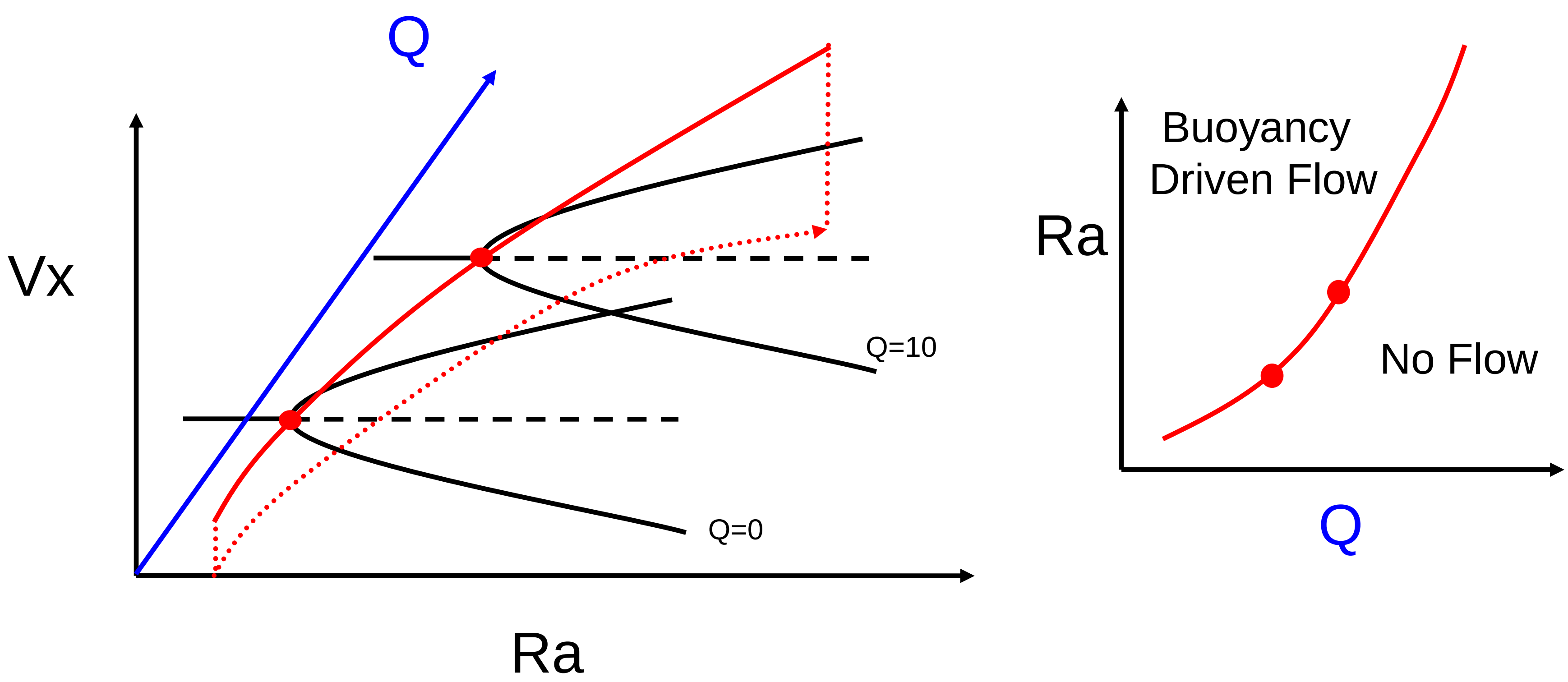
Design (Two-Parameter) Diagram



- “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):

$$\begin{bmatrix} J & 0 & f_p \\ (Jn)_x & J & J_p n \\ 0 & \phi^T & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta n \\ \Delta p \end{bmatrix} = \begin{bmatrix} -f \\ -Jn \\ 1 - \phi^T \cdot n \end{bmatrix}$$

- 4 linear solves per Newton iteration:

$$Ja = -f$$
$$Jb = -f_p$$
$$Jc = -(Jn)_x a - Jn$$
$$Jd = -(Jn)_x b - J_p n$$
$$\Delta p = (1 - \phi \cdot n - \phi \cdot c)/(\phi \cdot d)$$
$$\Delta n = c + \Delta p d$$
$$\Delta x = a + \Delta p b$$

Minimally Augmented

- Widely used algorithm for small systems:

$$\begin{bmatrix} \boldsymbol{J} & \boldsymbol{a} \\ \boldsymbol{b}^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{v} \\ s \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \begin{bmatrix} \boldsymbol{J}^T & \boldsymbol{b} \\ \boldsymbol{a}^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ t \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$
$$\Longrightarrow s = t = -\boldsymbol{u}^T \boldsymbol{J} \boldsymbol{v}$$

- J is singular if and only if s = 0

- Turning point formulation (N+1):

$$\boldsymbol{f}(\boldsymbol{x}, p) = 0$$
$$s(\boldsymbol{x}, p) = 0$$

- Newton's method:

$$\begin{bmatrix} \boldsymbol{J} & \boldsymbol{f}_p \\ \boldsymbol{s}_x & s_p \end{bmatrix} \begin{bmatrix} \Delta \boldsymbol{x} \\ \Delta p \end{bmatrix} = - \begin{bmatrix} \boldsymbol{f} \\ s \end{bmatrix},$$
$$\boldsymbol{s}_x = -(\boldsymbol{u}^T \boldsymbol{J} \boldsymbol{v})_x = -(\boldsymbol{u}^T \boldsymbol{J})_x \boldsymbol{v}.$$

- 3 linear solves per Newton iteration

Extension to large-scale iterative solvers

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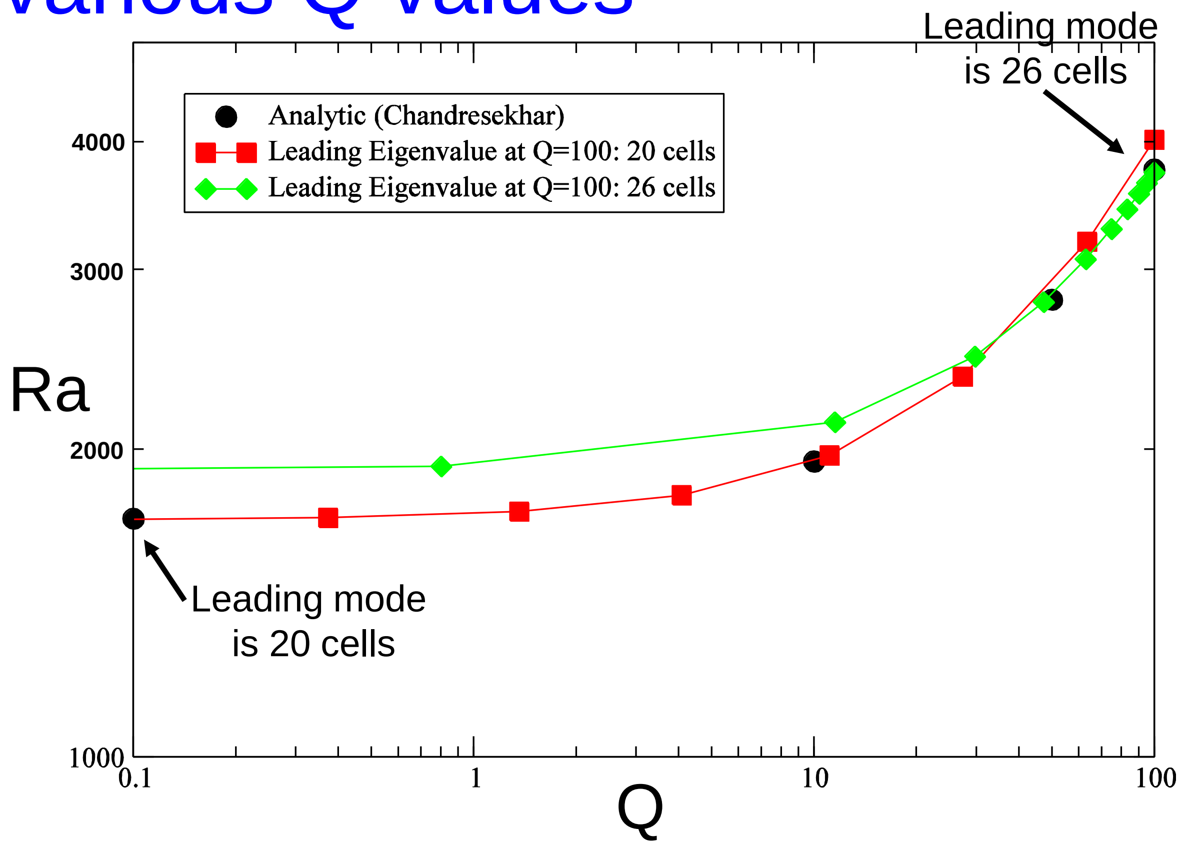
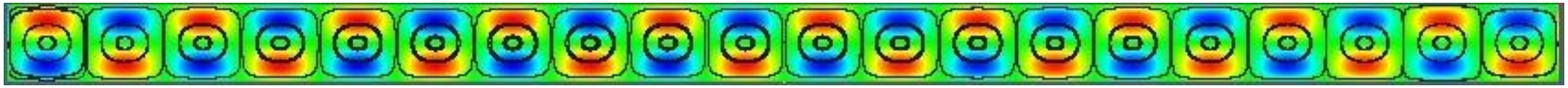
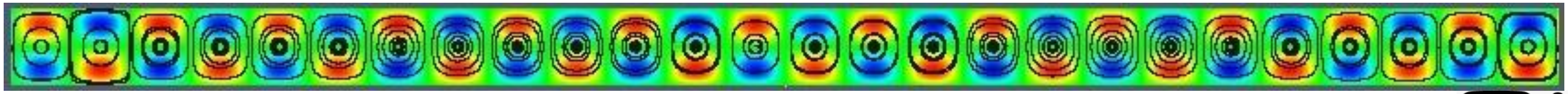
Leading Mode is different for various Q values

- 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

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SEACISM: Parallel Glimmer-CISM2

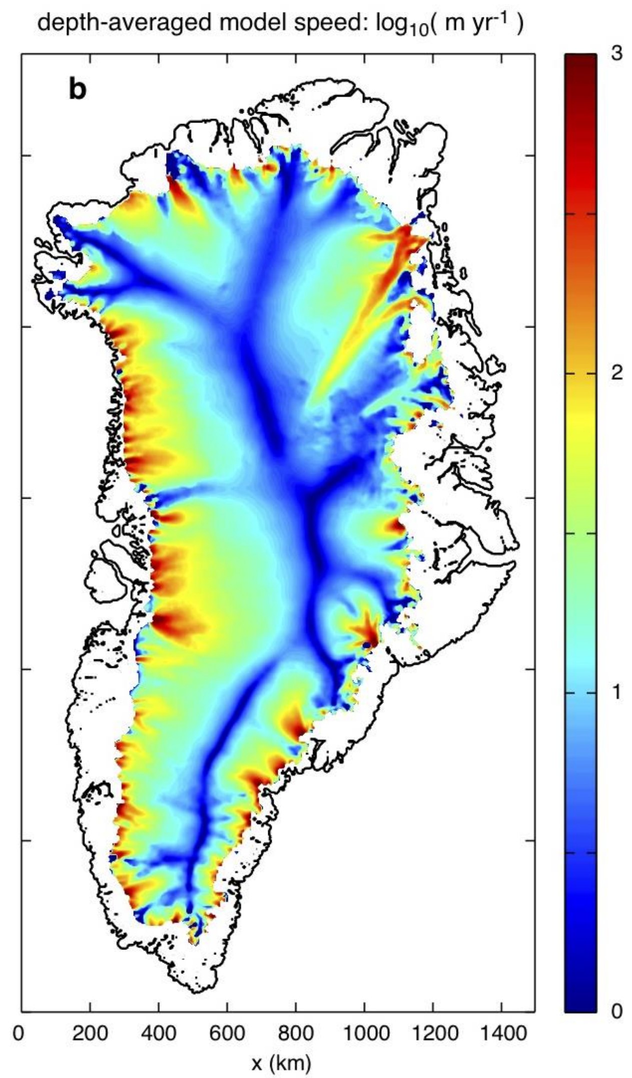
Evans, Worley, Nichols, Norman (ORNL)
Price, Lipscomb, Hoffman (LANL)
Salinger, Kalashnikova, Tuminaro (SNL)
Lemieux (NYU), Sachs (NCAR)

Glimmer Code ~2009:

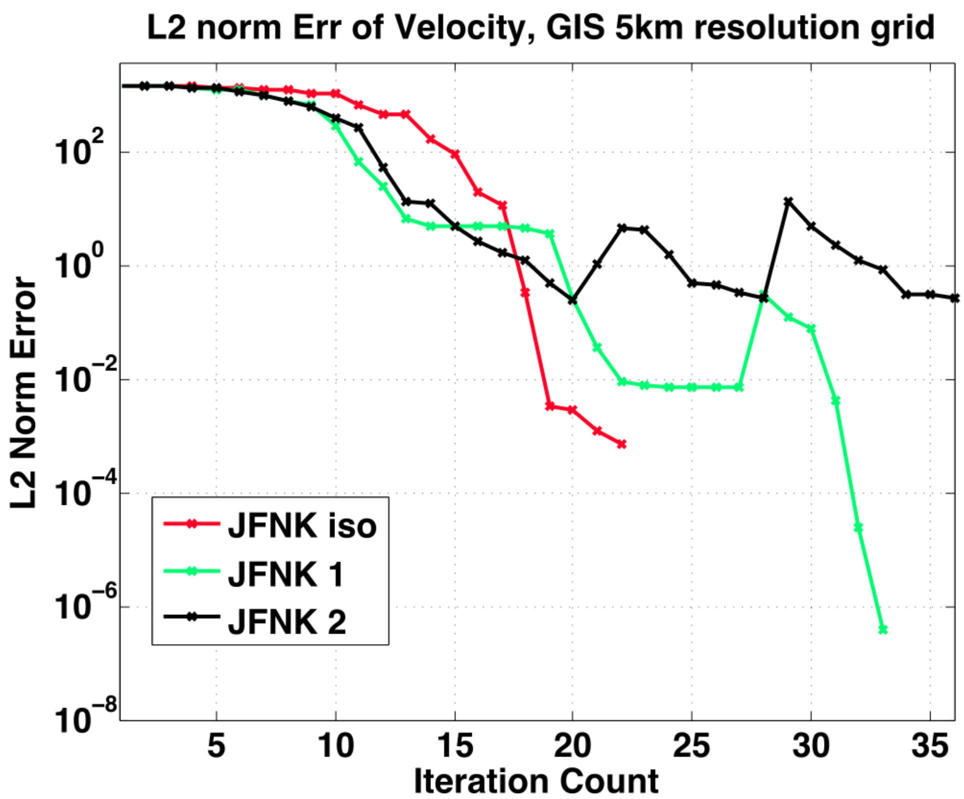
- First-Order Approx to Stokes: 3D for [U,V]
- Structured Grid
- Finite Difference
- Serial
- Picard Solver
- Autoconf

Glimmer Code ~2013:

- Parallel Assembly
- Parallel Solve
- Newton Solver
- Cmake
- Built in CESM development branch



Convergence is not adequately robust reliable for Greenland problems



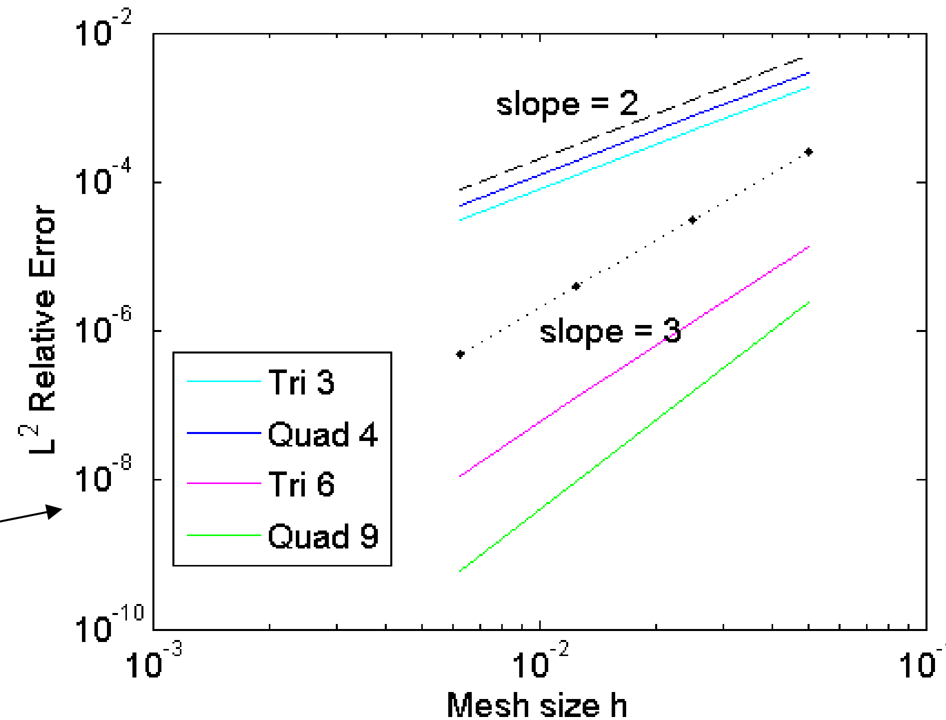
Why the poor robustness?

- 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[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

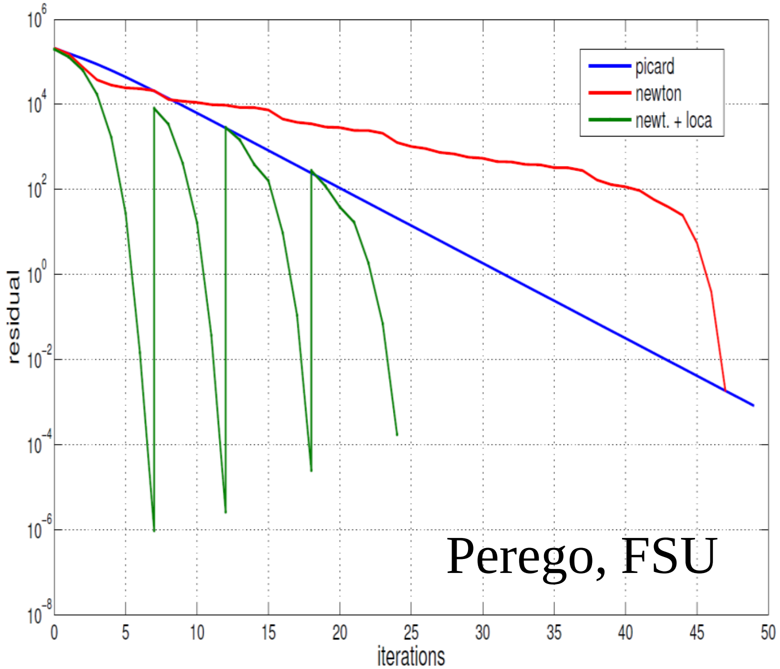


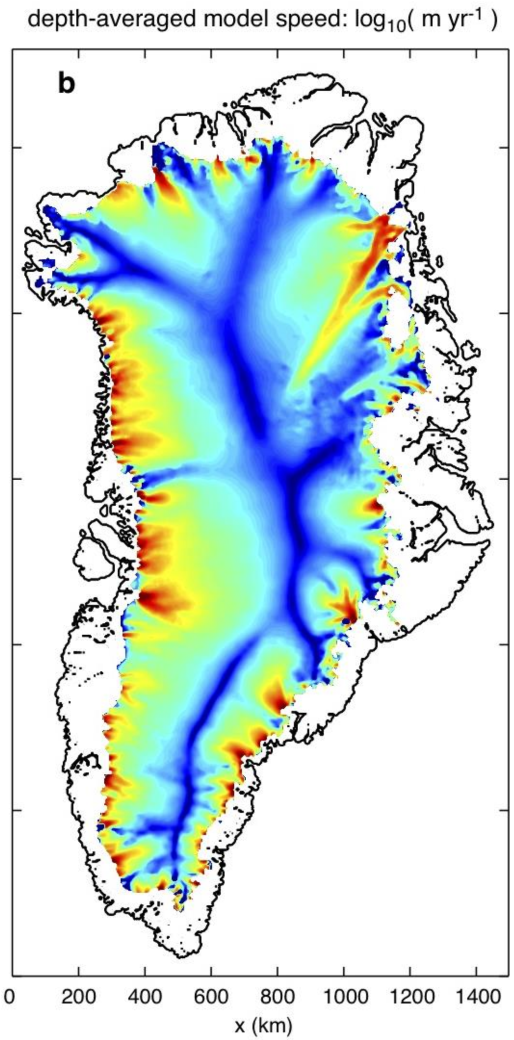
Manufactured Solution

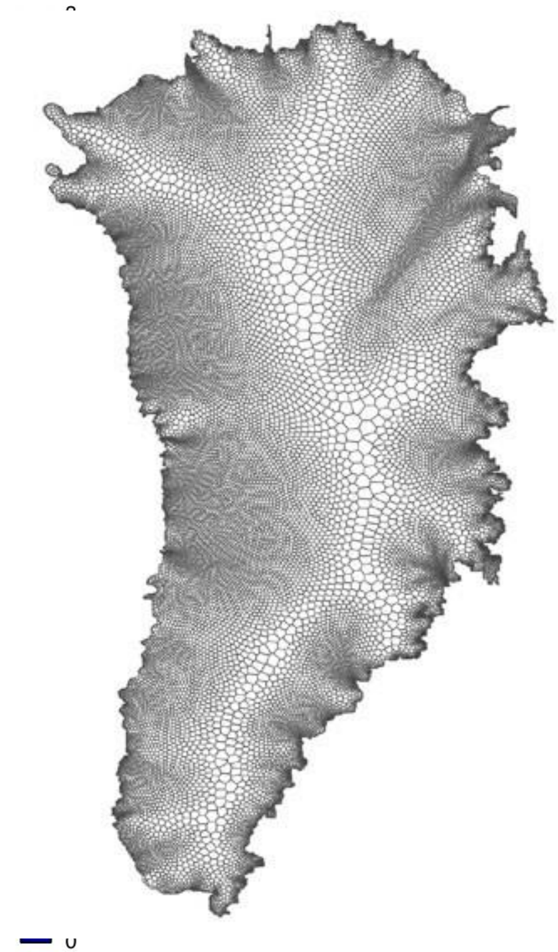
$$
\begin{aligned}
u &= \sin(2\pi x)\cos(2\pi y) + 3\pi x, \\
v &= -\cos(2\pi x)\sin(2\pi y) - 3\pi y
\end{aligned}
$$

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







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