Building an Open-source Multiphysics PDE Research Tool using Trilinos

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Outline

- Introduction
  - Motivation
  - History
- An example driving application: CASL GTRF Challenge Problem
- Code Design and Algorithms
- GTRF Results
- *A Users(?) Perspective on Trilinos*
- Conclusions

Focus

- Question:
  - If I need to build a multiphysics simulation capability, how much can we leverage Trilinos and how much do I have to develop?
- “Power User Session”: This talk is about pushing the Trilinos open source software stack to it’s limits.
- Hope to Convey: With the right tools in place, you can make significant progress very quickly on very complex physics with advanced software designs!

Motivation

Mathematical /Computational 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 response**
  - Evolve a solution on a **long time scale relative to component time scales**
  - Balance to produce **steady-state** behavior.

e.g. Nuclear Fission / Fusion Reactors; Conventional /Alternate Energy Systems; High Energy Density Physics; Electro-magnetic Launch; 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.

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History

- Research on Discretizations and Implicit Solution Technology for Large-scale PDE Simulation
  - Funding: DOE/SC/ASCR, NNSA/ASC, AFRL
  - Reacting flows, CFD, MHD, Aerosol, Semiconductor Drift Diffusion
- Foundational solvers work that contributed to many Trilinos packages
- Current simulation tool (Charon) will not meet our needs for FY12+:
  - ASCR funding requires new technology that doesn't easily fit the framework
  - ASC Target Problems are more complex
  - Export control restrictions
  - TPL dependencies on commercial software (e.g. Chemkin)
  - Monolithic framekwork
- Redesign for future research and production efforts in a collection of Trilinos packages

Research Requirements

A Research Tool for DOE/OS: ASCR/AMR, ASCR/UQ

- **Formulations: fully coupled fully implicit Newton-Krylov, semi-implicit, FCT**
- **Compatible discretizations:**
  - Mixed basis for DOFs within element block
  - Arbitrary element types (not restricted to nodal basis)
- **Multiphysics:**
  - Fully coupled systems composed of different equation sets in different element blocks
  - Preconditioning: Approximate block factorization/physics based
- **Supports advanced analysis techniques:**
  - Supports Template-based Generic Programming
  - Adjoint-based error analysis
  - Stability, bifurcation, embedded (SAND) optimization, embedded uncertainty quantification (Stokhos/PCE)
- **Open-source (collaborations)**
- **Exascale integration (Tpetra, Kokkos::MDArray)**

Production Requirements

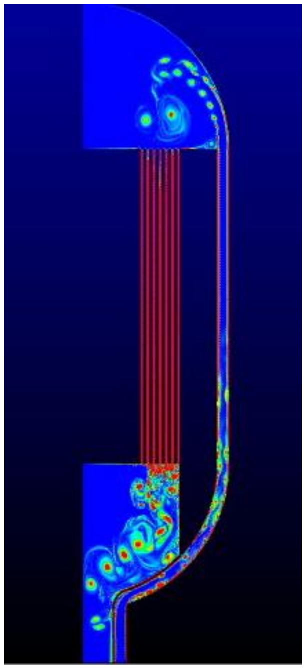
Production Quality Software (ASC, CASL)

- Strict and extensive unit testing (TDD), system testing, automated nightly and CI testing
- Application is a library (for multiphysics coupling)
- Integration with legacy code components
- NOT restricted to any mesh database or I/O format
- Control over granularity of assembly process (efficiency vs flexibility)
- Production Applications:
  - **ASC**: Semiconductor Device (Next-generation Charon) for QASPR
  - **CASL**: Drekar CFD component for VERA simulator

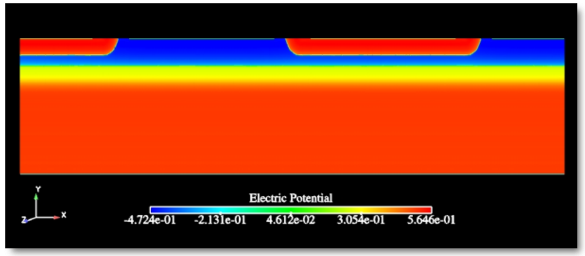
DOE / NNSA

Rapid Development of New Physics

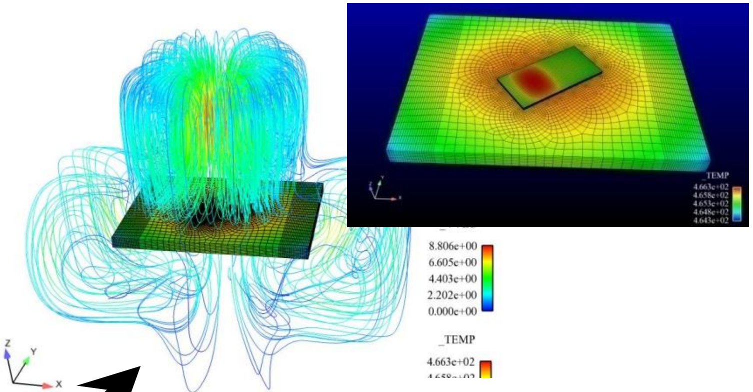
(Single driver and collection of interchangeable physics models)



NGNP Reactor

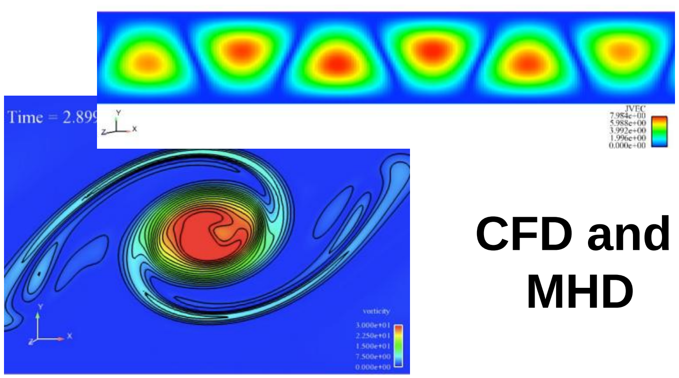


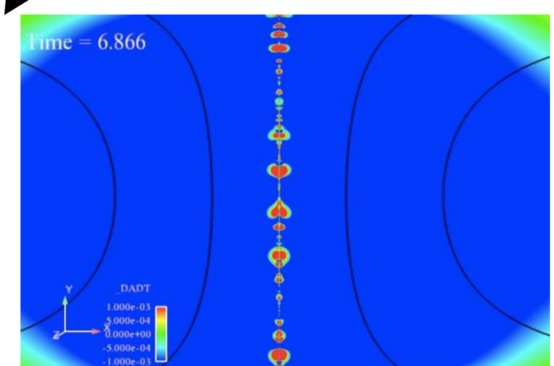
Semiconductor Drift Diffusion



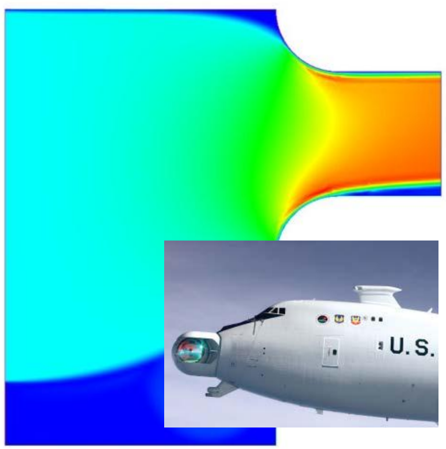
Chemicurrent

CHARON





CFD and MHD



Multi-phase Chemically Reacting Aerosol

Our Philosophy

- Leverage all of Trilinos
- Where appropriate, generalize your application code into Trilinos packages!
  - Object-oriented, lightweight, flexible components that can be swapped out according to bleeding edge research in Trilinos (Exascale)!
- Relevant Trilinos packages:
  - Trilinos/Phalanx: (Template-based Generic Programming Tools)
    - Developed in 2009
  - Trilinos/Panzer: General Finite Element Assembly Engine
    - Started Oct 2010
  - Drekar (Trilinos package in external repository)
    - Started late December 2010
- A Target application: CASL Grid-to-Rod Fretting:
  - Code V&V, Initial demonstration runs, and VUQ analysis
  - Due June 30th 2011

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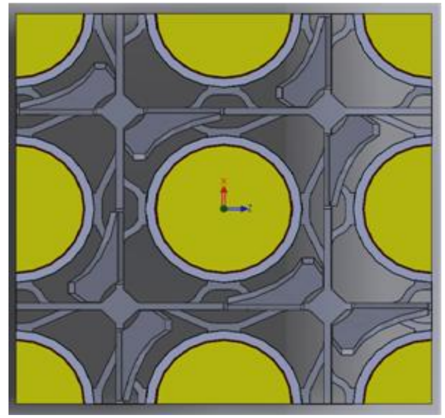
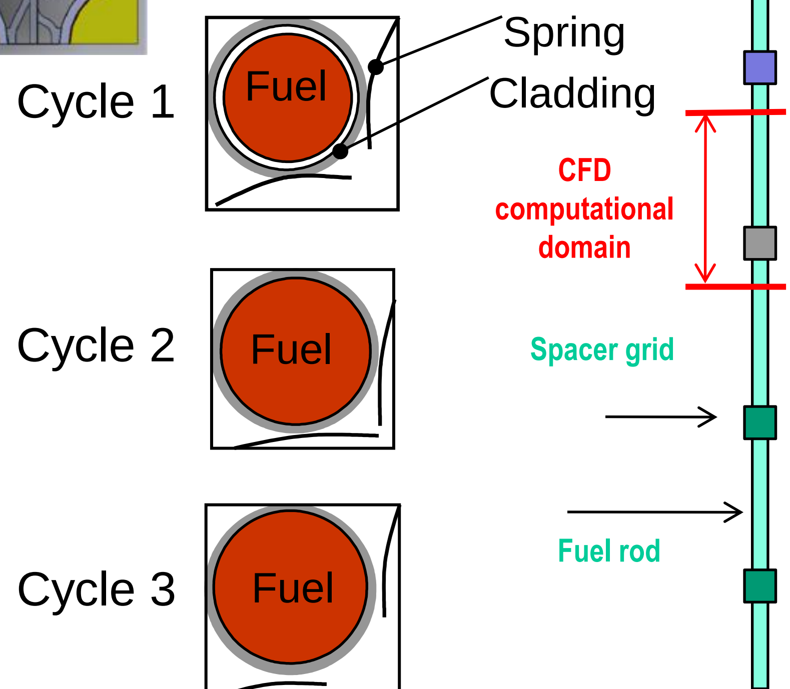
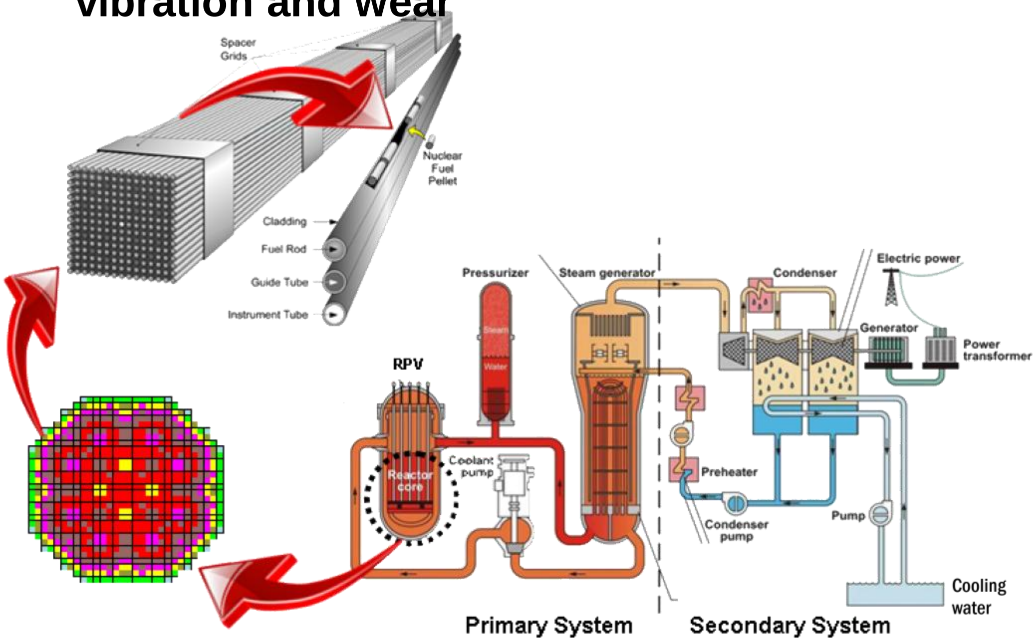
Challenge Problem: Grid-to-Rod Fretting

- Cladding failure can occur as the result of flow induced vibration
- Mixing vanes on spacer grid are used to produce turbulence to improve heat transfer between rod and fluid
- High-fidelity, FSI to predict gap, turbulent flow excitation, rod vibration and wear



Spacer grid cell





Governing Equations
(Unsteady Single-phase, Isothermal, Incompressible Flow)

- Navier-Stokes with spatially filtered LES

Momentum $$R_{\mathbf{u}} = \frac{\partial(\bar{\rho}\bar{\mathbf{u}})}{\partial t} + \nabla \cdot (\bar{\rho}\bar{\mathbf{u}} \otimes \bar{\mathbf{u}} - \mathbf{T})$$

Continuity $$R_p = \frac{\partial \bar{\rho}}{\partial t} + \bar{\rho} \nabla \cdot \bar{\mathbf{v}}$$

over bar denotes spatial filtering in LES

$$\mathbf{T} = -\bar{P}\mathbf{I} + \mu_{eff}(\nabla \bar{\mathbf{u}} + \nabla \bar{\mathbf{u}}^T)$$

$$\mu_{eff} = \mu + \mu_t$$ (molecular and eddy viscosity)

$$\mu_t = \bar{\rho}\nu_t$$

$$\bar{\mathbf{S}}_{ij} = \frac{1}{2}\left(\frac{\partial \bar{\mathbf{u}}_i}{\partial \mathbf{x}_j} + \frac{\partial \bar{\mathbf{u}}_j}{\partial \mathbf{x}_i}\right) \quad \bar{\Omega}_{ij} = \frac{1}{2}\left(\frac{\partial \bar{\mathbf{u}}_i}{\partial \mathbf{x}_j} - \frac{\partial \bar{\mathbf{u}}_j}{\partial \mathbf{x}_i}\right)$$

$$\nu_t = (C_w \Delta)^2 \frac{\left(\bar{\mathbf{S}}^d_{ij}\bar{\mathbf{S}}^d_{ij}\right)^{3/2}}{\left(\bar{\mathbf{S}}_{ij}\bar{\mathbf{S}}_{ij}\right)^{5/2} + \left(\bar{\mathbf{S}}^d_{ij}\bar{\mathbf{S}}^d_{ij}\right)^{5/4}}$$

$$\bar{\mathbf{S}}^d_{ij} = \bar{\mathbf{S}}_{ik}\bar{\mathbf{S}}_{kj} + \bar{\Omega}_{ik}\bar{\Omega}_{kj} - \frac{1}{3}\delta_{ij}\left[\bar{\mathbf{S}}_{mn}\bar{\mathbf{S}}_{mn} + \bar{\Omega}_{mn}\bar{\Omega}_{mn}\right]$$

- Wall Adapting Local Eddy-viscosity model (WALE)
  - Nicoud, F. and Ducros, F., “Subgrid-Scale Stress Modelling on the Square of the Velocity Gradient Tensor,” Flow Turbulence and Combustion, Vol. 62, 1999, pp. 183-200.
- Modified Smagorinsky eddy-viscosity model
  - Filter width is based on the square of the deviatoric stress tensor
  - Requires only "local data" to construct.
  - Recovers the proper near-wall scaling for the eddy viscosity so that it inherently decays to zero as the wall is approached without using a dynamic procedure or wall model

Spatial Discretization

- Stabilized Galerkin Finite Element 2nd order (2nd-8th available)
- PSPG allows equal order interpolation of velocity and pressure
- SUPG operator to limit oscillations in high grid Re flows.

$$\mathbf{F}_{\mathbf{m}i} = \underbrace{\int_{\Omega} \Phi R_{u_i} d\Omega}_{\text{Galerkin}} + \underbrace{\sum_e \int_{\Omega_e} \tau_m \left(\bar{\mathbf{u}} \cdot \nabla \Phi\right) R_{u_i} d\Omega}_{\text{SUPG}}$$

$$\mathbf{F}_{\mathbf{p}} = \underbrace{\int_{\Omega} \Phi R_p d\Omega}_{\text{Galerkin}} + \underbrace{\sum_e \int_{\Omega_e} \bar{\rho} \tau_m \left(\nabla \Phi \cdot R_u\right) d\Omega}_{\text{PSPG}}$$

- Future work will extend to full VMS-LES models
  - T.J.R. Hughes, L. Mazzei, K.E. Jansen, Large eddy simulation and the variational multiscale method, Comput. Vis. Sci. Vol. 3, 2000, pp. 47-59

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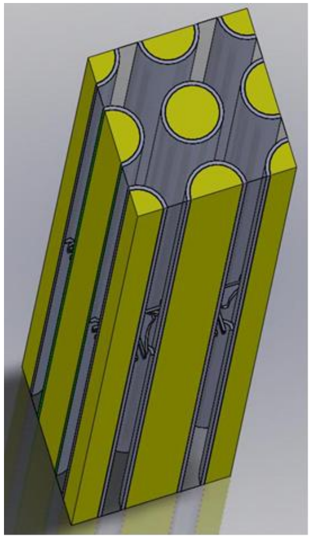
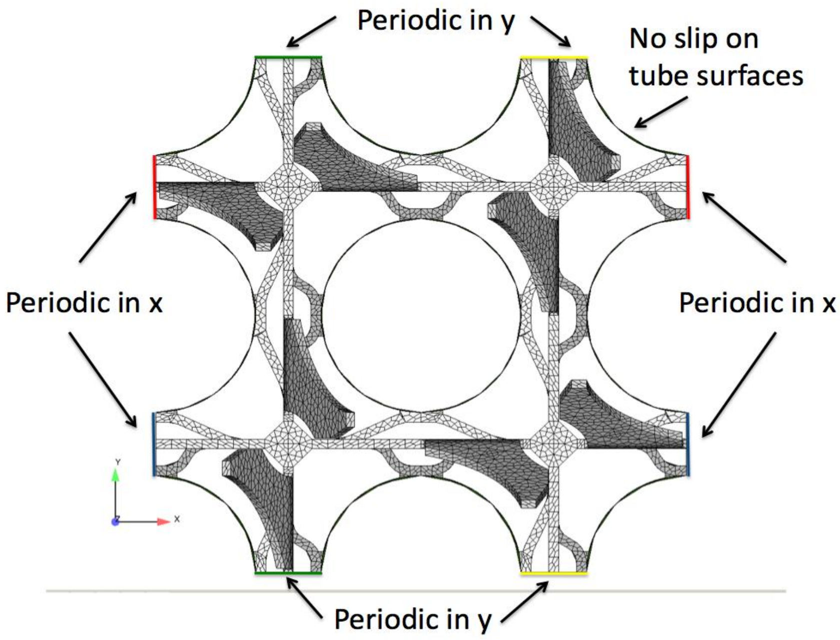
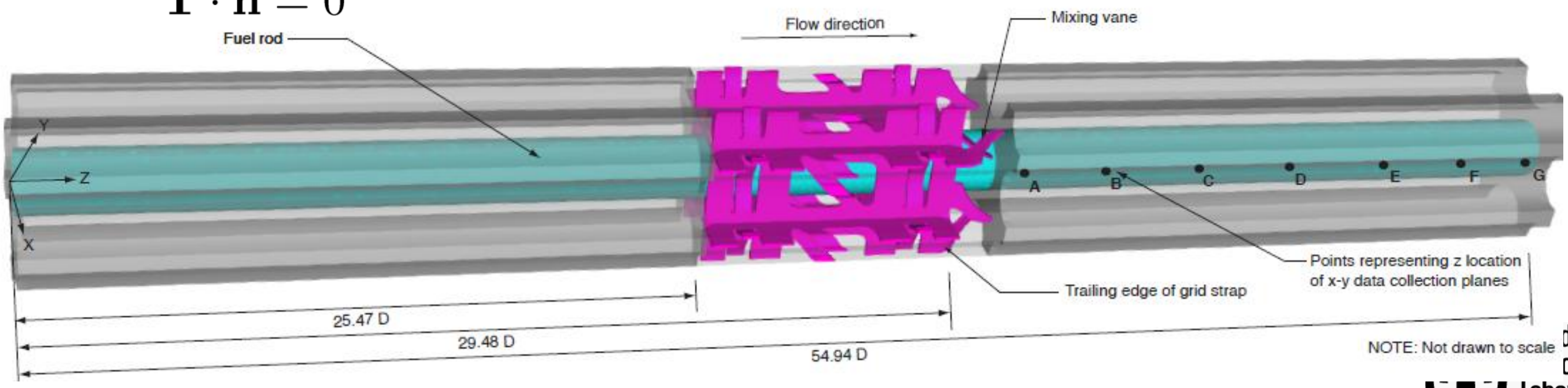
Problem Description (3x3 Rod Bundle)

- Isothermal
- Fluid: Water
  - T: 394K
  - Viscosity: 2.32×10^{-4} Pa sec
  - Density: 924 kg/m^3
- Re ~ 2x10^5
- Symmetry on sides
- No slip (v=0) on rods
- Inflow on bottom
  - 5 m/sec
- Outflow on top:

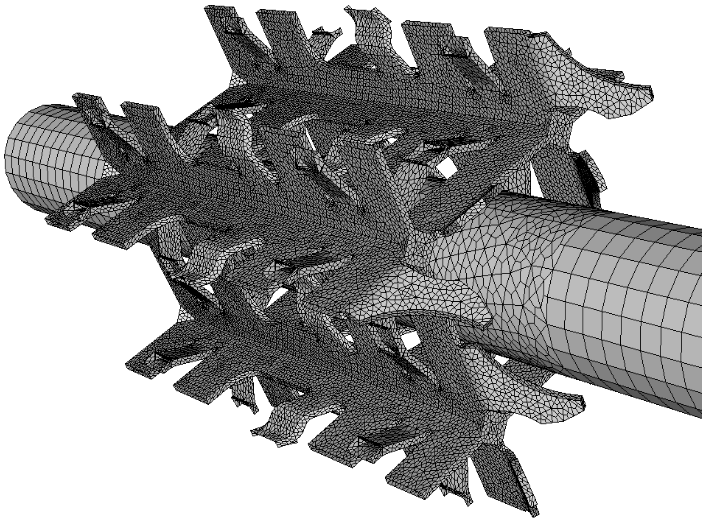
$$\mathbf{T} \cdot \mathbf{n} = 0$$

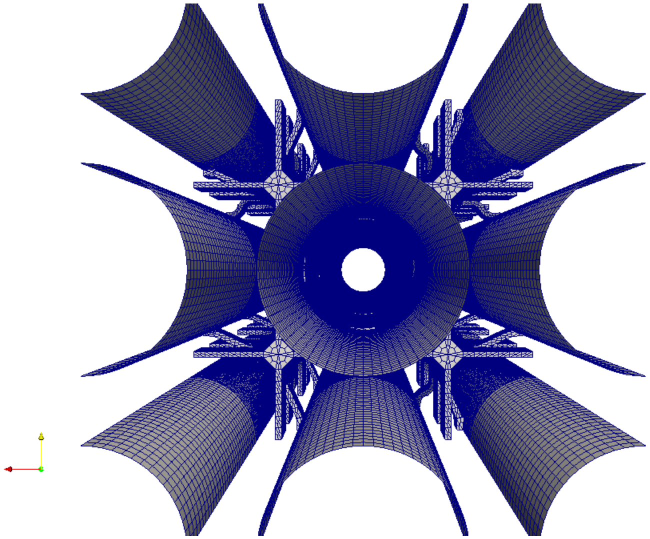


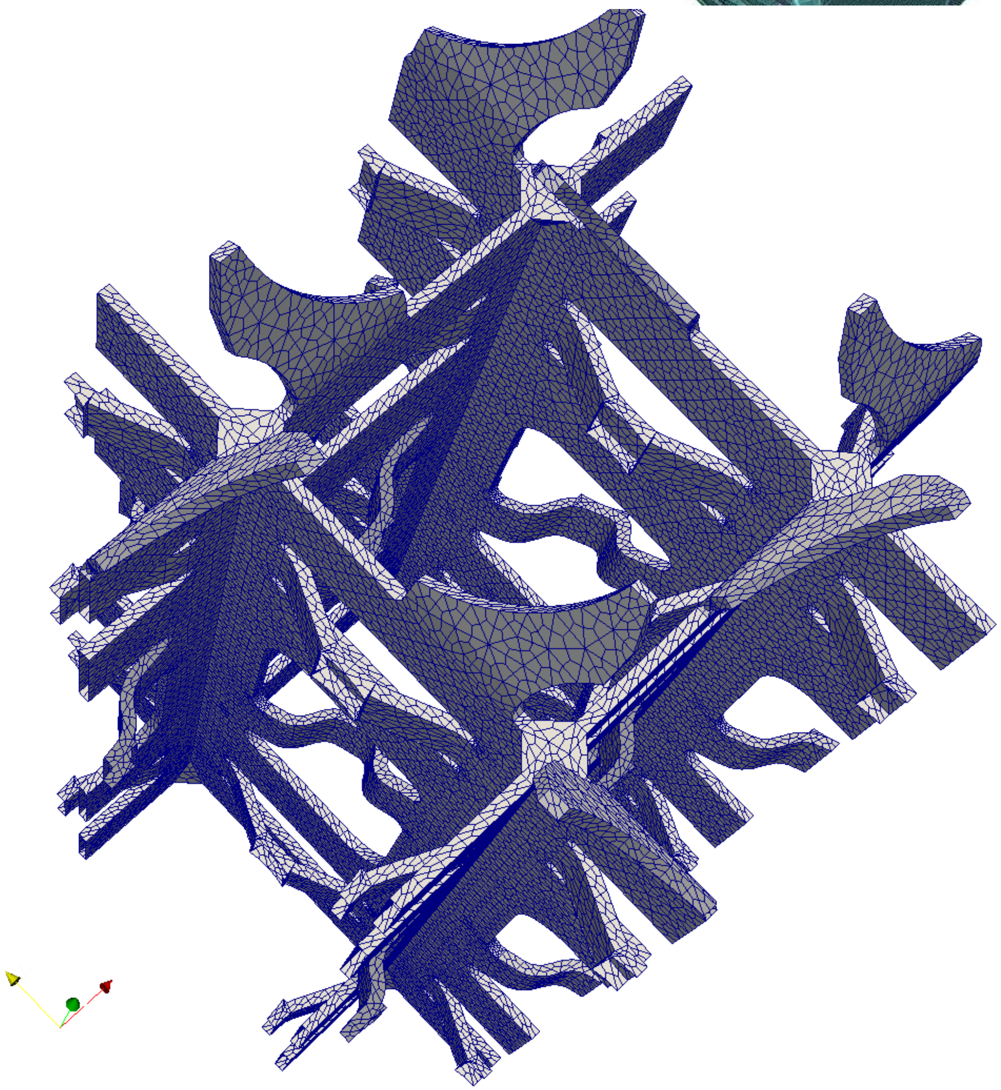




Geometry
(Hexahedral Elements)







Code Design

Agile Components (A. Salinger): Trilinos has a coordinated integration effort (ASC) to support all aspects of a simulation!

Analysis Tools (*non-invasive*)
- Optimization
- Parameter Studies
- UQ (non-invasive)
- V&V, Calibration
- OUU, Reliability
- Computational Steering

Analysis Tools (*invasive*)
- Nonlinear Solver
- Time Integration
- Continuation
- Sensitivity Analysis
- Stability Analysis
- Constrained Solves
- Optimization
- UQ Solver

Linear Algebra
- Data Structures
- Iterative Solvers
- Direct Solvers
- Eigen Solver
- Preconditioners
- Matrix Partitioning
- Architecture-Dependent Kernels

Mesh Tools
- Mesh I/O
- Inline Meshing
- Partitioning
- Load Balancing
- Adaptivity
- Remeshing
- Grid Transfers
- Mesh Quality

Mesh Database
- Mesh Database
- Geometry Database
- Solution Database

Local Fill

Discretizations
- Discretization Library
- Variable Manager

Derivative Tools
- UQ / PCE Propagation
- Derivatives
- Sensitivities

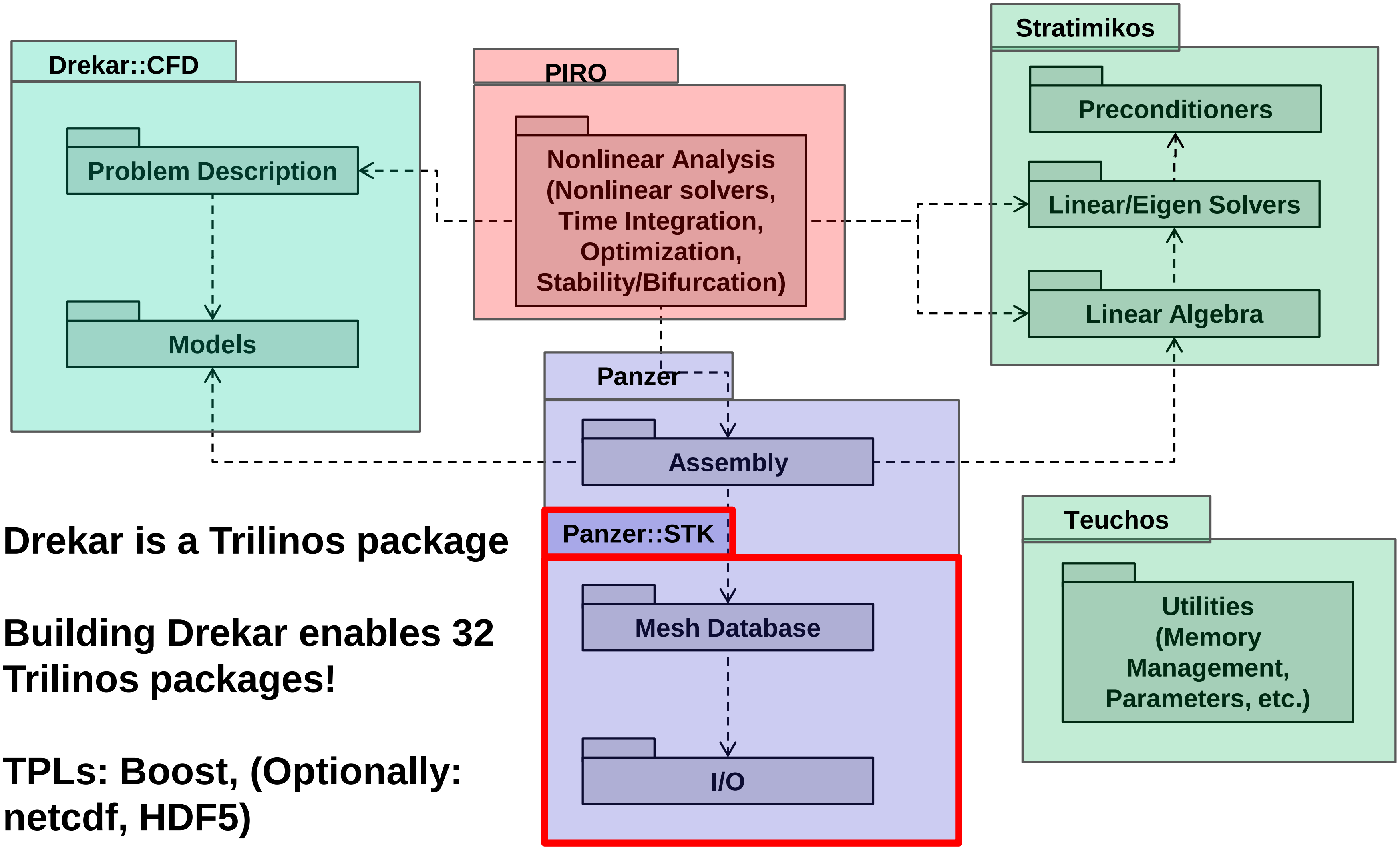
Physics Fill
- Element Level Fill
- Material Models
- Objective Function
- Constraints
- Error Estimates
- MMS Source Terms

Composite Physics
- MultiPhysics Coupling
- Solution Control
- System Models
- System UQ

Utilities
- Input File Parser
- Parameter List
- I/O Management
- Memory Management
- Communicators
- Runtime Compiler
- MultiCore Parallelization Tools

PostProcessing
- Visualization
- Verification Tools
- Feature Extraction
- Data Reduction
- Model Reduction

Software Design
(Composition of Trilinos Packages)



- **Drekar is a Trilinos package**
- **Building Drekar enables 32 Trilinos packages!**
- **TPLs: Boost, (Optionally: netcdf, HDF5)**

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Introducing Drekar

(Named for the Viking Longship)

- A **light-weight front end** "Trilinos package" that provides Stabilized Galerkin CFD and MHD physics
- Provides mathematical kernels to evaluate the discretized PDEs using TBGP concepts
- Panzer/Drekar package dependencies:
  - 10 required
  - 9 optional
- Indirect dependencies: 32 enabled packages (including Drekar itself)

Panzer and Drekar

Trilinos Discretization Tool Stack

(Pawlowski,Cyr, Shadid, Smith)

PIRO (Solvers)
NOX
Rythmos
MOOCHO
LOCA
LIME

Thyra Model Evaluator

Drekar::CFD

- Input ParameterList
- Equation Set Factory
- BC Factory
- Evaluator Factory

Phalanx (TBGP)

Intrepid (FE Basis/IR)

Shards (Cell Topology)

Stokhos (UQ)

Sacado (AD)

Panzer

- **Multiphysics Assembly Engine:**
  - Fully coupled Multiphysics
  - Compatible discretizations
  - Multiple Equation sets
  - Arbitrary BCs
- **DOF Manager**
  - Mapping DOFs
  - ConnectionManager

FEI (DOF Mapping Strategy)

STK (Mesh Database)

SEACAS (I/O, Partitioning)

Assembly Engine

- The assembly engine is the core of the multiphysics support
  - Supplies the residuals, Jacobians, etc. required for fully-coupled/implicit solution methods
  - Supplies physics specific preconditioner operators
- This was discussed in the talk on Panzer this morning!

Graph-based Assembly Process

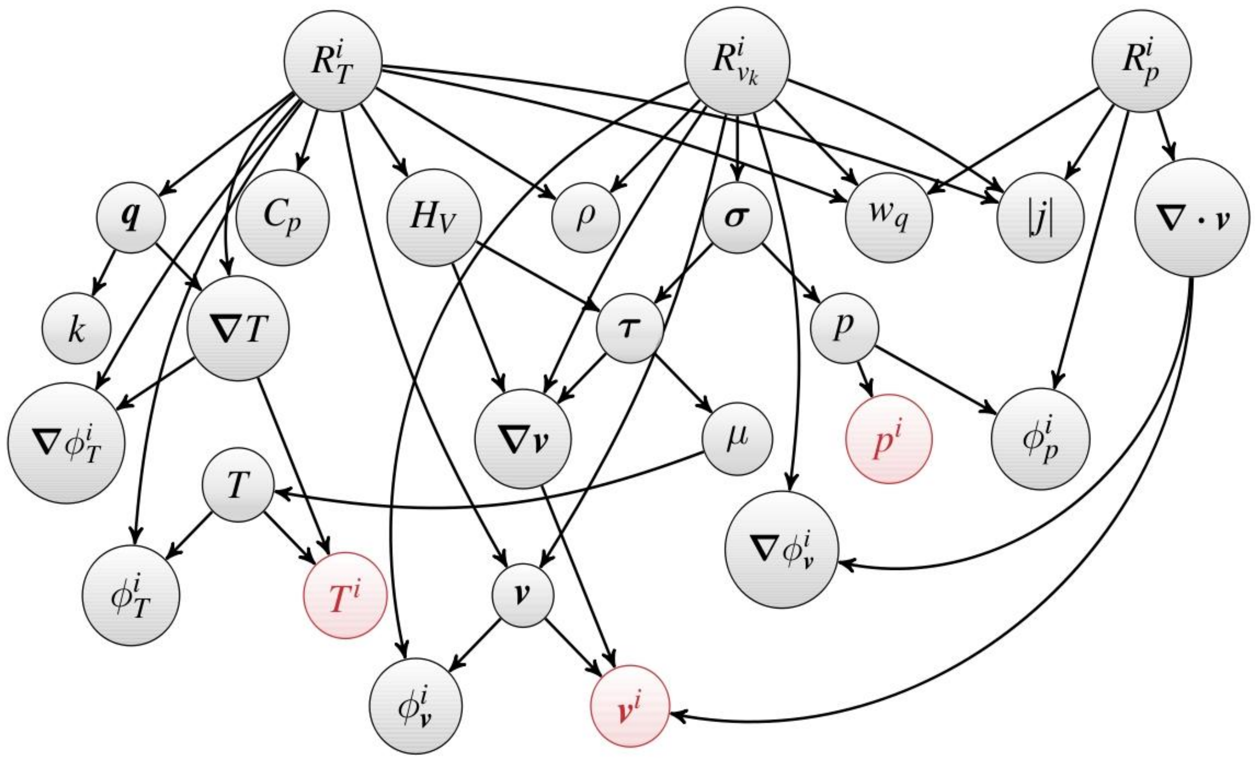
(Notz, Pawlowski, Sutherland; submitted to TOMS)

- Phalanx package
- Graph-based equation description
  - Automated dependency tracking (Topological sort to order the evaluations)
  - Each node is a point of extension that can be swapped out
  - Easy to add equations
  - Easy to change models
  - Easy to test in isolation
- Ideal for multiphysics
  - More equations → adding more nodes to graph
  - Reuse fields
- Multi-core research:
  - Spatial decomposition (Kokkos::MDArray)
  - Algorithmic decomposition

$$R_T^i = \sum_{e=1}^{N_e}\sum_{q=1}^{N_q}\left[\left(\rho C_p \boldsymbol{v}\cdot\nabla T - H_V\right)\phi_T^i - \boldsymbol{q}\cdot\nabla\phi_T^i\right] w_q|j| = 0$$

$$R_{v_k}^i = \sum_{e=1}^{N_e}\sum_{q=1}^{N_q}\left[\rho\boldsymbol{v}\cdot\nabla\boldsymbol{v}\phi_{\boldsymbol{v}}^i + \boldsymbol{\sigma} : \nabla\left(\phi_{\boldsymbol{v}}^i\boldsymbol{e}_k\right)\right] w_q|j| = 0$$

$$R_p^i = \sum_{e=1}^{N_e}\sum_{q=1}^{N_q}\nabla\cdot\boldsymbol{v}\phi_p^i w_q|j| = 0$$



Solution Algorithm Complexity

- Forward solves using implicit methods (Newton-based):

Find $x_* \in \mathbb{R}^n$ **such that** $F(x_*) = 0$ **where** $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$

  – Requires Jacobian or Jacobian vector product (JFNK):

$$J(x)_{ij} = \frac{\partial F_i}{\partial x_j} \qquad J(x) \in \mathbb{R}^{n \times n} \qquad Jv$$

- SAND: PDE Const. Optimization, Stability Analysis, Bifurcation Analysis:
  – Parameter sensitivities
  – Hessian

$$\frac{\partial F}{\partial p} \qquad \frac{\partial^2 F}{\partial x_i \partial x_j}$$

- Concept: Template-Based Generic Programming
  – Decouple the physics description from the requirements of the solution/analysis capabilities
  – The key: in c++, template the *scalar type and overload math operators using expression templates*

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Generic Programming Example: Templating the Scalar Type

$$f_0 = 2x_0 + x_1^2$$
$$f_1 = x_0^3 + sin(x_1)$$

```
// double version
void computeF(double* x, double* f)
{
  f[0] = 2.0 * x[0] + x[1] * x[1];
  f[1] = x[0] * x[0] * x[0] + sin(x[1]);
}
```

```
void computeJ(double* x, double* J)
{
  // J(0,0)
  J[0] = 2.0;
  // J(0,1)
  J[1] = 2.0 * x[1];
  // J(1,0)
  J[2] = 3.0 * x[0] * x[0];
  // J(1,1)
  J[3] = cos(x[1]);
}
```

Writing derivatives in the context of multiphysics systems with changing dependency chains is difficult and error prone!

```
// ad version
template <typename ScalarT>
void computeF(ScalarT* x, ScalarT* f)
{
  f[0] = 2.0 * x[0] + x[1] * x[1];
  f[1] = x[0] * x[0] * x[0] + sin(x[1]);
}
```

ScalarT → double	Residual
ScalarT → Dfad<double>	Jacobian

Machine precision accuracy: No FD involved!

Generic Programming

(using data types from Trilinos/Sacado: E. Phipps)

Field Manager is templated on Evaluation Type

Concept: Evaluation Types

- **Residual** $F(x,p)$ — `double`
- **Jacobian** $J = \frac{\partial F}{\partial x}$ — `DFad<double>`
- **Hessian** $\frac{\partial^2 F}{\partial x_i \partial x_j}$ — `DFad< DFad<double> >`
- **Parameter Sensitivities** $\frac{\partial F}{\partial p}$ — `DFad<double>`
- **Jv** Jv — `DFad<double>`
- **Stochastic Galerkin Residual** — `Sacado::PCE::OrthogPoly<double>`
- **Stochastic Galerkin Jacobian** — `Sacado::Fad::DFad< Sacado::PCE::OrthogPoly<double> >`

Scalar Types

(listed beside each evaluation type above)

NOTES:

1. Not tied to double (can do arbitrary precision)
2. Not tied to any one scalar type can use multiple scalar types in any evaluation type!

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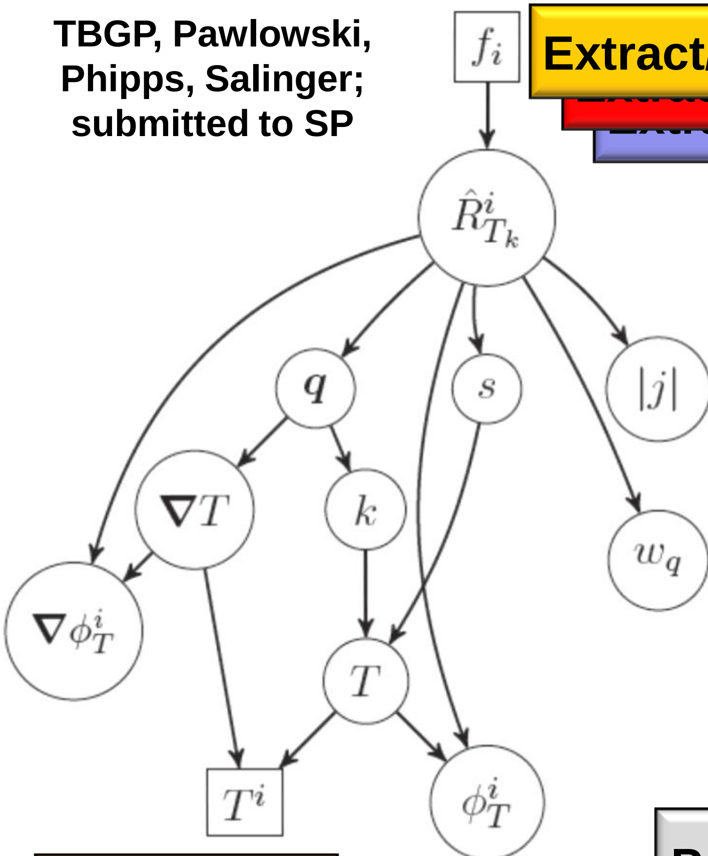
Phalanx Handles Multiphysics Complexity using Template-based Generic Programming

TBGP, Pawlowski, Phipps, Salinger; submitted to SP

Extract/Scatter



Gather/Seed

$$f(x) = \sum_{k=1}^{N_w} f_k = \sum_{k=1}^{N_w} Q_k^T \hat{R}^i_{T_k}(P_k x)$$

$$\hat{R}^i_T = \sum_{e=1}^{N_e} \sum_{q=1}^{N_q} \left[-\nabla \phi^i_T \cdot q + \phi^i_T s \right] w_q |j| = 0$$

Evaluation Type	Scalar Type
$f(x,p)$	`double`
$J = \frac{\partial f}{\partial x}$	`DFad<double>`
$\frac{\partial^2 f}{\partial x_i \partial x_j}$	`DFad< DFad<double> >`

Param. Sens., Jv, Adjoint, PCE (SGF, SGJ), Arb. Prec.

`PCE::OrthogPoly<double>`

`DFad<PCE::OrthogPoly<double> >`

Take Home Message:
Reuse the same code base!
Equations decoupled from algorithms!
Machine precision accuracy!

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Flexibility of Evlauation Types

```
struct Traits : public PHX::TraitsBase  {

  // ***************************************************************
  // *** Scalar Types
  // ***************************************************************
  typedef double RealType;
  typedef Sacado::Fad::DFad<RealType> FadType;

  #ifdef HAVE_STOKHOS
    typedef Stokhos::StandardStorage<int,RealType> SGStorageType;
    typedef Sacado::PCE::OrthogPoly<RealType,SGStorageType> SGType;
    typedef Sacado::Fad::DFad<SGType> SGFadType;
  #endif

  // ***************************************************************
  // *** Evaluation Types
  // ***************************************************************
  struct Residual { typedef RealType ScalarT; };
  struct Jacobian { typedef FadType ScalarT;  };

  #ifdef HAVE_STOKHOS
    struct SGResidual { typedef SGType ScalarT; };
    struct SGJacobian { typedef SGFadType ScalarT;  };
  #endif
```

```
// ***************************************************************
// *** MPL Vector of Evaluation Types
// ***************************************************************

typedef Sacado::mpl::vector<Residual, Jacobian
                     #ifdef HAVE_STOKHOS
                       , SGResidual, SGJacobian
                     #endif
                    > EvalTypes;
```

Jacobian-Free Newton-Krylov (JFNK)

$$x_{k+1} = x_k + \alpha \Delta x$$

$$J_k \triangle x = -F_k$$

<u>**Iterative Linear Solver – GMRES**</u>

Krylov Subspace of the form:

$$\mathcal{K}(A, v) \equiv \text{span}\{v, Av, A^2 v, ..., A^{m-1} v\}$$

In the inner iteration of the linear solve, we only need the action of the Jacobian on a vector:

$$Jv \approx \frac{F(x + \delta v) - F(x)}{\delta}$$

Only require an explicit matrix for preconditioning – does NOT have to be exact!

Advantages:

- <u>**Same as Newton, but no Jacobian is required**</u>**!**
- **Residual Based!**

Disadvantage:

- **Accuracy/convergence issues due to scalar perturbation factor:**

$$\delta = \lambda \left(\lambda + \frac{||\mathbf{x}||}{||\mathbf{v}||} \right)$$

- **Solution vector scaling is critical**

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Example: JFNK
(2D Diffusion/Rxn System: 2 eqns)

- **JFNK (FD)**

$$Jv \approx \frac{F(x+\delta v) - F(x)}{\delta}$$

$$t \approx (\text{num\_Its}) * cost(F)$$

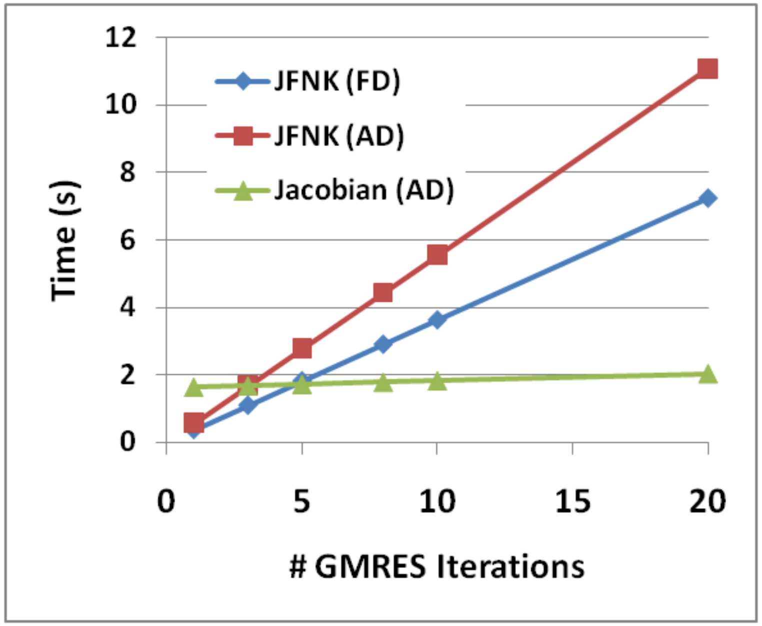
- **JFNK (AD)**
  - **Machine precision accurate**
  - **Ex: Solution varies 10^12 over domain**

$$Jv \leq 2.5 * cost(F)$$
$$t \approx 1.53 * (num\_Its) * cost(F)$$

- **Explicit Jacobian (AD generated)**
  - **Machine precision accurate**
  - **Complexity ideas allow for storing individual operators for preconditioning!**
  - **Larger memory requirements**

$$J(x) \leq 13 * cost(F)$$
$$t \approx 4.45 + (num\_Its) * cost(Mv)$$

	Relative times	
JFNK (AD)	F(x)	1.00
Explicit J (AD)	J(x)	4.45
JFNK (AD)	Jv (AD)	1.53
Explicit J (AD)	Mv (matvec)	0.06



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Build System

- Panzer and Drekar are both Trilinos packages
  - Panzer will be released as official Trilinos package
- Reside in separate git repository
  - Uses external Trilinos package support
- Leverage the build and testing infrastructure
- Under CI, nightly testing as part of CASL

Utilities

- Memory Management
  - **Teuchos** memory management classes: RCP, ArrayRCP, …
  - Has some important features missing in boost/tr1
    - Array view semantics, extra data
  - Common look and feel with Trilinos packages

- Input Objects are constructed with Teuchos ParameterLists
  - Validation is critical for robust usage
  - Common look and feel with Trilinos packages

- Boost (Phalanx Assembly)
  - Template metaprogramming library (MPL)
  - Graph library
  - Tokenizer (for one input path)
  - Hash Table

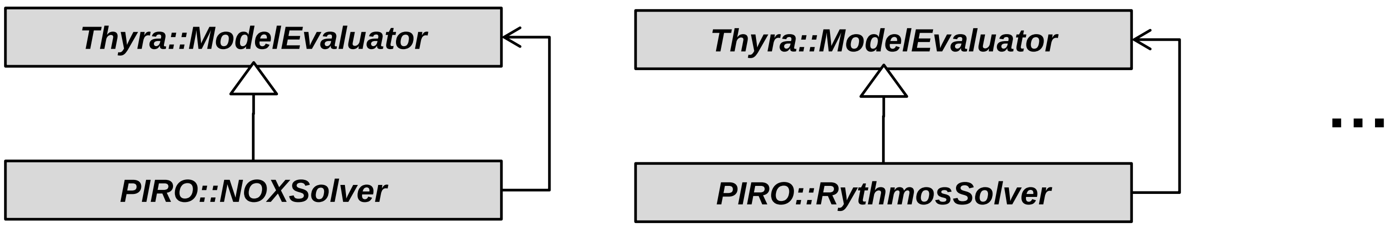
Problem Description

- Driven by Teuchos::ParameterList
  - Runtime configurable database
  - Let developers write their own front end to populate:
    - XML (automatically supported)
    - GUI (Trilinos/Optika/QT)
    - Traditional text parsing (boost::tokenizer)

- Issues
  - ParameterList XML reader does not preserve ordering (not standards compliant)
  - Validation doesn't quite support our use case
    - Dynamic (user defined) trees: sublist names are designated by the user at runtime

Nonlinear Analysis

- We use the PIRO package to interface to nonlinear analysis tools
  - Gives access to NOX, LOCA, Rythmos, and MOOCHO through a single interface
  - Model evaluator driven
  - **ParameterList + ModelEvaluator (+ optional observers) = Solver**



Building a Nonlinear Analysis Model Evaluator is this Simple!

```
RCP<Teuchos::ParameterList> piro_params =
  Teuchos::rcp(new Teuchos::ParameterList(solncntl_params));

RCP<Thyra::ModelEvaluatorDefaultBase<double> > piro;

if (solver=="NOX") {
  piro = Teuchos::rcp(new Piro::NOXSolver<double>(piro_params, drekar_me));
}
else if (solver=="Rythmos") {
  piro = Teuchos::rcp(new Piro::RythmosSolver<double>(piro_params, drekar_me,
            observer_factory->buildRythmosObserver(mesh,dofManager,ep_lof)));
}
else {
```

Why Newton-Krylov Methods?

Newton-Krylov

Direct-to-steady-state

Fully-implicit transient

Convergence properties

- Strongly coupled multi-physics often requires a strongly coupled nonlinear solver
- Quadratic convergence near solutions (backtracking, adaptive convergence criteria)
- Often only require a few iterations to converge, if close to solution, independent of problem size

$$\mathbf{F}(\mathbf{x}, \lambda_1, \lambda_2, \lambda_3, ..) = \mathbf{0}$$

Inexact Newton-Krylov

Solve $\mathbf{J}\mathbf{p}_k = -\mathbf{F}(\mathbf{x}_k)$; until $\dfrac{\|\mathbf{J}\mathbf{p}_k + \mathbf{F}(\mathbf{x}_k)\|}{\|\mathbf{F}(\mathbf{x}_k)\|} \le \eta_k$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \Theta \mathbf{p}_k$$

Jacobian Free N-K Variant

$$\mathbf{M}\mathbf{p}_k = \mathbf{v}$$

$$\mathbf{J}\mathbf{p}_k = \frac{\mathbf{F}(\mathbf{x} + \delta \mathbf{p}_k) - \mathbf{F}(\mathbf{x})}{\delta}\ ;\ \text{or by AD}$$

See e.g. Knoll & Keyes, JCP 2004

Why Newton-Krylov Methods?

Newton-Krylov

Direct-to-steady-state

Fully-implicit transient

$$\mathbf{F}(\dot{\mathbf{x}},\mathbf{x},\lambda_1,\lambda_2,\lambda_3,..)=\mathbf{0}$$

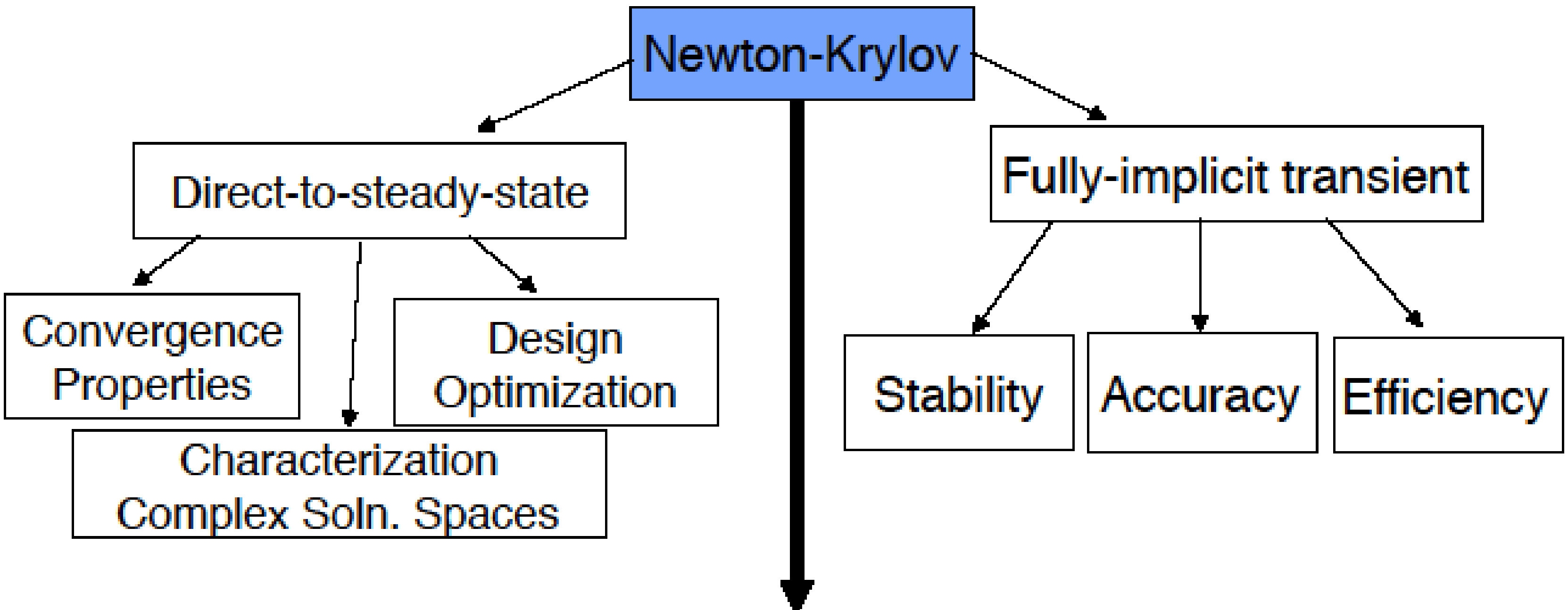
e.g.

$$\left.\frac{\partial c}{\partial t}\right|^{n+1}+\nabla\bullet\left(\left[\rho c\mathbf{u}\right]^{n+1}\right)-\nabla\bullet\left[D^{n+1}\nabla c^{n+1}\right]+S_c^{n+1}=0$$

<u>Stability and Accuracy Properties</u>

- Stable (stiff systems)
- High order methods
- Variable order techniques
- Local and global error control possible
- Can be stable and accurate run at the dynamical time-scale of interest in multiple-time-scale systems (e.g. Knoll et. al., Brown & Woodward., Chacon and Knoll, Ropp & S.)

Why Newton-Krylov Methods?

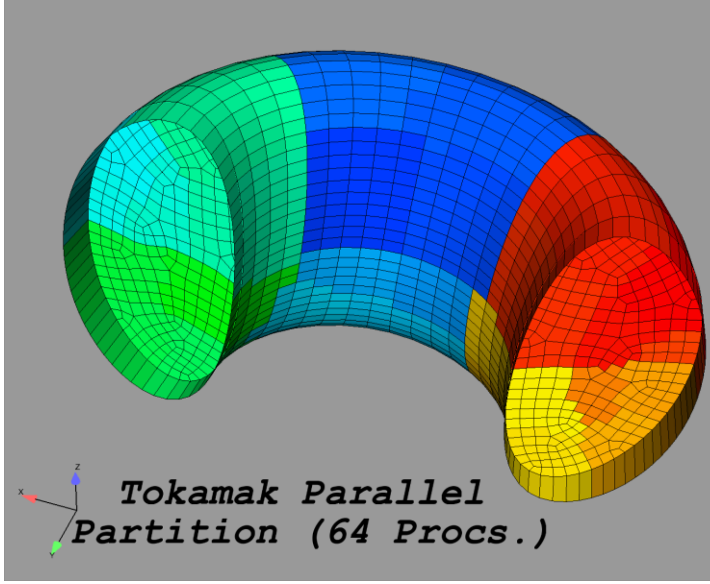


Very Large Problems -> Parallel Iterative Solution of Sub-problems

Krylov Methods - Robust, Scalable and Efficient Parallel Preconditioners

- Approximate Block Factorizations
- Physics-based Preconditioners
- Multi-level solvers for systems and scalar equations

Preconditioning



Three variants of preconditioning

1. Domain Decomposition (Trilinos/Aztec & IFPack)

- ILU(k) Factorization on each processor (with overlap)
- High parallel efficiency, non-optimal algorithmic scalability

2. Multilevel methods: Trilinos/ML Package

Fully-coupled Algebraic Multilevel methods

- Consistent set of DOF at each node (stabilized FE)
- Aggregation rate chosen to fix coarse grid size
- Jacobi, GS, ILU(k) as smoothers
- Can provide optimal algorithmic scalability

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

3. Approximate Block Factorization / Physics-based: Trilinos/Teko package

- Applies to mixed interpolation (FE) or staggered (FV) discretization approaches
- Applied to systems where AMG is difficult or might fail
- Can provide optimal algorithmic scalability

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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
$\begin{pmatrix} F & B^T \\ \hat{B} & -C \end{pmatrix} \begin{pmatrix} \Delta \mathbf{u}_k \\ \Delta p_k \end{pmatrix} = \begin{pmatrix} \mathbf{g}_\mathbf{u}^\mathbf{k} \\ g_p^k \end{pmatrix}$	$\begin{pmatrix} I & 0 \\ \hat{B}F^{-1} & I \end{pmatrix} \begin{pmatrix} F & 0 \\ 0 & -S \end{pmatrix} \begin{pmatrix} I & F^{-1}B^T \\ 0 & I \end{pmatrix}$ $S = C + \hat{B}F^{-1}B^T$	$\begin{bmatrix} I & 0 \\ \hat{B}H_1 & I \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & -\hat{S} \end{bmatrix} \begin{bmatrix} I & H_2B^T \\ 0 & I \end{bmatrix}$

Precond. Type	H_1	H_2	$\hat{S}$	References
Pres. Proj; 1st Term Nuemann Series	$\mathbf{F}^{-1}$	$(\mathbf{\Delta t I})^{-1}$	$\mathbf{C} + \mathbf{\Delta t \hat{B} B^T}$	Chorin(1967);Temam (1969); Perot (1993): Quateroni et. al. (2000) as solvers
SIMPLEC	$\mathbf{F}^{-1}$	$(\mathbf{diag}(\sum \lvert\mathbf{F}\rvert))^{-1}$	$\mathbf{C} + \hat{\mathbf{B}}(\mathbf{diag}(\sum \lvert\mathbf{F}\rvert))^{-1}\mathbf{B^T}$	Patankar et. al. (1980) as solvers; Pernice and Tocci (2001) smothers/MG
Pressure Convection / Diffusion	0	$\mathbf{F}^{-1}$	$\mathbf{A_p F_p^{-1}}$	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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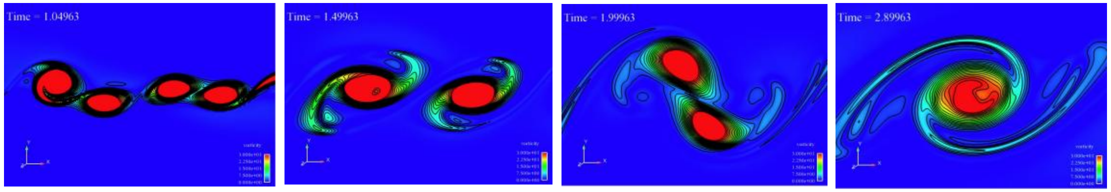
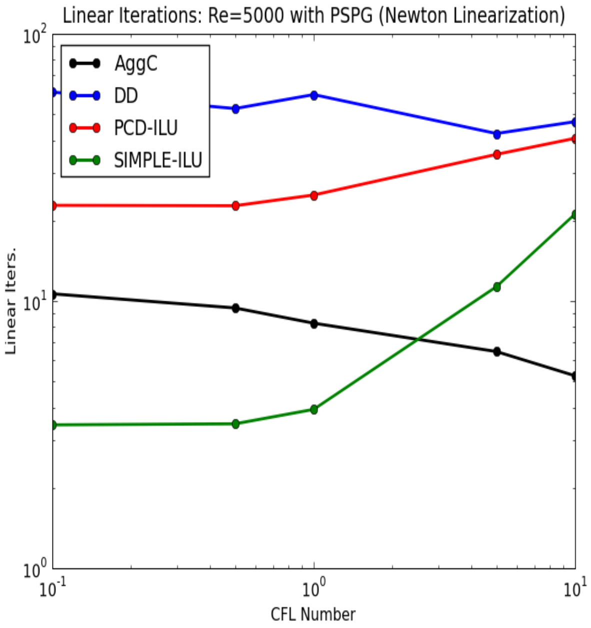
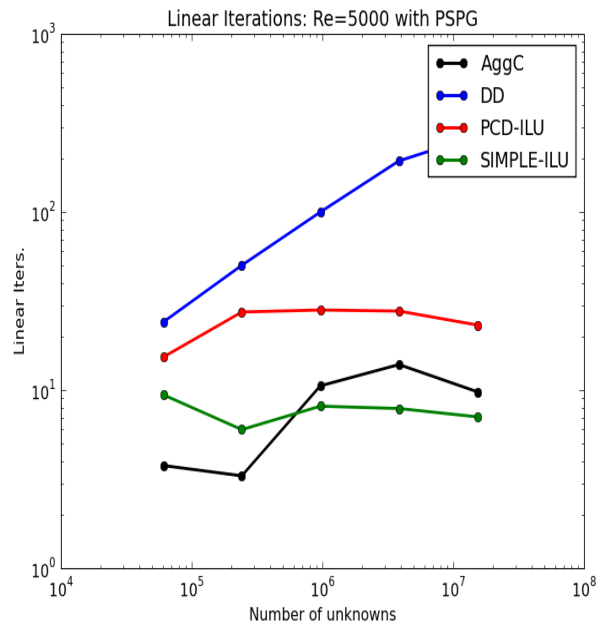
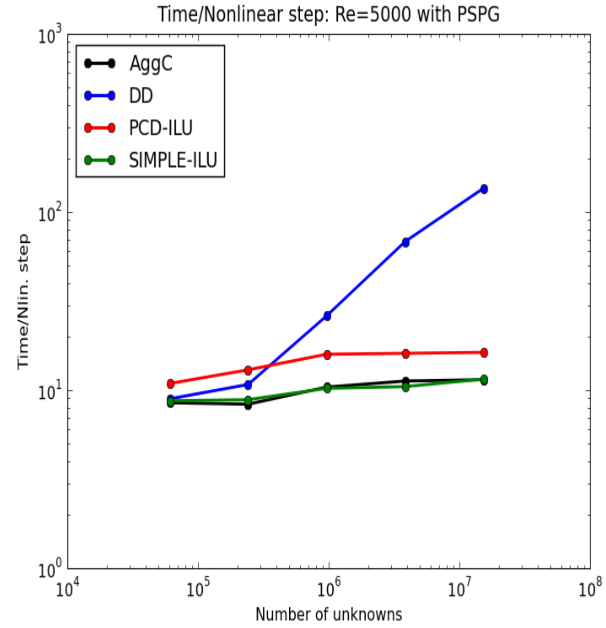
Transient Kelvin-Helmholtz









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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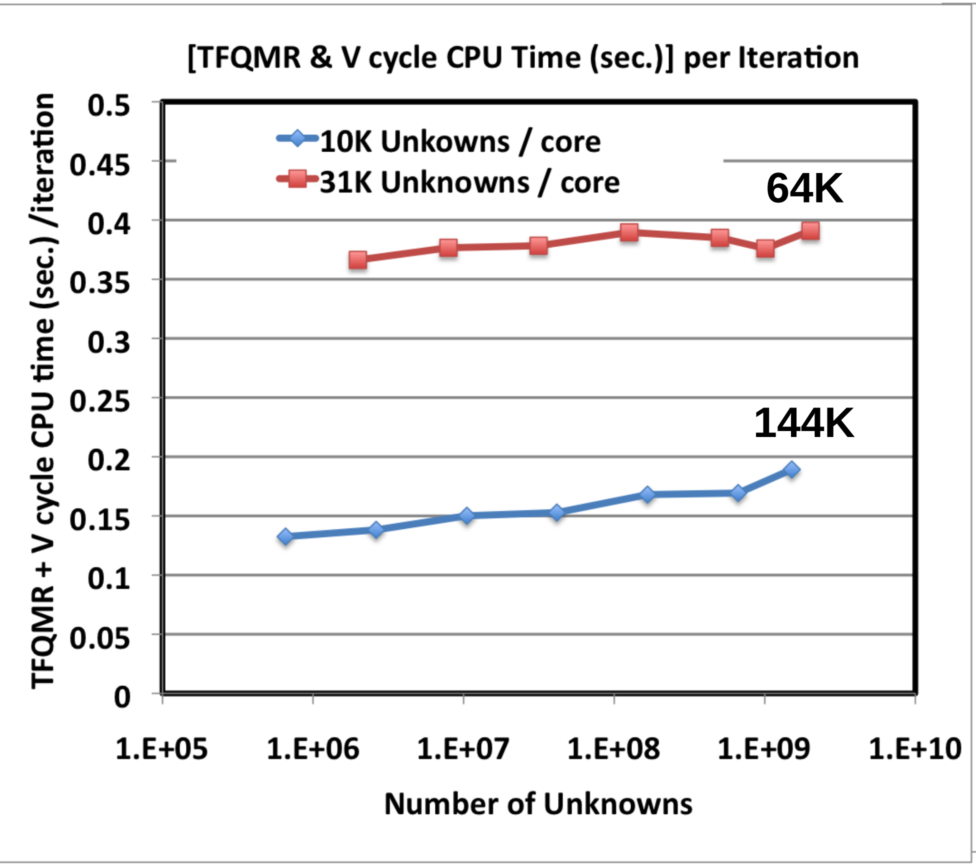
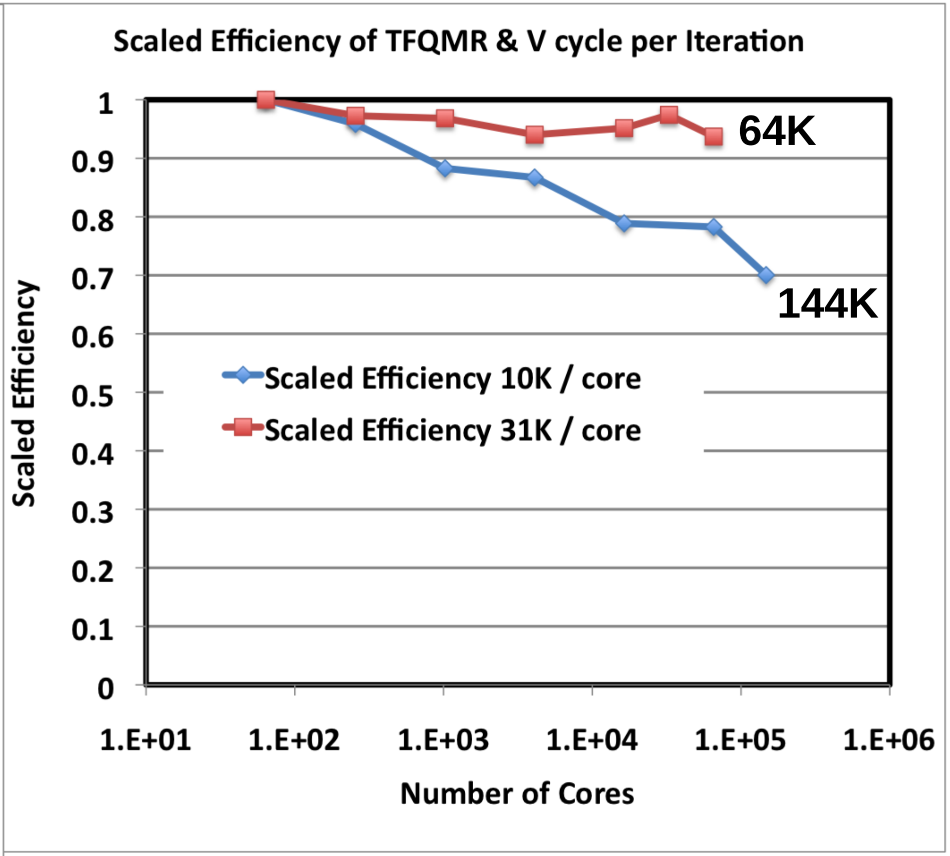
Weak Scaling Uncoupled Aggregation Scheme: Time/iteration on BlueGene/P (Drift – Diffusion BJT: P. Lin)





- 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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Linear and Eigen Solvers

- We use the Stratimikos package for linear solvers
  - ParameterList driven assembly of all linear solvers and eigensolvers in Trilinos
    - AztecOO, Belos, Amesos
    - "Linear Operator with Solve" (LOWS)
    - Preconditioner support included (Ifpack, ML, Teko, …)
  - Assembles Thyra objects:
- Anasazi (Eigensolver) is accessed
  - Indirectly via LOCA stability analysis

Building a linear solver is this simple!

```
Stratimikos::DefaultLinearSolverBuilder linearSolverBuilder;

linearSolverBuilder.setParameterList(strat_params);

RCP<Thyra::LinearOpWithSolveFactoryBase<double> > lowsFactory =
    createLinearSolveStrategy(linearSolverBuilder);

RCP<Thyra::ModelEvaluatorDefaultBase<double> > thyra_me =
  Thyra::epetraModelEvaluator(ep_me,lowsFactory);
```

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Linear Algebra Layer

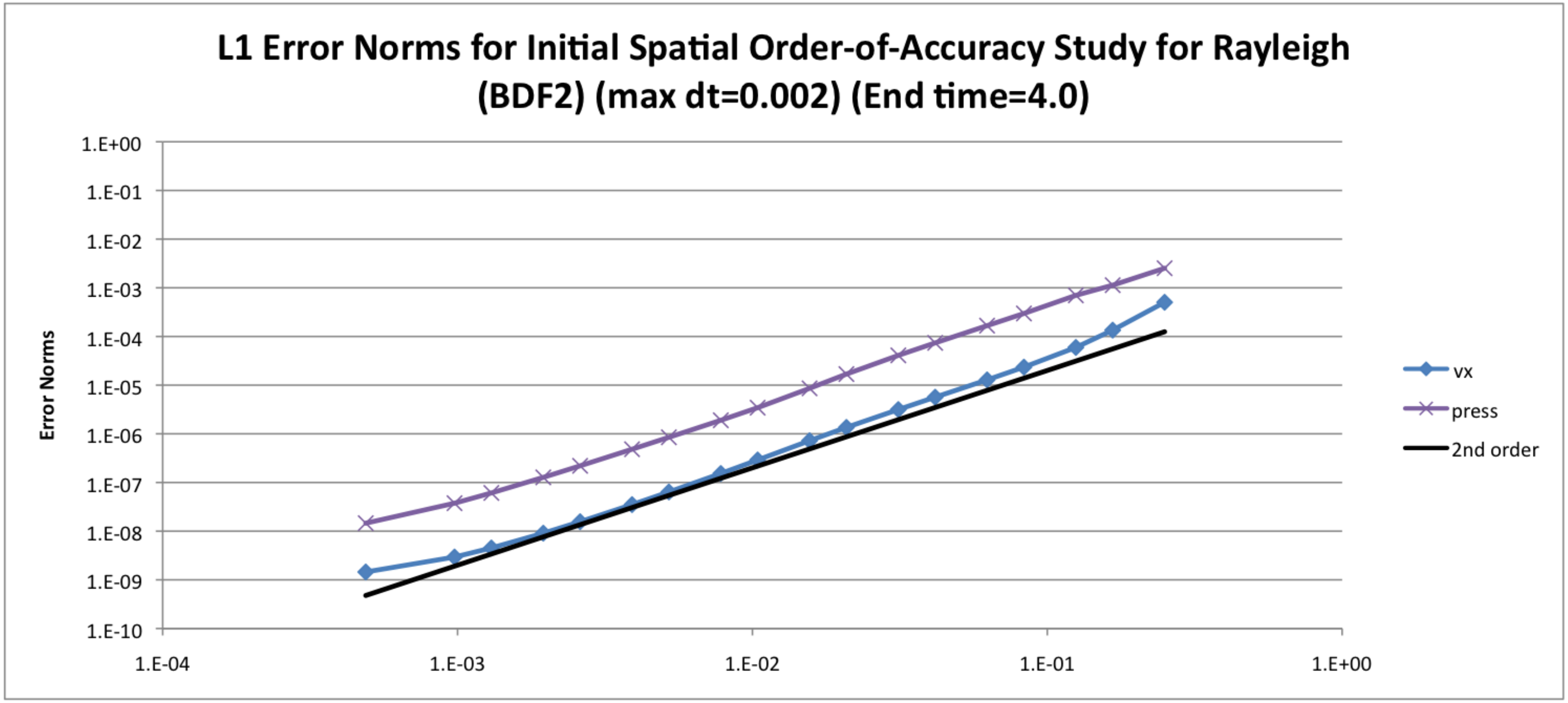
- Pass Thyra vector and operator objects throughout code
  - At the lowest level we cast to concrete type to fill object
  - Plan to use Tpetra, but not all pieces are present in the “2nd Generation” stack
    - MueLu
    - NOX/LOCA
  - For now we use Epetra for concrete LA type

Mesh Database and I/O

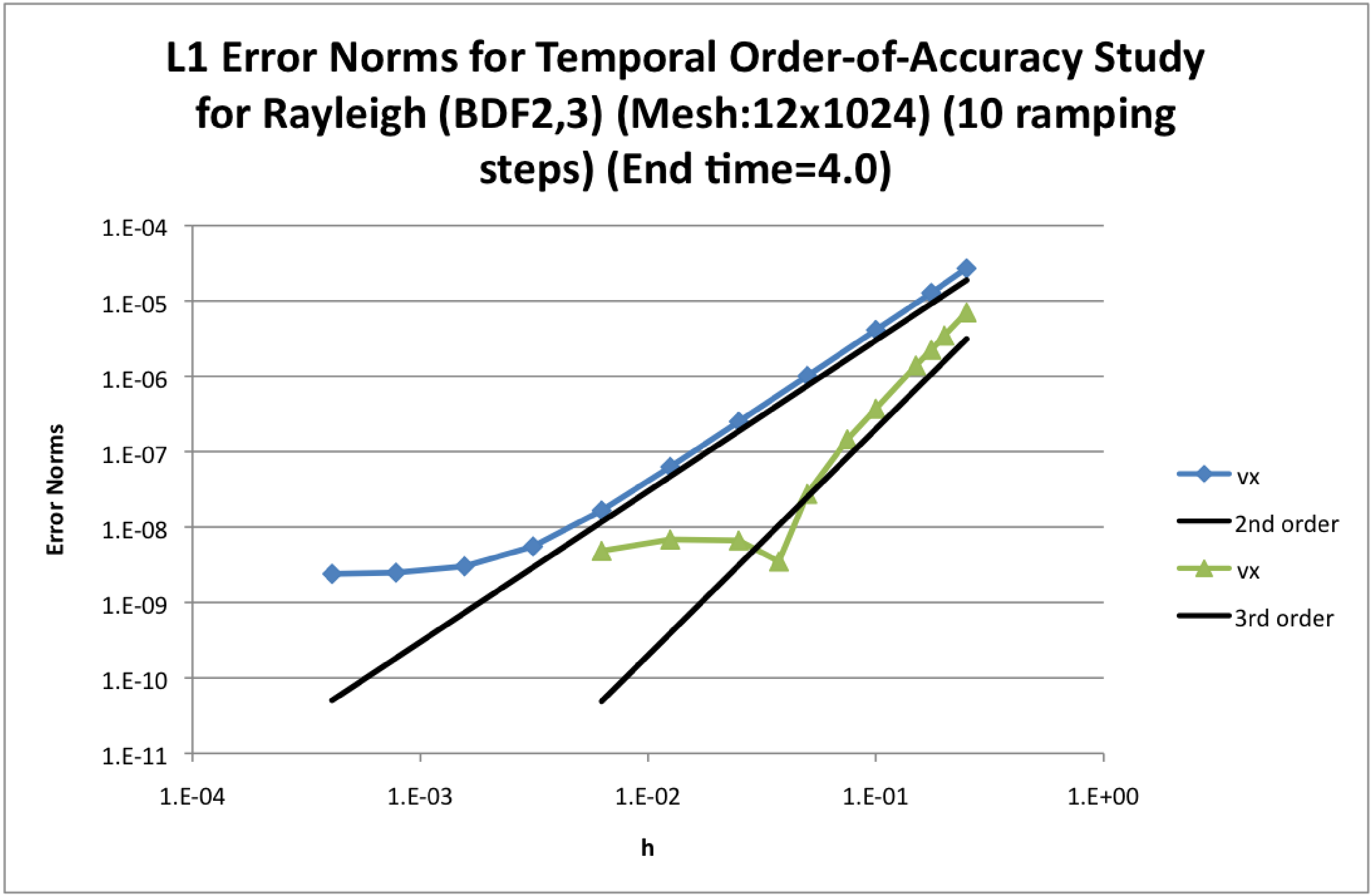
- Any mesh database or I/O format can be used, must implement a Panzer::ConnectionManager to use with the assembly engine
- Panzer conatins a concrete Implementation to **STK::mesh**
  - A ConnectionManager implementation to STK for DOF mapping
- SEACAS
  - I/O uses Exodus format
  - Apps are now in Trilinos (exodiff)
- Panzer provides Observers for NOX and Rythmos to write Exodus file on triggered events (e.g. successful time steps)

Results

Spatial Error Verification



Temporal Error Verification



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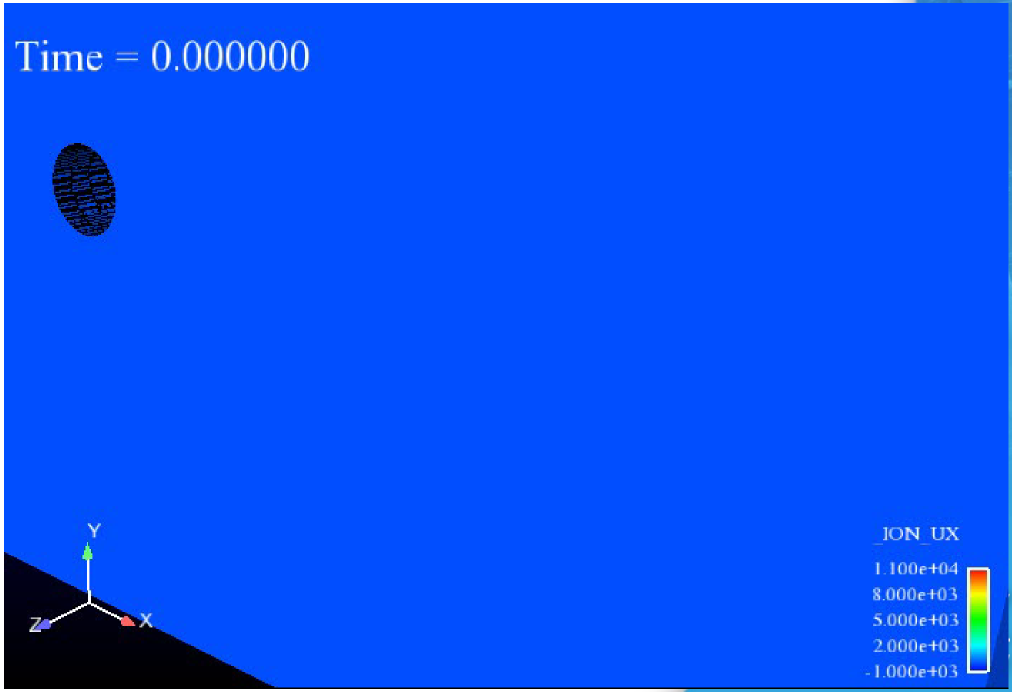
VUQ Coordination for solution verification and validation (with B. Rider)

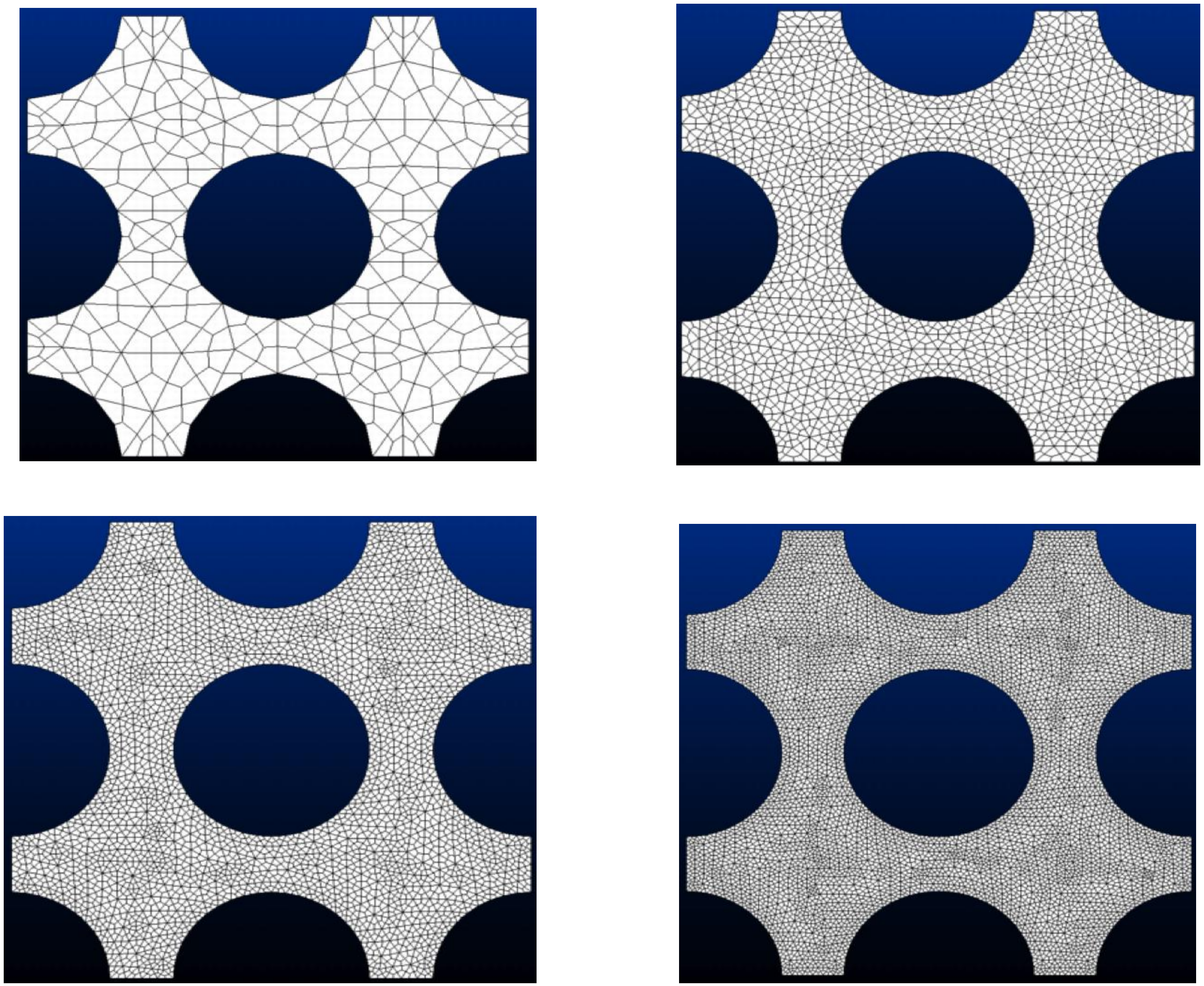
Vortex shedding over cylinder

Method	Experimental Data	Salsa Data	Drekar Data
Re=60	$.136 \pm .006$	0.132	$.134 \pm .004$
Re=100	$.164 \pm .005$	0.163	$.163 \pm .005$
Re=200	$.185 \pm .007$	0.189	$.189 \pm .004$
Re=400	$.205 \pm .005$		$.209 \pm .005$
Re=600	$.210 \pm .006$	0.218	$.218 \pm .006$
Re=1000	$.212 \pm .006$		$.222 \pm .007$
Re=5000	$.212 \pm .006$		$.220 \pm .010$



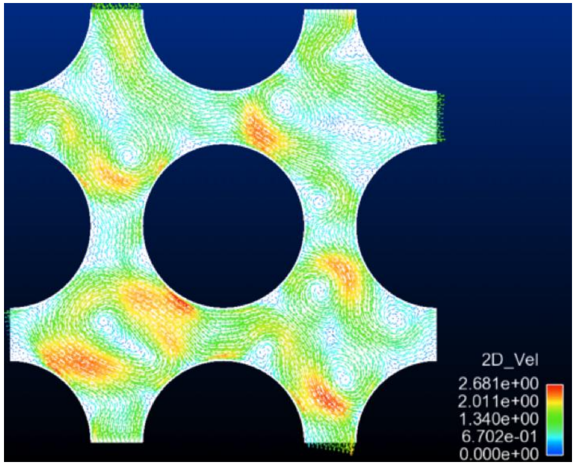
Verification on Multiple Meshes

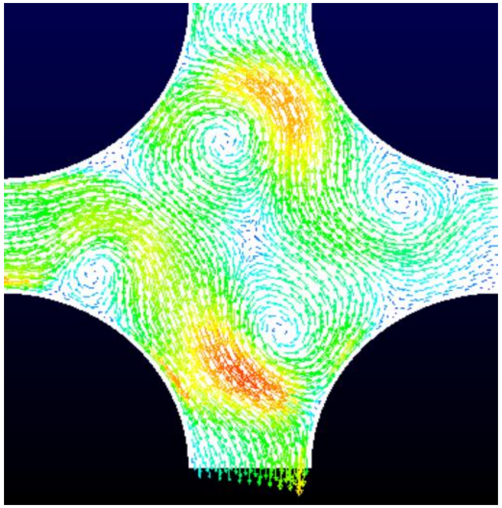
(Hex mesh ranging from 700K to 6M elements)

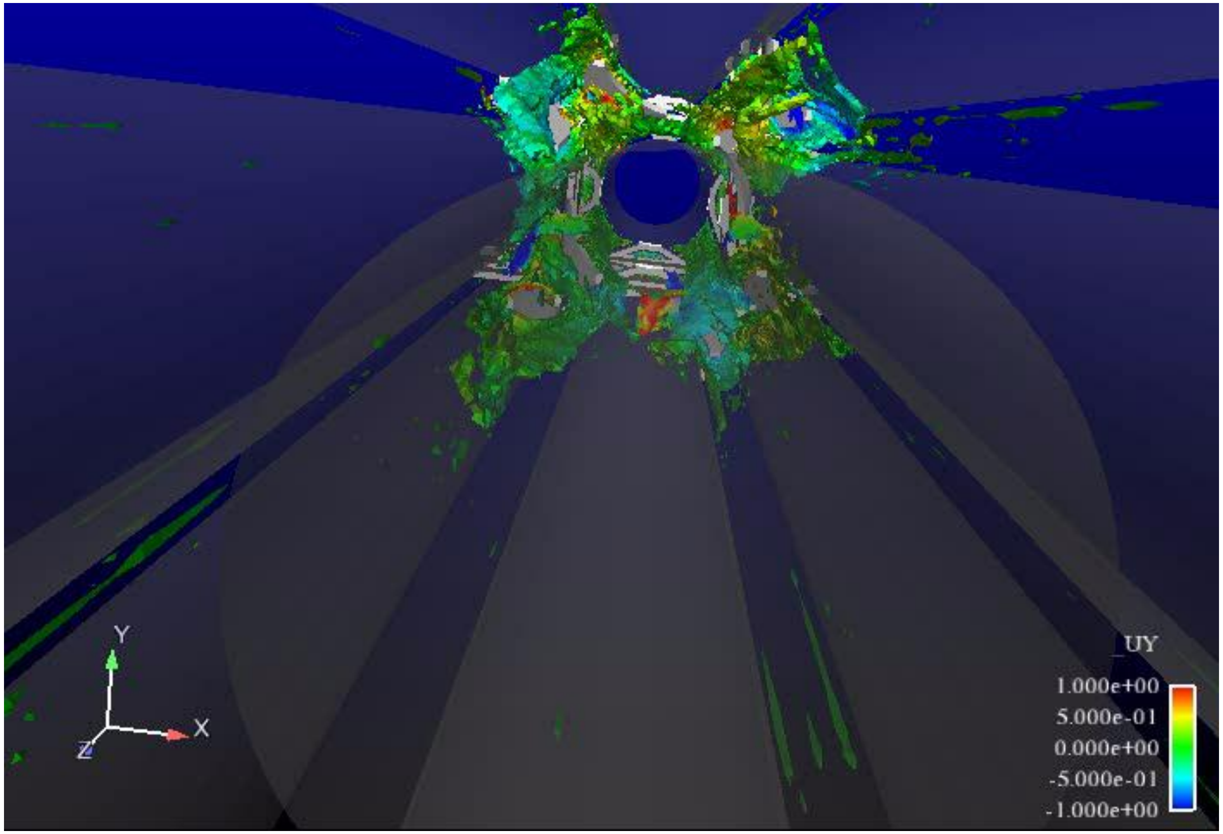


Solution Profiles

- Sandia Redsky platform, 256-1024 processes
- Oak Ridge Jaguar platform, 1200-9600 processes
- 2^{nd} order BFD2 time integration
- Linear Lagrange elements (2^{nd} order in space)







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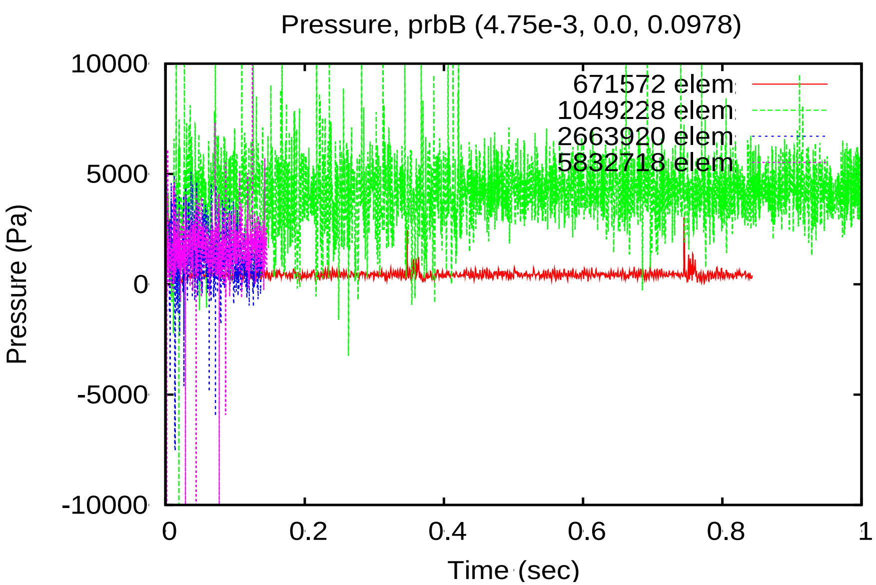
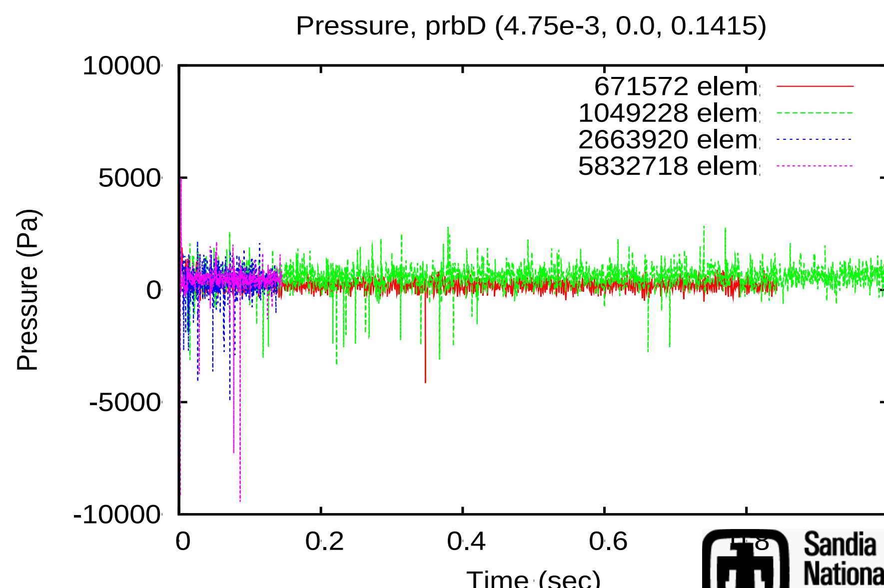
Transient Pressure Profiles

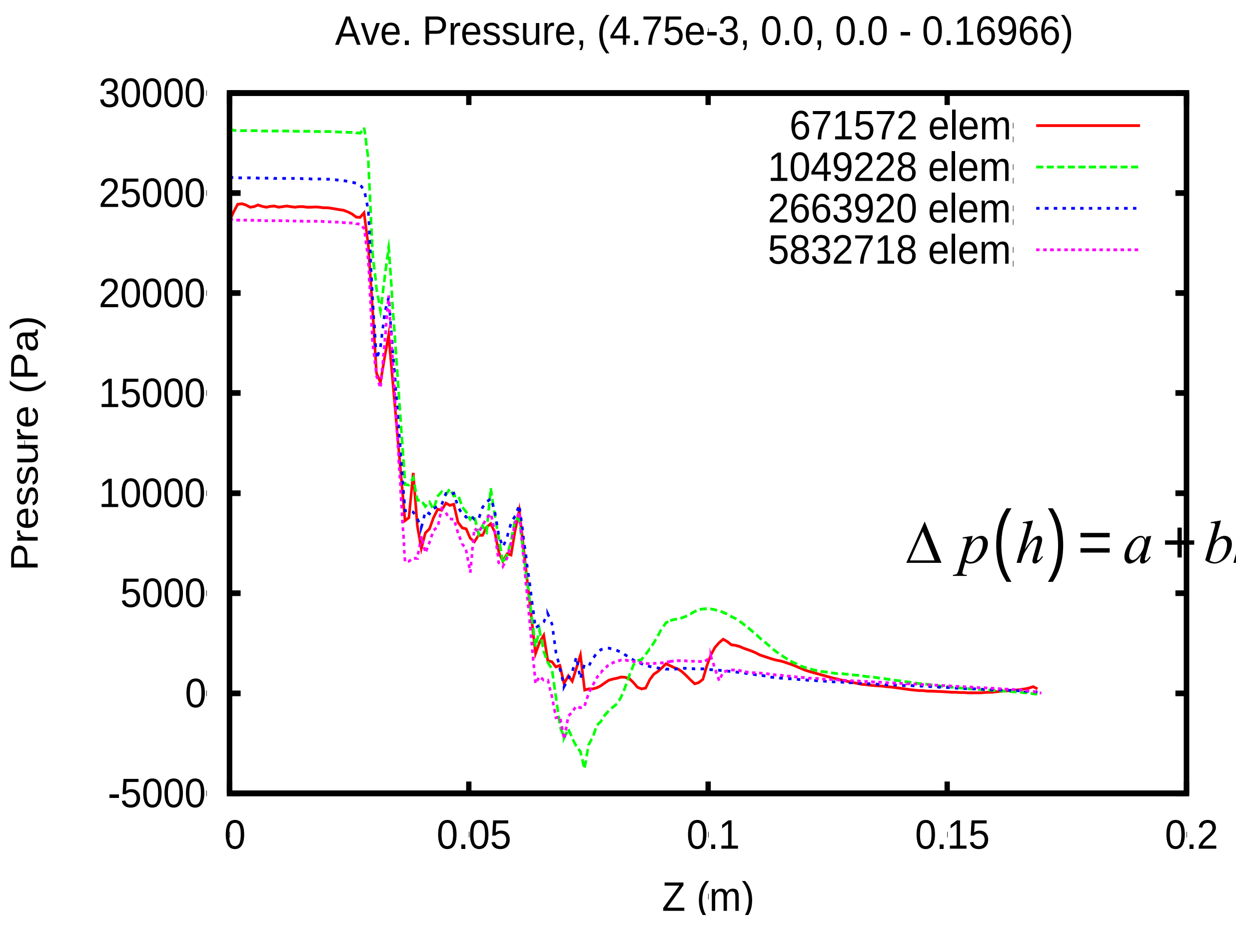
Mesh	# of Elements	Simulated Time (sec.)	Flow through times	Δt	CFL ave. (section1/section3)	Y+ ave.
672K (Red)	671,572	0.88	26	5.0×10^{-5}	9.6/1.3	26
1M (Green)	1,049,288	1.11	33	5.0×10^{-5}	11.1/2.9	19
3M (Blue)	2,663,920	0.2	6	2.0×10^{-5}	5.9/2.1	16
6M (Purple)	5,832,718	0.32	9	2.0×10^{-5}	7.9/2.2	13





Time Averaged Pressure Profiles Across Spacer Grid

- Coarsest mesh is inadequate for simulation
- 3 finer meshes show signs of convergence

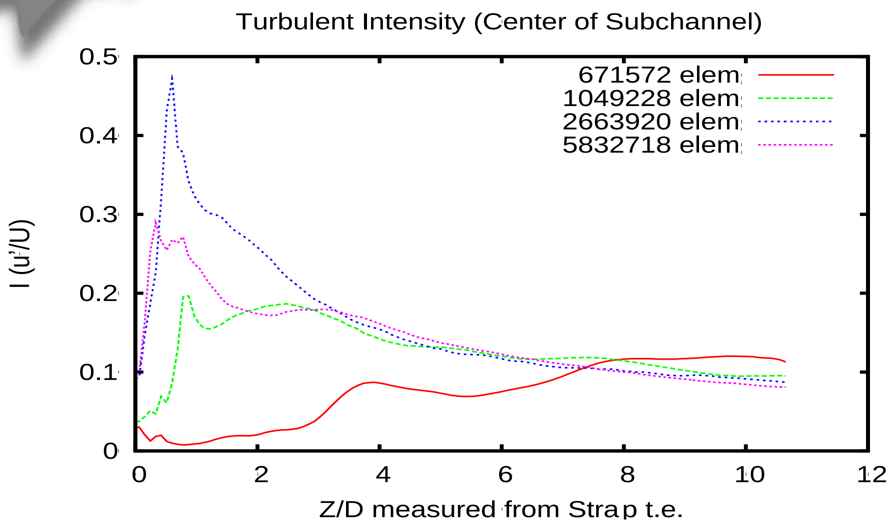


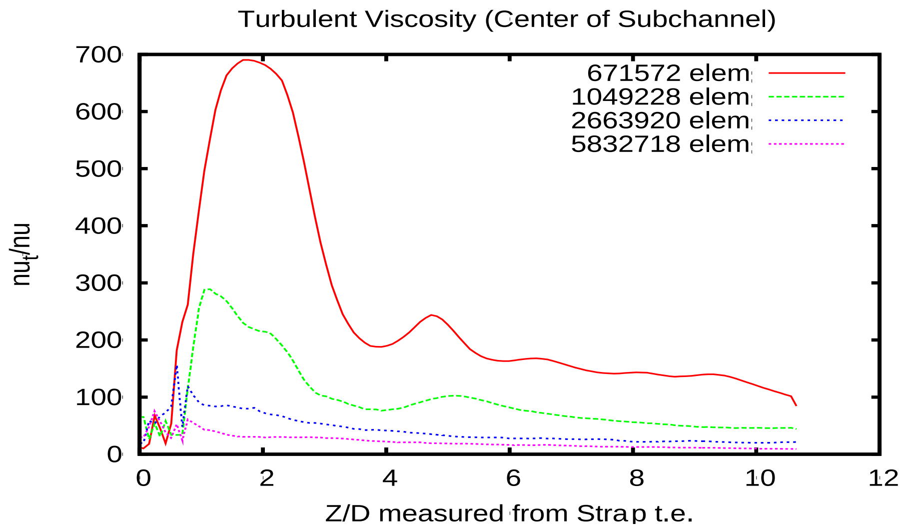
Mesh	Mean Pressure Drop (Pa)
677K	23,400
1M	26,780
3M	23,800
6M	22,042

$$\Delta p(h) = a + bh^c = 17.42 - 163.7h^{1.234}$$

- **Pressure drop value**
- **Coarse mesh solutions not yet in asymptotic range**
- **Already > 1st order!**

Turbulence Characteristics

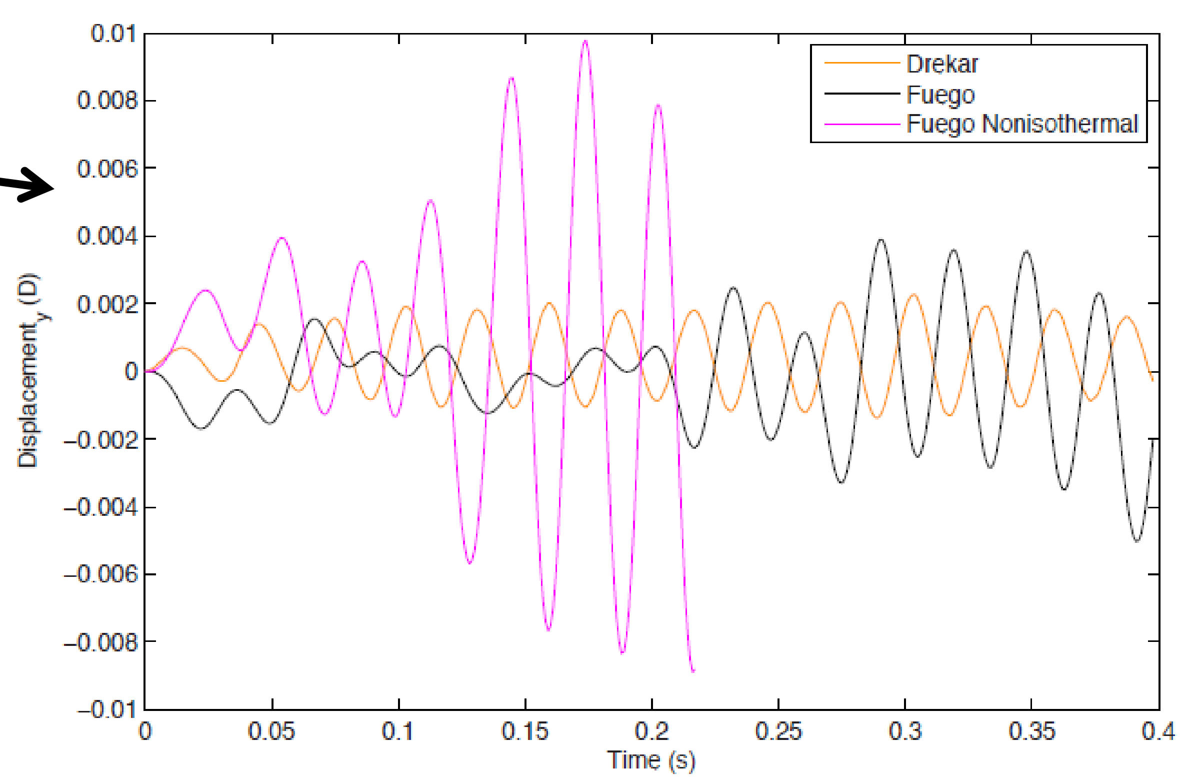


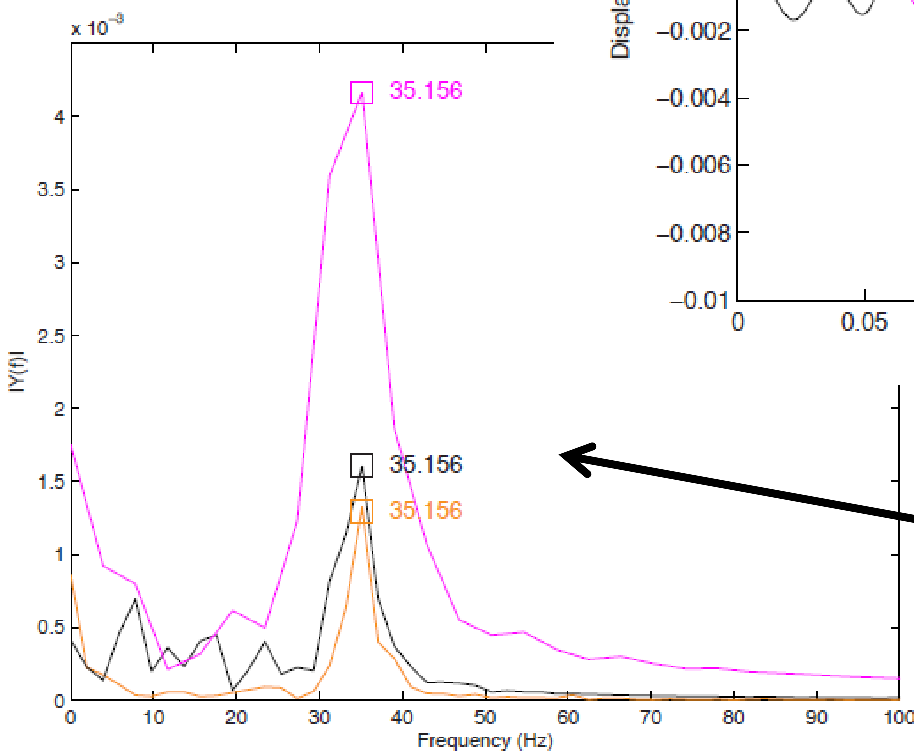


- 672K mesh is inadequate to resolve behavior near spacer grid.
- Non-monotonic behavior in turbulent intensity:
  - Converges 3 diameters downstream as turbulence subsides
  - Suggests under-resolution of mesh near spacer grid
- Turbulent intensity comparison to Benhamadouche *et al.* 2009:
  - At 3 diameters downstream, Drekar: 18%, Ben.: 11%
  - At 10 diameters downstream, Drekar: 10%, Ben.: 8.5%
- Monotonic decrease in amount of eddy-viscosity with refined mesh shows correct behavior (reduced contribution of subgrid model).

Demo of Forcing of Structural Vibration (Sierra/Presto). Solid Zircaloy Rod

Rod displacement in y-direction produced by fluid loads





FFT on displacement yields same frequency.

Impact

- TBGP w/ Phalanx and Panzer allows for rapid development and integration of advanced physics (Using Agile Components)
  - **Drekar went from drawing board to milestone completion in 6 months**
  - **Implementation + verification + validation + production runs!**
- New capabilities to propel ASCR research:
  - Multiphysics: Mixed equation sets (e.g. conjugate heat transfer)
  - Mixed basis and higher order methods (compatible disc. For MHD)
- Drekar has been adopted as one of two TH/CFD codes for CASL.
  - Integrated into VERA simulation suite.
  - First official release to CASL in FY12/Q2
- Community Adoption:
  - ASC/QASPR: Next-generation Charon now under development using Panzer (Suzey Gao)
  - Phalanx is the backbone of FE assembly in Albany(~10 different physics).
- Being considered for “Joule metric” code (ASCR OMB metric)

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A Users Perspective

- Trilinos is not a uniform code base:
  - Many developers with varying opinions on software quality
  - Good documentation vs good tests (sometimes both or neither)
- Confusion in a package maturity level:
  - PS and SS do not mean **hardened** code! Is there a better way to describe a code's status?
  - Additional capabilities required: PIRO and Rythmos
- Pushing new interfaces/capabilities through Thyra layers can be difficult.
  - The answer can't always be go to Ross!
- Would not have advanced this far this fast without expertise that spans a large part of Trilinos.
  - High entry bar to Trilinos

Conclusions

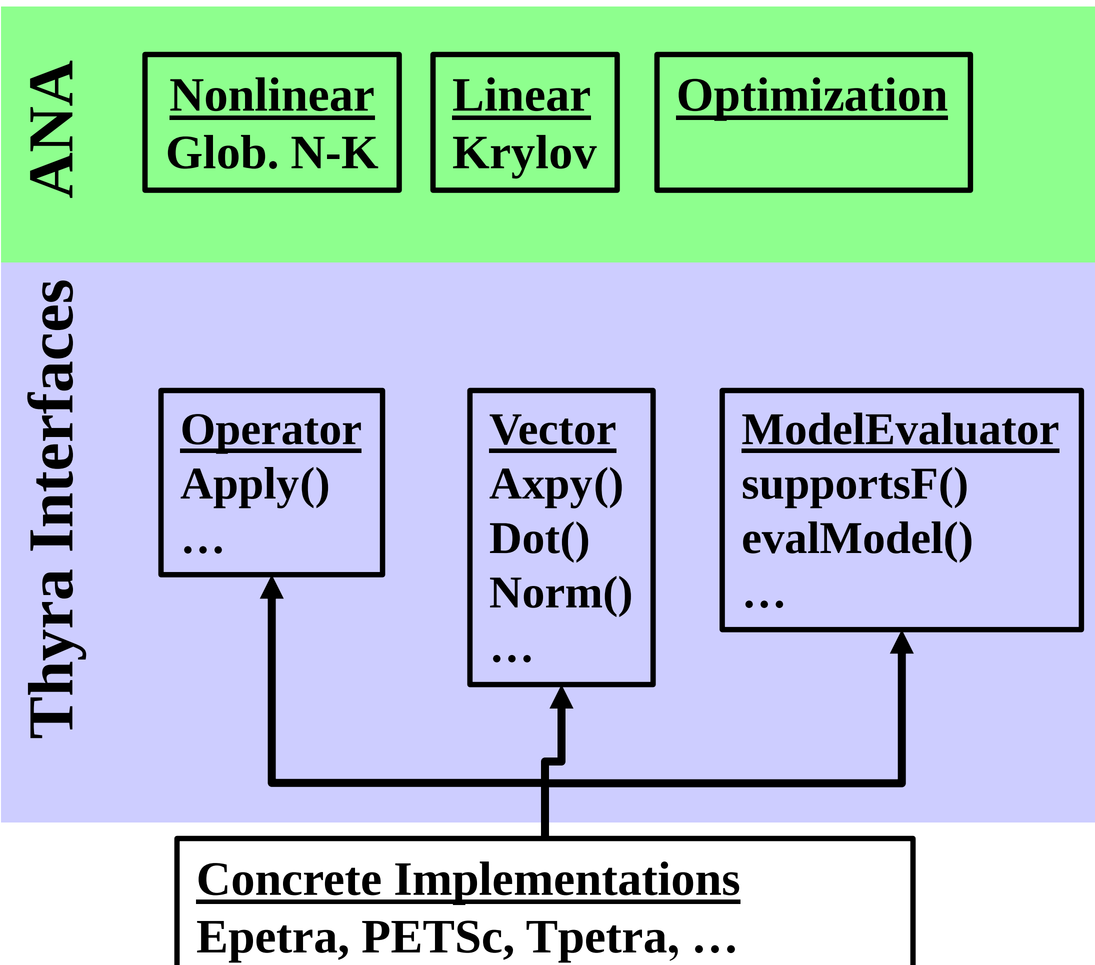
- Successfully stood up a new code in 6 months!
- Leveraged a significant portion of Trilinos
- Not all packages fit perfectly, but it is preferable to rolling your own (technical debt)
- Lightweight front end physics description
- Decoupled from solution/analysis procedures

Extra Slides

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:

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

Block Factorization Preconditioners:

$$\begin{bmatrix} I & 0 \\ \hat{B}H_1 & I \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & -\hat{S} \end{bmatrix} \begin{bmatrix} I & H_2 B^T \\ 0 & I \end{bmatrix}$$

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

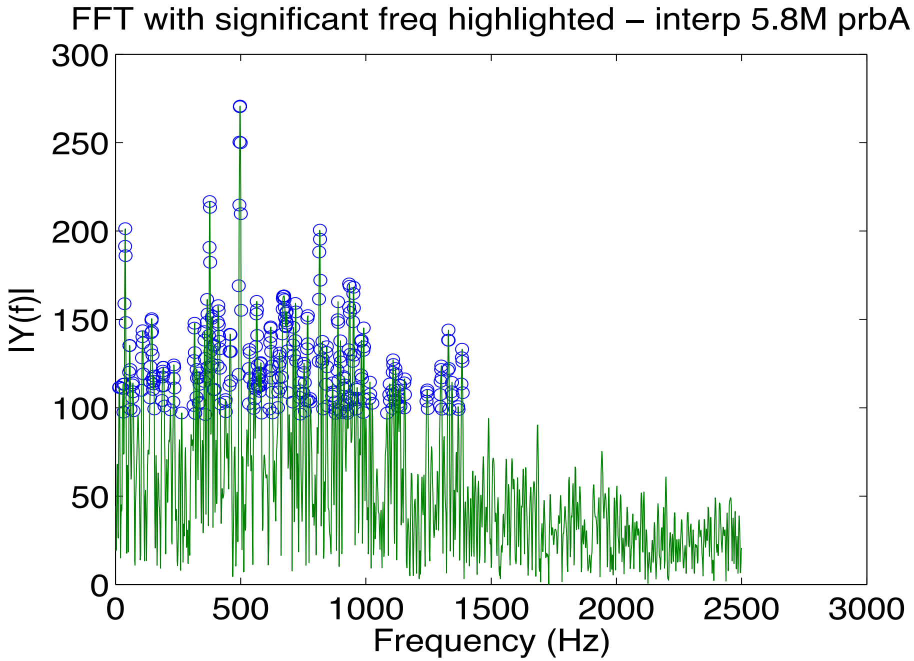
Wish List

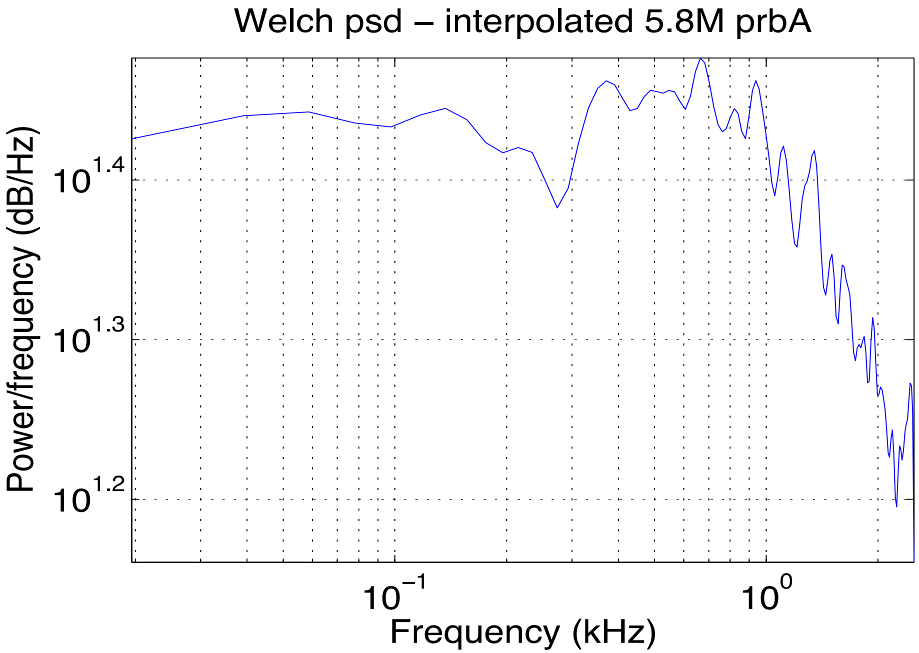
- Order preserving ParameterList xml parser
- ParameterList Validators for our use case
- Improved support for Thyra

- Rythmos support for better startup and ramping
- Intrepid:
  - 0D quadratures need to be supported for 1D code!
  - Cylindrical coordinates (3D physics on a 2D mesh)
- Improved TPL support: versioning!
  - STK, ML, Zoltan: Parmetis 3 → 4

- When code should be made into a general Trilinos package?

FFT and PSD on Center Rod





- Maximum frequency of the FFT is roughly the Nyquist frequency.
- Characteristic turbulent cascade is evident in the PSD (just starting to analyze this).

Drekar::CFD

trilinos.sandia.gov

- **Massively Parallel: MPI**
- **2D & 3D Unstructured Stabilized FE**
- **Fully Coupled Globalized Newton-Krylov solver**
  - **Sensitivities: Template-based Generic Programminc for Automatic Differentiation (Sacado), UQ, Arb. Prec.**
  - **GMRES (AztecOO, Belos)**
  - **Additive Schwarz DD w/ Var. Overlap (Ifpack, AztecOO)**
  - **Aggressive Coarsening Graph Based Block Multi-level [AMG] for Systems (ML w/Amesos for coarse solve)**
  - **Physics-based/Block Factorization (Teko)**
- **Fully-implicit: 1st-5th variable order BDF (Rythmos) & TR**
- **Direct-to-Steady-State (NOX), Continuation, Linear Stability and Bifurcation (LOCA / Anasazi), PDE Constrained Optimization (Moocho)**