Phalanx: An Flexible and Extensible Assembly/Field Evaluation Kernel For Handling Complexity in Simulation

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Trilinos User Group Meeting
November 4, 2009

SAND2009-7348P

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000

Acknowledgements

- Phalanx Contributors
  - Eric Phipps
  - Carter Edwards
  - Pat Notz
- Consulting
  - Roscoe Bartlett
  - Pavel Bochev
  - Dennis Ridzal
  - Andy Salinger

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Motivation

- Assembly for general FE/FV PDE discretizations gets quite complex when supporting arbitrary equation sets.

- Issues to Address:
  - Compact and uniform user interface for extensibility
  - Flexibility to easily swap equation sets, material models and material properties while maintaining efficiency
  - Support for user defined data types
  - Support for embedded technology
  - Good OO-design/Code reuse

- Generalization and unification of:
  - Expression Manager in SIERRA/Aria
  - Variable Manager in Charon

Overview

- Phalanx is a local field evaluation kernel designed for assembly of arbitrary equation sets (i.e. evaluating residuals and Jacobians).
  - Equation sets, material models might change drastically
- Decompose a complex problem into a number of simpler problems with managed dependencies
  - Supports rapid development and extensibility
  - Consistent evaluation of fields as dependencies change
- Phalanx supports arbitrary user defined data types and evaluation types through template metaprogramming.
  - Flexibility for direct integration with user applications
  - Provides extensive support for embedded technology such as automatic differentiation for sensitivities and uncertainty quantification.
- Efficient evaluation of fields using worksets and memory management for efficient use of cache.

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Complex Dependency Chains

Momentum $$\frac{\partial(\rho\mathbf{v})}{\partial t} + \nabla\cdot(\rho\mathbf{v}\otimes\mathbf{v} + \mathbf{T}) - \rho\mathbf{g} = 0$$

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

Energy $$\rho C_p\frac{\partial T}{\partial t} + \nabla\cdot(\rho C_p T\mathbf{v} - \mathbf{q}) + s = 0$$

Species $$\rho\frac{\partial y_i}{\partial t} + \nabla\cdot(\rho\mathbf{v}y_i + \mathbf{j}_k) + W_i\dot{\omega}_i \qquad i = 1 \ldots N_{sp}$$

$$\mathbf{T} = P\mathbf{I} + \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I} - \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T) \qquad \mathbf{q} = -k\nabla T$$

$$\mathbf{j}_k = \rho y_k \frac{1}{x_k\bar{W}}\sum_{j=1}^{K} W_j D_{kj}\nabla x_j$$

- Complexity spirals when we add new equations, operators, use subsets, etc…
  - Swap eqns/models at runtime (no complex if/switch statements)
- **Automatically adjust the dependency tree** $\rho(T,P) \Rightarrow \rho(y_i,P,T)$
- Separate fields so that they are evaluated only once (density)

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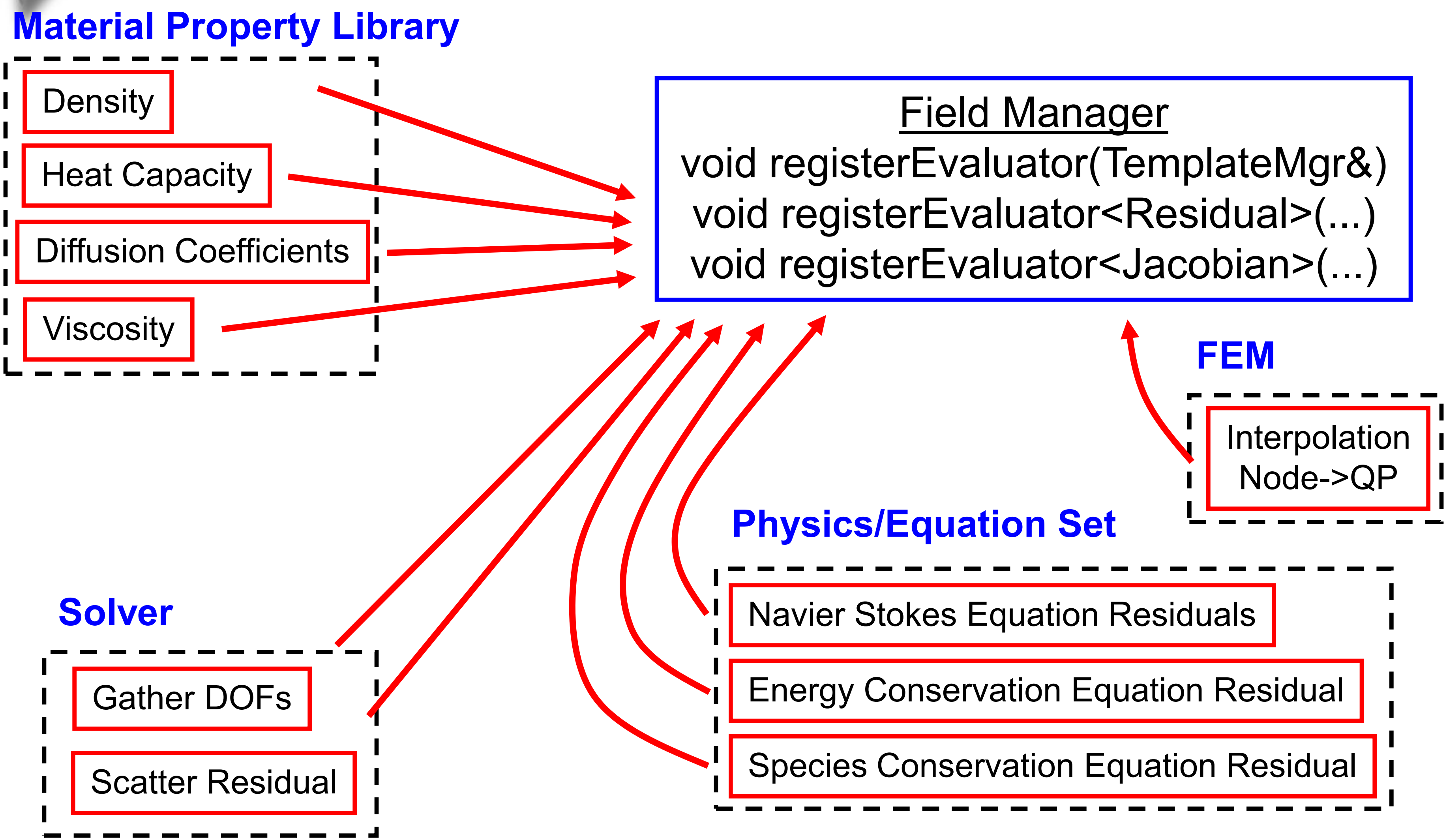
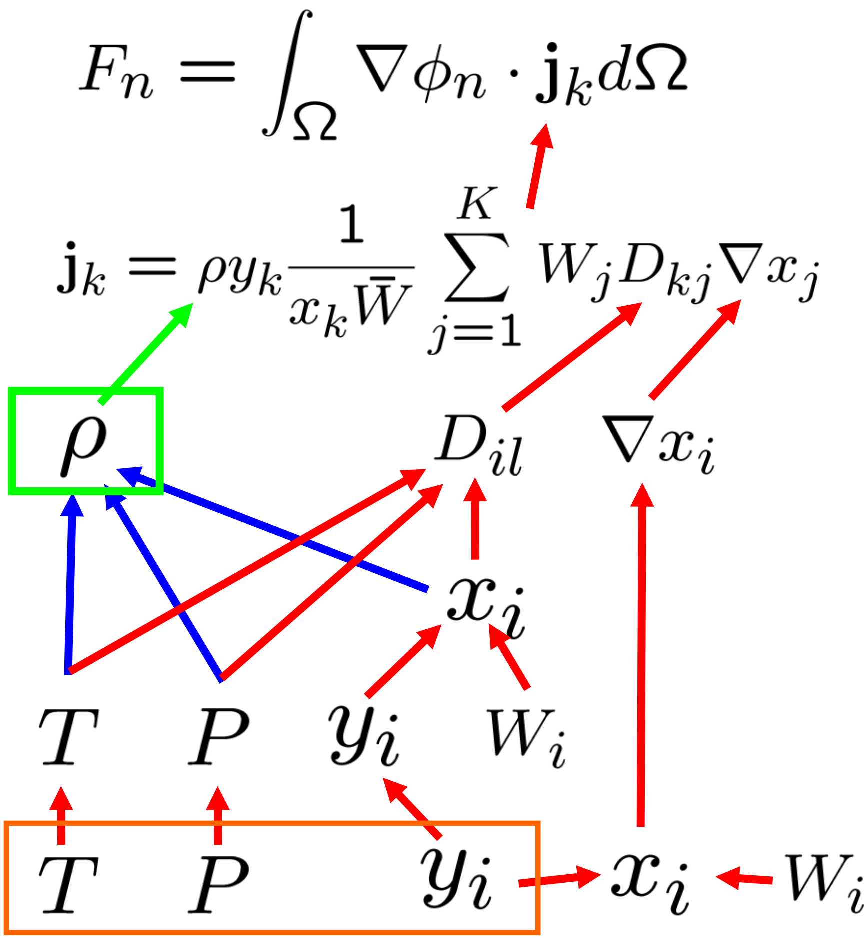
Idea: Evaluators (Expressions)



Evaluators can be registered anytime before postRegistrationSetup()

Evaluator Anatomy

$$\rho\frac{\partial y_i}{\partial t} + \nabla\cdot(\rho\mathbf{v}y_i) + \nabla\cdot\mathbf{j}_k + W_i\dot{\omega}_i \Rightarrow F_n = \int_\Omega \nabla\phi_n\cdot\mathbf{j}_k d\Omega$$



@ node points

@ integration points

@ integration points

@ integration points

@ integration points

@ basis points

- Evaluates one or more fields
- Depends on one or more fields
- CTOR: Size the fields
- Setup Method: Get pointers to memory
- Evaluate Method: Evaluate the field(s)
- Intrepid package does the final integration

Idea: Chain of Evaluators

- Phalanx FieldManager will
  - Determine which evaluators to call
  - The order to call the evaluators for consistency
  - Perform the evaluation on a workset

```
field_manager.evaluateFields<Residual>(workset);

field_manager.evaluateFields<Jacobian>(workset);
```

Evaluators: Simple for Users

- We must simplify interfaces for analysts to implement
  - Don't expose entire equation set to users
  - Hide advanced c++ (i.e. templating) from analysts looking to add new equations and material models
  - Don't have to know about derivatives/solver techniques

$$\mathbf{q} = -\rho k \nabla T$$

```
PHX_EVALUATOR_CLASS(EnergyFlux)

  Field< MyVector<ScalarT> > flux;

  Field< ScalarT > density;
  Field< ScalarT > k;
  Field< MyVector<ScalarT> > grad_temp;

  int points_per_cell;

PHX_EVALUATOR_CLASS_END
```

```
PHX_EVALUATE_FIELDS(EnergyFlux,workset)
{
  int size = workset.num_cells * points_per_cell;

  for (int i = 0; i < size; ++i)
    flux[i] = -density[i] * k[i] * grad_temp[i];
}
```

Skipped CTOR (field sizing),
Setup (get pointers to memory)

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Workset/Memory Management

- Break work up into worksets
  - Chunk of cells in finite element/volume calculation
- Memory allocation of all fields of all scalar types for an evaluation type is done in a single contiguous array!
  - Possibly fit all fields in cache
  - User defined allocators (template parameter in Traits)
- Leverage BLAS in evaluators

What does this buy you?

- Consistent Evaluations: Dependencies are ensured to be up-to-date
- Evaluate each field once per cell
  - No recalculation of temporaries
- Flexible and Extensible: each simpler piece becomes an extension point that can be swapped out with different implementations
- Easier to craft code because each piece is simpler, more focused and easier to test in isolation
- Minimal interface: isolate users from bulk of assembly process
- Efficient: use of worksets
  - Block evaluations → Blas
  - Possibly fits into cache

Embedded Technology!!!

Field Manager is templated on Evaluation Type

Concept: Evaluation Types		Scalar Types
• **Residual**	$F(x,p)$	`double`
• **Jacobian**	$J = \frac{\partial F}{\partial x}$	`Sacado::FAD::DFad<double>`
• **Tangent**	$\frac{\partial F}{\partial p}$	`Sacado::FAD::DFad<double>`
• **Stochastic Galerkin Residual**		`Sacado::PCE::OrthogPoly<double>`
• **Stochastic Galerkin Jacobian**		`Sacado::Fad::DFad< Sacado::PCE::OrthogPoly<double> >`

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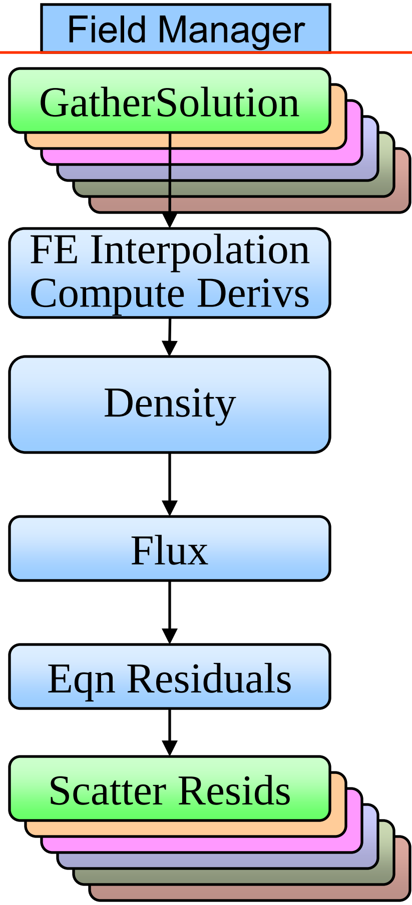
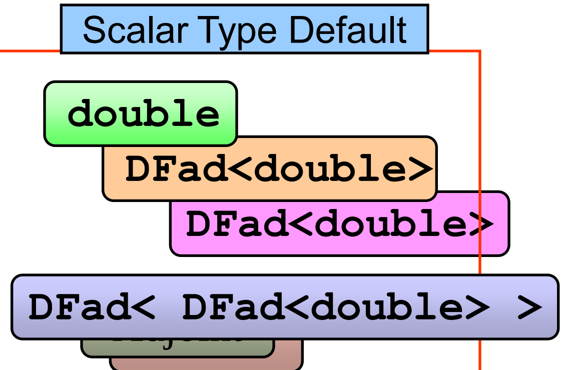
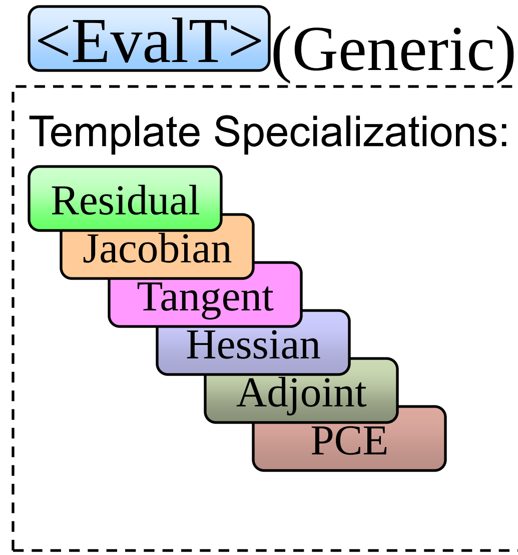
Transformational PDE Assembly using Agile Components





Take Home Message:

1. Reuse the same code base
2. Never write Jacobians manually



Rapid, Transformational, Scalable

<u>Packages / Libraries:</u>

Sacado: Automatic Differentiation
Phalanx: Field Manager, Evaluators
Intrepid: Compatible Discretizations
iTAPS: Mesh interface

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Example Traits

```
struct MyTraits : public PHX::TraitsBase {

  typedef double RealType;
  typedef Sacado::Fad::DFad<double> FadType;

  struct Residual { typedef RealType ScalarT; };
  struct Jacobian { typedef FadType ScalarT; };

  typedef boost::mpl::vector<Residual, Jacobian> EvalTypes;

  // Residual (default scalar type is RealType)
  typedef boost::mpl::vector< RealType,
                              MyVector<RealType>,
                              MyMatrix<RealType>
  > ResidualDataTypes;

  // Jacobian (default scalar type is Fad<double>)
  typedef boost::mpl::vector< FadType,
                              MyVector<FadType>,
                              MyMatrix<FadType>
  > JacobianDataTypes;

  // Maps the key EvalType a vector of DataTypes
  typedef boost::mpl::map<
    boost::mpl::pair<Residual, ResidualDataTypes>,
    boost::mpl::pair<Jacobian, JacobianDataTypes>
  >::type EvalToDataMap;
```

Declare Scalar Types

Declare Evaluation Types

Evaluation Types

Declare Residual Data Types

Declare Jacobian Data Types

Maps Evaluation Types to Data Types

Multidimensional Arrays

(Shards – C. Edwards next)

```
PHX_EVALUATOR_CLASS(EnergyFlux)

  Field< MyVector<ScalarT> > flux;

  Field< ScalarT > density;
  Field< ScalarT > k;
  Field< MyVector<ScalarT> > grad_temp;

  int points_per_cell;

PHX_EVALUATOR_CLASS_END
```

```
PHX_EVALUATE_FIELDS(EnergyFlux,workset)
{
  int size = workset.num_cells * points_per_cell;

  for (int i = 0; i < size; ++i)
    flux[i] = -density[i] * k[i] * grad_temp[i];
}
```

```
PHX_EVALUATOR_CLASS(EnergyFlux)

  MDField<ScalarT,Cell,QuadPoint,Dim> flux;

  MDField<ScalarT,Cell,QuadPoint> density;
  MDField<ScalarT,Cell,QuadPoint> dc;
  MDField<ScalarT,Cell,QuadPoint,Dim> grad_temp;

  int num_qp;
  int num_dim;

PHX_EVALUATOR_CLASS_END
```

```
PHX_EVALUATE_FIELDS(EnergyFlux,workset)
{
  int num_cells = workset.num_cells;

  for (int cell = 0; cell < num_cells; ++cell)
    for (int qp = 0; qp < num_qp; ++qp)
      for (int dim = 0; dim < num_dim; ++dim)
        flux(cell,qp,dim) =
            - density(cell,qp) * dc(cell,qp) * grad_temp(cell,qp,dim);
}
```

Optional compile time checked access

In closing...

- This package is very advanced
  - C++ templates and template metaprogramming
  - One developer will need to know templates to set up
  - Everyone else only needs to write evaluators (very minimal template code)
- Think hard before using
  - This is a hammer, its not right for every PDE code, especially if your equation set/models doesn't change
- "My understanding keeps changing..." – Andy Salinger
- Don't hesitate to ask for help!
- http://trilinos.sandia.gov/packages/phalanx: a very detailed users guide.

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Phalanx Summary

- Assembly kernel for cell based discretization of PDEs
- Breaks complex problems into simpler pieces
  - Automatically manage complex dependency chains
  - Easier to unit test
  - Don't expose fully complex system to the user – only expose exactly what they need to write a user defined function
- Supports rapid development and extensibility
  - Easily swap evaluation routines
  - Easily swap dependency trees
- Arbitrary user defined data types and evaluation types: C++ Template metaprogramming
- Embedded technology support