Building Hierarchical Toolchains for Nonlinear Analysis

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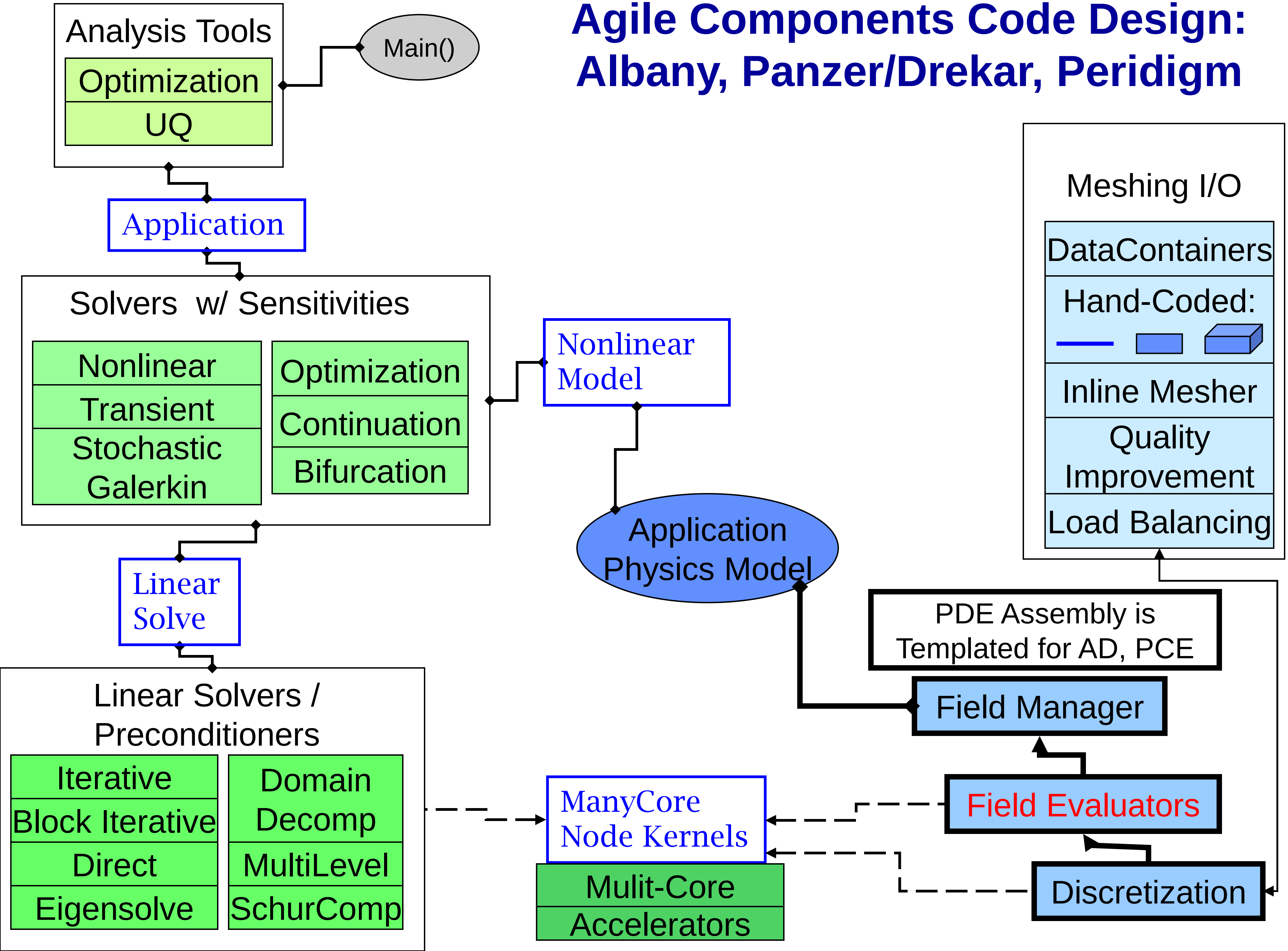
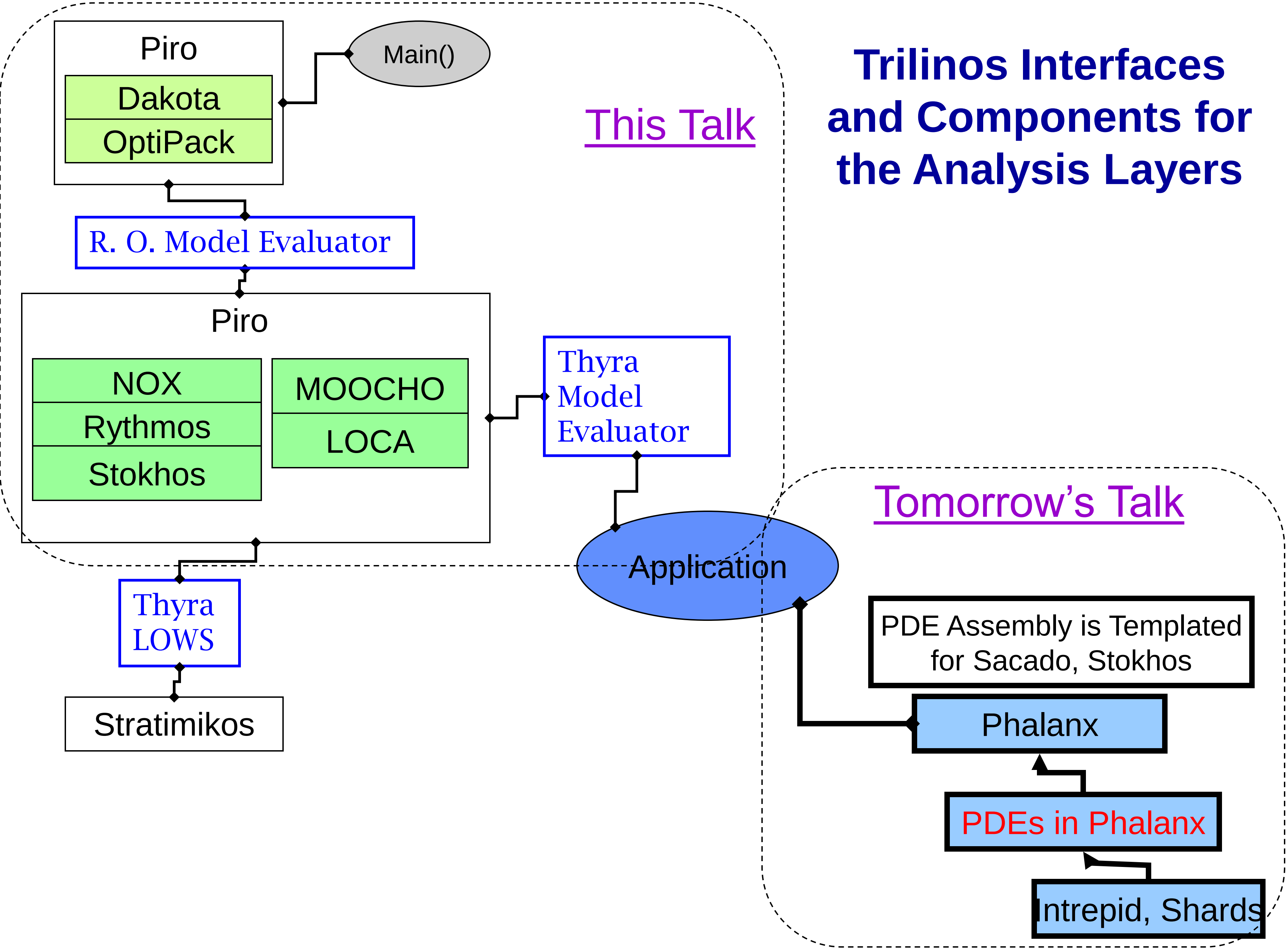
Embedded Nonlinear Analysis Capability Area

- Basic Capabilities:
  - TBGP Automatic Differentiation (Sacado)
  - (Globalized) Nonlinear solution methods (NOX)
  - Time Integration (Rythmos)
- Advance Analysis Capabilities:
  - (Multi-)Parameter Continuation (LOCA)
  - Stability analysis (LOCA)
  - Bifurcation analysis (LOCA)
  - Optimization (Aristos/ROL, MOOCHO, TriKota/DAKOTA)
  - Uncertainty Quantification (Stokhos TriKota/DAKOTA)
- Analysis beyond direct simulation:
  - Often a simple direct solve is not enough
  - Automate computational tasks that are often performed by application code users by trial-and-error or repeated simulation

Agile Components Code Design: Albany, Panzer/Drekar, Peridigm



Trilinos Interfaces and Components for the Analysis Layers



General Physics Model

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

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

$x \in \mathbb{R}^{n_x}$ 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,

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

$g_j(\dot{x}, x, \{p_l\}, t) : \mathbb{R}^{\left(2n_x + \left(\sum_{l=0}^{N_p - 1} n_{p_l}\right) + 1\right)} \to \mathbb{R}^{n_{g_j}}$ 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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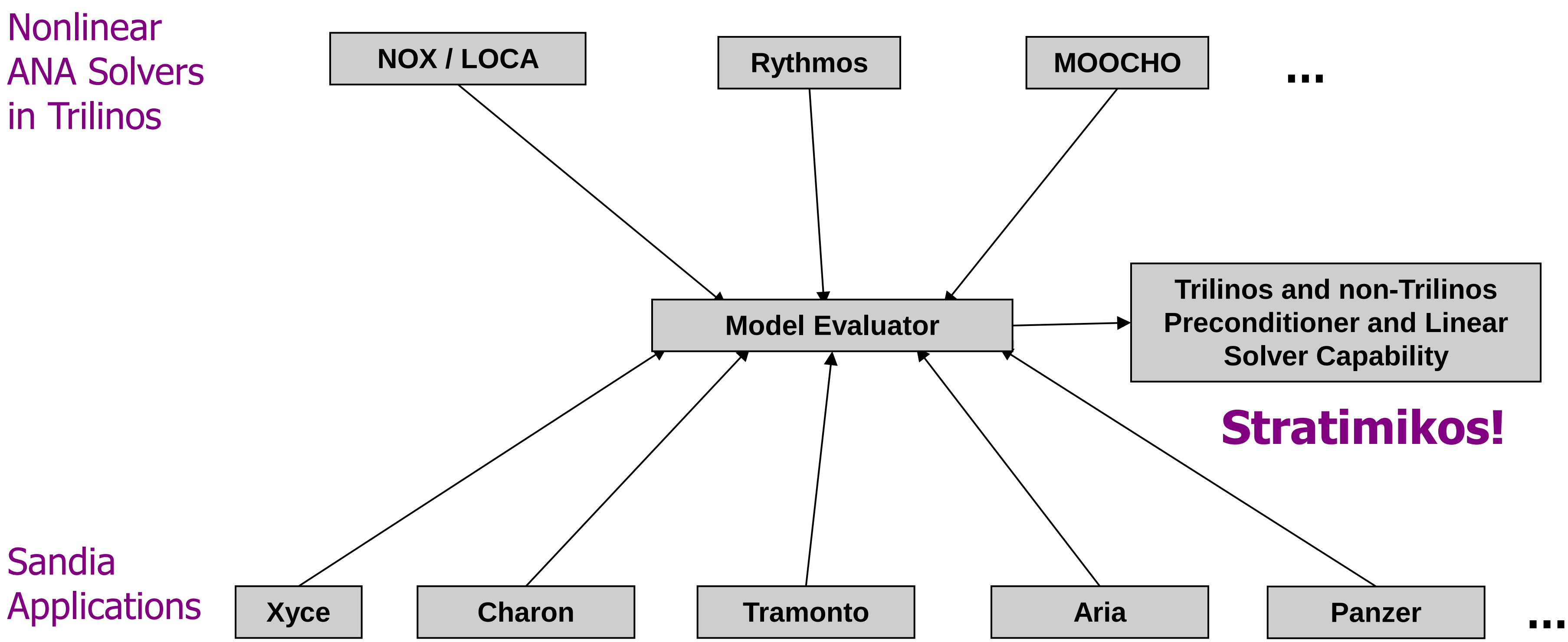
Some Examples of Nonlinear Analysis Supported by ModelEvaluator

Nonlinear equations:	Solve $f(x) = 0$ for $x \in \mathbf{R}^n$
Stability analysis:	For $f(x,p) = 0$ find space $p \in \mathcal{P}$ such that $\frac{\partial f}{\partial x}$ is singular
Explicit ODEs:	Solve $\dot{x} = f(x,t) = 0, t \in [0,T]$, $x(0) = x_0$, for $x(t) \in \mathbf{R}^n, t \in [0,T]$
DAEs/Implicit ODEs:	Solve $f(\dot{x}(t), x(t), t) = 0, t \in [0,T]$, $x(0) = x_0$, $\dot{x}(0) = x'_0$ for $x(t) \in \mathbf{R}^n, t \in [0,T]$
Explicit ODE Forward Sensitivities:	Find $\frac{\partial x}{\partial p}(t)$ such that: $\dot{x} = f(x,p,t) = 0, t \in [0,T]$, $x(0) = x_0$, for $x(t) \in \mathbf{R}^n, t \in [0,T]$
DAE/Implicit ODE Forward Sensitivities:	Find $\frac{\partial x}{\partial p}(t)$ such that: $f(\dot{x}(t), x(t), p, t) = 0, t \in [0,T]$, $x(0) = x_0$, $\dot{x}(0) = x'_0$, for $x(t) \in \mathbf{R}^n, t \in [0,T]$
Unconstrained Optimization:	Find $p \in \mathbf{R}^m$ that minimizes $g(p)$
Constrained Optimization:	Find $x \in \mathbf{R}^n$ and $p \in \mathbf{R}^m$ that: minimizes $g(x,p)$ such that $f(x,p) = 0$
ODE Constrained Optimization:	Find $x(t) \in \mathbf{R}^n$ in $t \in [0,T]$ and $p \in \mathbf{R}^m$ that: minimizes $\int_0^T g(x(t),p)$ such that $\dot{x} = f(x(t),p,t) = 0$, on $t \in [0,T]$ where $x(0) = x_0$

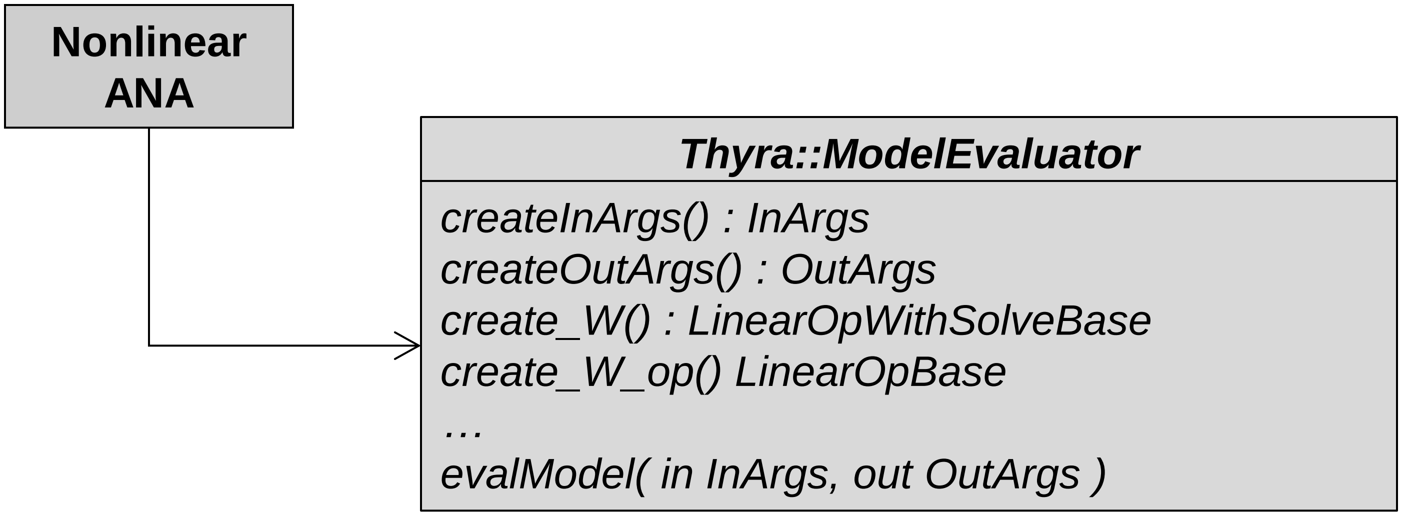
Nonlinear Algorithms and Applications : Thyra & Model Evaluator!



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

Model Evaluator : Thyra and EpetraExt Versions



- **Common interface for ANAs**
  - **Residuals, Jacobians, parameters, parameter sensitivities, response functions, stochastic Residuals/Jacobians**
- **Stateless model (All state passed in as parameters)**
- **Allows for efficient multiple shared calculations (e.g. automatic differentiation)**
- **Inputs and Outputs are extensible without requiring changes to user code**

ModelEvaluator and Response Only ModelEvaluator

Analysis Tools (*black-box*)

- Optimization
- UQ (sampling)

Response Only ModelEvaluator

$$p \rightarrow g(p)$$

InArgs	OutArgs
I can make use of:	I can compute:
p	g
	$\frac{dg}{dp}$

Analysis Tools (*embedded*)

- Time Integration
- Nonlinear Solver

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

Model Evaluator

Local Fill

I can make use of:	I can compute:
x	$f(\dot{x}, x, p, t)$
$\dot{x}$	$W = \alpha \frac{df}{d\dot{x}} + \beta \frac{df}{dx}$
p	$\frac{df}{dp}$
t	g
	$\frac{\partial g}{\partial x}$
	$\frac{\partial g}{\partial p}$

Piro::NOXSolver

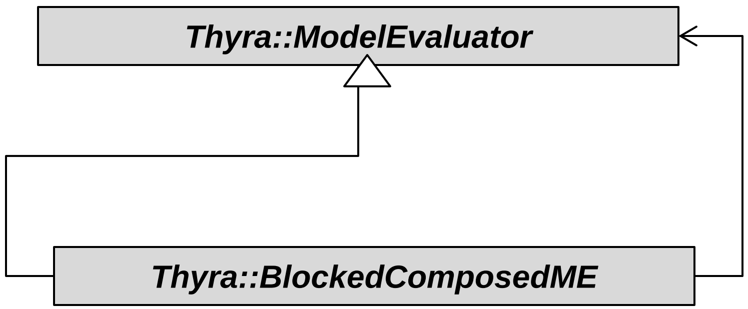
$$f(x, p) = 0$$

$$\frac{dg}{dp} = \frac{\partial g}{\partial x}^T \mathbf{J}^{-1} \frac{df}{dp} + \frac{\partial g}{\partial p}$$

f=residual; *x*=solution vec; *p*=parameters(properties); *g*=responses

Concept

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



- Model Evaluator Use Cases:
  1. Application Interface
  2. PIRO "Response Only Model Evaluators" with response sensitivities:
     - Nonlinear (NOX),
     - Time Integrator (Rythmos),
     - Optimization (MOOCHO), Param.
     - Continuation/Stability/Bifurcation (LOCA)
  3. Decorators:
     - Default Implementation (DelegatorBase)
     - Scaled
     - Jacobian-Free Newton-Krylov (JFNK)
     - Block Composite (LIME Multiphysics)

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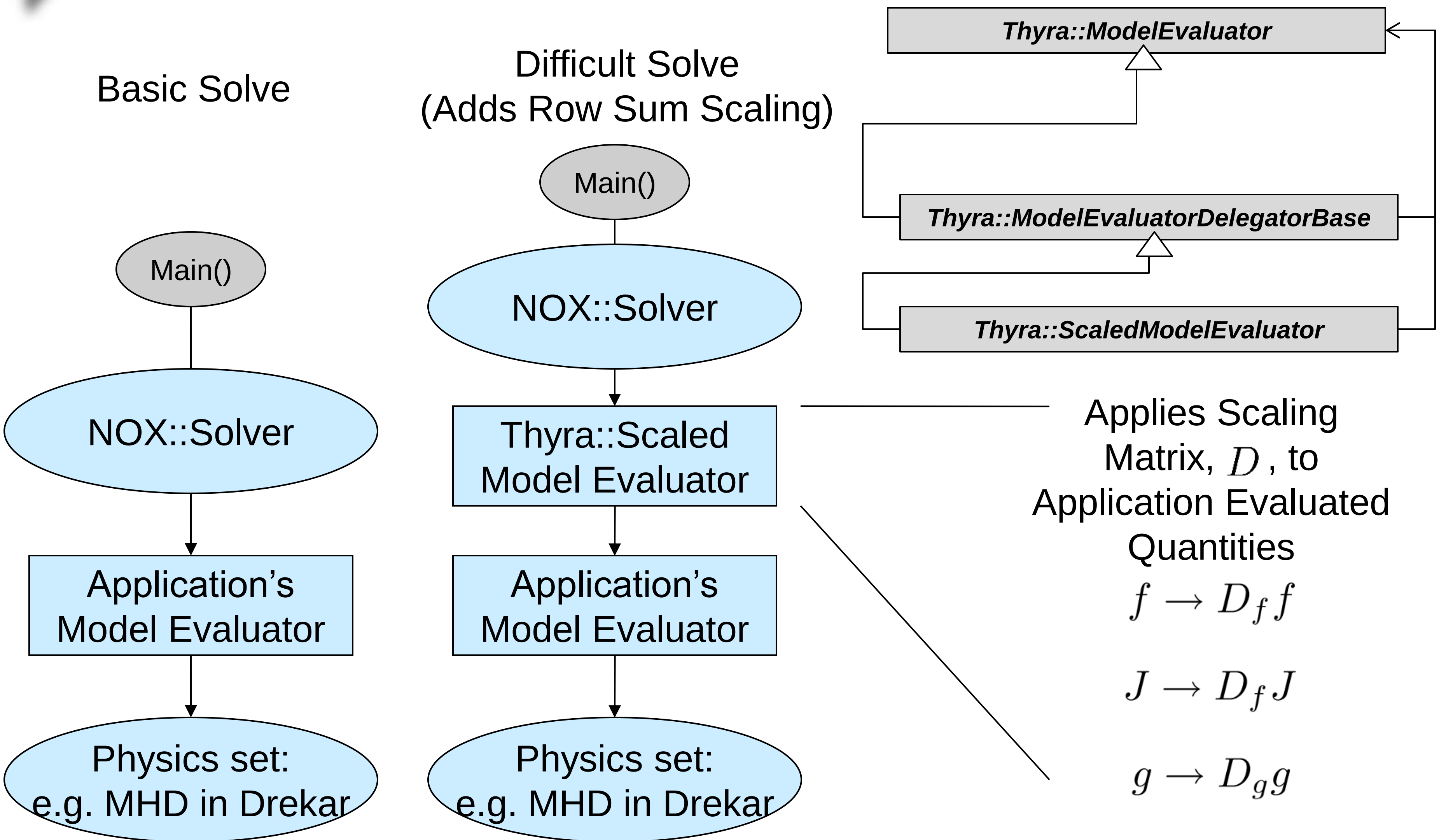
Uses **Decorator** to better condition a poorly scaled system of equations



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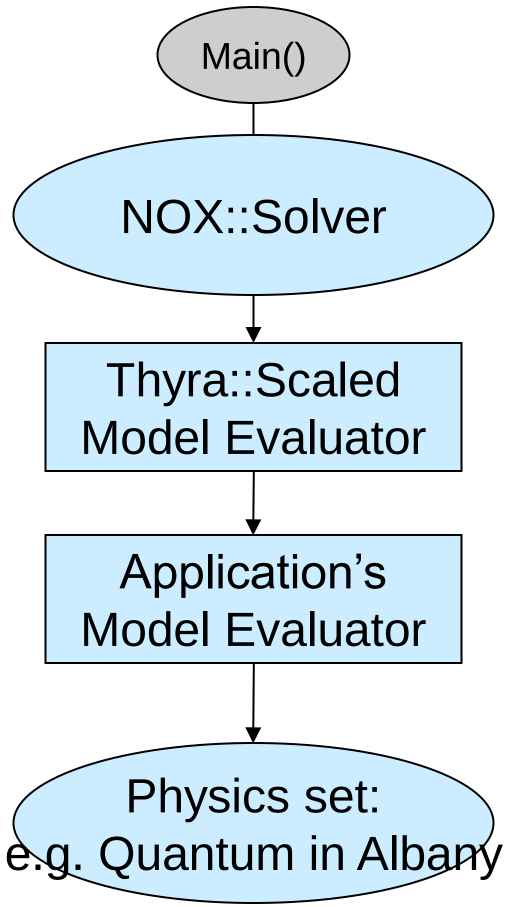
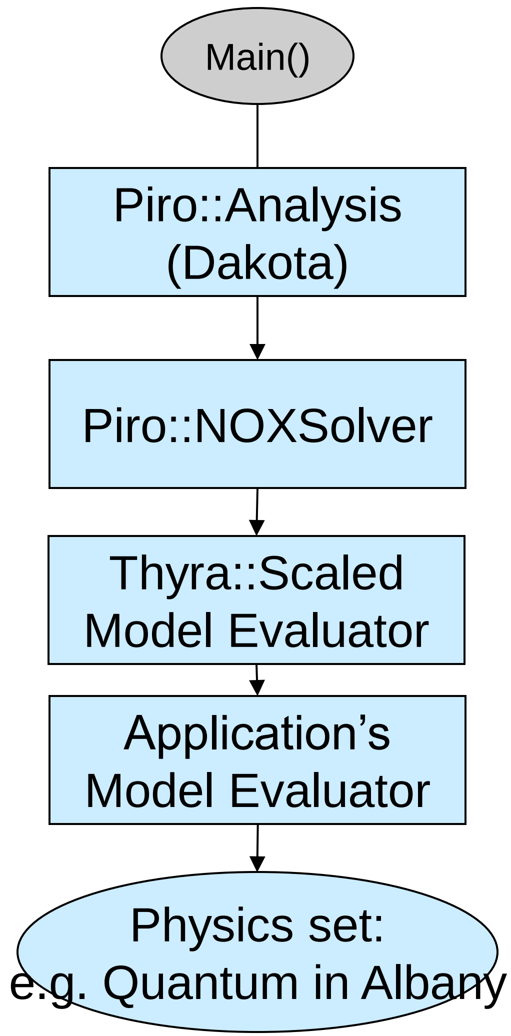
PIRO ROMEs Add direct support to Nonlinear Analysis Tools and Response Sensitivities

Difficult Solve



Analysis



$$p \longrightarrow g(p)$$

Piro::NOXSolver

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

$$\frac{dg}{dp} = \frac{\partial g}{\partial x}^T \mathbf{J}^{-1} \frac{df}{dp} + \frac{\partial g}{\partial p}$$

Piro::RythmosSolver

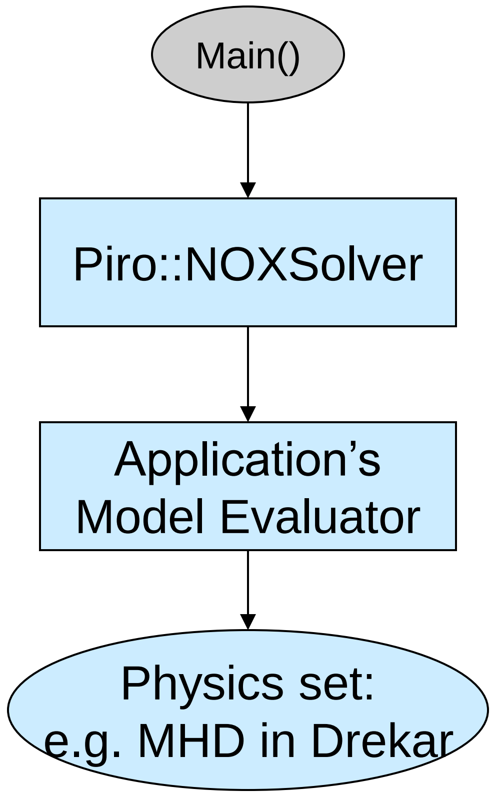
Piro::MOOCHOSolver

Piro::LOCASolver

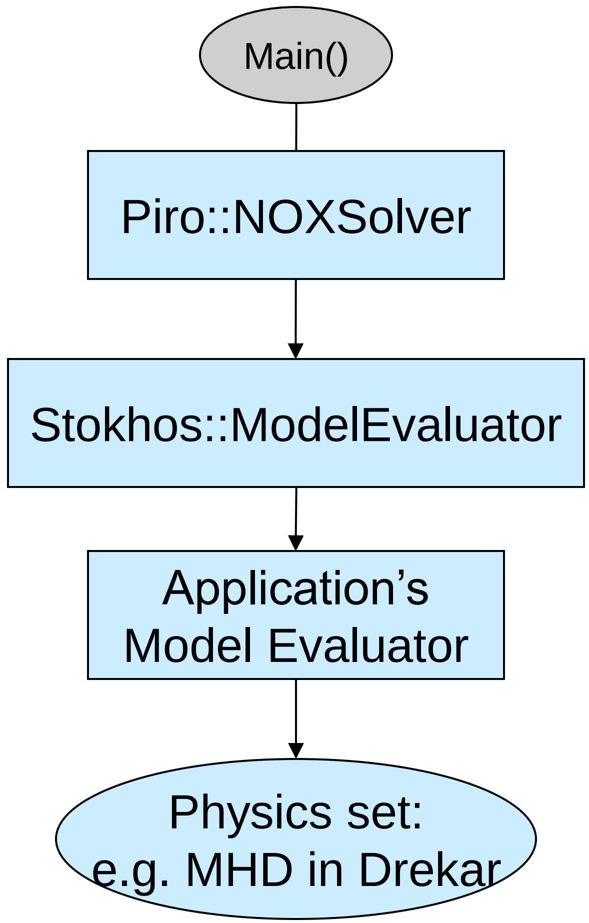
Piro::Analysis (Dakota)

Embedded UQ can be Inserted as a ME Decorator

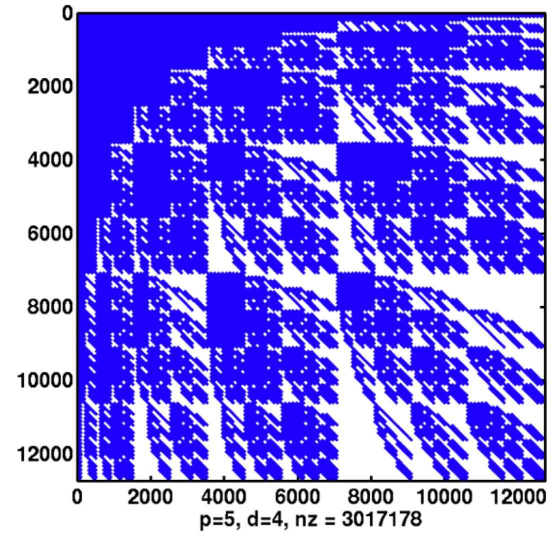
Basic Solve



Embedded UQ



Stokhos forms a block composite system



Each point is a block corresponding to a basic solve Jacobian

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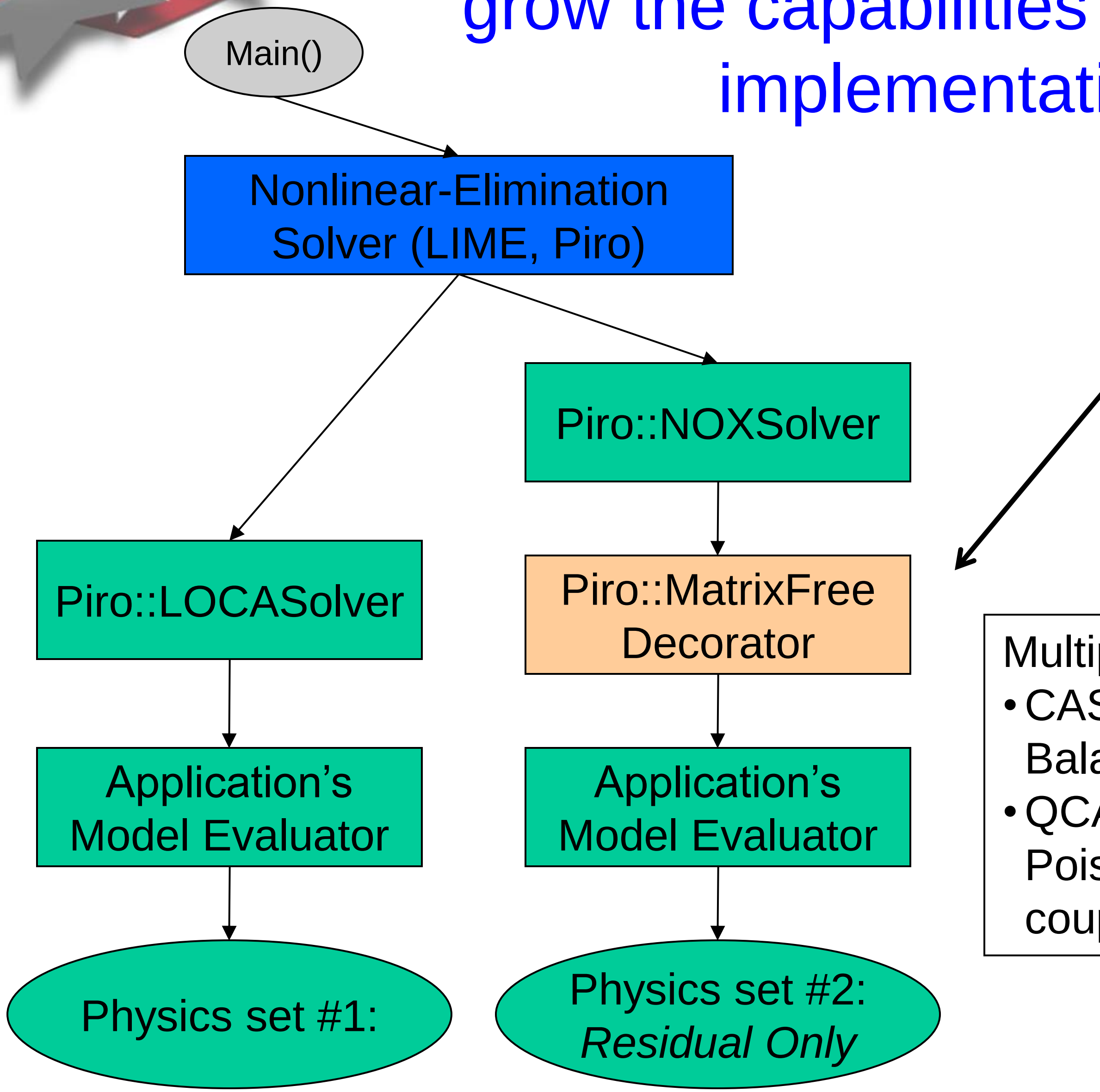
Decorators and multi-physics solvers grow the capabilities with generic implementations



6 Model Evaluators in 1 run

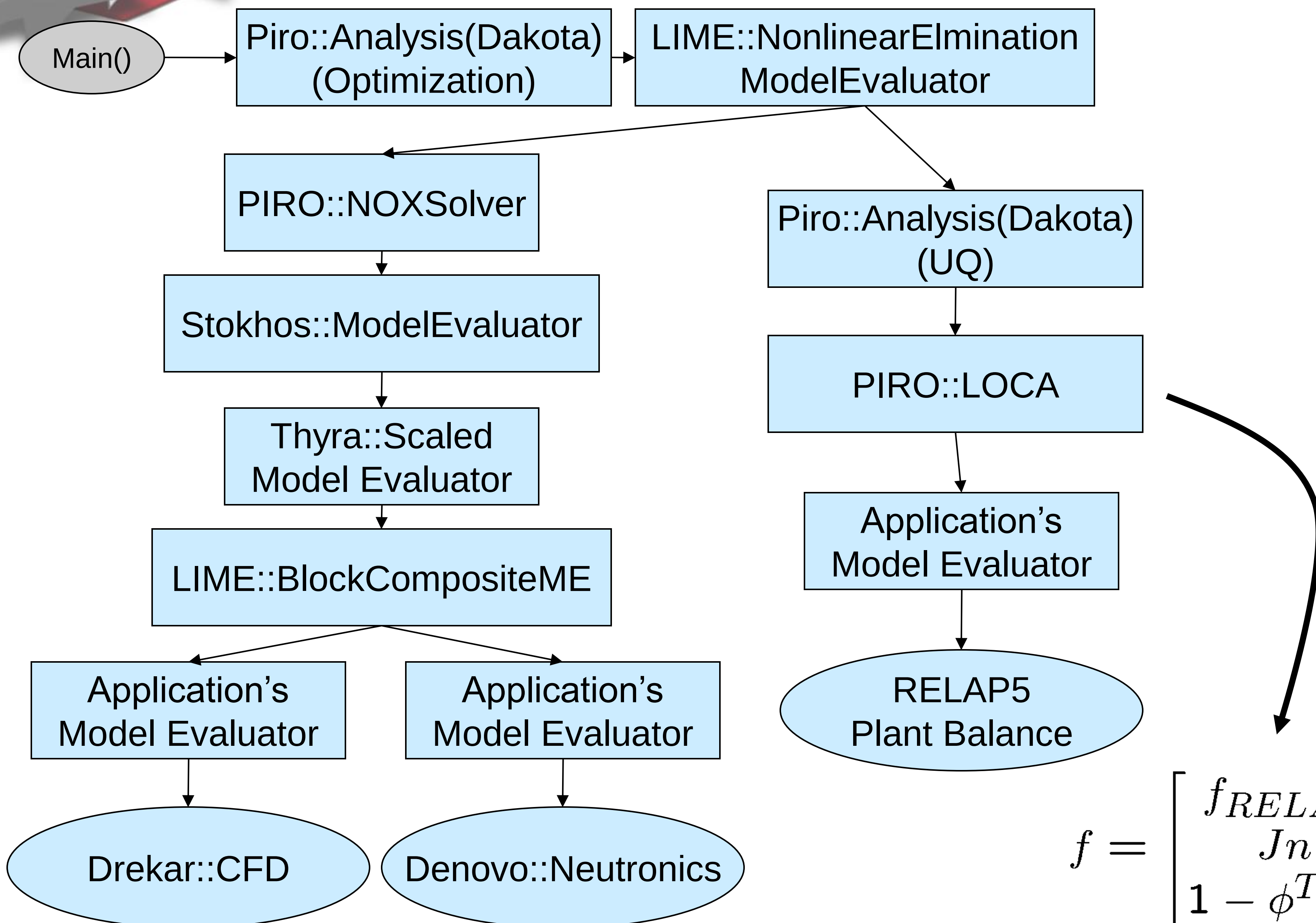
JFNK implemented as a decorator ME, implements: create_W_op()

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

Multiphysics coupling examples:

- CASL: CFD/Neutronics/Plant Balance
- QCAD: Coupled Schrodinger-Poisson (nonlinear solve coupled to eigensolve

Let Go Crazy!



$$f = \begin{bmatrix} f_{RELAP} \\ Jn \\ 1 - \phi^T \cdot n \end{bmatrix}$$

What’s Missing?

- Thyra::BlockComposed (Product) Model Evaluator
- Stochastic support in Thyra::ModelEvaluator
  - Currently only implemented in EpetraExt::ModelEvaluator

Current and Future Efforts

- Update Thyra::ModelEvaluator
    - *Many capabilities are EpetraExt-only*
    - “Ripen” Tpetra Adapters to Thyra implementations
- Refactor/Expansion of Model Evaluator interface
    - Usability
    - expand in/out args
    - handling of statefulness
    - usability (e.g. selection of parameters by string)
    - adaptivity-enabled (reset maps / vector spaces)
- System UQ (Phipps, Wildey)
- Thyra transition to kokkos
    - Currently only supports some operations relevant to belos GMRES solves.