Embedded Nonlinear Analysis Tools Capability Area

We are: top level algorithms (outermost loops)

- solution of nonlinear equations
- time integration
- bifurcation tracking / stability analysis
- parameter continuation
- optimization (PDE-constrained)
- uncertainty quantification

Governing Philosophy: "Analysis beyond Simulation,"

Goal: to automate many computational analysis and design tasks using good algorithms and good math, replacing trial-and-error or repeated simulation.

- parameter studies
- sensitivity analysis
- calibration
- optimization
- error control in transient integration
- locating instabilities
- performing UQ

Trilinos Strategic Goals that we align with:

1. **Full Vertical Coverage**
2. Hardened Solvers
3. Scalability

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Trilinos Packages in the Embedded Nonlinear Analysis Capability Area

Package Name	Quick Description	Point of Contact
NOX	Nonlinear Solver with Globalized Newton's methods	Roger Pawlowski
LOCA	Parameter Continuation, Bifurcation Tracking, 4D	Eric Phipps
Rythmos	Time integration algorithms	Todd Coffey
Moocho	Embedded (PDE-constrained) Optimization, rSQP	Roscoe Bartlett
Aristos	Full-space embedded optimization (not yet released)	Dennis Ridzal
Sacado	Automatic Differentiation using Expression Templates	Eric Phipps
Stokhos	Stochastic-Galerkin Uncertainty Quantification Tools	Eric Phipps
TriKota	Interface to Dakota for a Trilinos app (not yet released)	Andy Salinger

Related Efforts Outside of Trilinos

Dakota	Dakota is a mature and widely-used software toolkit at Sandia that delivers many related analysis capabilities using non-intrusive...
DemoApps	...a code project building a prototype PDE code primarily from Trilinos packages...

We are consolidating on a single expandable interface: the ModelEvaluator
- Application code must be stateless to let Analysis code do the driving!

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Brief Mathematical Description of Embedded Nonlinear Analysis Capabilities:

Nonlinear Solver (NOX): $\qquad\qquad f(x) = 0 \qquad$ solve for: x

Time Integration (Rythmos): $\quad f(\dot{x}, x, p, t) = 0 \qquad$ solve for: $x(t); \frac{dx}{dp}$

Bifurcation Tracking / Constraint Enforcement (LOCA):

$$F(X) = \left[\begin{array}{c} f(x,p) \\ [Real(\lambda)] \end{array} \right] = 0 \qquad F(X) = \left[\begin{array}{c} f(x,p) \\ h(x,p) \end{array} \right] = 0 \qquad \text{solve for: } X = (x,p)$$

Parameter Continuation (LOCA):

$$f(x,p) = 0 \qquad \text{solve for: } (x,p); \frac{dx}{dp}$$

Stability Analysis (LOCA→Anasazi):

$$Jz = \lambda M z \qquad \text{solve for: } (\lambda, z)$$

PDE-Constrained Optimization (Moocho/Aristos):

minimize $g(x,p)$ subject to $f(x,p) = 0 \qquad$ solve for: (x, p, g_{min})

Embedded UQ (Stokhos):

$$f(x(\xi), \xi) = 0 \qquad \text{solve for: } x(\xi)$$

Pop Quiz: What is the favorite Trilinos package among the developers in the Embedded Nonlinear Analysis Capability Area*?

1. Sacado (Automatic Differentiation → Analytic Derivatives)

2. Epetra (Distributed memory vector and matrix formats)

3. Teuchos::RCP (Reference Counted Pointers for memory management)

*Based on a statistical sample of 14% of the developers.

Active Areas of Research and Development

- Expand Rythmos Capabilities (today 2:45pm)
  - Error estimation and control
  - Adjoint integration with checkpointing
- Embedded UQ capability (today 3:45pm)
  - hybrid sampling / embedded
  - linear solves of stochastic systems
- System Modeling Capability
  - System-level Interfaces
  - Network builders
  - System Solvers (Born with AD/UQ)
- Single ENAT_Solver factory for NOX, LOCA, Rythmos, Moocho
- Improved Software Quality, e.g. exception handing
- Demonstrations of Transformational Embedded Nonlinear Analysis Capabilities (today: 4:10pm)

Roscoe Bartlett, Todd Coffey, Roger Pawlowski, Eric Phipps, Andy Salinger, Dennis Ridzal, Bart van Bloemen Waanders