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 (black-box, PDE-constrained, full-space)
- uncertainty quantification
- multi-physics coupling

Governing Philosophy: "Analysis beyond Simulation,"

Goal: to automate many computational analysis and design tasks, using applied math and algorithms to replace 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

Trilinos Packages in the Embedded Nonlinear Analysis Capability Area

Package Name	Quick Description	Point of Contact
Piro	Uniform Wrapper for most ENAT Capabilities	Andy Salinger
NOX	Nonlinear Solver with Globalized Newton's methods	Roger Pawlowski
LOCA	Parameter Continuation, Bifurcation Tracking, 4D	Eric Phipps
Rythmos	Time integration algorithms	**Curt Ober FY12**
Moocho	Embedded (PDE-constrained) Optimization, rSQP	Roscoe Bartlett
ROL/Aristos	Full-space embedded optimization	Dennis Ridzal
OptiPack	Nonlinear CG	Roscoe Bartlett
GlobiPack	Library of Line search methods for globalizations	Roscoe Bartlett
Sacado	Automatic Differentiation using Expression Templates	Eric Phipps
Stokhos	Stochastic-Galerkin Uncertainty Quantification Tools	Eric Phipps
TriKota	Interface to Dakota for a Trilinos app	Andy Salinger
LIME	Multi-Physics coupling framework	Hooper, Schmidt, Belcourt, Pawlowski, Bartlett

Related Efforts Outside of Trilinos

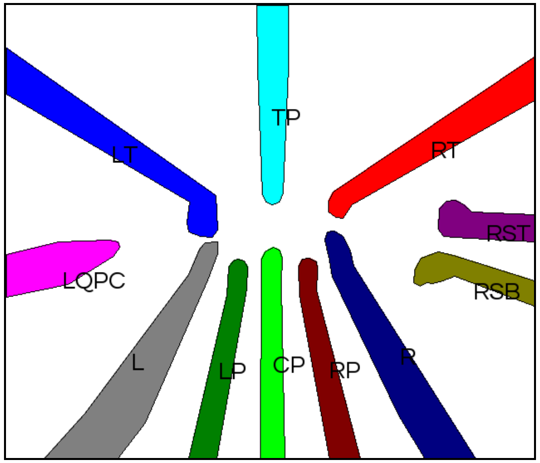
Dakota	Dakota is a mature and widely-used software toolkit that delivers many analysis capabilities using a non-intrusive (a.k.a. blackbox) interface...
Albany, Drekar	Code projects for building a PDE codes primarily from Trilinos packages, born with transformational capabilities.

ENAT Success Story: QCAD LDRD for Quantum Dot Design (Muller, Gao, Nielsen, Salinger, Young)

The unit of calculation is an ensemble of optimization runs!!!!

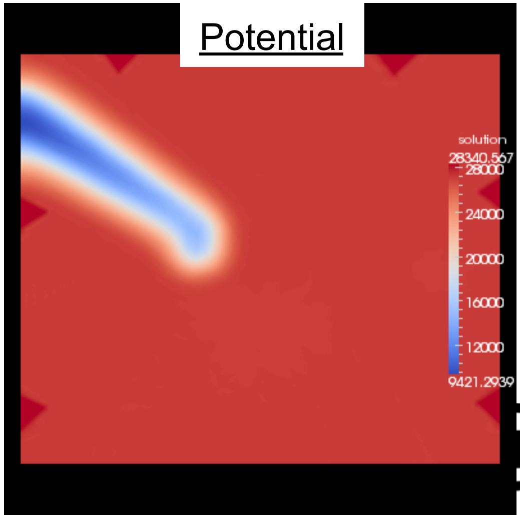
Q: Given this design of gates, each with a voltage as an operating parameter.

A: How well can this device be tuned for ~40 cases (# of free electrons in quantum region, barrier height between wells



Some Optimization run descriptions (QI=#of free electrons):

- QI=1, LTB on, vary AG TP LP LT
- QI=10, DB off, LQPCB on, vary AG TP CP LP-RP LT-RT L-R LQPC
- QI=100, DB on, LQPCB on, vary AG TP CP LP-RP LT-RT L-R LQPC
- QI=10, LTB on, vary AG TP



Uses: Dakota, Cubit, Exodus, Ioss, SEACAS tools, STK_Mesh, STK_IO, Sacado, Phalanx, Intrepid, Shards, Epetra, EpetraExt, Piro, NOX, LOCA, TriKota, Stratimikos, Thyra, Belos, Ifpack, Teuchos

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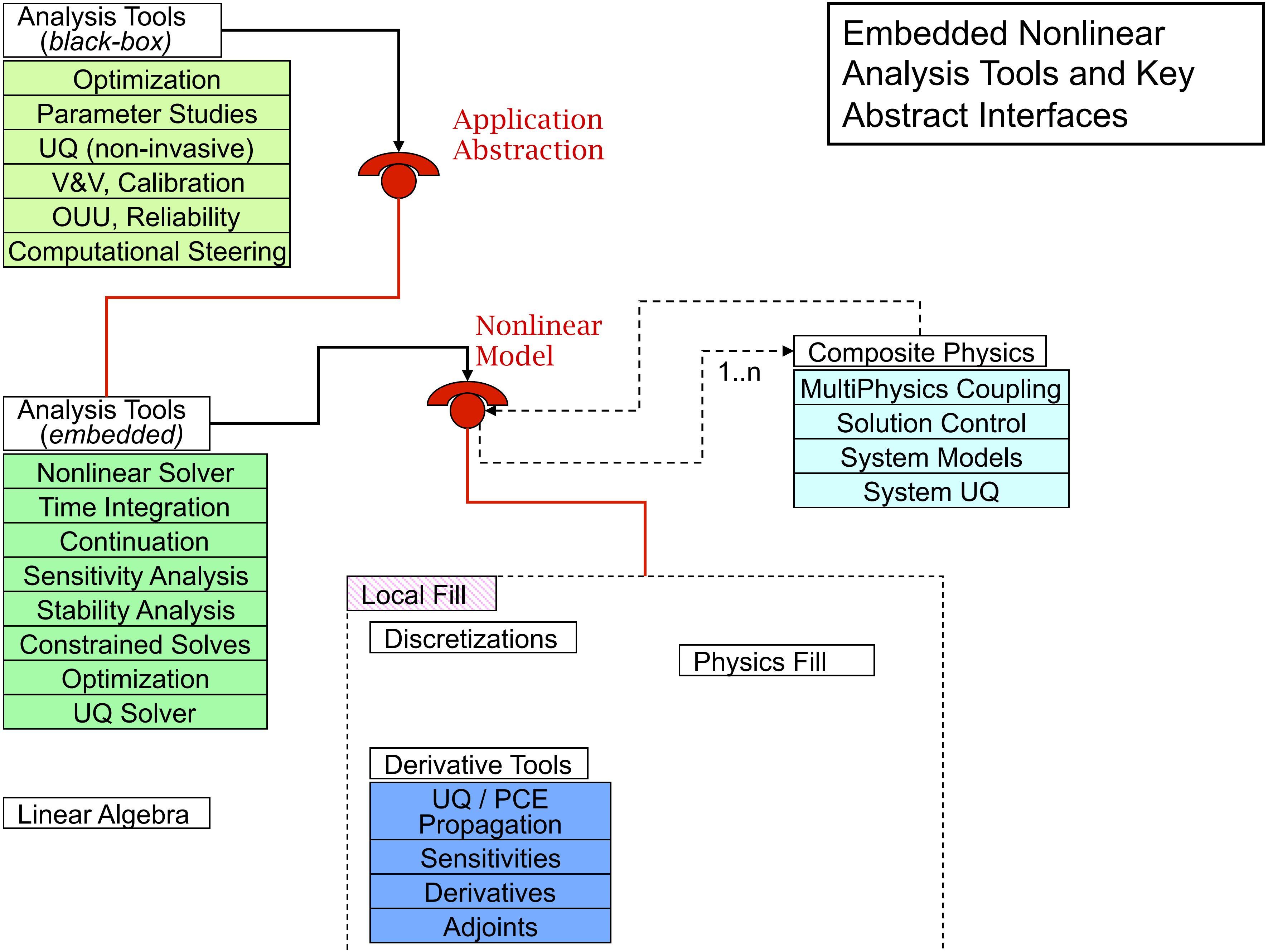
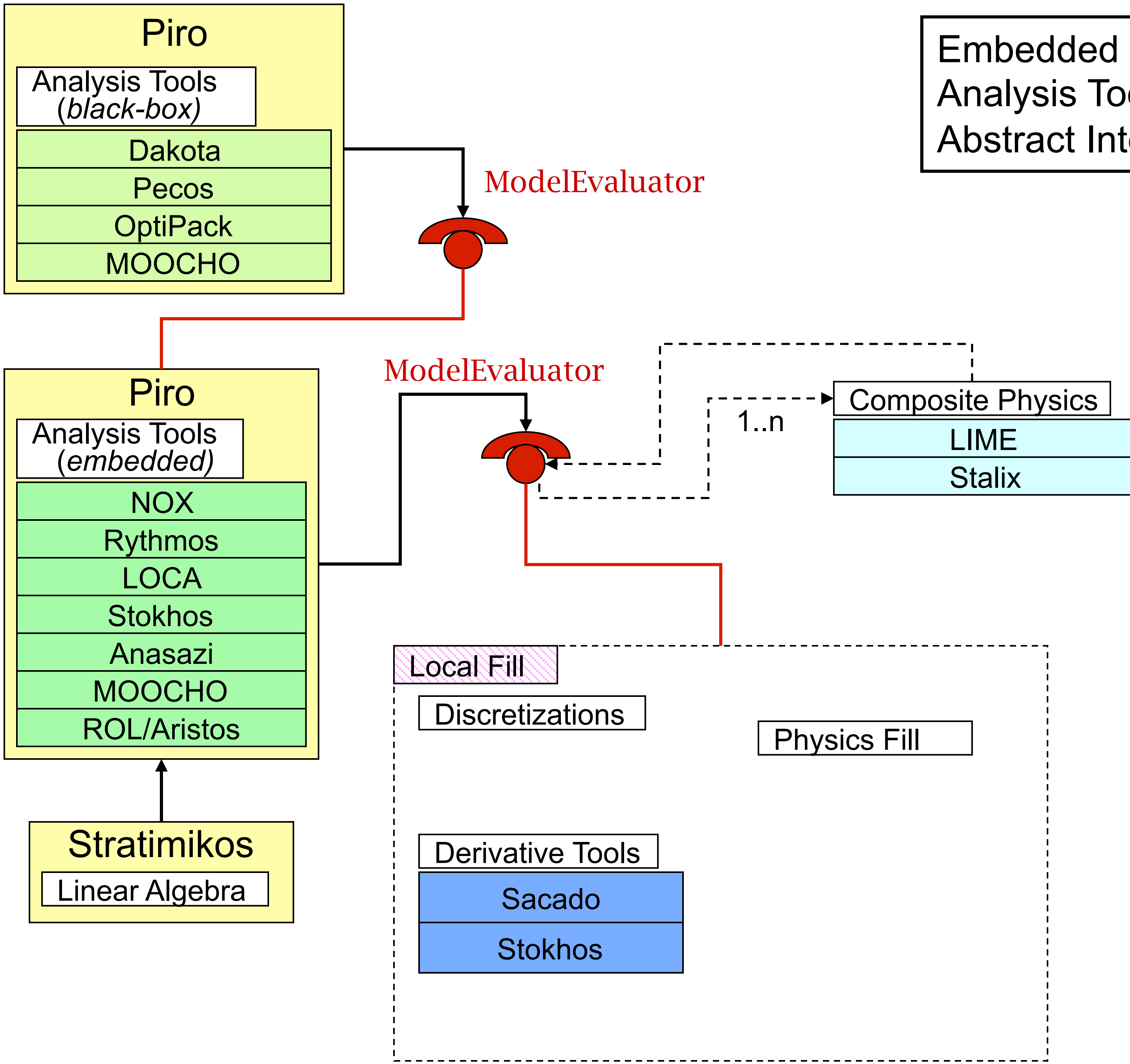
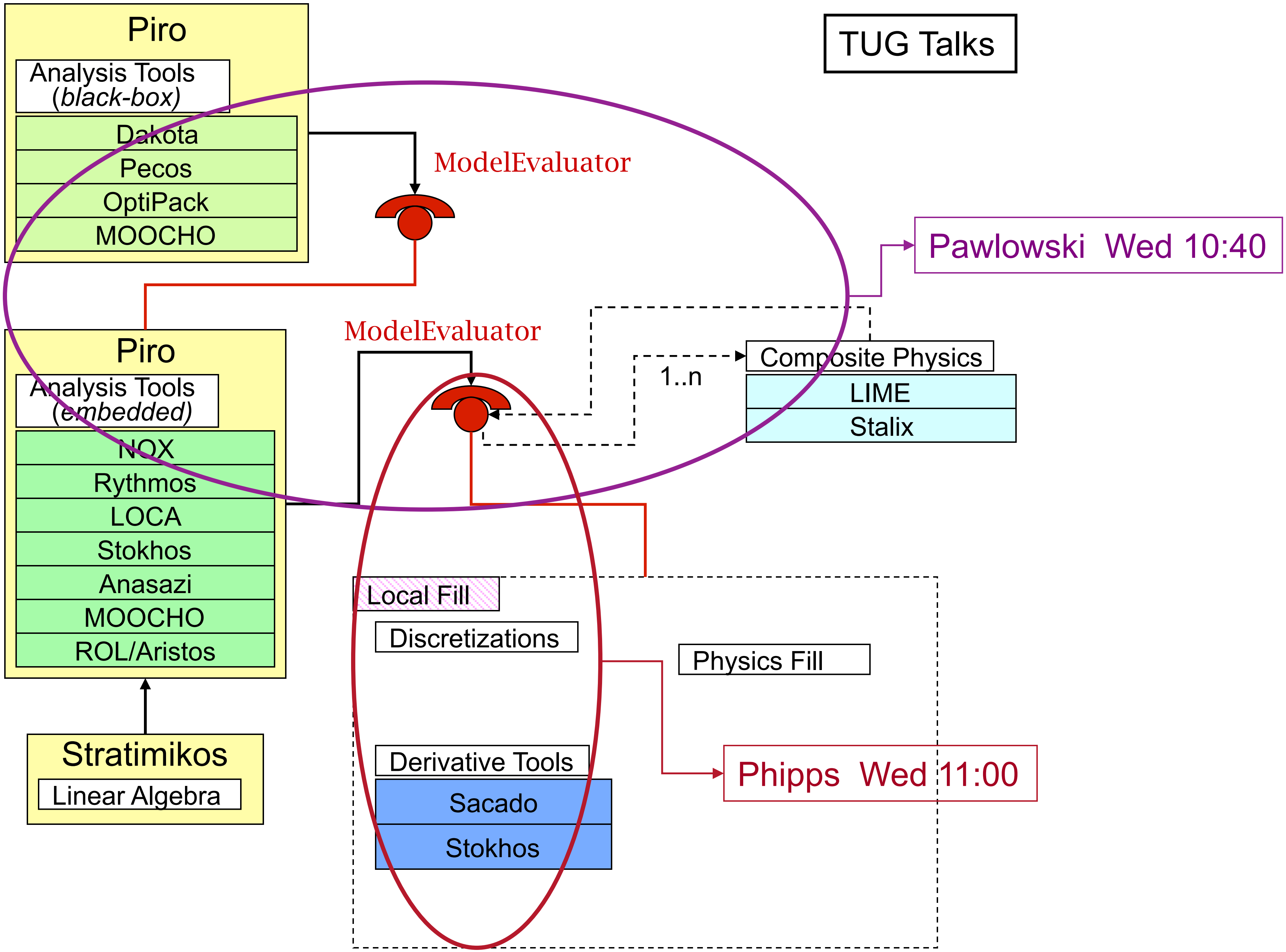


Embedded Nonlinear Analysis Tools and Key Abstract Interfaces
Analysis Tools (*black-box*)
Optimization
Parameter Studies
UQ (non-invasive)
V&V, Calibration
OUU, Reliability
Computational Steering
Application Abstraction
Nonlinear Model
Composite Physics
1..n
MultiPhysics Coupling
Solution Control
System Models
System UQ
Analysis Tools (*embedded*)
Nonlinear Solver
Time Integration
Continuation
Sensitivity Analysis
Stability Analysis
Constrained Solves
Optimization
UQ Solver
Local Fill
Discretizations
Physics Fill
Derivative Tools
UQ / PCE Propagation
Sensitivities
Derivatives
Adjoints
Linear Algebra

Embedded Nonlinear Analysis Tools and Key Abstract Interfaces





TUG Talks
Piro
Analysis Tools
(black-box)
Dakota
Pecos
OptiPack
MOOCHO
ModelEvaluator
Pawlowski Wed 10:40
ModelEvaluator
Piro
Analysis Tools
(embedded)
NOX
Rythmos
LOCA
Stokhos
Anasazi
MOOCHO
ROL/Aristos
Composite Physics
1..n
LIME
Stalix
Stratimikos
Linear Algebra
Local Fill
Discretizations
Physics Fill
Derivative Tools
Sacado
Stokhos
Phipps Wed 11:00

Embedded Nonlinear Analysis Capabilities: Active Areas of Research and Development

- Expanded Rythmos Capabilities (Curt Ober et al)
  - Usability
  - All varieties of Sensitivities
  - Adjoints
- Embedded UQ capability
  - Multi-Physics UQ
  - UQ and Multicore architectures
- Embedded Optimization with many Inequality Constraints
  - Full Space, reduced space
- Multi-Physics coupling layers (Piro,LIME)
- Full templated stack (NOX, LOCA, Piro)
  - Tpetra and Thyra support throughout
- More Demonstrations of Transformational Embedded Nonlinear Analysis Capabilities

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