

Embedded Nonlinear Analysis Tools Capability Area SAND2011-8316C

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



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

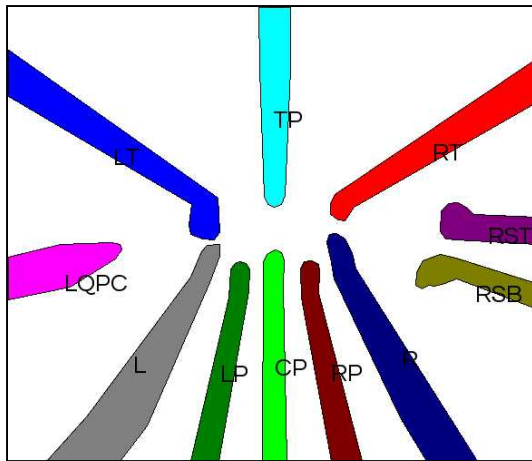
Dakota	Dakota is a mature and widely-used software toolkit that delivers many analysis capabilities using a non-intrusive (a.k.a. blackbox) interface...
Albany, Drekar	Code projects for building a PDE codes primarily from Trilinos packages, born with transformational capabilities.



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):

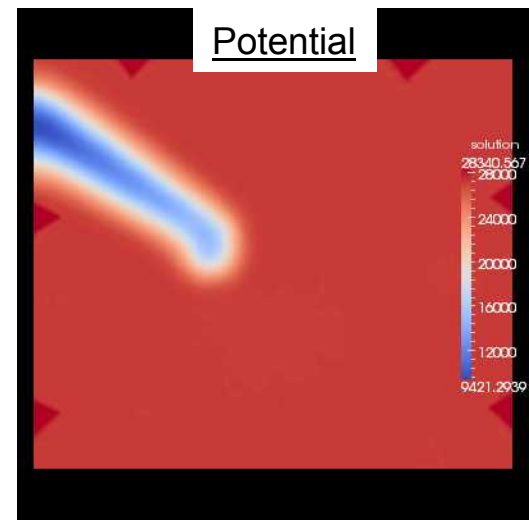
QI=1, LTB on, vary AG TP LP LT

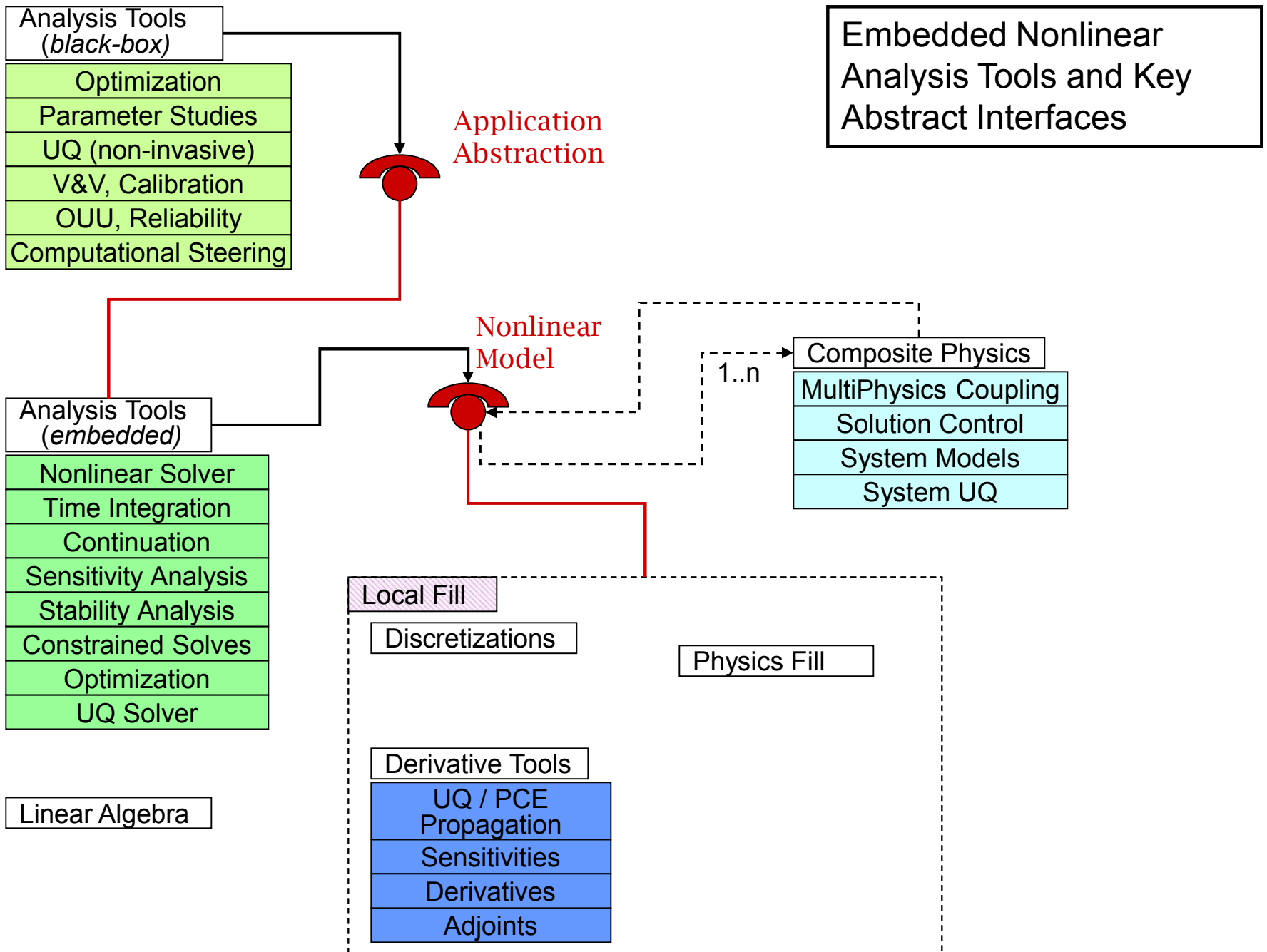
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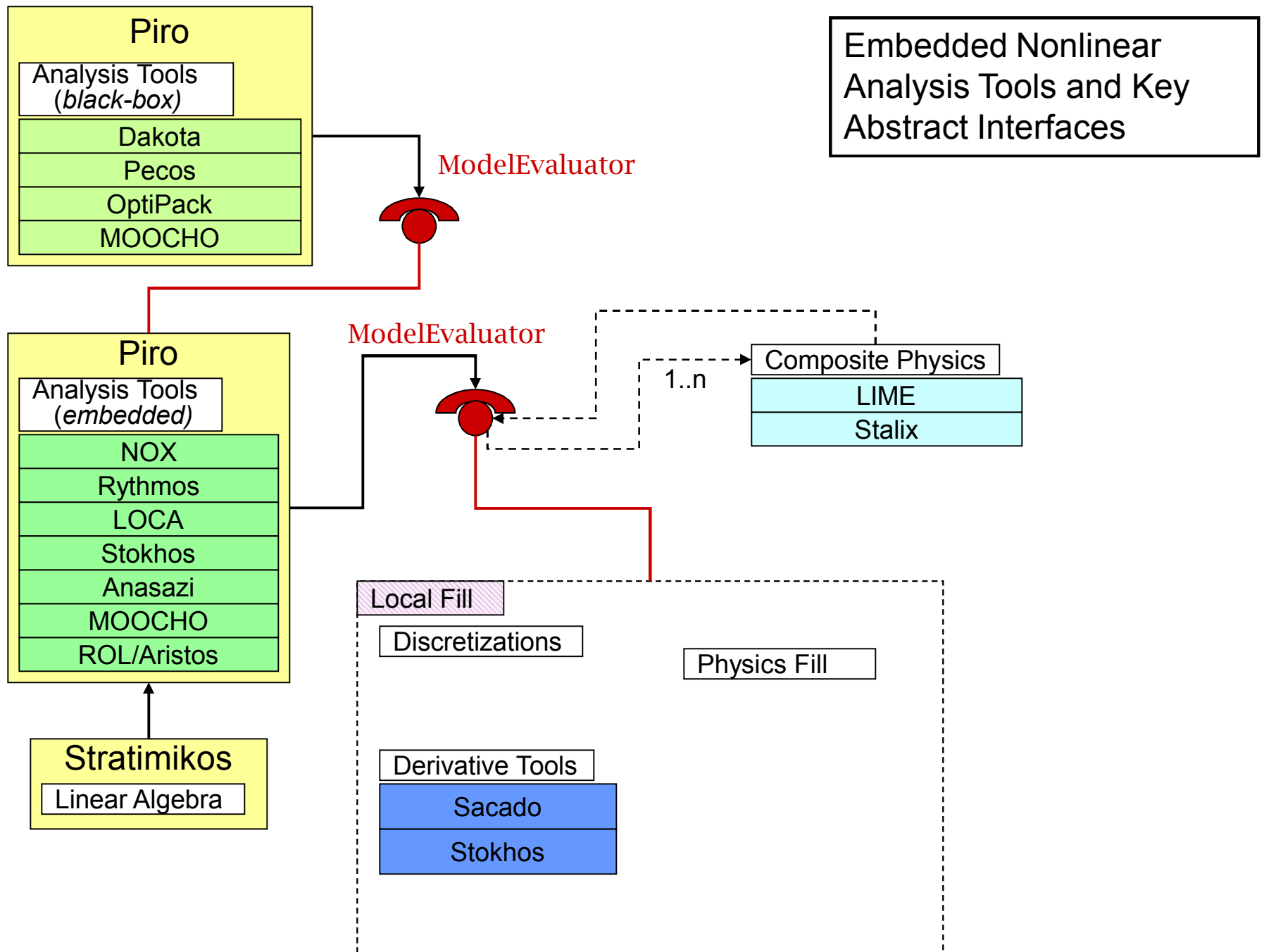
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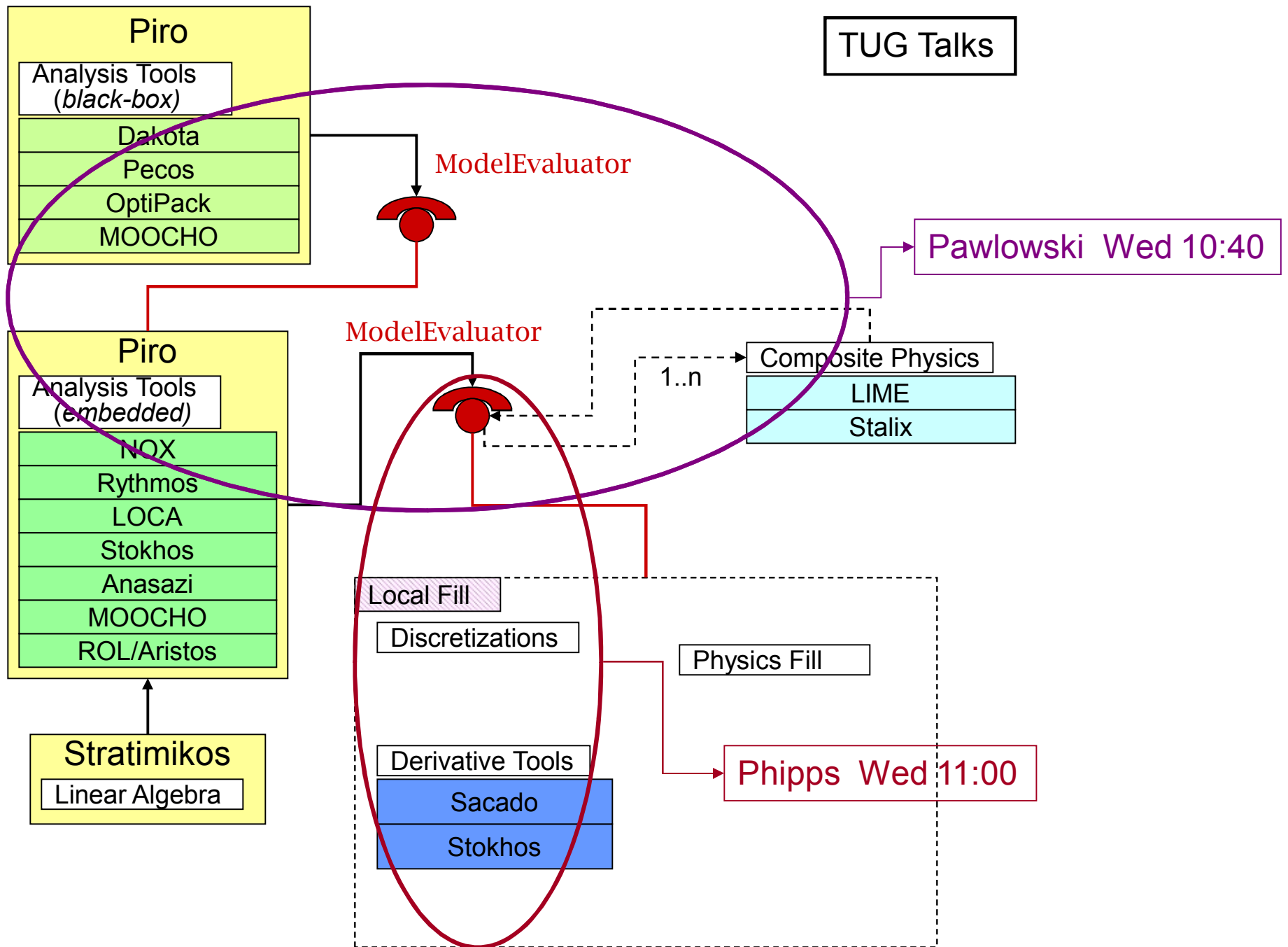
QI=10, LTB on, vary AG TP

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











Embedded Nonlinear Analysis Capabilities: Active Areas of Research and Development

- Expanded Rythmos Capabilities (Curt Ober et al)
 - Usability
 - All varieties of Sensitivities
 - Adjoint
- Embedded UQ capability
 - Multi-Physics UQ
- 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