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Foundational Capabilities for Computational Simulation

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Sandia National Laboratories

Computational Simulation Group

Presented to Goodyear

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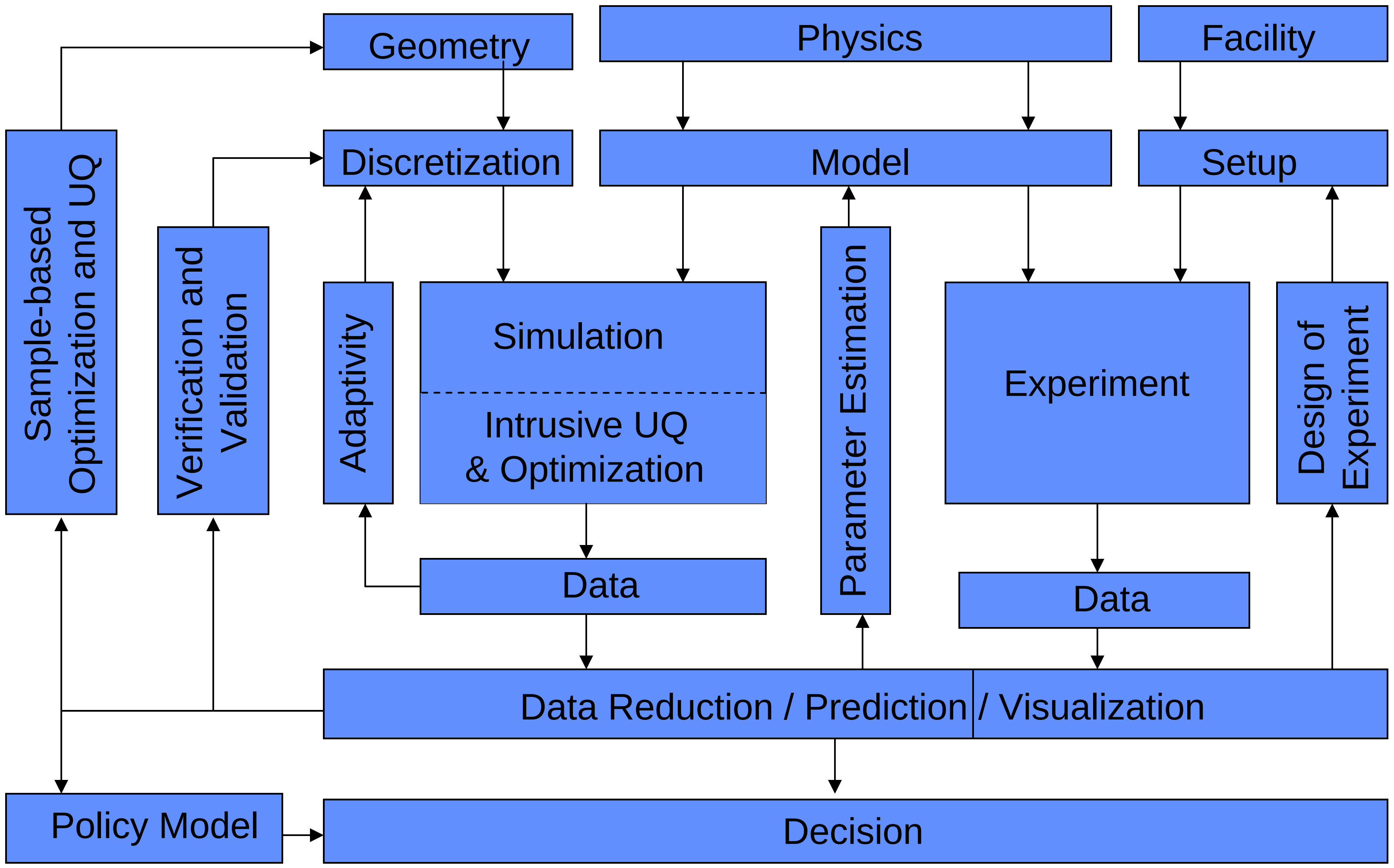
Modeling and Simulation "Workflow"



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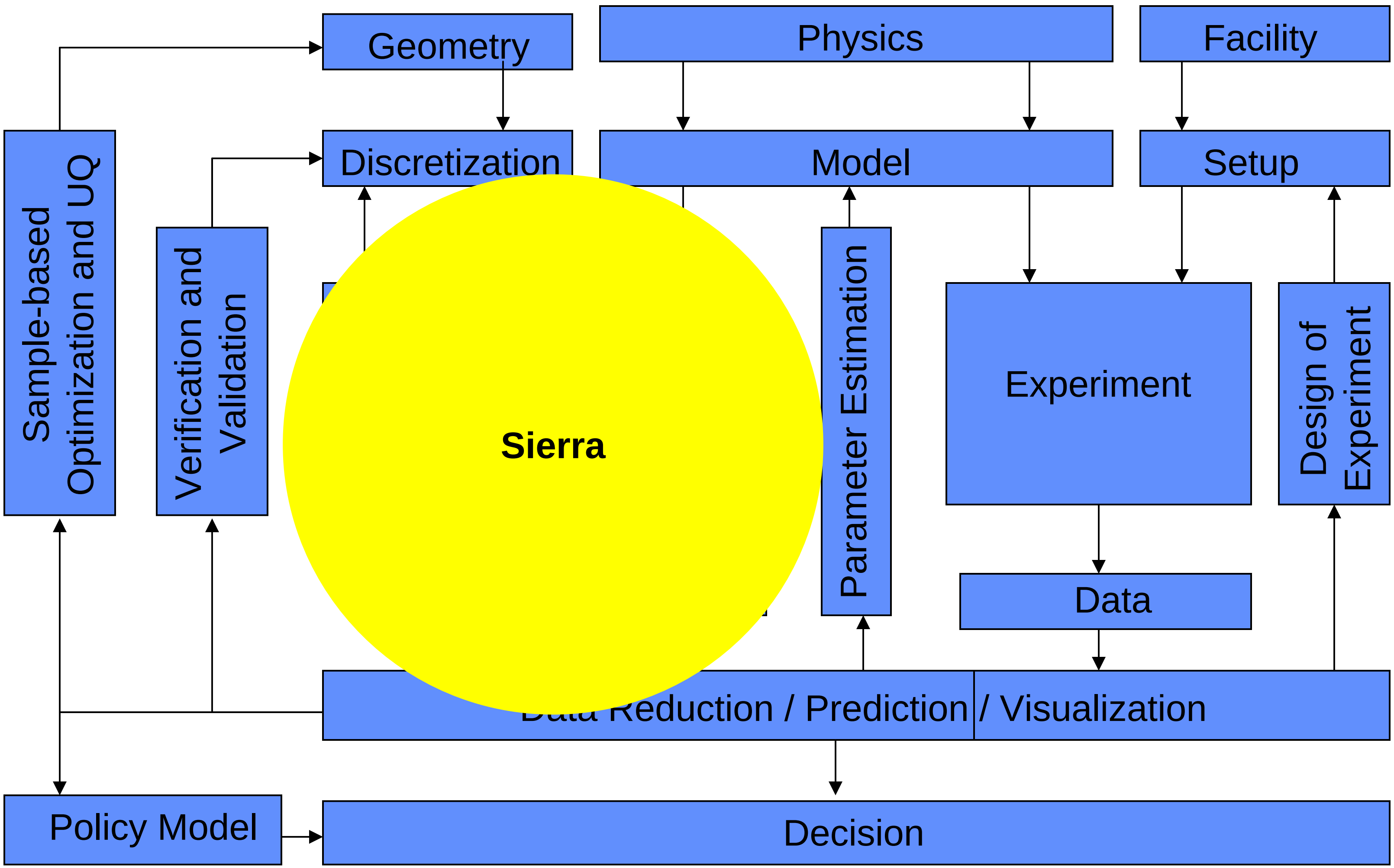
Modeling and Simulation "Workflow"



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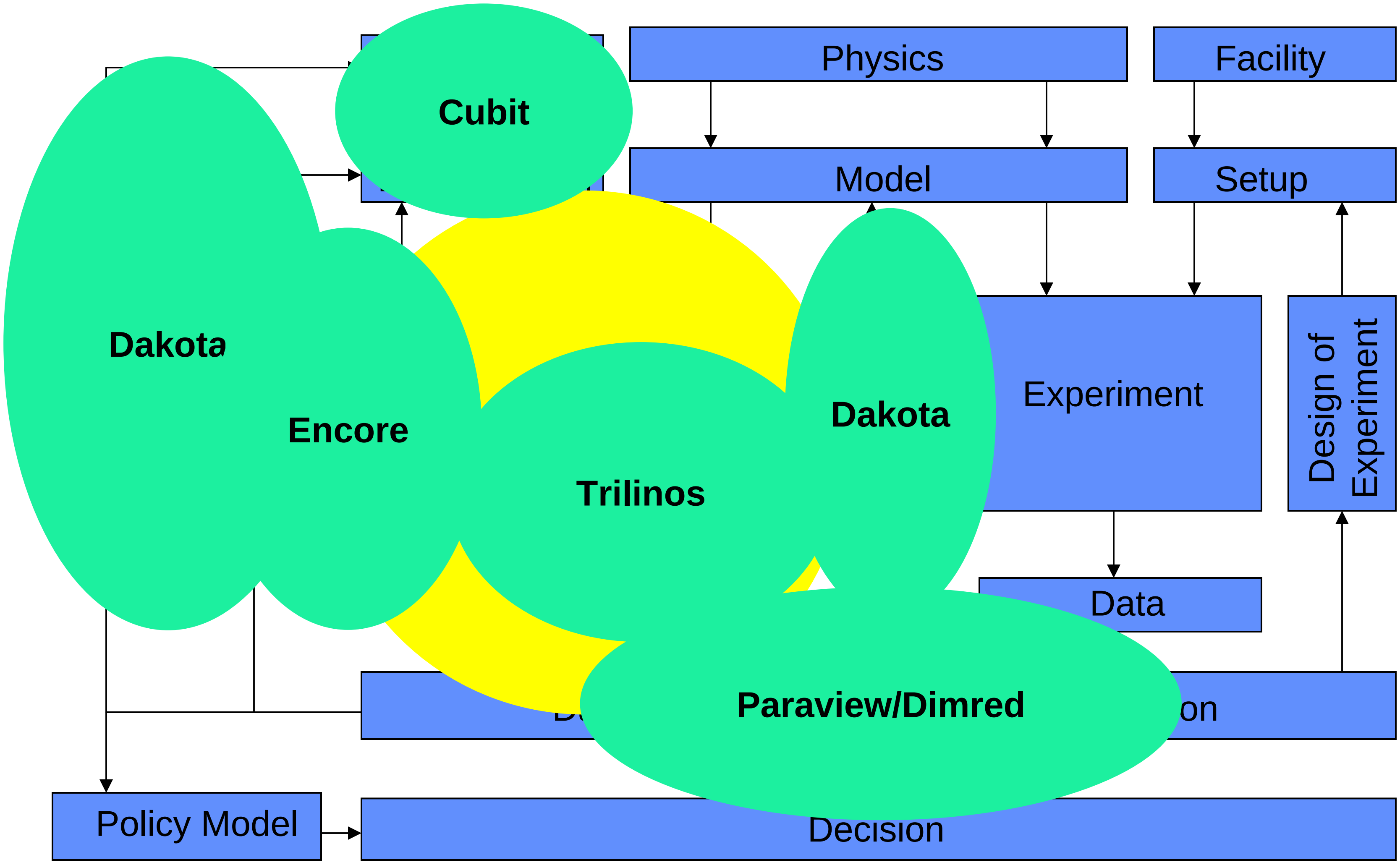
Modeling and Simulation "Workflow"



Evolving Trilinos Solution

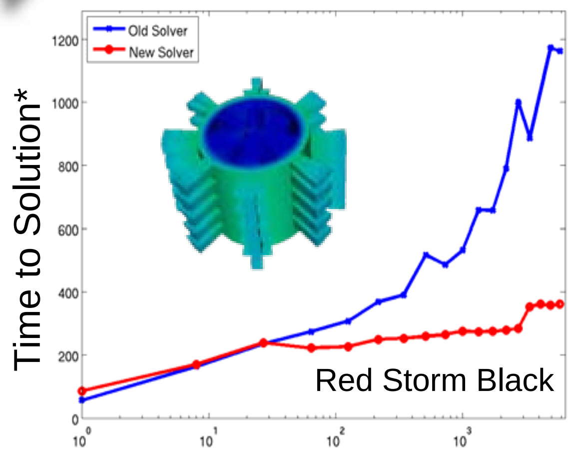
- Trilinos[1] is an evolving framework to address these challenges:
  - Fundamental atomic unit is a *package*.
  - Includes core set of vector, graph and matrix classes (Epetra/Tpetra packages).
  - Provides a common abstract solver API (Thyra package).
  - Provides a ready-made package infrastructure (new_package package):
    - Source code management (cvs, bonsai).
    - Build tools (autotools).
    - Automated regression testing (queue directories within repository).
    - Communication tools (mailman mail lists).
  - Specifies requirements and suggested practices for package SQA.
- In general allows us to categorize efforts:
  - Efforts best done at the Trilinos level (useful to most or all packages).
  - Efforts best done at a package level (peculiar or important to a package).
  - Allows package developers to focus only on things that are unique to their package.

1. Trilinos loose translation: "A string of pearls"

Trilinos Package Summary

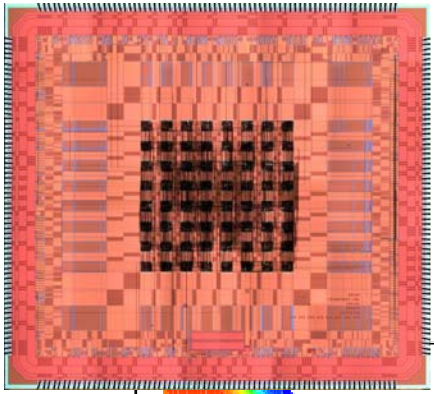
	Objective	Package(s)
Discretizations	Meshing & Spatial Discretizations	phdMesh, Intrepid, Pamgen, Sundance
	Time Integration	Rythmos
Methods	Automatic Differentiation	Sacado
	Mortar Methods	Moertel
Core	Linear algebra objects	Epetra, Jpetra, Tpetra
	Abstract interfaces	Thyra, Stratimikos, RTOp
	Load Balancing	Zoltan, Isorropia
	"Skins"	PyTrilinos, WebTrilinos, Star-P, ForTrilinos, CTrilinos
	C++ utilities, I/O, thread API	Teuchos, EpetraExt, Kokkos, Triutils, TPI
Solvers	Iterative (Krylov) linear solvers	AztecOO, Belos, Komplex
	Direct sparse linear solvers	Amesos
	Direct dense linear solvers	Epetra, Teuchos, Pliris
	Iterative eigenvalue solvers	Anasazi
	ILU-type preconditioners	AztecOO, IFPACK
	Multilevel preconditioners	ML, CLAPS
	Block preconditioners	Meros
	Nonlinear system solvers	NOX, LOCA
	Optimization (SAND)	MOOCHO, Aristos
	Stochastic PDEs	Stokhos

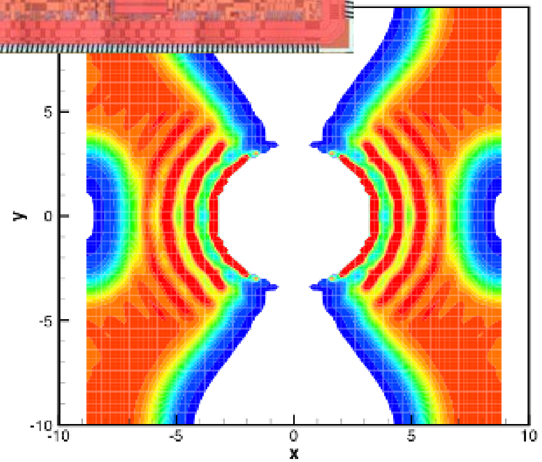
Example Applications

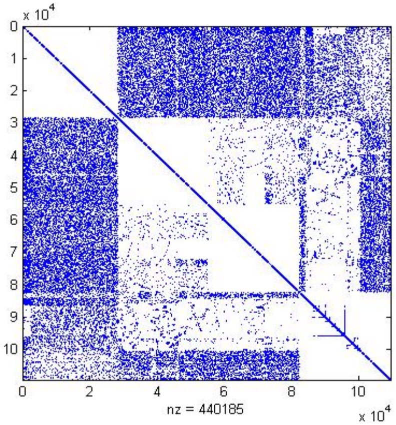


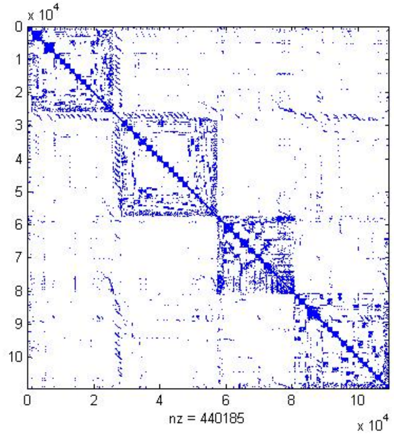
Number of Processors

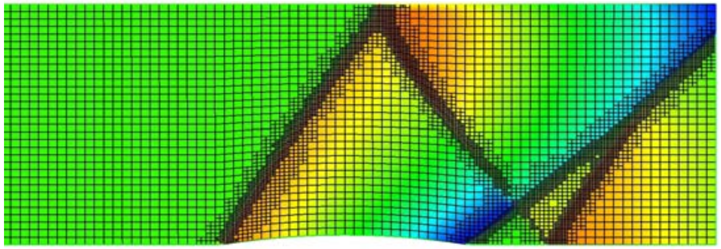
Number of Processors











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Embedded Algorithms will Drive Tomorrow's M&S Tools

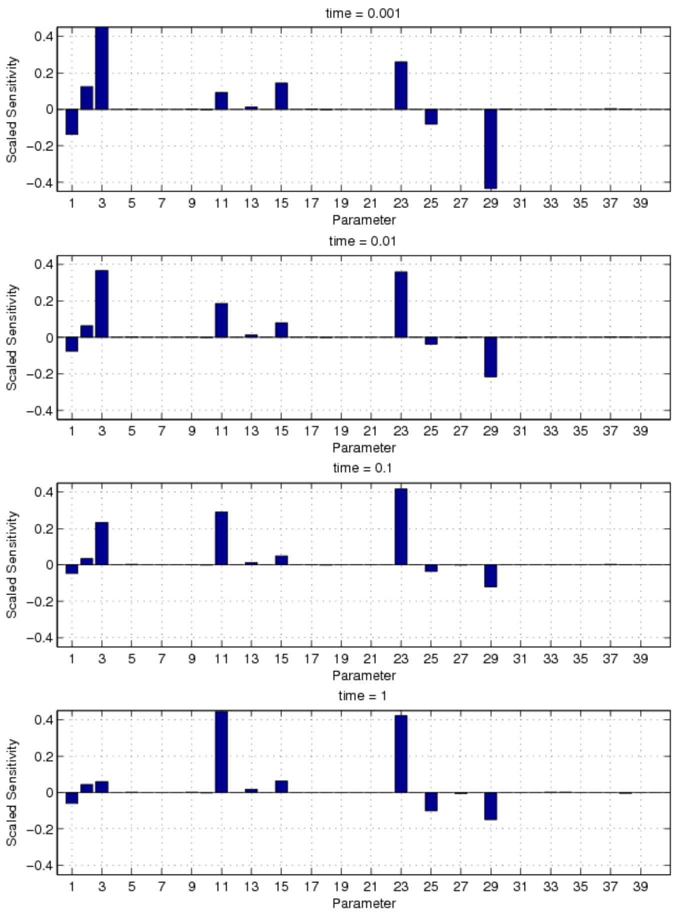
- Algorithm Infrastructure
  - Automatic Differentiation (AD)
  - Adjoint solution technology

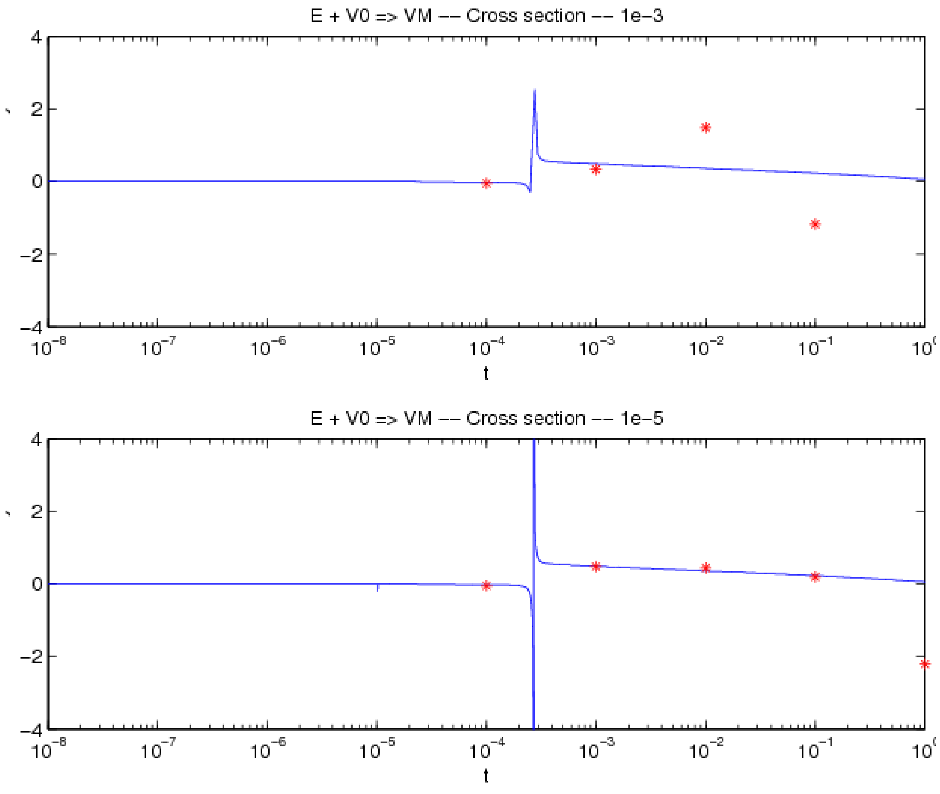
- Applications of *Embedded Algorithms*
  - Sensitivity analysis
  - Uncertainty Quantification
  - Goal-oriented (adjoint-based) error estimation

Adjoints and AD are key capabilities for increased efficiency and accuracy!

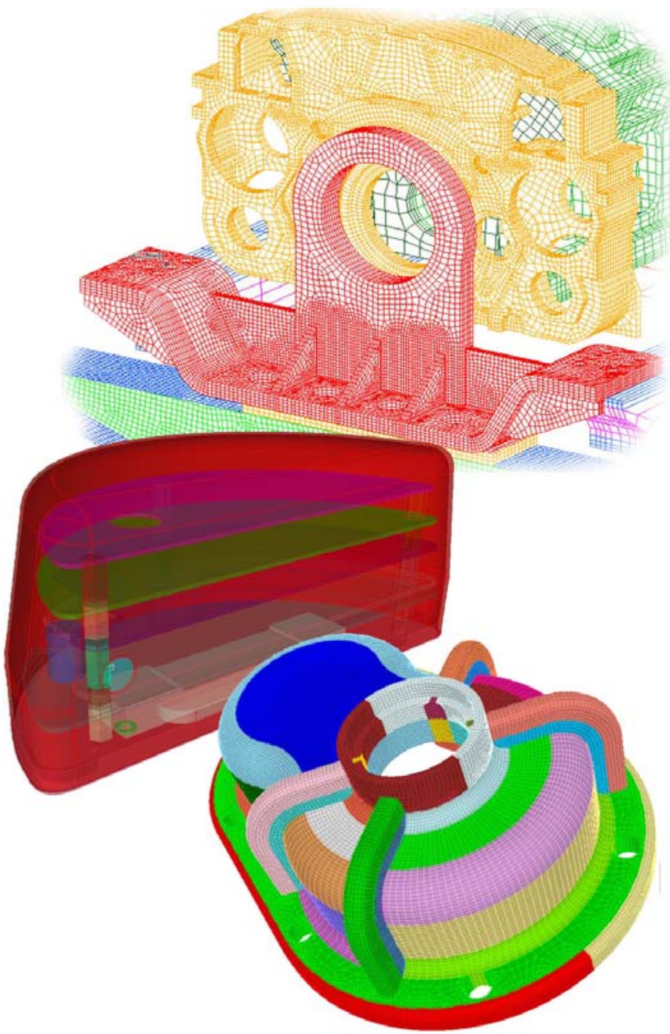
The Power of “Embedded Algorithms”

Direct calculations of transient sensitivities in semiconductor devices

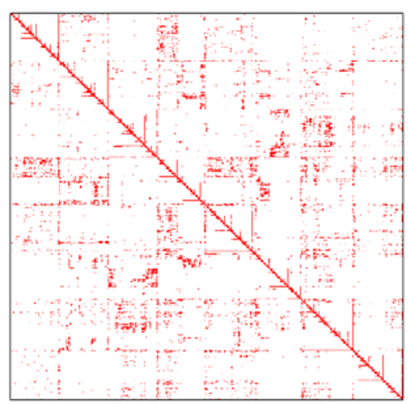


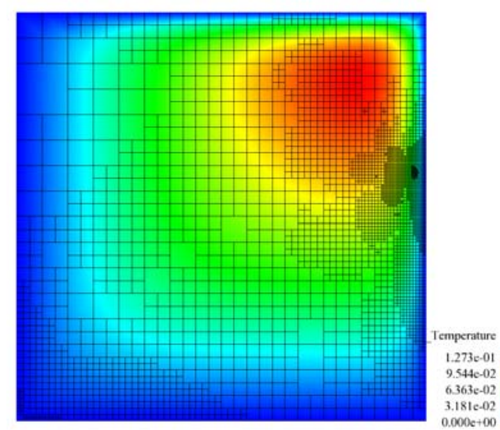


Partitioning and Load Balancing



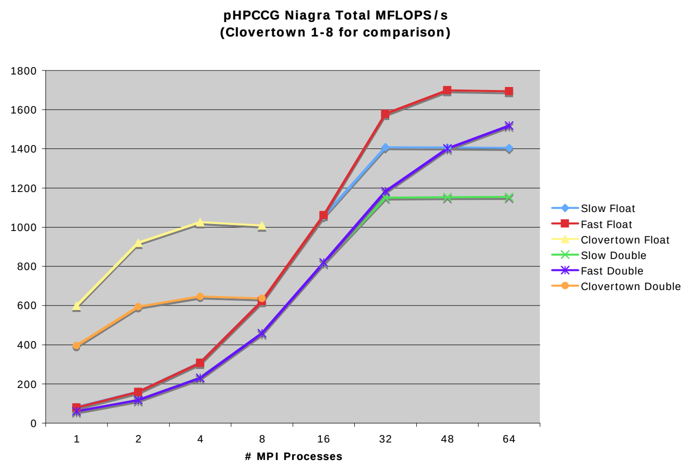
- **Parallel hypergraph partitioning in Zoltan has advantages over graph partitioning**
  - **Supports rectangular systems (ParPCx, Trilinos)**
  - **Supports highly connected, non-symmetric systems (Tramonto, Xyce, Trilinos)**
- **More accurate communication model**
  - **Up to 48% reduction in communication volume**



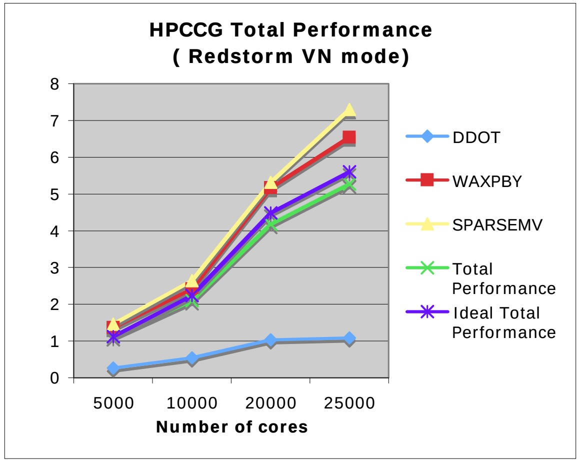


Taking A New Look At Algorithm and Application Performance

- Three types of packages:
  - Microapps
  - Microdrivers
  - Prolego: Parametrized, composable fragment collection to mimic real apps.



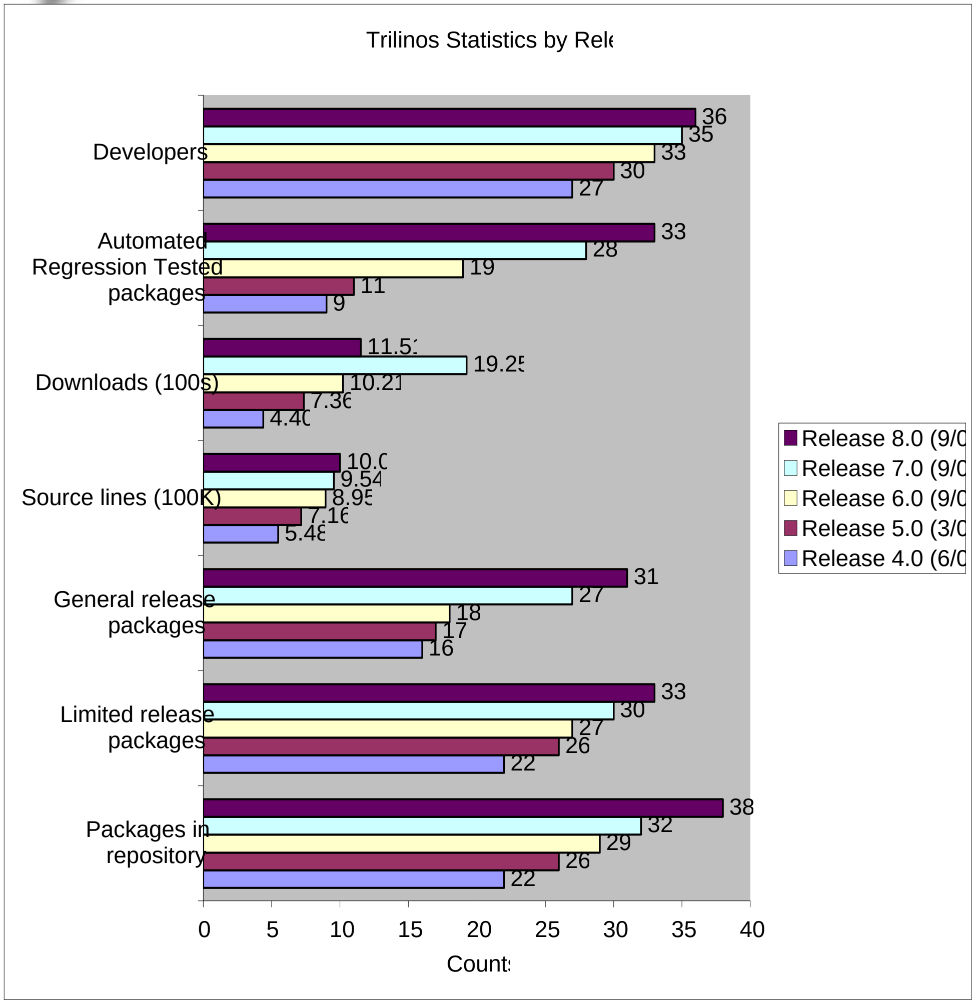
- Goals:
  - Predict performance of real applications in new situations and in new architectures
  - Aid in system design decisions: Proxies for real apps.
  - Guide application and library developers

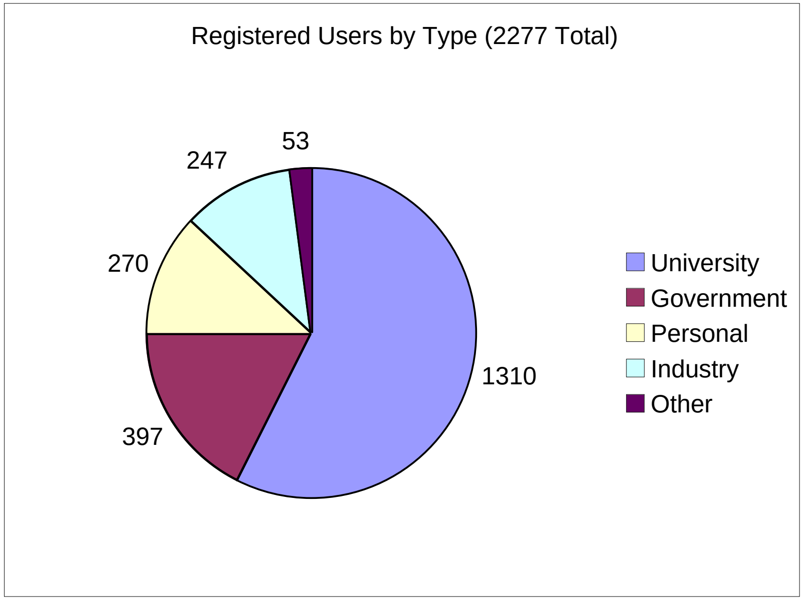


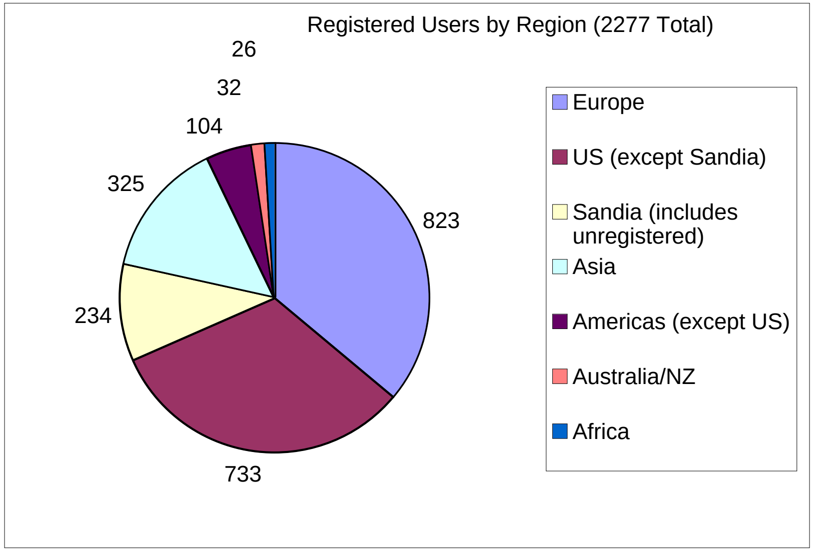
- HPCCG developed and showing results

* Greek: augur, guess, predict, presage

Trilinos Statistics

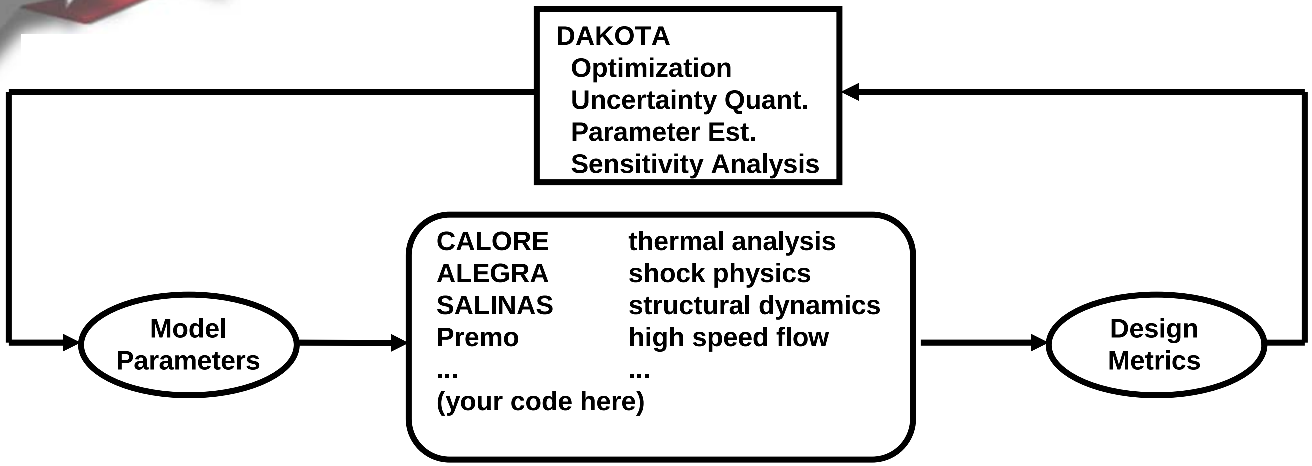




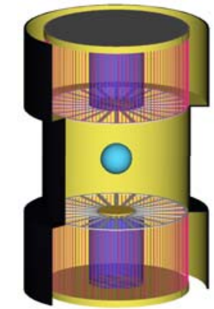


Stats: Trilinos Download Page 02/06/2008.

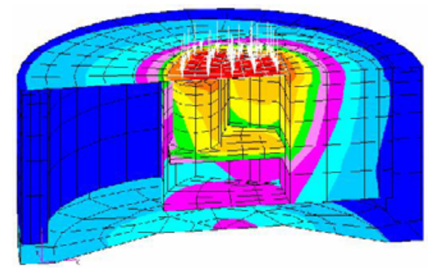
DAKOTA Overview



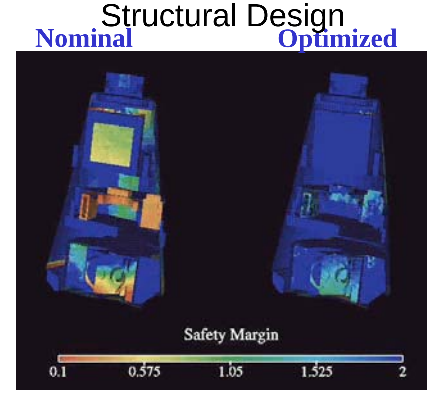
- Answer fundamental engineering questions:
  - What is the best design?
  - How safe is it?
  - How much confidence in my answer?
- Enables sensitivity analysis, optimization, and uncertainty quantification w/ high-fidelity simulation tools on massively-parallel supercomputers
- Works with just about any simulation code
  - Typically in “black box” mode with file reading/writing
  - DAKOTA contains math & stats methods – no physics!
- Exploits large-scale/massively parallel computing platforms
- Freely available worldwide via GNU General Public License
  - ~4400 downloads

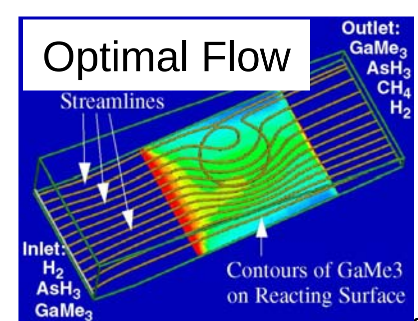


Worst Case Fire Safety



Structural Design

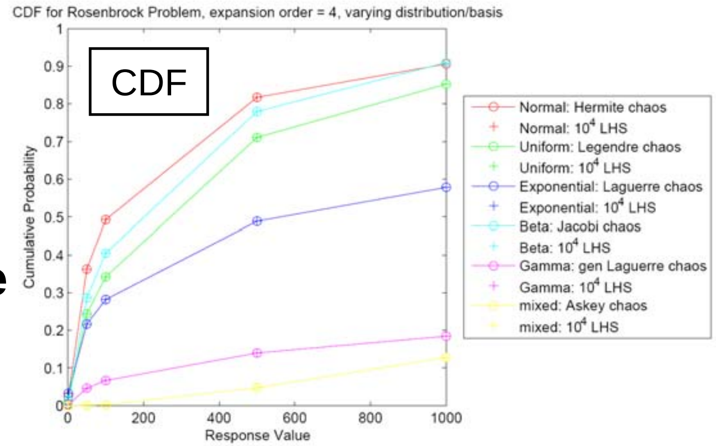




New Capabilities In Dakota Target UQ

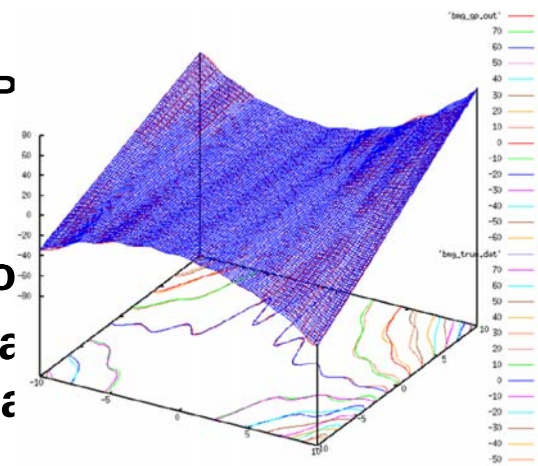
Major emphasis on new UQ methods

- **Methods that provide a more effective balance between accuracy and efficiency than current methods**
  - **Towards smart, adaptive UQ with verifie accuracy**



New OUU algorithms

- **New UQ algorithms previously reported**
  - **Efficient Global Reliability Analysis (EGRA)**
  - **Wiener-Askey generalized Polynomial Chaos Expansions (P**
- **This quarter, new Optimization Under Uncertainty algorithms tailored to these new UQ methods**
  - **Nested, sequential, and all-at-once RBDO based o**
  - **PCE-based OUU with mixed variable expansions a analytic design sensitivities for moments and relia**



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DAKOTA UQ Algorithms

New methods bridge robustness/efficiency gap

	Production	New (Version 4.1)	Under dev.	Planned	Collabs.
Sampling	LHS/MC, QMC/CVT	IS/AIS/MMAIS, Incremental LHS		Bootstrap, Jackknife	Gunzburger
Reliability	1st/2nd-order local: MVFOSM/SOSM, x/u AMV/AMV^2/ AMV+/AMV^2+, x/u TANA, FORM/SORM	Global: EGRA			Renaud, Mahadevan
Polynomial Chaos		Wiener-Askey gPC: sampling, quadrature, pt collocation	Cubature	Adaptivity, Wiener-Haar	Ghanem
Other probabilistic				Dimension reduction	Youn
Epistemic	Second-order probability	Dempster-Shafer evidence theory		Bayesian, Imprecise probability	Higdon, Williams, Ferson
Metrics	Importance factors, Partial correlations	Main effects, Variance-based decomposition	Stepwise regression		Storlie

PECOS:
Random Field/Stochastic Process Modeling Toolkit

Random Fields/Stochastic Processes (RF/SP)

Power spectral density (PSD) → space/time random inputs

$$g(\omega) = \frac{1}{\pi}\int_0^\infty r(\tau)\,\cos(\omega\tau)\,\mathrm{d}\tau,\ \ \omega \geq 0,$$

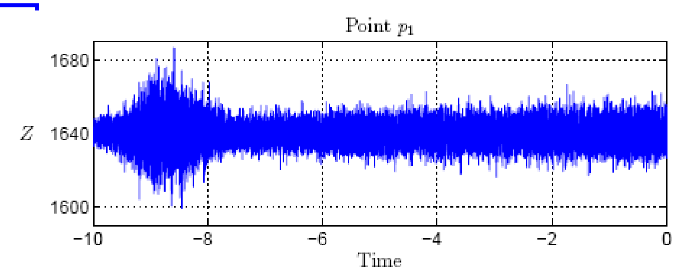
PSD Corr. fn.

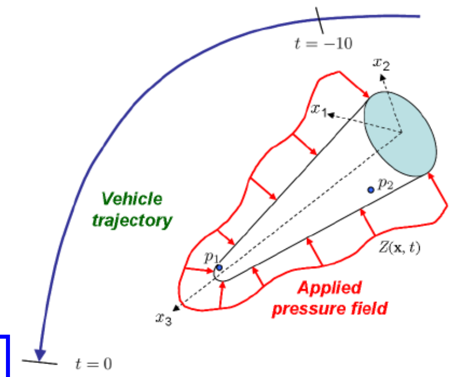
- Spectral representations, Karhunen-Loeve, et al.
- Support Gaussian/non-Gaussian, stationary/nonstationary

Simulate complex random environments:

- Re-entry: turbulent boundary layers, turbulence transition, storms
- Materials: foam densities, heterogeneous/non-continuum

Replaces MATLAB file-based approach with scalable library





Initial C++ Library has been created

- PECOS: *Parallel Environment for Creation Of Stochastics*
- Collects distribution transformation routines from DAKOTA/UQ
- Adds FFT codes for PSD → space/time-domain realizations
- For export to both DAKOTA and Trilinos and import into application codes

Initial application target is Salinas

Encore: Toolkit for Verification

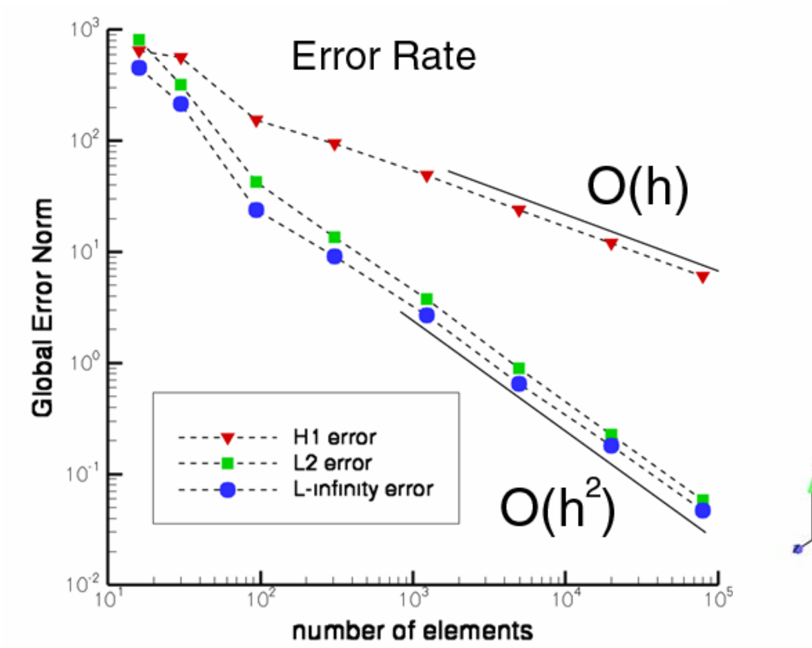
- Strategic goal: *To enable predictive simulations*
  - Unified, modular services for *code and solution verification*
  - Bridge between application codes (e.g., SIERRA Mechanics, RAMSES) and UQ tools (Trilinos, DAKOTA)

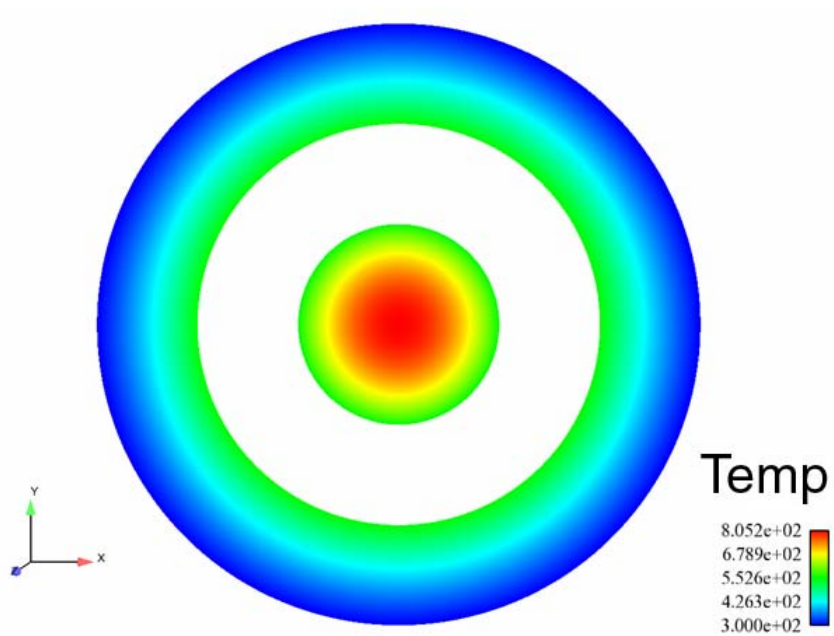
- Code verification
  - Analytical and manufactured solutions
  - Grid transfers (for comparing solutions)
  - Norms, derived quantities of interest

- Solution verification
  - Developing support for *adjoint-based* error estimators
  - Flexible, user-driven adaptivity system

Encore Example:
Code Verification in SIERRA Mechanics

- **Application: Coupled conduction/enclosure radiation.**
- **Using an analytical solution, the error in each global norm can be calculated, and the order of convergence verified.**





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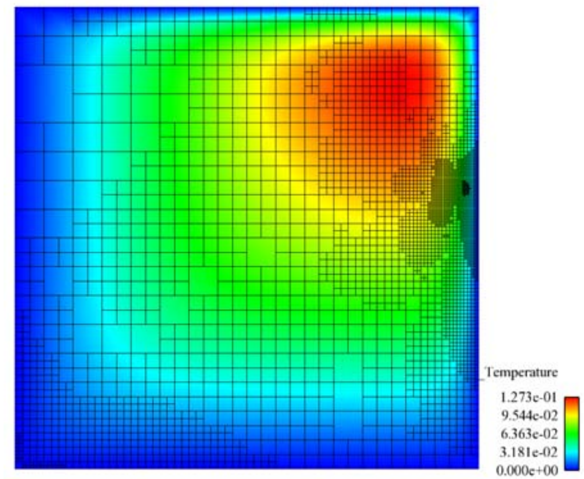
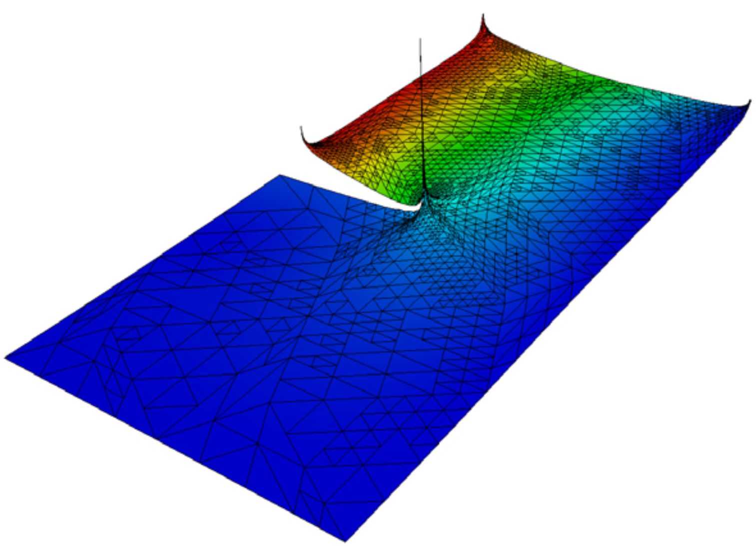
Adjoint-Based Error Estimators and Adaptivity in SIERRA Mechanics

- Temperature field from thermal advection-diffusion example.
- *Quantity of interest:* Temperature at a point near the right boundary.
- The adjoint error estimator produces adaptivity that is optimal for this output.

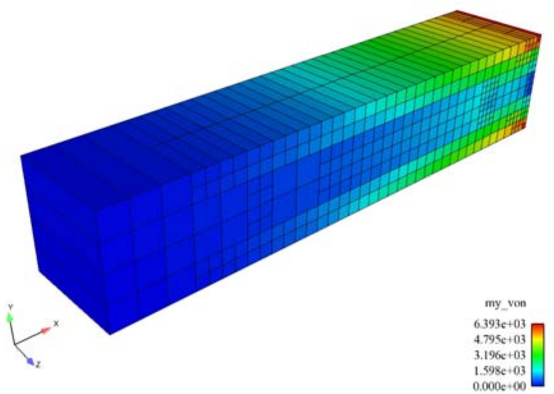




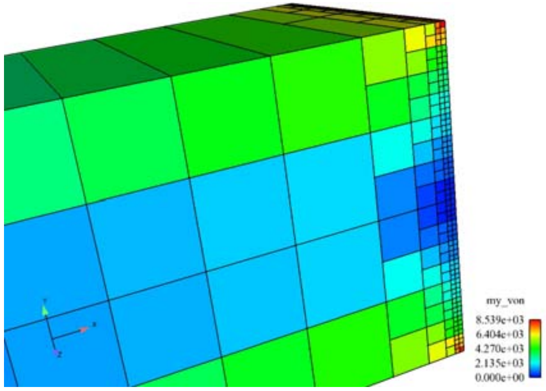
- Nonlinear quasi-statics example.
- Elevation of Von Mises stress field colored by magnitude of adjoint displacement field.
- *Quantity of interest:* Integral surface traction on the upper left surface.
- The adaptivity resolves stress singularities critical to calculation of an accurate force-displacement curve.

Using Encore with SIERRA/Adagio

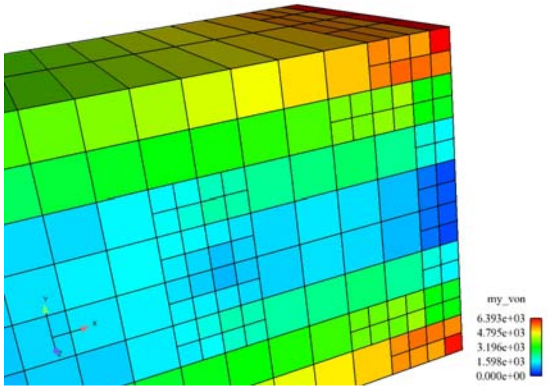
- *Example:* **Cantilever beam with Linear Elastic Material**
- **Encore's flexible adaptivity system allows for both feature and error-based indicators**



Von Mises Stress – adapted mesh



Feature-based adaptivity (surface)



Error-based adaptivity

We are beginning a more rigorous evaluation to establish the confidence we have in our analyses

Predictive Capability Maturity Model (PCMM)

ELEMENT \ MATURITY	Maturity Level 0 Low Consequence, Minimal M&S Impact, e.g., Scoping Studies	Maturity Level 1 Moderate Consequence, Some M&S Impact, e.g., Design Support	Maturity Level 2 High-Consequence, High M&S Impact, e.g., Qualification Support	Maturity Level 3 High-Consequence, Decision Making Based on M&S, e.g.. Qualification or Certification
Representation and Geometric Fidelity What features are neglected because of simplifications or stylizations?	• Judgment only • Little or no representational or geometric fidelity for the system and boundary conditions (BCs)	• Significant simplification or stylization of the system and BCs • Geometry or representation of major components is defined	• Limited simplification or stylization of major components and BCs • Geometry or representation is well defined for major components and some minor components • Some peer review conducted	• Essentially no simplification or stylization of components in the system and BCs • Geometry or representation of all components is at the detail of "as built," e.g., gaps, material interfaces, fasteners • Independent peer review conducted
Physics and Material Model Fidelity How fundamental are the physics and material models and what is the level of model calibration?	• Judgment only • Model forms are either unknown or fully empirical • Few, if any, physics-informed models • No coupling of models	• Some models are physics based and are calibrated using data from related systems • Minimal or ad hoc coupling of models	• Physics-based models for all important processes • Significant calibration needed using separate-effects tests (SETs) and integral-effects tests (IETs) • One-way coupling of models • Some peer review conducted	• All models are physics based • Minimal need for calibration using SETs and IETs • Sound physical basis for extrapolation and coupling of models • Full, two-way coupling of models • Independent peer review conducted
Code Verification Are algorithm deficiencies, software errors, and poor SQE practices corrupting the simulation results?	• Judgment only • Minimal testing of any software elements • Little or no SQE procedures specified or followed	• Code is managed by SQE procedures • Unit and regression testing conducted • Some comparisons made with benchmarks	• Some algorithms are tested to determine the observed order of numerical convergence • Some features & capabilities (F&Cs) are tested with benchmark solutions • Some peer review conducted	• All important algorithms are tested to determine the observed order of numerical convergence • All important F&Cs are tested with rigorous benchmark solutions • Independent peer review conducted
Solution Verification Are numerical solution errors and human procedural errors corrupting the simulation results?	• Judgment only • Numerical errors have unknown or large effect on simulation results	• Numerical effects on relevant SRQs are qualitatively estimated • Input/output (I/O) verified only by the analysts	• Numerical effects are quantitatively estimated to be small on some SRQs • I/O independently verified • Some peer review conducted	• Numerical effects are determined to be small on all important SRQs • Important simulations are independently reproduced • Independent peer review conducted
Model Validation How carefully is the accuracy of the simulation and experimental results assessed at various tiers in a validation hierarchy?	• Judgment only • Few, if any, comparisons with measurements from similar systems or applications	• Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest • Large or unknown experimental uncertainties	• Quantitative assessment of predictive accuracy for some key SRQs from IETs and SETs • Experimental uncertainties are well characterized for most SETs, but poorly known for IETs • Some peer review conducted	• Quantitative assessment of predictive accuracy for all important SRQs from IETs and SETs at conditions/geometries directly relevant to the application • Experimental uncertainties are well characterized for all IETs and SETs • Independent peer review conducted
Uncertainty Quantification and Sensitivity Analysis How thoroughly are uncertainties and sensitivities characterized and propagated?	• Judgment only • Only deterministic analyses are conducted • Uncertainties and sensitivities are not addressed	• Aleatory and epistemic (A&E) uncertainties propagated, but without distinction • Informal sensitivity studies conducted • Many strong UQ/SA assumptions made	• A&E uncertainties segregated, propagated, and identified in SRQs • Quantitative sensitivity analyses conducted for most parameters • Numerical propagation errors are estimated and their effect known • Some strong assumptions made • Some peer review conducted	• A&E uncertainties comprehensively treated and properly interpreted • Comprehensive SAs conducted for parameters and models • Numerical propagation errors are demonstrated to be small • No significant UQ/SA assumptions made • Independent peer review conducted

Enabling Technologies Strategic Directions

- **Simulation capabilities**
  - **High efficiency and scalability on new platforms**
  - **Flexible and agile software architectures**
  - **Multi-scale and multi-physics couplings**
  - **Embedded algorithms**

- **Decision making**
  - **Tightly coupled optimization and design capabilities**
  - **Uncertainty quantification, error estimation and adaptivity**
  - **Integrated verification and validation capabilities**