Albany

A Component-Based Trilinos App

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Trilinos User's Group Meeting
October 31, 2012
CSRI, Sandia-NM

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SAND 2012-9337P

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What is Albany?

A parallel, implicit, unstructured-grid finite element code,

that demonstrates the AgileComponents vision by using, maturing, and spinning-off reusable libraries and abstract interfaces,

that is an friendly early adopter of cutting-edge technology from Trilinos, SierraToolKit, and Dakota,

that is a model for a Trilinos-App,

that demonstrates transformational analysis spanning template-based generic programming, optimization, UQ, adaptivity, and model order reduction,

that serves as an attractive environment for the development of open-source application codes and research,

and is the code base underlying LCM, QCAD, and FELIX applications.

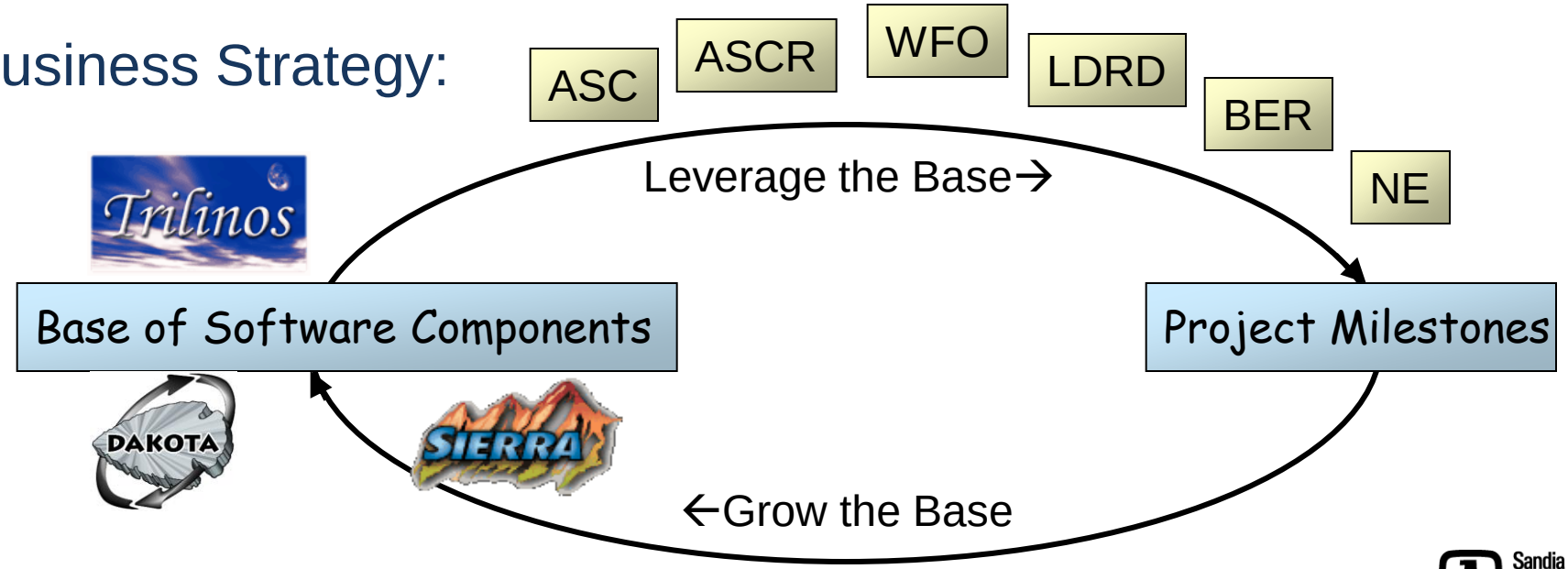
What is AgileComponents?

Technical Strategy: Projects create, use, and improve a common base of modular, independent-yet-interoperable, software components

"Components" = ☑ Libraries ☑ Software Quality Tools ☑ Interfaces ☑ Demonstration Applications

White Paper: "Component-Based Scientific Application Development"

Business Strategy:



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The Components Effort is Large (~100 modular pieces)

Analysis Tools (*black-box*)
- Optimization
- UQ (sampling)
- Parameter Studies
- V&V, Calibration
- OUU, Reliability

Analysis Tools (*embedded*)
- Nonlinear Solver
- Time Integration
- Continuation
- Sensitivity Analysis
- Stability Analysis
- Constrained Solves
- Optimization
- UQ Solver

Linear Algebra
- Data Structures
- Iterative Solvers
- Direct Solvers
- Eigen Solver
- Preconditioners
- Matrix Partitioning

Architecture-Dependent Kernels
- Multi-Core
- Accelerators

Composite Physics
- MultiPhysics Coupling
- System Models
- System UQ

Mesh Tools
- Mesh I/O
- Inline Meshing
- Partitioning
- Load Balancing
- Adaptivity
- Remeshing
- Grid Transfers
- Quality Improvement
- DOF map

Utilities
- Input File Parser
- Parameter List
- Memory Management
- I/O Management
- Communicators

PostProcessing
- Visualization
- Verification
- Model Reduction

Mesh Database
- Mesh Database
- Geometry Database
- Solution Database

Local Fill

Discretizations
- Discretization Library
- Field Manager

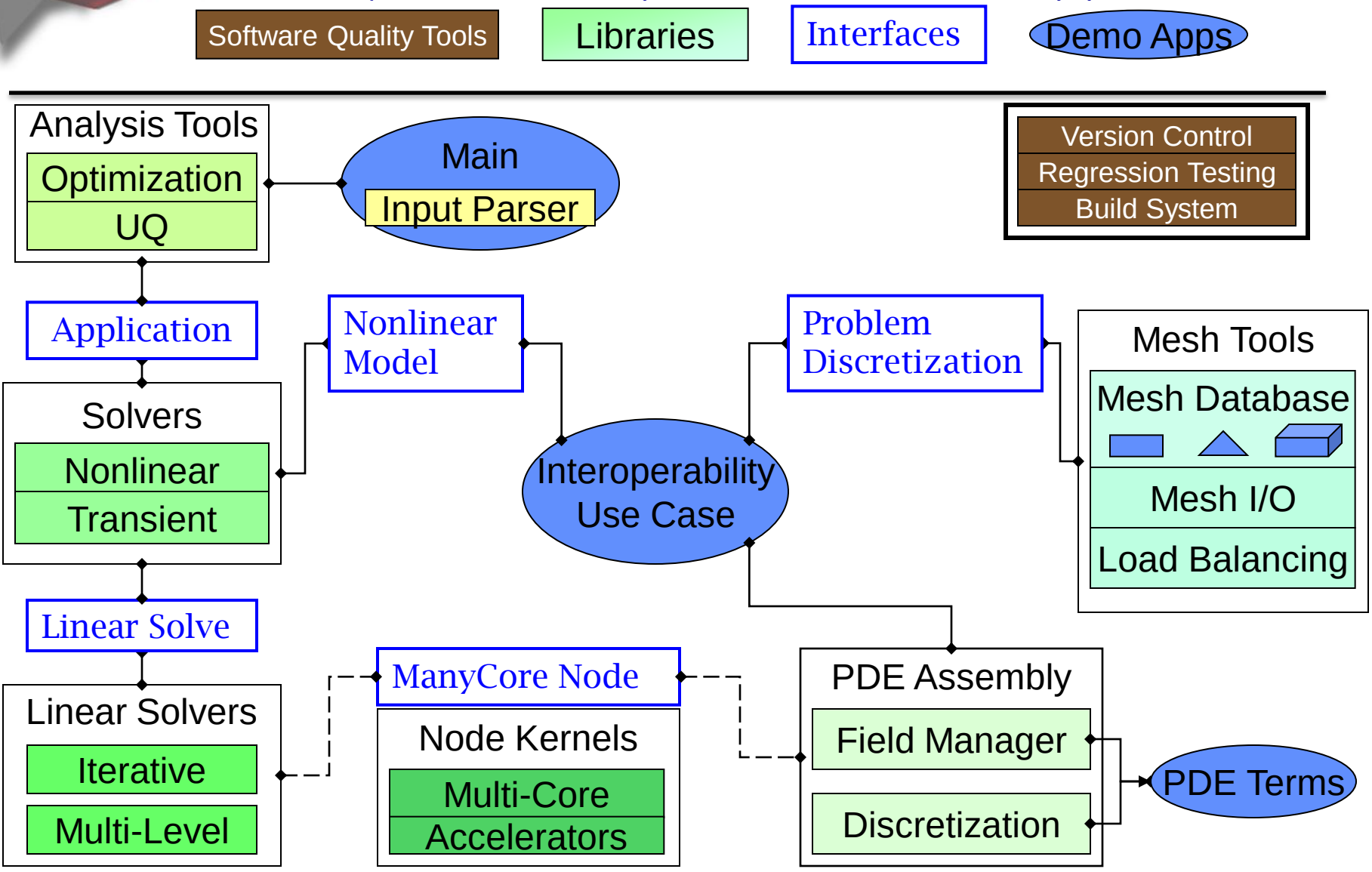
Derivative Tools
- Sensitivities
- Derivatives
- Adjoints
- UQ / PCE Propagation

Physics Fill
- Element Level Fill
- Material Models
- Objective Function
- Constraints
- Error Estimates
- MMS Source Terms

Data-Centric Algs
- Graph Algorithms
- SVDs
- Map-Reduce
- Linear Programming
- Network Models

Software Quality
- Version Control
- Regression Testing
- Build System
- Backups
- Verification Tests
- Mailing Lists
- Unit Testing
- Bug Tracking
- Performance Testing
- Code Coverage
- Porting
- Web Pages
- Release Process

Anatomy of a Component-Based Application:



Albany's Evolving Role

Mini-Project

FY08-10: A mechanism to articulate and drive AgileComponents vision:

1. Evaluate and mature capabilities
2. Define new interfaces
3. Prototype a "Trilinos Application"
4. Demonstrate Transformation
   - Optimization, UQ, Sensitivities,…

Disposable: migrate success into Trilinos, publications

Co-op

FY10-11: A mechanism to drive AgileComponents vision and strategy

1. LCM ←
2. QCAD ←
3. Embedded / System UQ Research

No longer fully Disposable

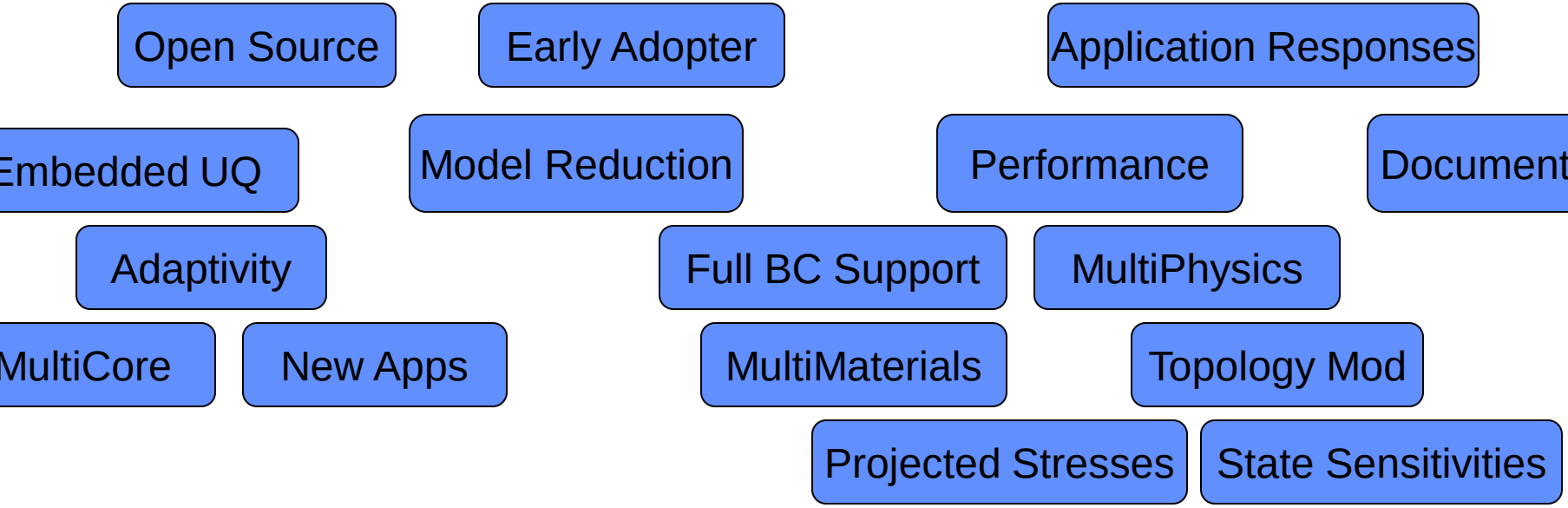
FY12-13:

4. NEAMS Hydride problem
5. Tpetra templated software stack maturation
6. Nuclear Waste Disposal (ended)
7. Model Order Reduction
8. LAMENT Development
9. FELIX: Finite Element Land Ice eXperiments ←
10. Peridynamics-LCM Coupling

Tension from Albany's Diverse Roles

Agility
Research
Generality

Usability
Usefulness
Application-Specific



Albany fills a role between
Trilinos examples / mini-Apps ←→ Production codes Sierra/Alegra

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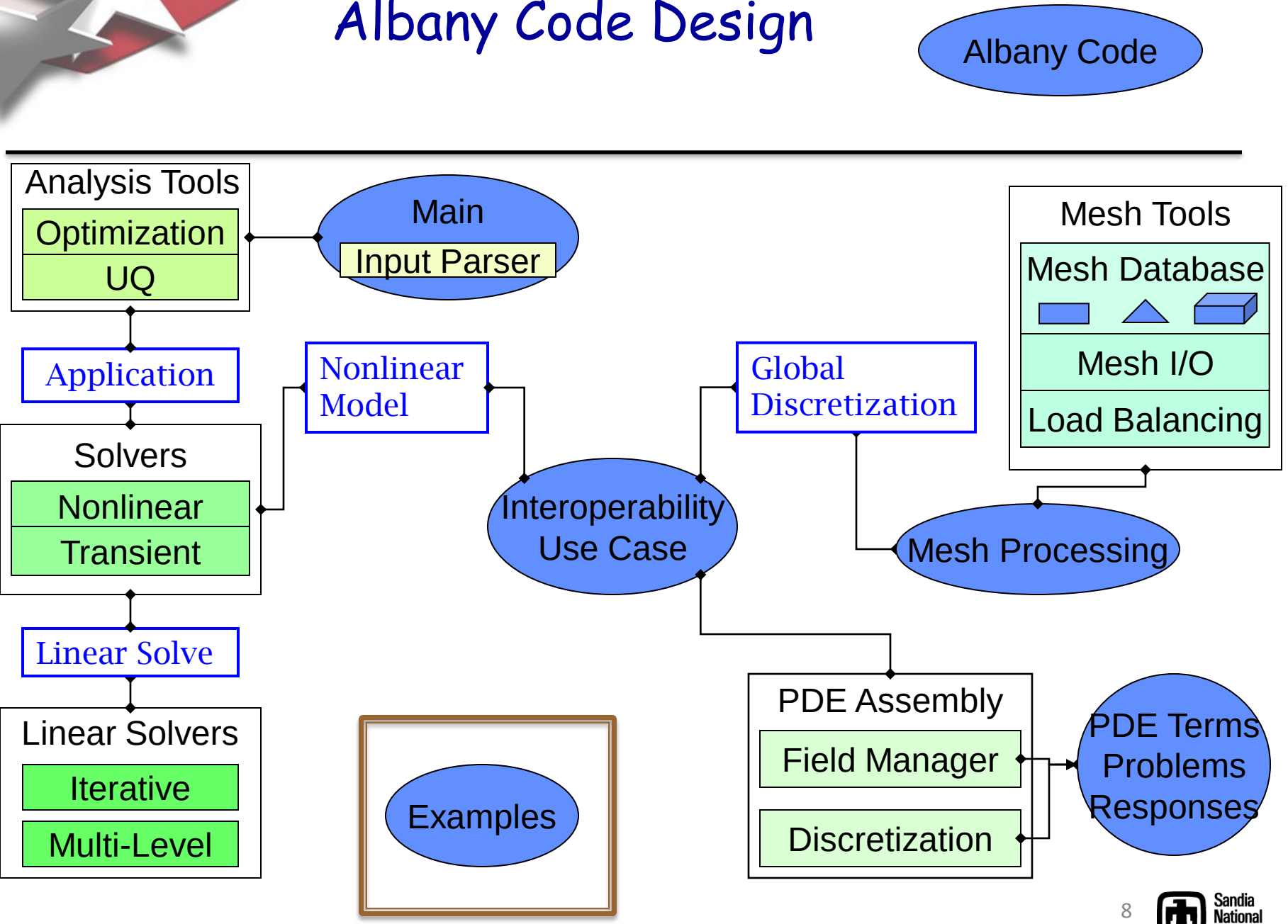
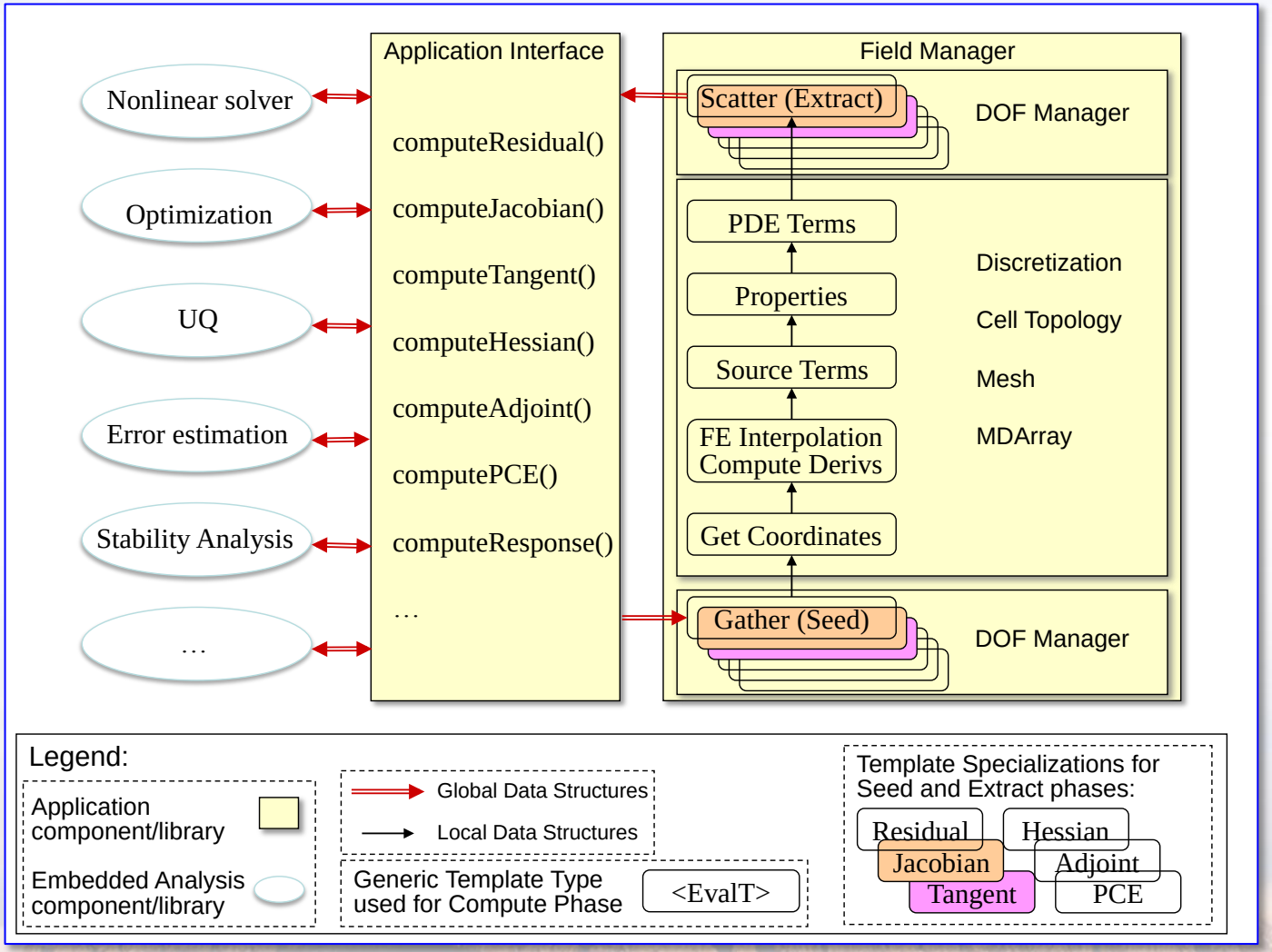
Albany Code Design



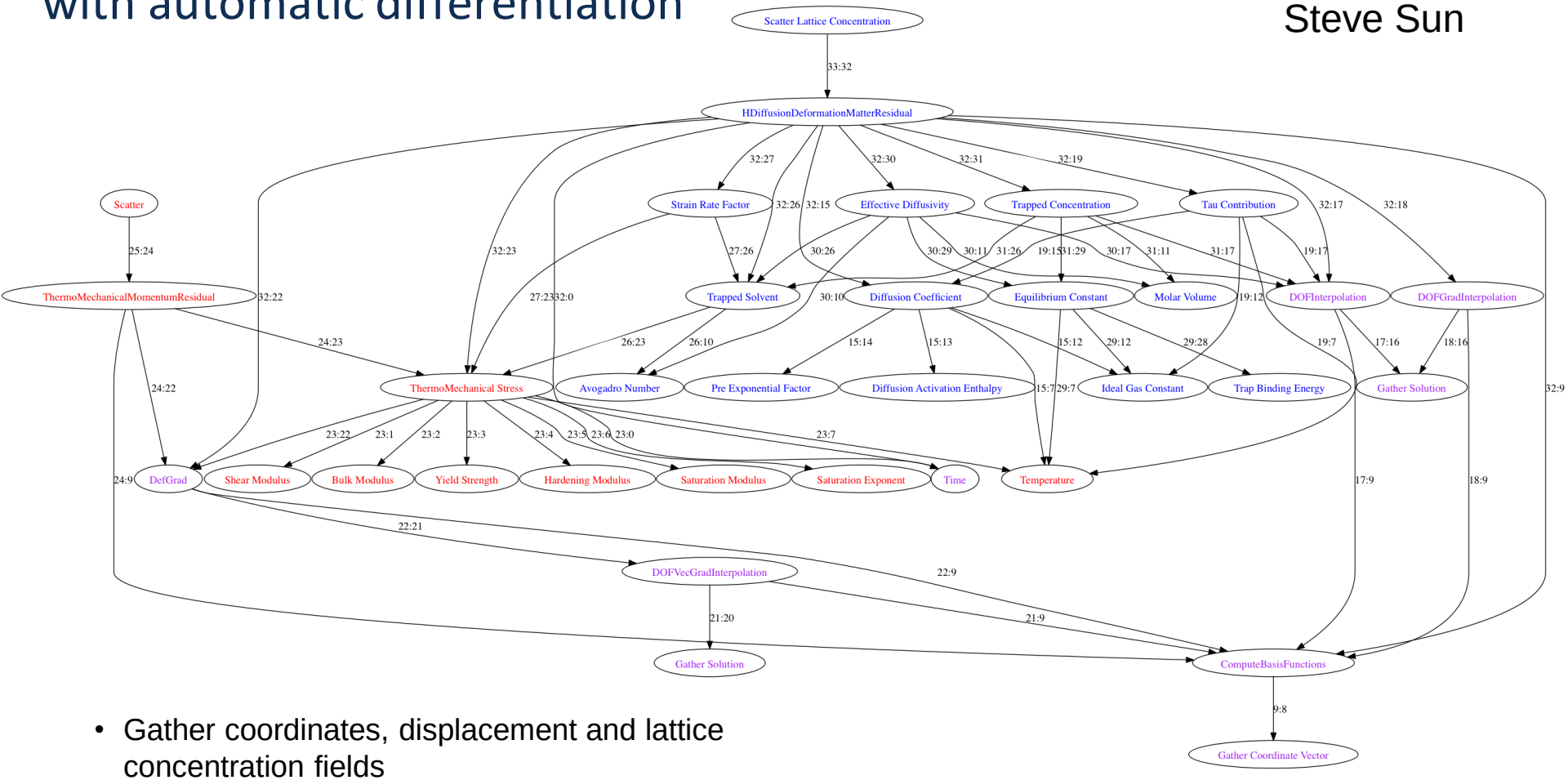
Templated Components Orthogonalize Physics and Embedded Algorithm R&D ("TBGP")



Phalanx
Sacado
Stokhos
Intrepid
Shards
*Petra
Teuchos

Implementation of Hydrogen Diffusion-Mechanics Problem with automatic differentiation

Steve Sun



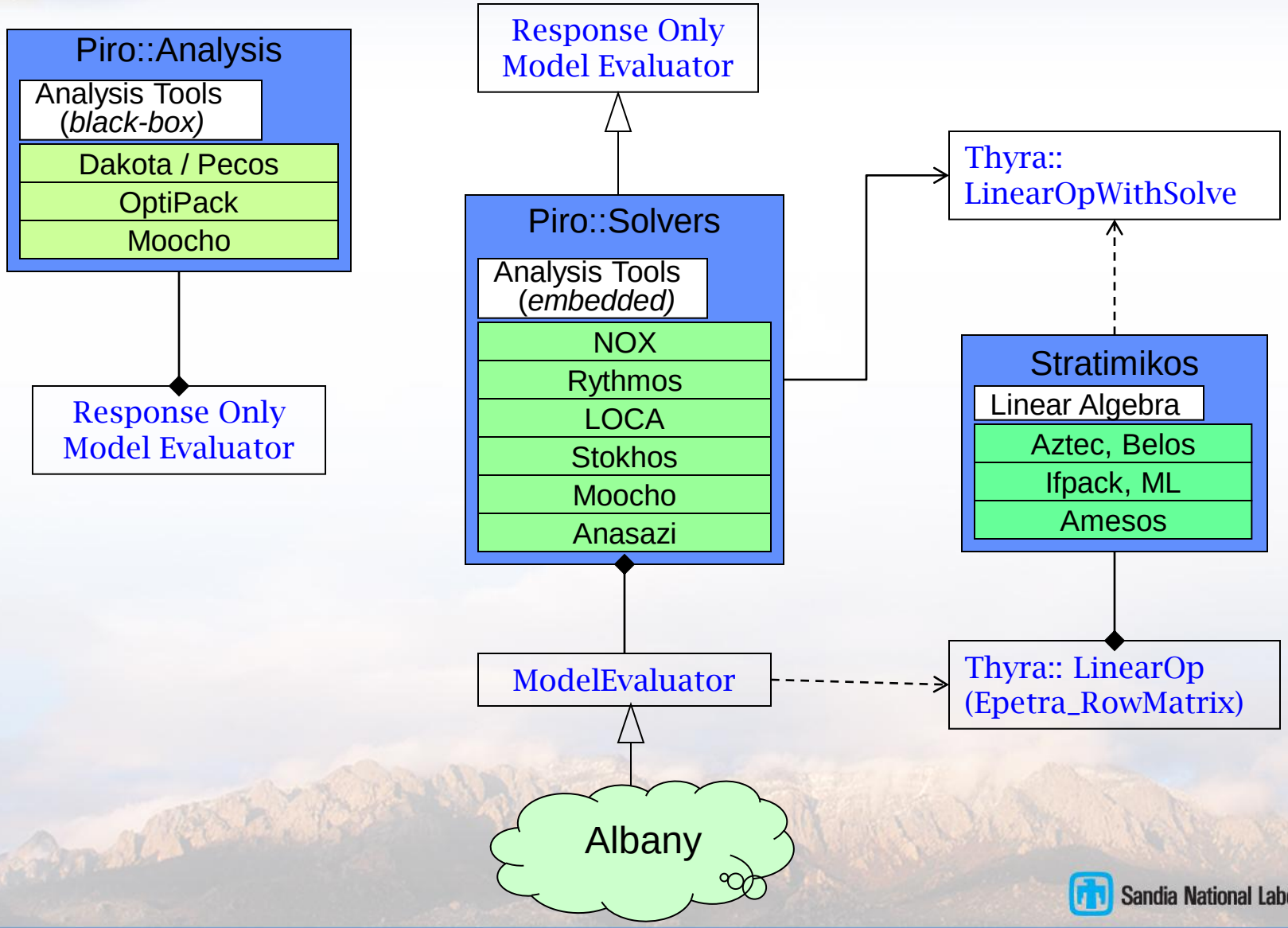
- Gather coordinates, displacement and lattice concentration fields
- Interpolate fields and gradients to integration points
- Chain together Evaluators to compute Momentum and Conservation of Hydrogen Residuals
- Scatter back to the global system of equations

Blue = Hydrogen Transport

Red = Solid Mechanics (J2 Plasticity)

Purple = coupled terms

Embedded Nonlinear Analysis Tools



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libstk_util_env.a
libstk_util_util.a
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libdakota_src_fortran.a
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libpecos.a
libpecos_src.a
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libconmin.a
libdace.a
libanalyzer.a
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libjega_fe.a
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libeutils.a
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librtop.a
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libtpi.a
libteuchos.a

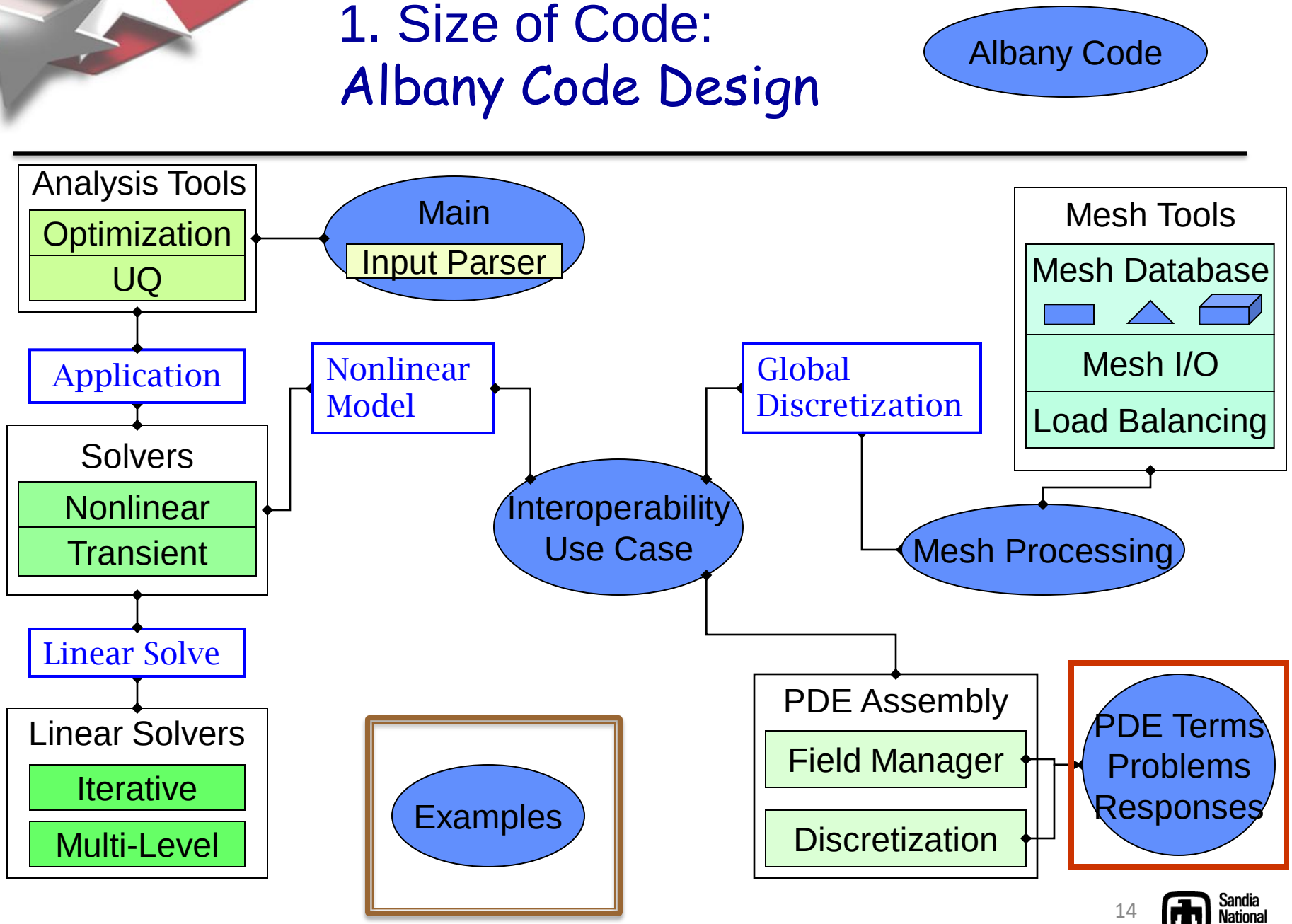
Albany: State of the Code

1. Size of Code
2. Funding and Release History
3. Current Projects
4. Documentation
5. Current and Future Work

Team Size:

- 22 “git push”-ers
- 6+ pair-programming contributors

1. Size of Code: Albany Code Design



Albany State of the Code

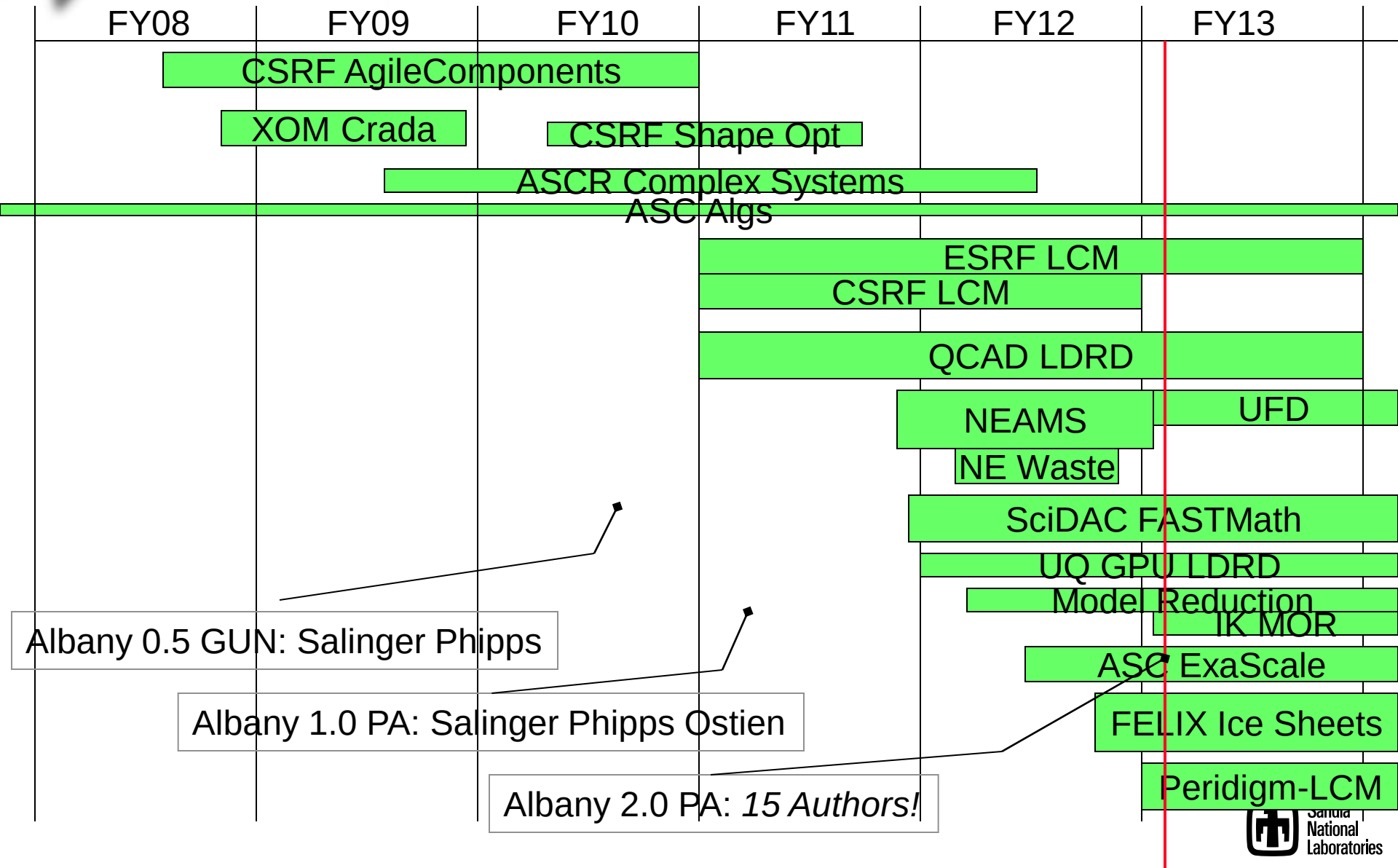
1. Albany Code Size: 140K Lines, 43K Semicolons

Main	`src/Main*:`	8 files;	546 semicolons
Interoperability Use Case	`src/*:`	41 files;	3650 semicolons
Mesh Processing	`src/stk:`	16 files;	1584 semicolons
PDE Terms Problems Responses	All `problems/evaluators/responses`:	593 files;	30681 semicolons
	[*LCM:*	*298 files;*	*16573 semicolons*]

>80% of Albany/src is implementation of PDEs!

Examples	`examples:`	128 regression tests, 183 example input files

Albany State of the Code
2. Funding and Release History



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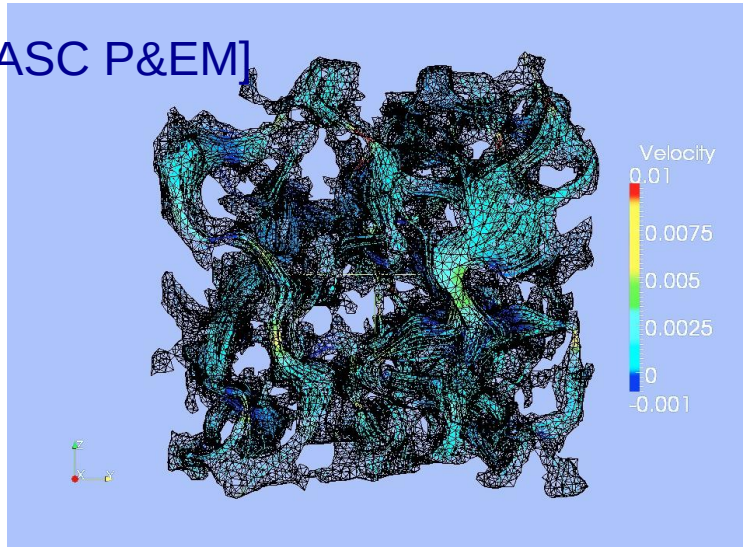
Albany State of the Code
3. Current Projects

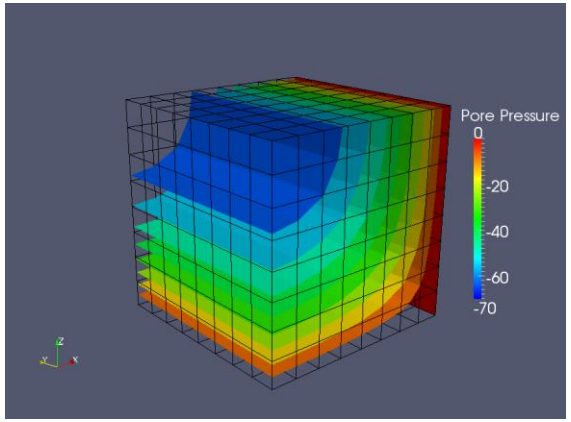
Applications:

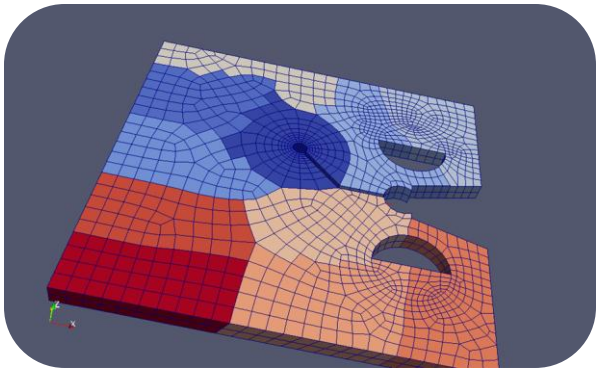
- LCM Laboratory for Computational Mechanics [ASC P&EM]
- QCAD Quantum dot design [LDRD]
- Nuclear fuels degradation [NEAMS,UFD]
- GPAM [Used Fuel Disposition] {ended}
- FELIX Ice Sheet Dycore [SciDAC-BER]
- Peridym/LCM Coupling [FY13 LDRD, WFO?]

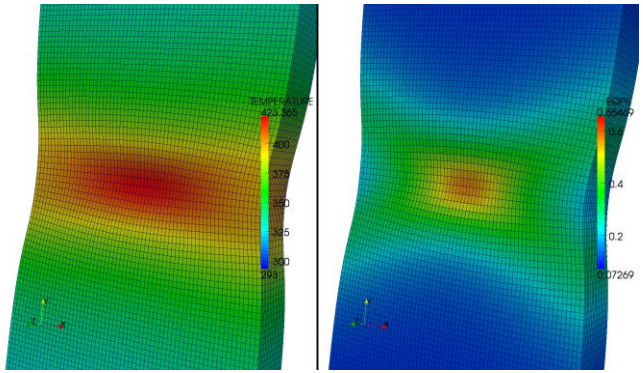


Algorithms and Software:

- UQ System Research [ASCR] {ended}
- Templated stack maturation testbed [ASC Algs]
- Adaptivity-Solver interactions [SciDAC ASCR]
- Model Order Reduction [Truman LDRD, IK-LDRD]







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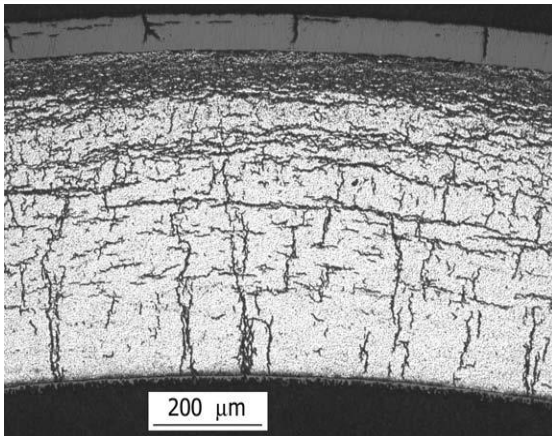
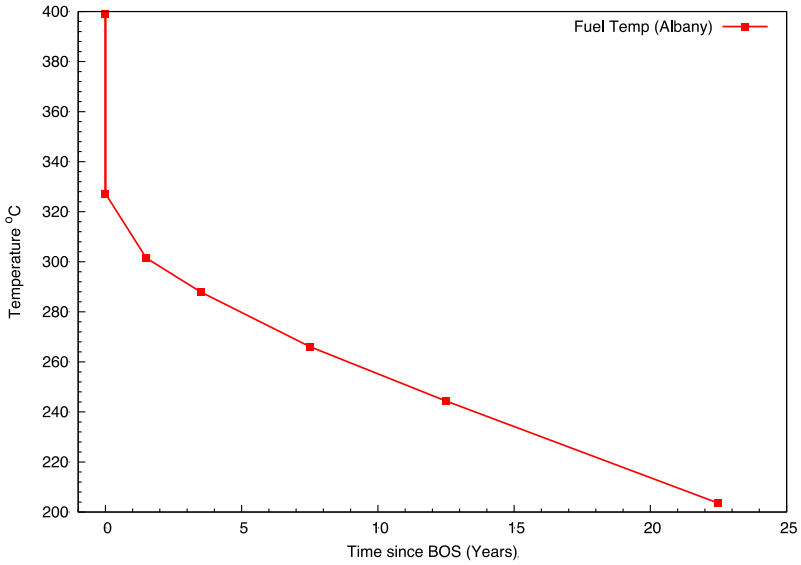
Modeling of Hydride Formation in Spent Nuclear Fuel Rods: Hansen, Chen, Ostien

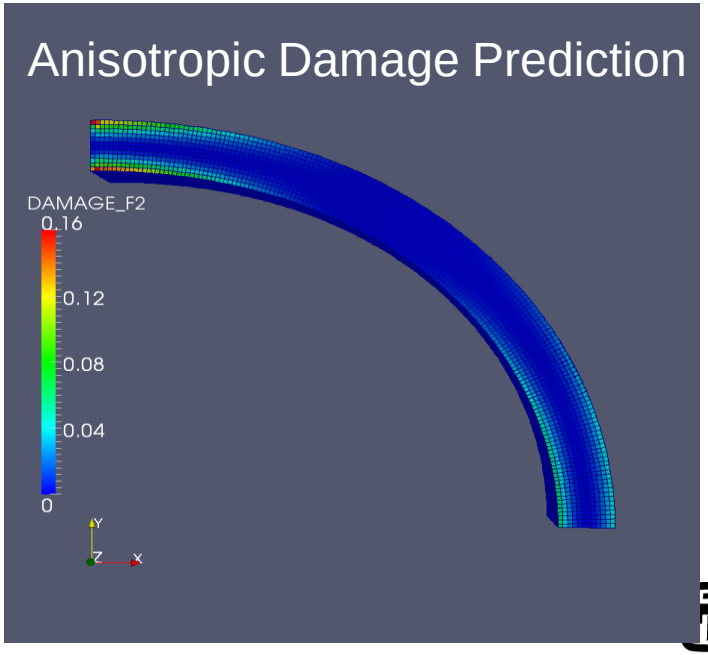
- **Normal storage periods are ~20 years in duration**
- **Will issues develop that could affect safe handling of fuel if this dry storage period is increased to 100 years? 300 years?**
- **Degradation mechanism: Radial hydrides formed during drying process.**



Temperature History Prediction



Anisotropic Damage Prediction



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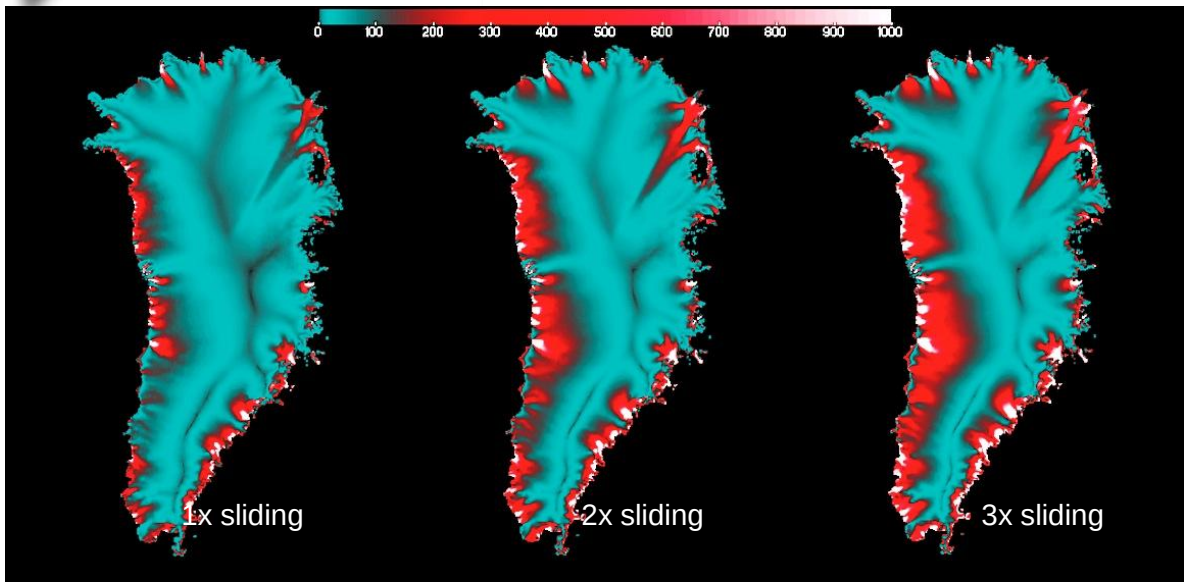
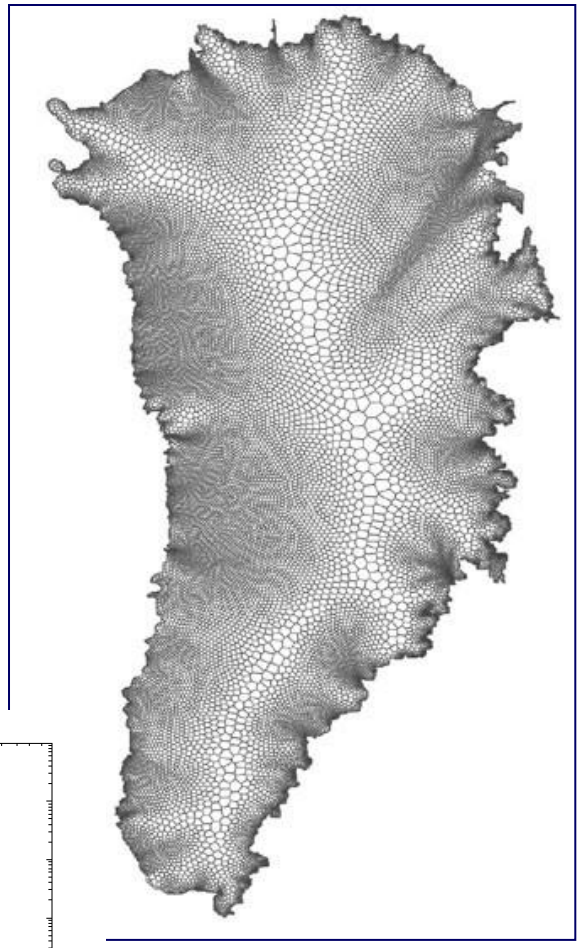
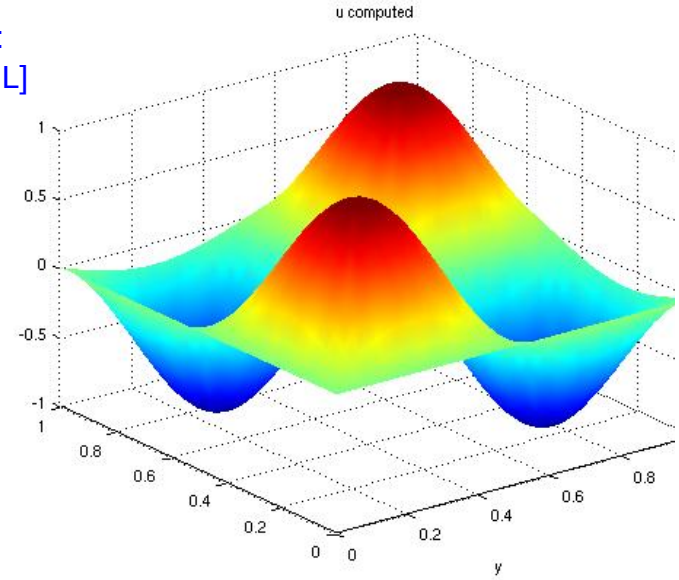
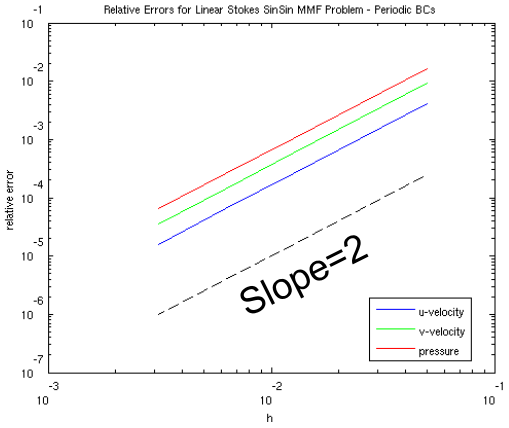
FELIX Ice Sheet Code (SciDAC-BER) 5yrs





Courtesy:
Price [LANL]





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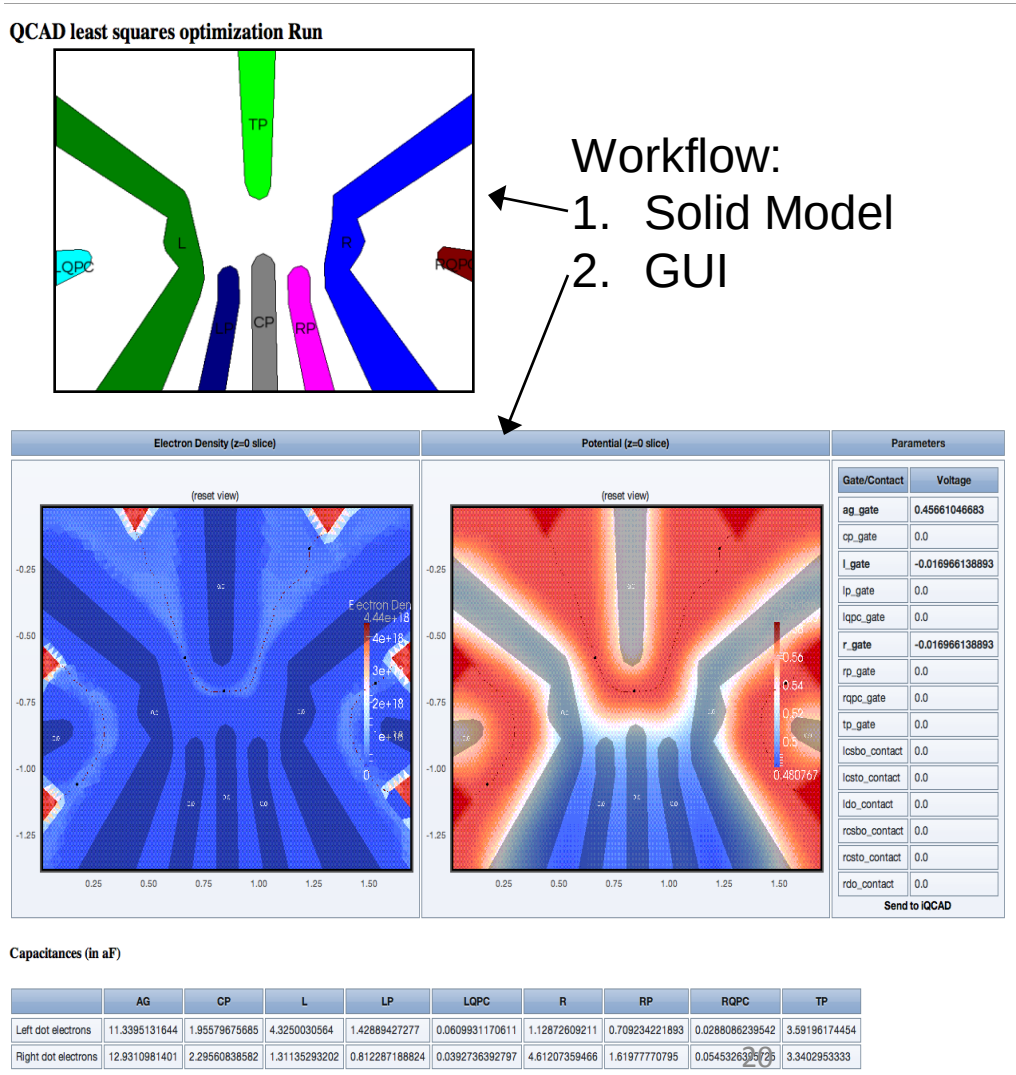
Nielsen: 1:30 Today!

Success Story: Rapid Stand-Up of a World-Class Quantum Device Design Tool

"I thought I was being ambitious in the proposal, and we finished most of the 3-year milestones in the first year." [PI: Muller]

- Sandia has world-class experimental facilities (CINT) for quantum device fabrication, for quantum computing
- Quantum device computational design tool built from components:
  - Nonlinear-Poisson + Schrödinger
  - 30+ Trilinos packages
  - Dakota optimization
  - Unit of computation:
    - ~30 optimization runs for every design
  - GUI for Experimentalists



	AG	CP	L	LP	LQPC	R	RP	RQPC	TP
Left dot electrons	11.3395131644	1.95579675685	4.3250030564	1.42889427277	0.0609931170611	1.12872609211	0.709234221893	0.0288086239542	3.59196174454
Right dot electrons	12.9310981401	2.29560838582	1.31135293202	0.812287188824	0.0392736392797	4.61207359466	1.61977770795	0.0545326395726	3.3402953333

Albany State of the Code
4. Documentation

SANDIA REPORT

SAND20XX-????
Unlimited Release
Printed ??

Albany Development: Getting Started

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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- QCAD Project
- FELIX Project
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- Albany Presentations
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Albany 2nd Developers Meeting, October 2, 2012.

Meeting Agenda:
Albany 2nd Developers Meeting Agenda (pdf).

Overviews:
Salinger: Albany Overview (pdf).
Phipps: Algorithms Research Overview (pdf).

LCM Talks:
Ostien: LCM Overview (pdf).
Sun: MultiPhysics Applications (pdf).
Chen: Constitutive Modeling (pdf).
Mota: Multiscale Coupling (pdf).
Mota: Continuum-Continuum Coupling (pdf).
Littlewood: LAMENT Material Library (pdf).
Hansen: Hydride Modeling for Fuel Rods (pdf).

QCAD Talks:
Muller: QCAD Overview (pdf).
Gao: Schrodinger-Poisson (pdf).
Nielsen: Quantum Dot Design (pdf).

New Initiatives Session:
Hansen: Progress Towards Adaptivity (pdf).
Cortial: Model Order Reduction (pdf).
Littlewood: Peridym-LCM LDRD (pdf).
Salinger/Kalashnikova: FELIX Ice Sheet Dynamics (pdf).

Developers Discussion Summary:
Albany 2nd Developers Meeting Discussion Summary (pdf).

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development.sandia.gov/Albany

Albany State of the Code
5. Current / Future Generic Code Work

Current/Future/Desired Code Infrastructure Work:

- Software Quality:
  - Documentation (Developers guide; Doxygen)
  - SEMS improvements
    - Scalability/performance/coverage tests
    - Code refactors – scientific programming
- Internal Algorithms:
  - Sensitivities/Uncertainties of States
  - Adjoints for Distributed Parameters
  - Mixed Discretization *using* DOFManager (*Cyr*)
- Early Adopter of Libraries
  - Finish Tpetra/Thyra Branch (Kalashnikova/Cortial)
  - Early Adopter of Kokkos for New Architectures?
  - UQ on GPU (Phipps *et al*.)
  - MOR ROM R&D
- smAlbany? Official Trilinos DemoApp

Thanks!

Albany Questions?

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