Albany
A Component-Based Trilinos App

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Trilinos User’s Group Meeting
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CSRI, Sandia-NM
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:

Base of Software Components ➔ Project Milestones

Leverage the Base ➔

←Grow the Base

ASC  ASCR  WFO  LDRD  BER  NE

Trilinos

Dakota

Sierra
The Components Effort is Large (~100 modular pieces)
## Albany’s Evolving Role

<table>
<thead>
<tr>
<th>FY08-10: A mechanism to articulate and drive AgileComponents vision:</th>
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<tbody>
<tr>
<td>1. Evaluate and mature capabilities</td>
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<tr>
<td>2. Define new interfaces</td>
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<td>3. Prototype a “Trilinos Application”</td>
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<td>4. Demonstrate Transformation</td>
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<td>• Optimization, UQ, Sensitivities,…</td>
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**Disposable:** migrate success into Trilinos, publications

<table>
<thead>
<tr>
<th>FY10-11: A mechanism to drive AgileComponents vision and strategy</th>
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<tbody>
<tr>
<td>1. LCM ➔</td>
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<td>2. QCAD ➔</td>
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<td>3. Embedded / System UQ Research</td>
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**No longer fully Disposable**

<table>
<thead>
<tr>
<th>FY12-13:</th>
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<tr>
<td>4. NEAMS Hydride problem</td>
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<td>5. Tpetra templated software stack maturation</td>
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<td>6. Nuclear Waste Disposal (ended)</td>
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<td>7. Model Order Reduction</td>
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<td>8. LAMENT Development</td>
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<tr>
<td>9. FELIX: Finite Element Land Ice eXperiments ➔</td>
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<td>10. Peridynamics-LCM Coupling</td>
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Tension from Albany’s Diverse Roles

Albany fills a role between Trilinos examples / mini-Apps ↔ Production codes Sierra/Alegra
Templated Components Orthogonalize Physics and Embedded Algorithm R&D (“TBGP”)

Legend:
- Application component/library
- Embedded Analysis component/library
- Global Data Structures
- Local Data Structures
- Generic Template Type used for Compute Phase
- Template Specializations for Seed and Extract phases:
  - Residual
  - Jacobian
  - Hessian
  - Adjoint
  - Tangent
  - PCE

Nonlinear solver
Optimization
UQ
Error estimation
Stability Analysis

Application Interface
- computeResidual()
- computeJacobian()
- computeTangent()
- computeHessian()
- computeAdjoint()
- computePCE()
- computeResponse()

Field Manager
- Scatter (Extract)
- DOF Manager
- PDE Terms
- Properties
- Source Terms
- FE Interpolation Compute Derivs
- Get Coordinates
- Gather (Seed)
- DOF Manager

Phalanx
Sacado
Stokhos
Intrepid
Shards
*Petra
Teuchos
Implementation of Hydrogen Diffusion-Mechanics Problem with automatic differentiation

- 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

- Dakota / Pecos
- OptiPack
- Moocho

- NOX
- Rythmos
- LOCA
- Stokhos
- Moocho
- Anasazi

- Thyra::LinearOp (Epetra_RowMatrix)
- Thyra::LinearOpWithSolve
- Aztec, Belos
- Ifpack, ML
- Amesos

- Albany

- Response Only Model Evaluator
- Analysis Tools (black-box)
- Analysis Tools (embedded)
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

Analysis Tools
- Optimization
- UQ

Application

Solvers
- Nonlinear
- Transient

Linear Solve

Linear Solvers
- Iterative
- Multi-Level

Main
- Input Parser

Nonlinear Model

Interoperability Use Case

Global Discretization

Mesh Tools
- Mesh Database
- Mesh I/O
- Load Balancing

Mesh Processing

Examples

PDE Assembly
- Field Manager
- Discretization

PDE Terms
- Problems
- Responses

Albany Code

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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

<table>
<thead>
<tr>
<th>FY08</th>
<th>FY09</th>
<th>FY10</th>
<th>FY11</th>
<th>FY12</th>
<th>FY13</th>
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<tr>
<td>CSRF AgileComponents</td>
<td>XOM Crada</td>
<td>CSRF Shape Opt</td>
<td>ASCR Complex Systems</td>
<td>ASC Algs</td>
<td>ESRF LCM</td>
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<td>CSRF LCM</td>
<td>QCAD LDRD</td>
<td>NEAMS</td>
<td>UFD</td>
<td>NE Waste</td>
<td>SciDAC FASTMath</td>
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<td>ASC ExaScale</td>
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<td>FELIX Ice Sheets</td>
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<td>Peridigm-LCM</td>
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Albany 0.5 GUN: Salinger Phipps

Albany 1.0 PA: Salinger Phipps Ostien

Albany 2.0 PA: 15 Authors!
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]
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**

- **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.
FELIX Ice Sheet Code (SciDAC-BER) 5yrs

Courtesy: Price [LANL]
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

Workflow:
1. Solid Model
2. GUI

Nielsen: 1:30 Today!
Albany State of the Code
4. Documentation

SANDIA REPORT
SAND20XX-????
Unlimited Release
Printed ??

Albany Development: Getting Started

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Approved for public release; further dissemination unlimited.
Albany 2nd Developers Meeting, October 2, 2012.

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

Overviews:
Salinger: Albany 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).

QCAD Talks:
Muller: QCAD Overview (pdf).
Gao: Schrodinger-Poisson (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).
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
  - Adjoint 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?