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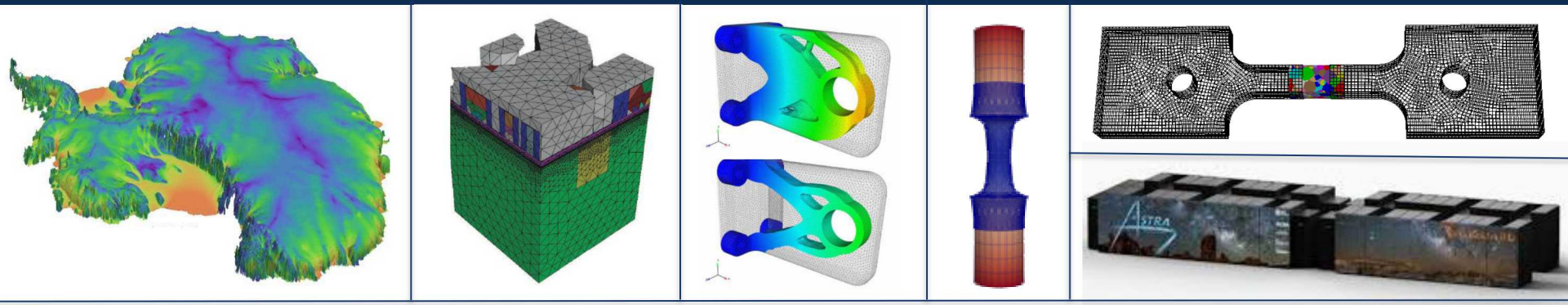

Albany : a Trilinos-based multi-physics partial differential equation research tool created using the AgileComponents code development strategy

Irina Tezaur

Quantitative Modeling & Analysis Dept., Sandia National Laboratories, Livermore, CA.

SIAM CSE 2019 Spokane, WA Feb. 25-Mar. 1 2019

U.S. DEPARTMENT OF ENERGY | NNSA National Nuclear Security Administration

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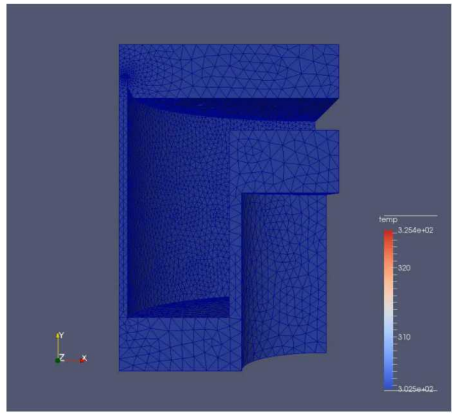
- Andy Salinger [SNL]

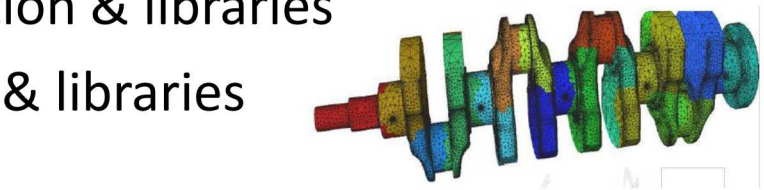
Albany contributors (58, from github):

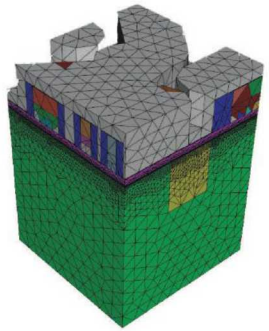
- I. Tezaur [SNL]
- A. Mota [SNL]
- D. Ibanez [RPI/SNL]
- G. Hansen [SNL]
- M. Perego [FSU/SNL]
- L. Bertagna [FSU/SNL]
- A. Bradley [SNL]
- J. Ostien [SNL]
- B. Granzow [RPI/SNL]
- A. Salinger [SNL]
- D. Littlewood [SNL]
- J. Foulk [SNL]
- C. Alleman [SNL]
- J. Overfelt [SNL]
- E. Nielsen [SNL]
- I. Demeshko [LANL]
- O. Guba [SNL]
- M. Juha [U de La Sabana]
- E. Phipps [SNL]
- J. Frederick [SNL]
- J. Watkins [SNL]
- J. Robbins [SNL]
- T. Smith [SNL]
- R. Jones [SNL]
- B. Spotz [SNL]
- S. Besu [RPI]
- J. Foucar [SNL]
- Q. Chen [Clemson]
- P. Lindsay [SNL]
- J. Fike [SNL]
- S. Gao [SNL]
- J. Redhorse [SNL]
- S. Bova [SNL]
- P. Bosler [SNL]
- H. Yuan [Tokyo]
- C. Siefert [SNL]
- T. Voth [SNL]
- T. Wildey [SNL]
- C. Smith [RPI]
- J. Clough [USC]
- W. Sun [Columbia]
- Z. Wang [USC]
- T. Fuller [SNL]
- A. Vacanti [Kitware]
- R. Tuminaro [SNL]
- M. Parks [SNL]
- J. Robbins [SNL]
- M. Hoffman [LANL]
- R. Pawlowski [SNL]
- M. Bloomfield [RPI]
- G. Phlipot [CalTech]
- B. Perschbacher [SNL]
- J. Willenbring [SNL]
- …

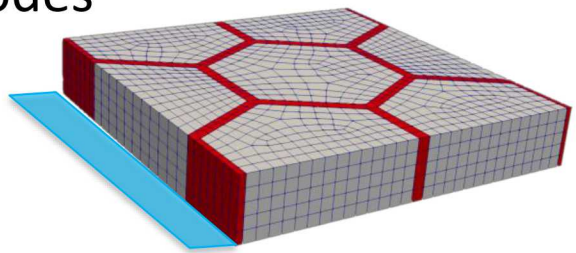
Outline

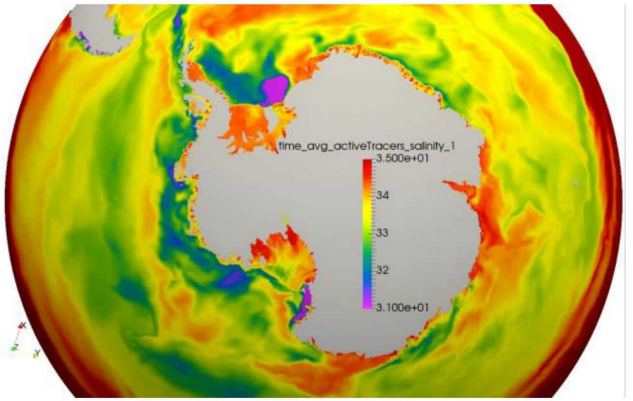


1. AgileComponents code-development strategy
2. What is Albany?
3. Albany code design
   - Global discretization & libraries
   - Problem abstraction & finite element assembly
   - Nonlinear model abstraction & libraries
   - Linear model abstraction & libraries
   - Software quality tools
4. Applications hosted by Albany
5. Algorithmic projects hosted by Albany
6. Coupling with other codes
7. Work in progress
8. Summary









AgileComponents: a PDE code strategy

Strategic Goal: To enable the **rapid** development of new **production** codes embedded with **transformational** capabilities.

- ***Technical strategy:*** projects create, use, and improve a common base of modular, independent-yet-interoperable, software **components**
  - **2012 white paper by A. Salinger**: "Component-Based Scientific Application Development" (right).

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Trilinos SIERRA DAKOTA PUMI

Base of Software Components

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ASC NNSA National Nuclear Security Administration | Office of Science U.S. Department of Energy | SciDAC Scientific Discovery through Advanced Computing | LDRD | ECP Exascale Computing Project

Trilinos | SIERRA | DAKOTA | PUMI Parallel Unstructured Mesh Infrastructure

Base of Software Components

Projects

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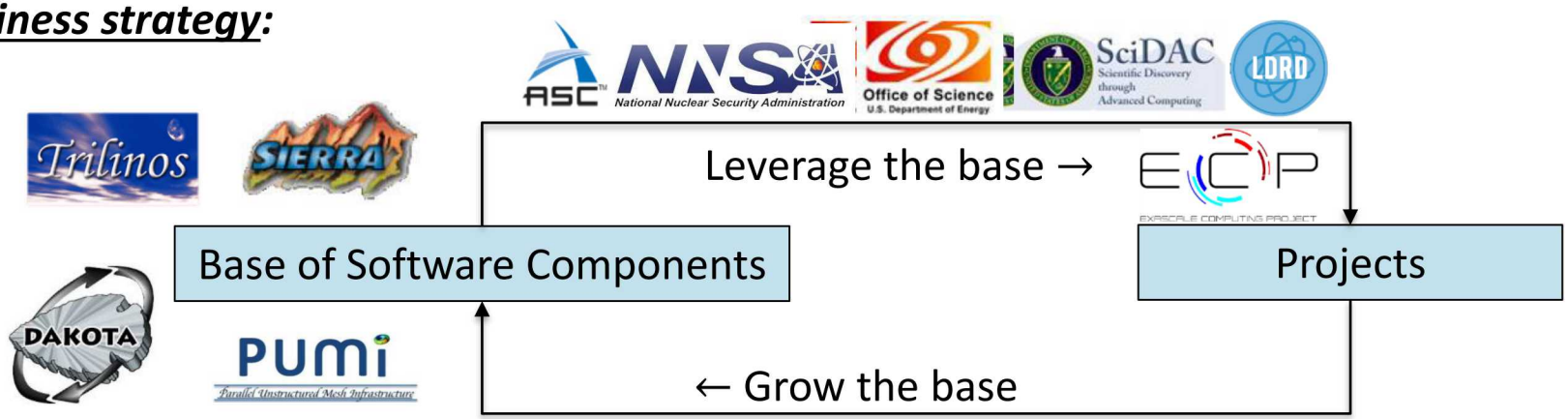

What is Albany? (high-level description)

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"**Components**" =

- ☑ Libraries
- ☑ Software Quality Tools
- ☑ Interfaces
- ☑ **Demonstration Applications**

2008

What is Albany? (high-level description)

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Albany: open-source*, parallel, C++, unstructured-grid, mostly-implicit multi-physics finite element code that demonstrates **AgileComponents** vision.

*** Albany github repo:** https://github.com/SNLComputation/Albany.

What is Albany? (high-level description)

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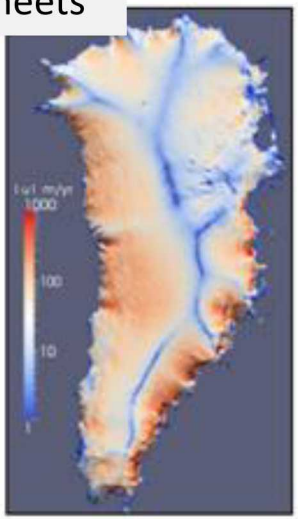
Albany: open-source*, parallel, C++, unstructured-grid, mostly-implicit multi-physics finite element code that demonstrates **AgileComponents** vision.

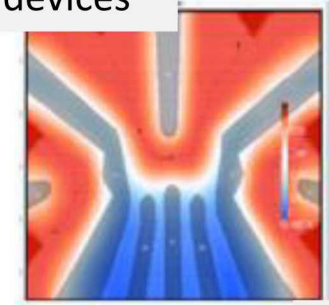
Distinguishing features of Albany:

- Houses a variety of **diverse algorithmic projects** and **applications**:

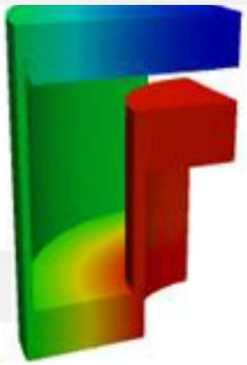
Ice sheets



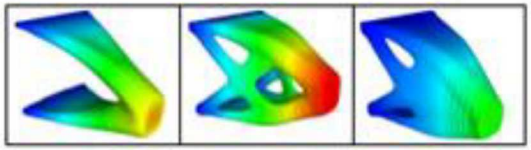
Quantum devices



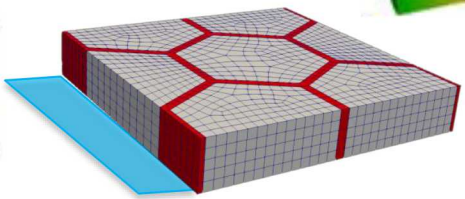
Computational mechanics



Additive manufacturing



Arctic costal erosion



- **Funded** entirely **by applications** residing within.
- Both a **"sand-box"** for prototyping **new algorithms/applications** and a **production** code.

* **Albany github repo:** https://github.com/SNLComputation/Albany.

The components effort: libraries & tools

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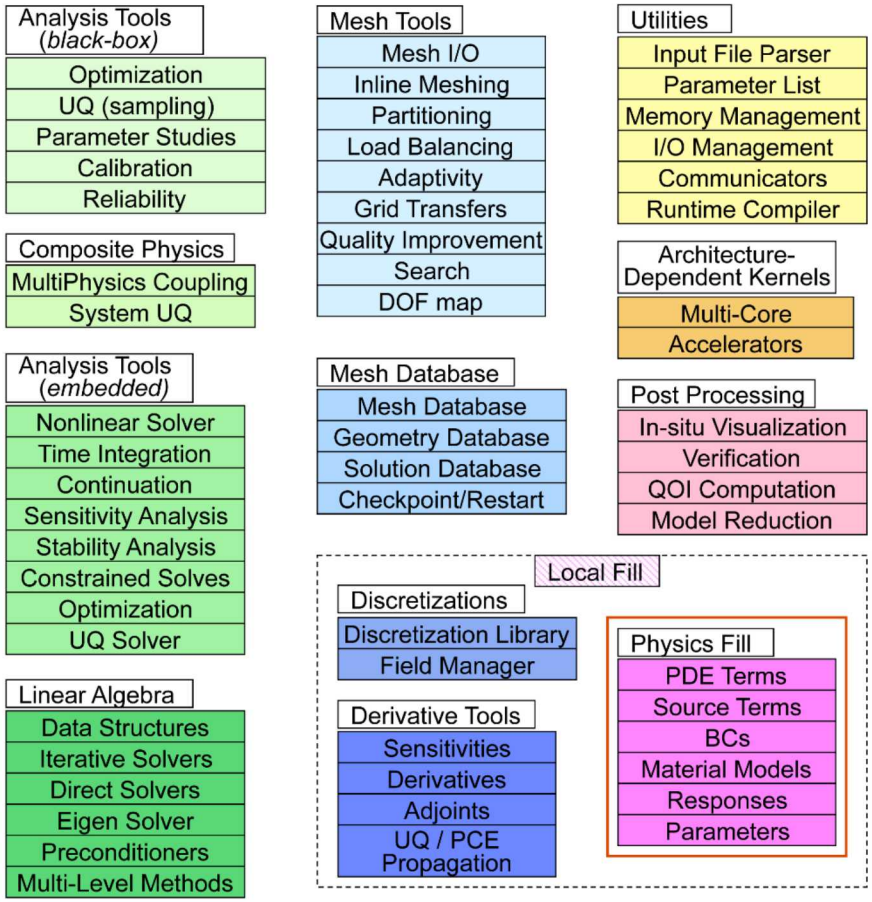
Components in Albany = cutting-edge technology from Trilinos, SCOREC, SierraToolKit, DAKOTA, FASTMath, QUEST, Kitware, etc.

Many components are **Trilinos* packages**:

- Distributed linear algebra (*Tpetra*)
- Mesh tools (*STK*)
- Discretization tools (*Intrepid2*)
- Nonlinear solver (*NOX*)
- Linear solver (*Belos*)
- Preconditioners (*Ifpack2*)
- Automatic differentiation (*Sacado*)
- Shared memory parallelism (*Kokkos*)
- Optimization (*ROL*)
- *Many more…*



Trilinos : 40+ packages; 120+ libraries

* **Trilinos github repo:** https://github.com/trilinos/Trilinos.

What is Albany? (under-the-hood)

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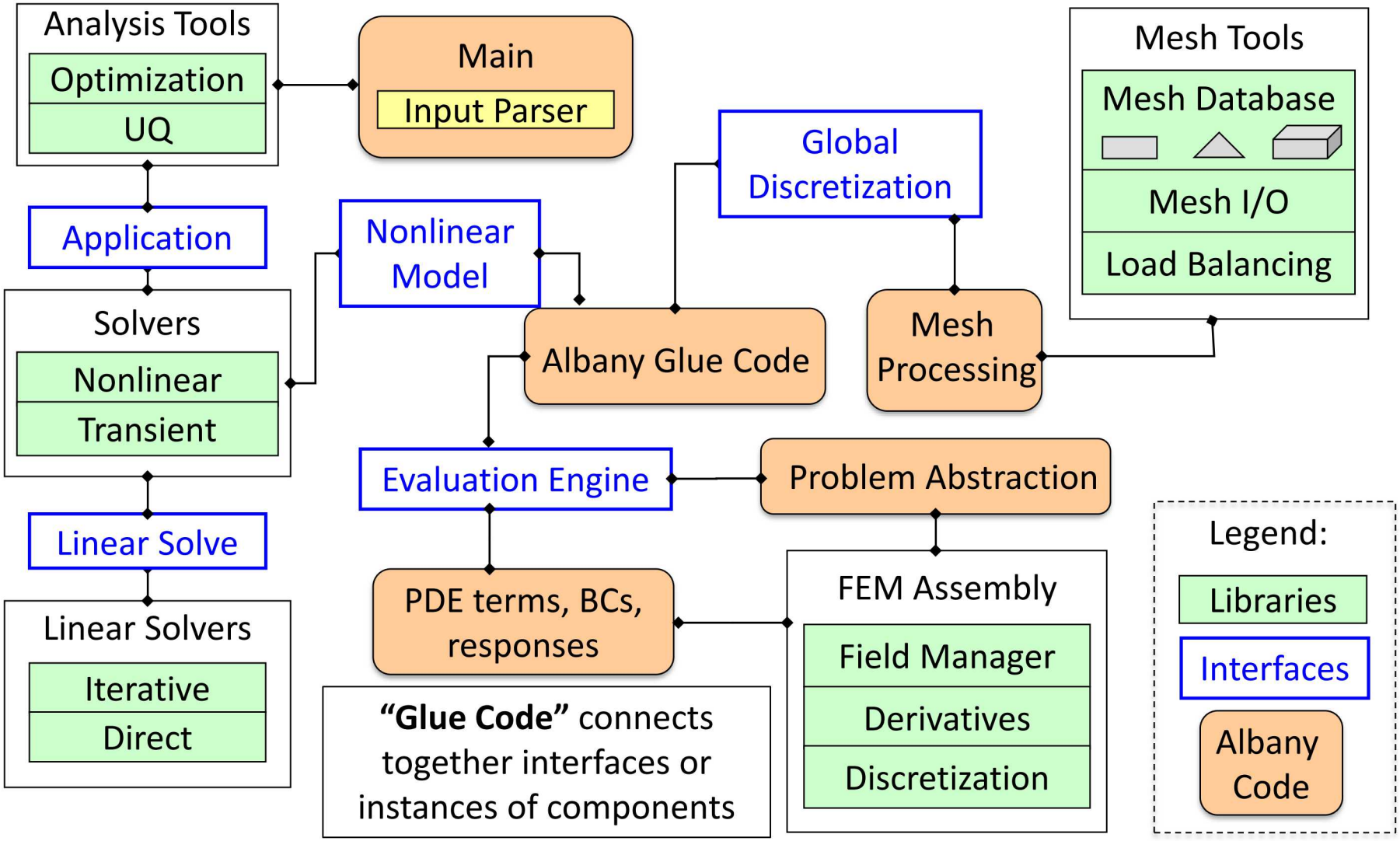
Albany = Component Libraries + Abstract Interfaces + "Glue Code"



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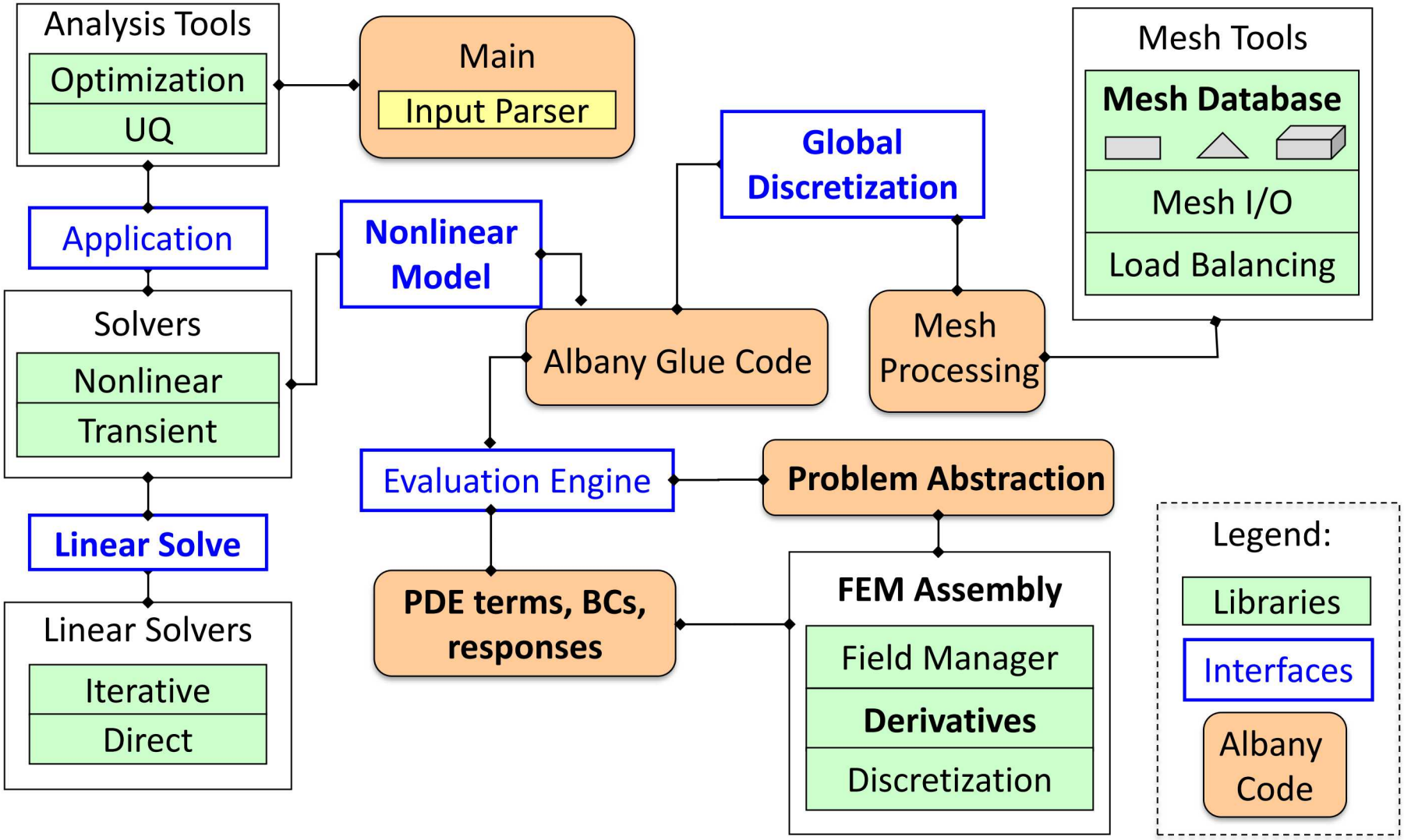

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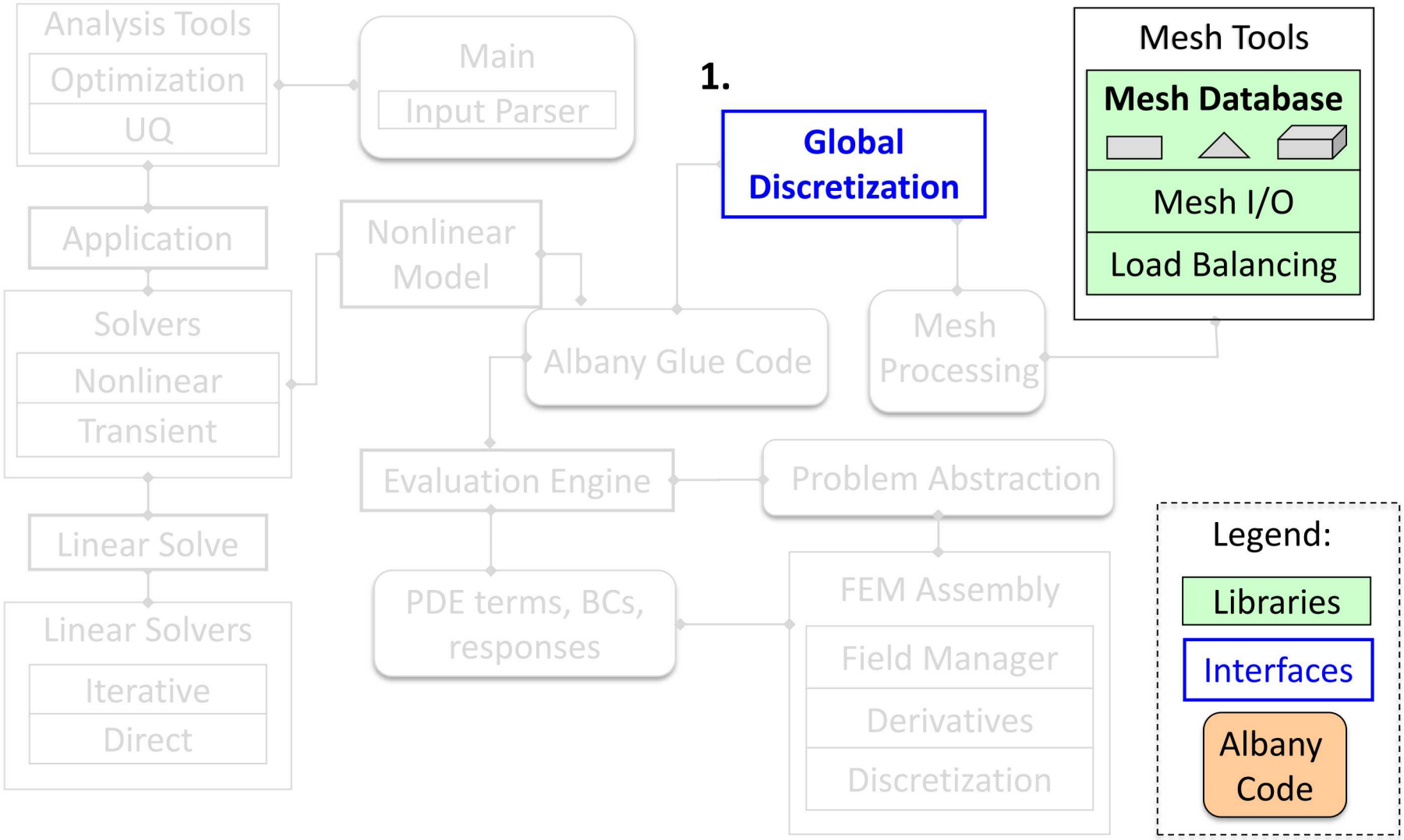

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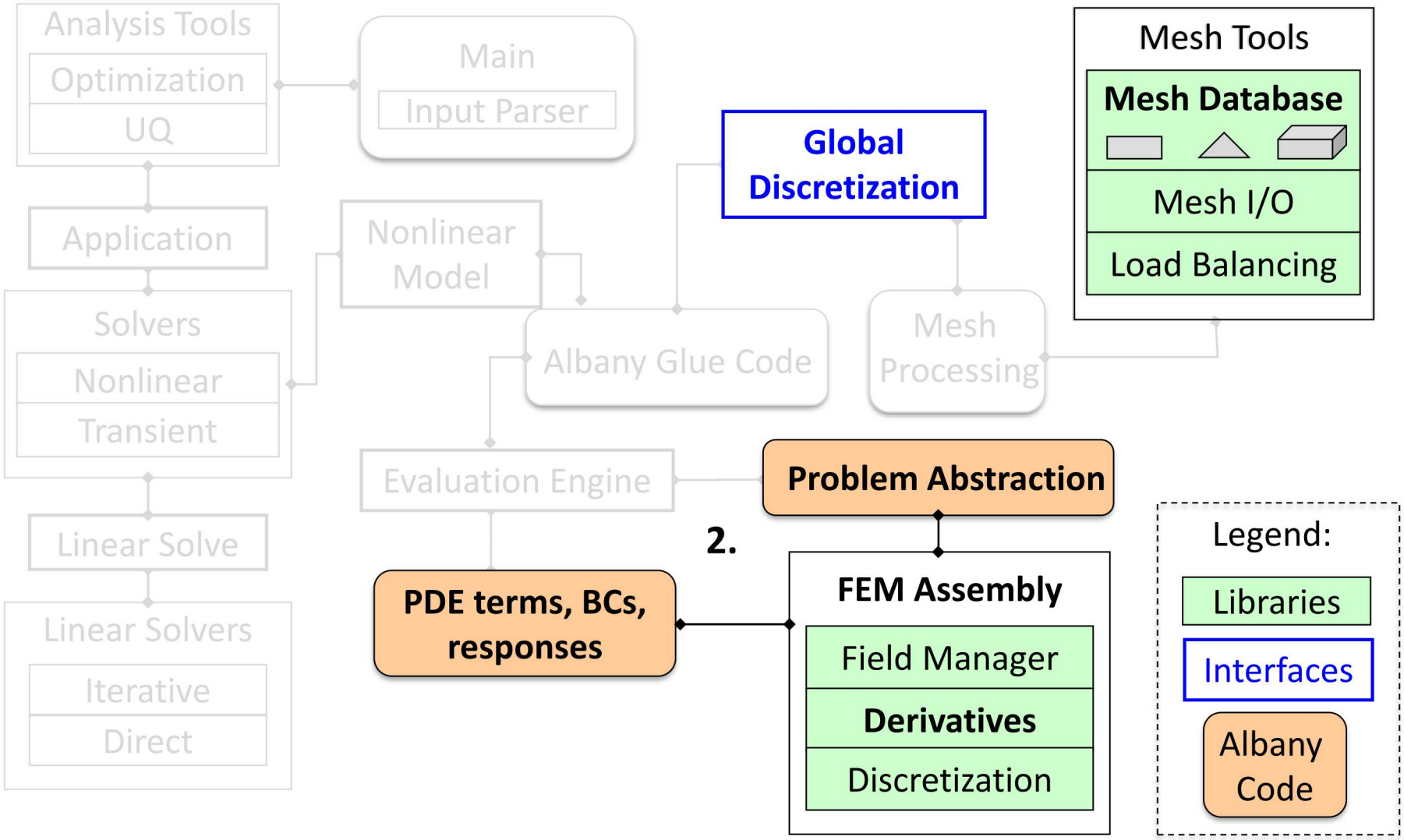

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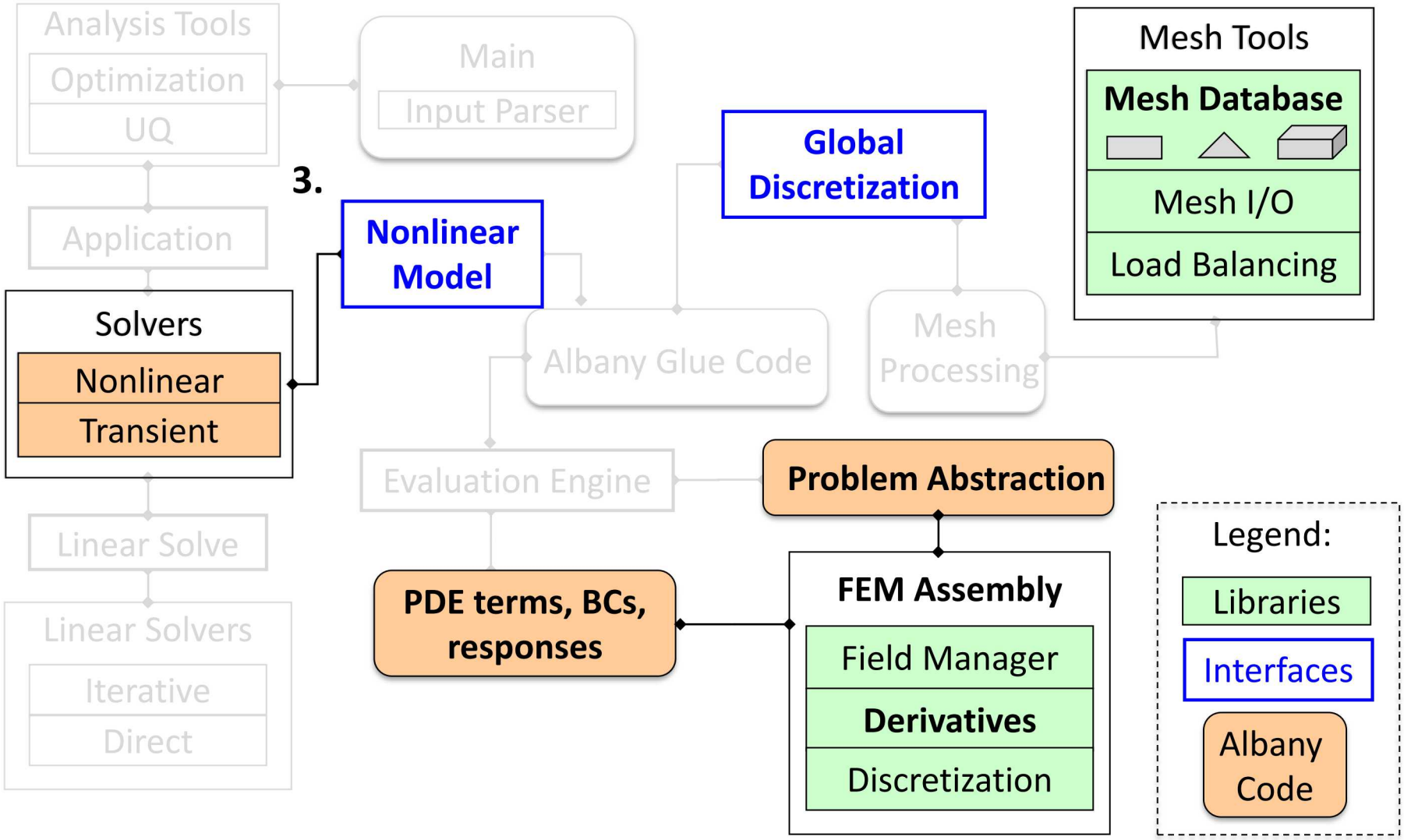

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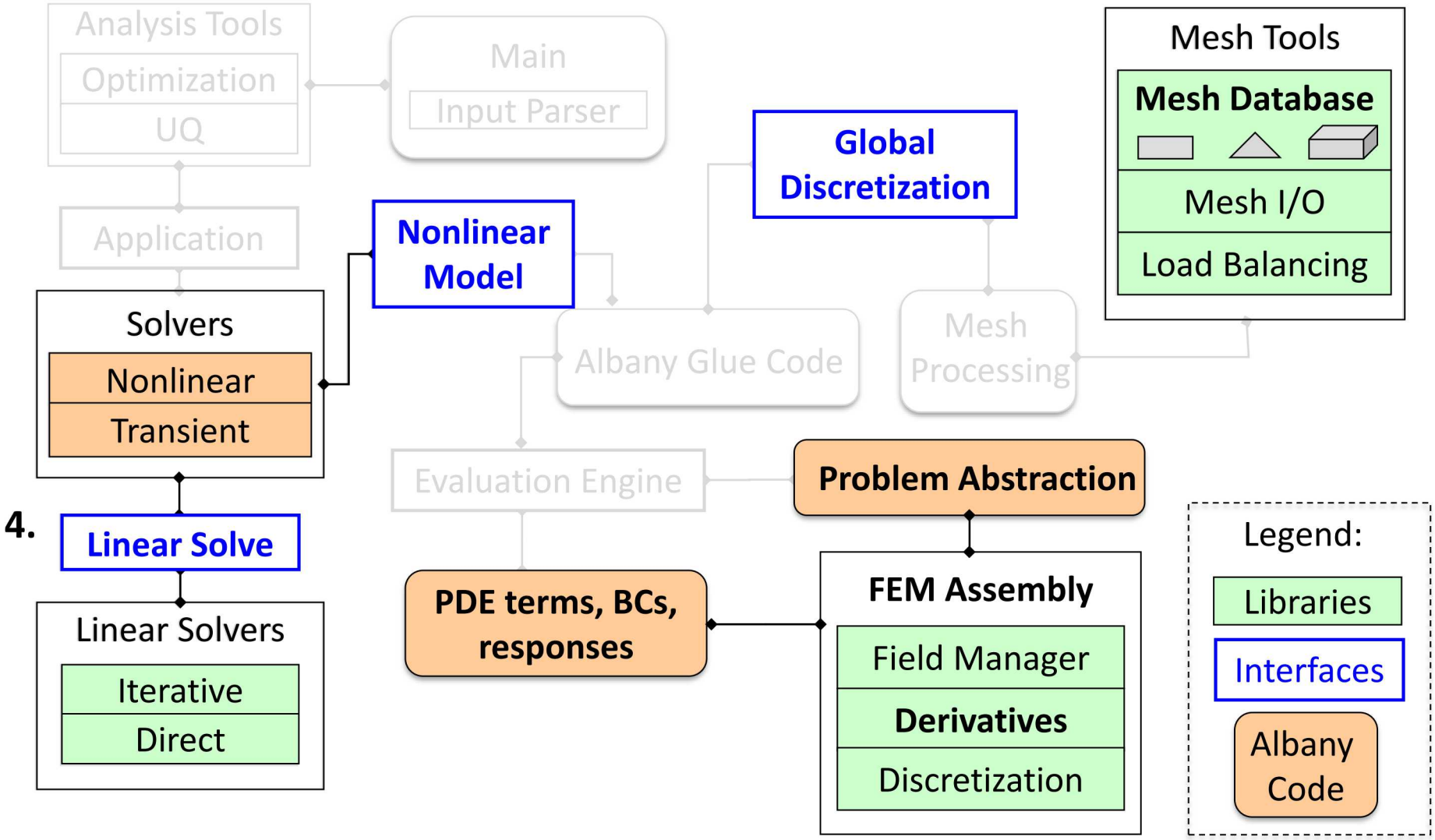

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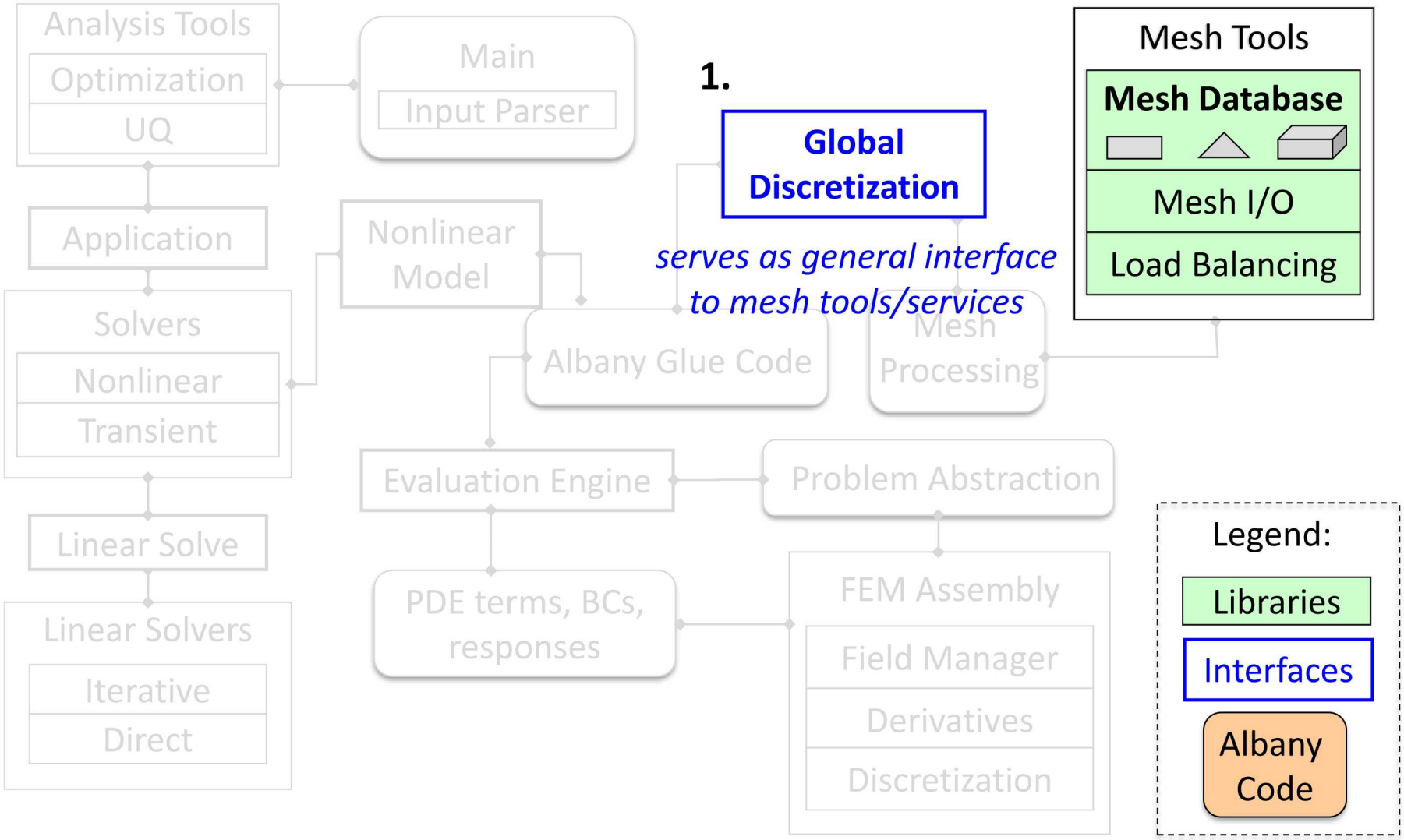

Global discretization abstraction & libraries

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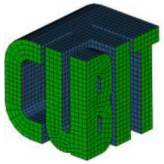
Discretization interface: currently has ***two independent implementations***

1. **SierraToolKit (STK)** package in Trilinos.
   - Supports reading in **Exodus** mesh files (e.g., from CUBIT), **inline meshing** via Pamgen, **simple rectangular meshes** constructed in Albany.
   - Meshes can be **structured/unstructured** but are **static**.
2. **Parallel Unstructured Mesh Interface (PUMI)** package, developed at the Scientific Computation Research Center (SCOREC) at RPI.
   - Supports **VTK mesh files** (generated by Symmetrix).
   - Goal-oriented generalized **error estimation** and **in-memory mesh adaptation**.



S. Seol *et. Al.* PUMI, *High Performance Computing, Networking, Storage and Analysis (SCC), 2012.*

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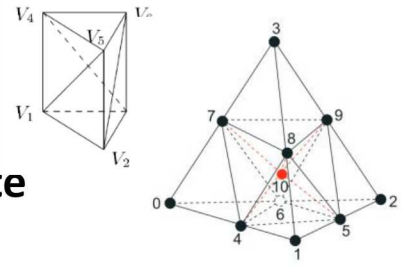
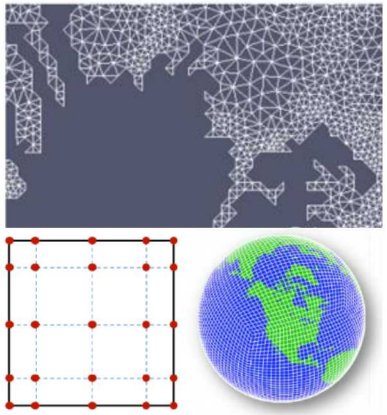
Element types: variety of element types supported, with basis functions/quadrature routines from ***Intrepid2*** Trilinos library:

- **Isoparametric** elements (tet, hex, wedge, …).
- 2D **spectral elements** of arbitrary orders.
- Some physics-specific elements, e.g., **composite 10-node tetrahedron** for solid mechanics.





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Albany is a **Continuous Galerkin (CG)** unstructured grid finite element code.

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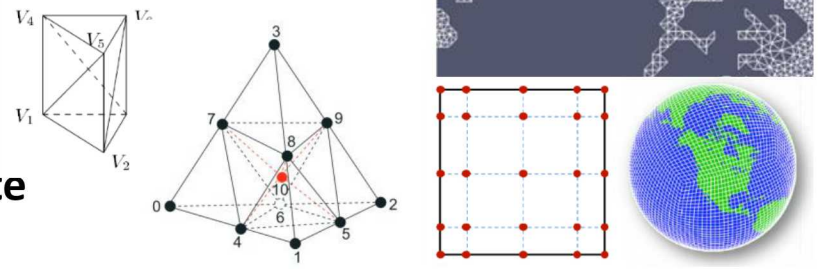
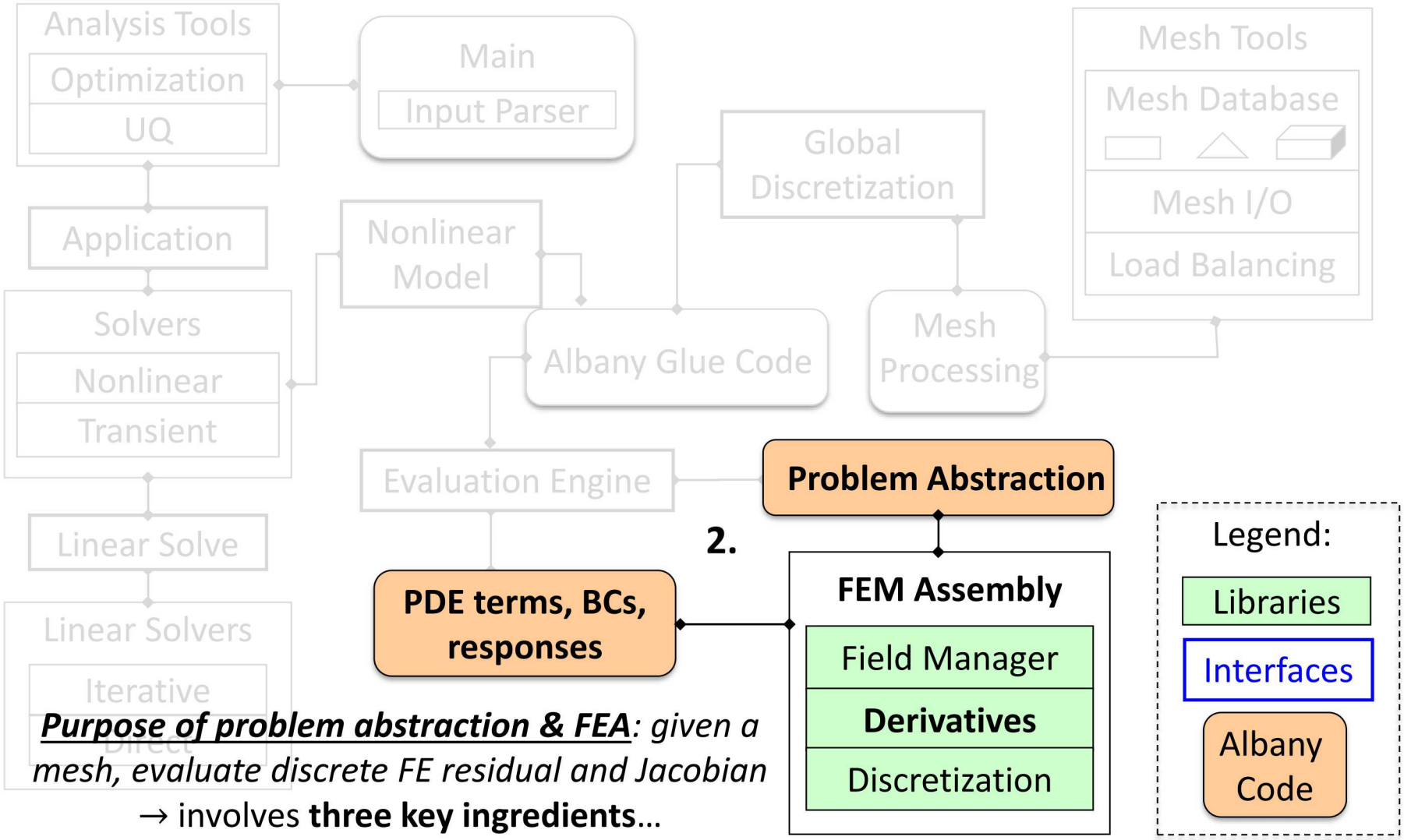


What is Albany? (under-the-hood)

Albany = Component Libraries + Abstract Interfaces + "Glue Code"



***Purpose of problem abstraction & FEA**: given a mesh, evaluate discrete FE residual and Jacobian*

→ involves **three key ingredients**…

1. Templated-based automatic differentiation

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Automatic differentiation (AD) provides exact derivatives without time/effort of deriving and hand-coding them.

- Template equation implementation on scalar type.
- Libraries (Sacado) provides new scalar types that ***overload the math operators*** to propagate embedded quantities via chain rule.
  - *Derivatives:* DFad<double>
  - *Hessians*: DFad<SFad<double,N>>
  - *Stochastic Galerkin resid*: PCE<double>
  - *Stochastic Galerkin Jac*: DFad<PCE<double>
  - *Sensitivities*: DFad<double>

No finite difference truncation error!

- Great for ***multi-physics codes*** (e.g., many Jacobians) and ***advanced analysis*** (e.g., sensitivities, optimization)

Operation	double	Overloaded AD impl DFad<double>
$c = a \pm b$		$\dot{c} = \dot{a} \pm \dot{b}$
$c = ab$		$\dot{c} = a\dot{b} + \dot{a}b$
$c = a/b$		$\dot{c} = (\dot{a} - c\dot{b})/b$
$c = a^r$		$\dot{c} = ra^{r-1}\dot{a}$
$c = \sin(a)$		$\dot{c} = \cos(a)\dot{a}$
$c = \cos(a)$		$\dot{c} = -\sin(a)\dot{a}$
$c = \exp(a)$		$\dot{c} = c\dot{a}$
$c = \log(a)$		$\dot{c} = \dot{a}/a$

```
template <typename ScalarT>
void computeF(ScalarT* x, ScalarT* f)
{
  f[0] = 2.0 * x[0] + x[1] * x[1];
  f[1] = x[0] * x[0] * x[0] + sin(x[1]);
}
```

```
double* x;
double* f;
…
computeF(x,f);
```

```
DFad<double>* x;
DFad<double>* f;
…
computeF(x,f);
```

E. Phipps *et. al*. Efficient expression templates for operator overloading-based AD, LNCSE, 309–319, 2012.

2. Template-based generic programming (TBGP)

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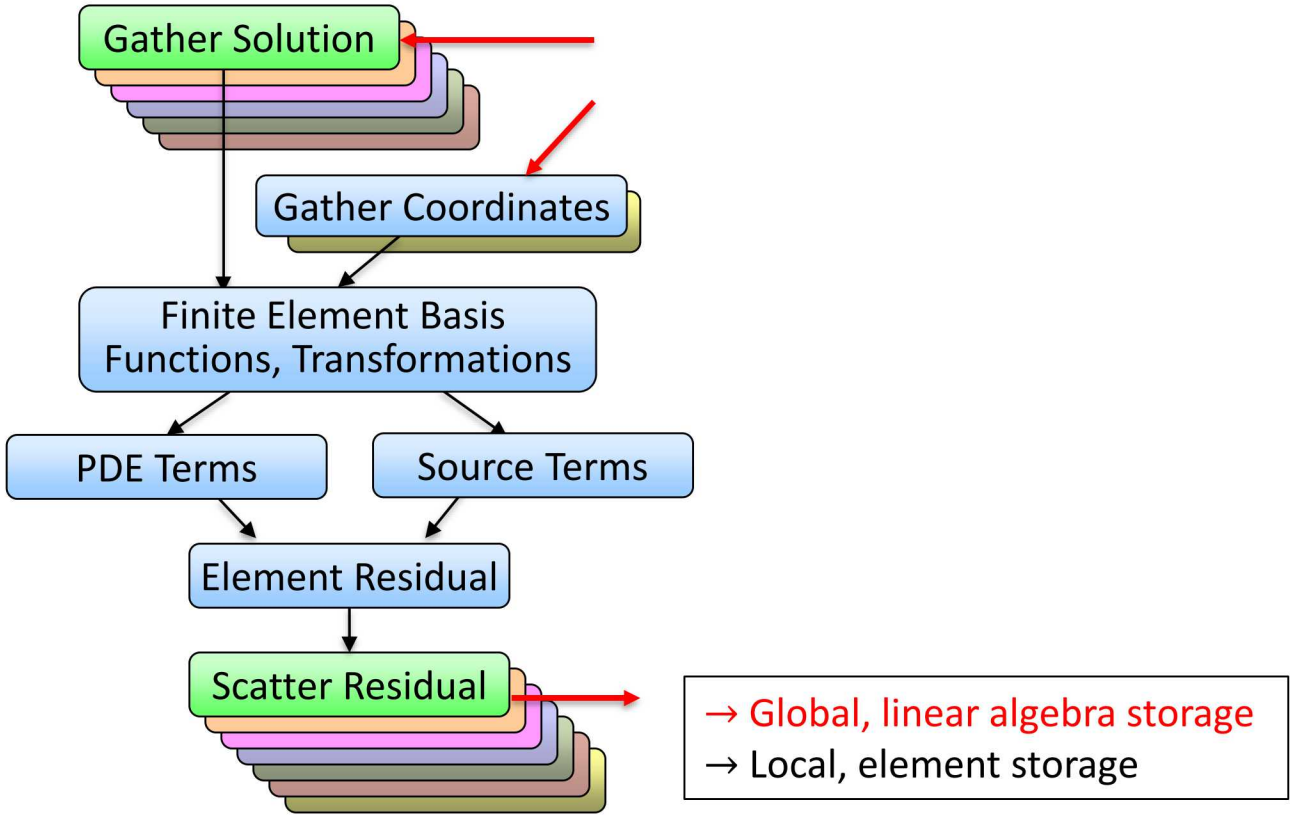
Albany Finite Element Assembly (FEA):



- **Gather Solution** extracts values from global structures, puts in element local structures
- **Evaluators** operate on element local data structures
- **Scatter** adds local contributions to global structures

2. Template-based generic programming (TBGP)

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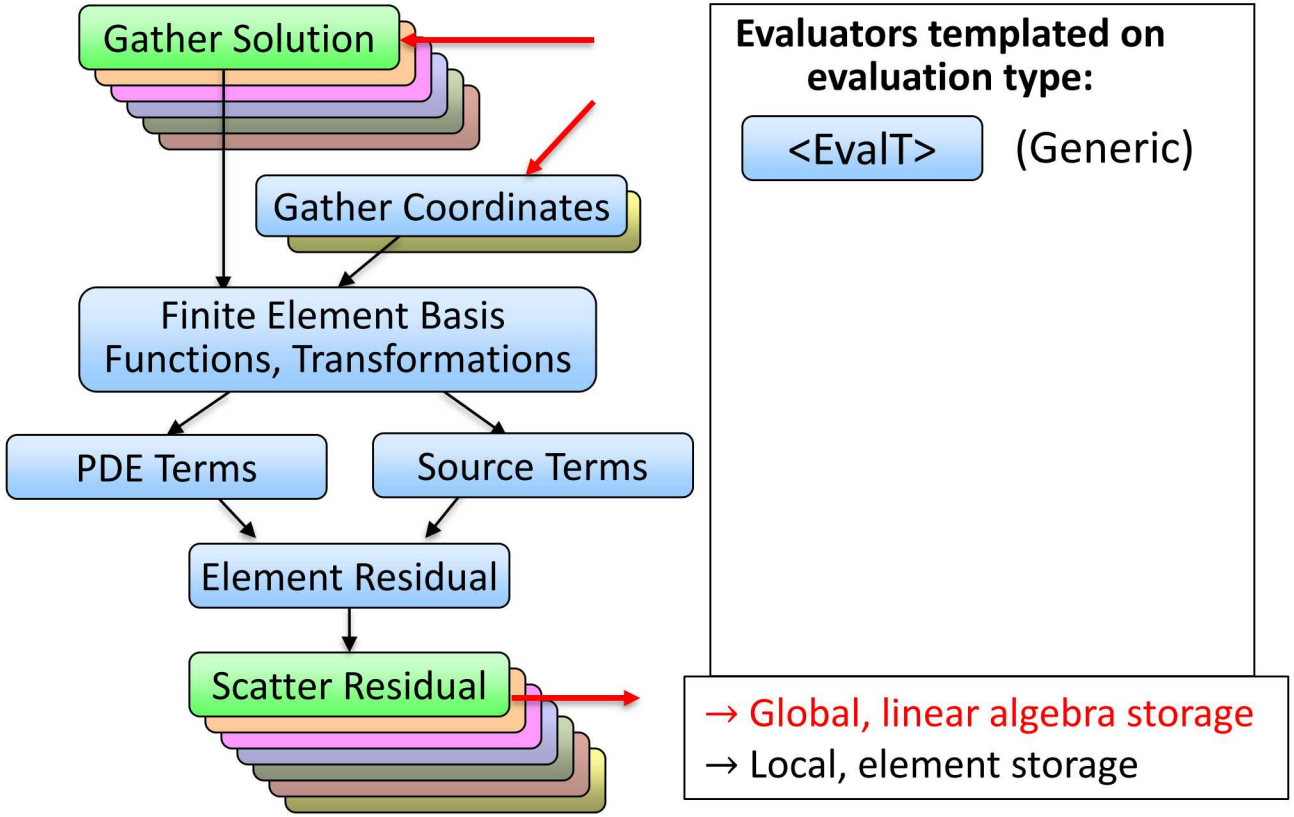

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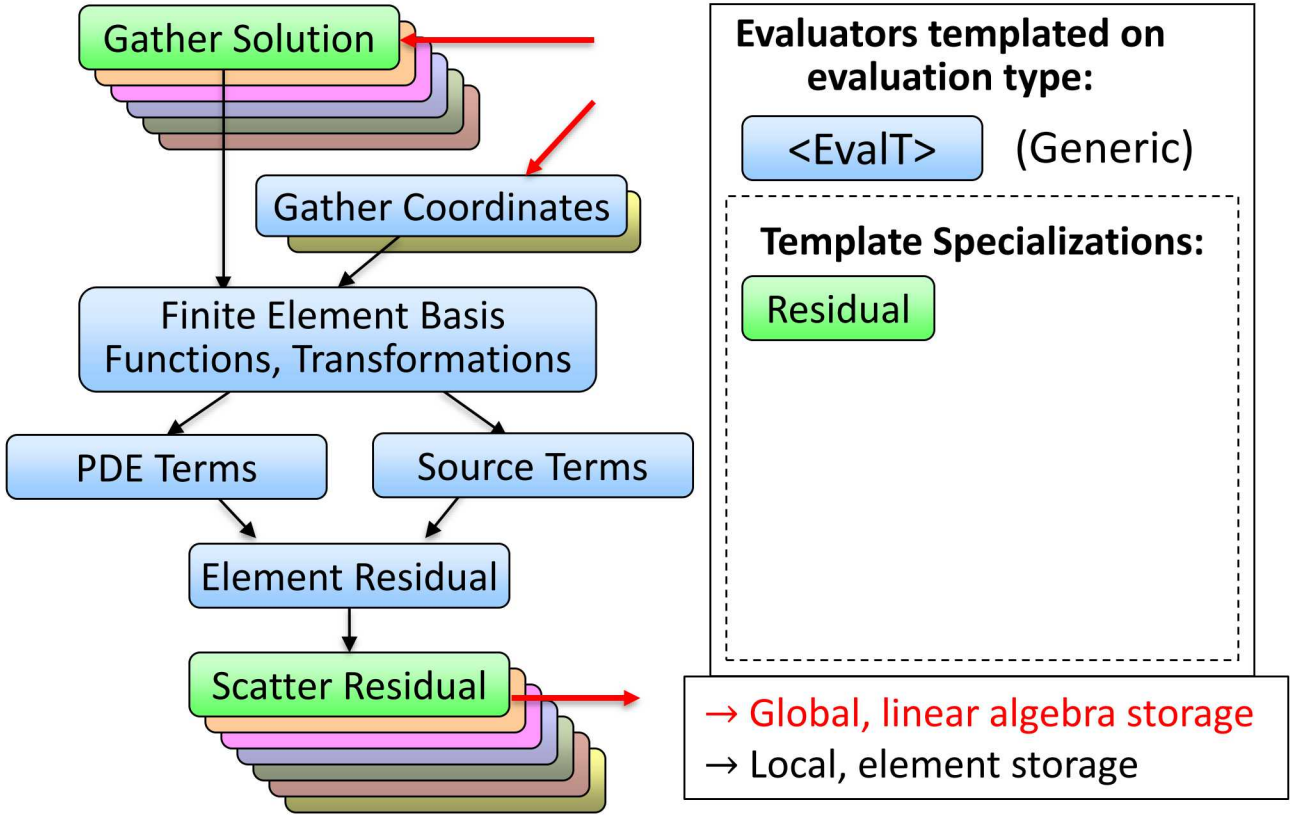

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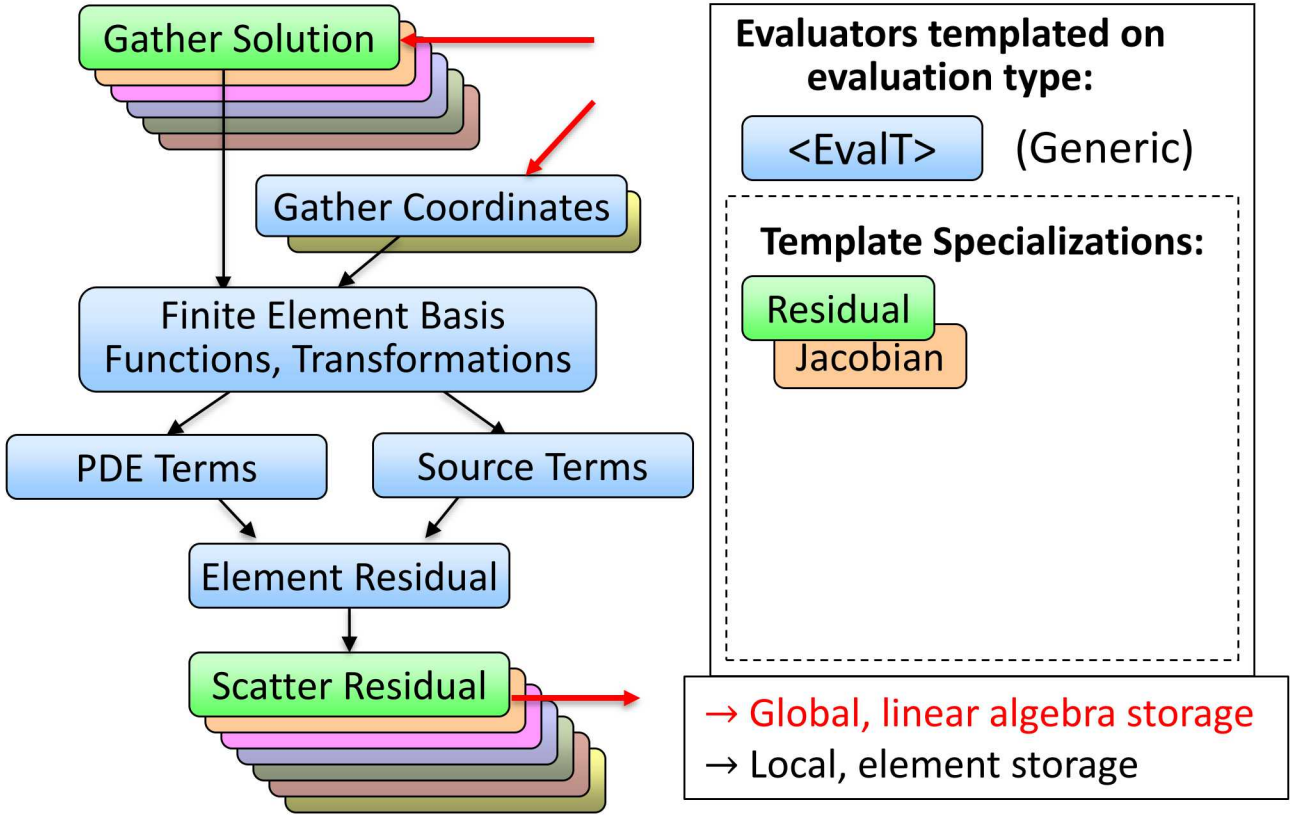
2. Template-based generic programming (TBGP)

Sandia National Laboratories

Albany Finite Element Assembly (FEA):



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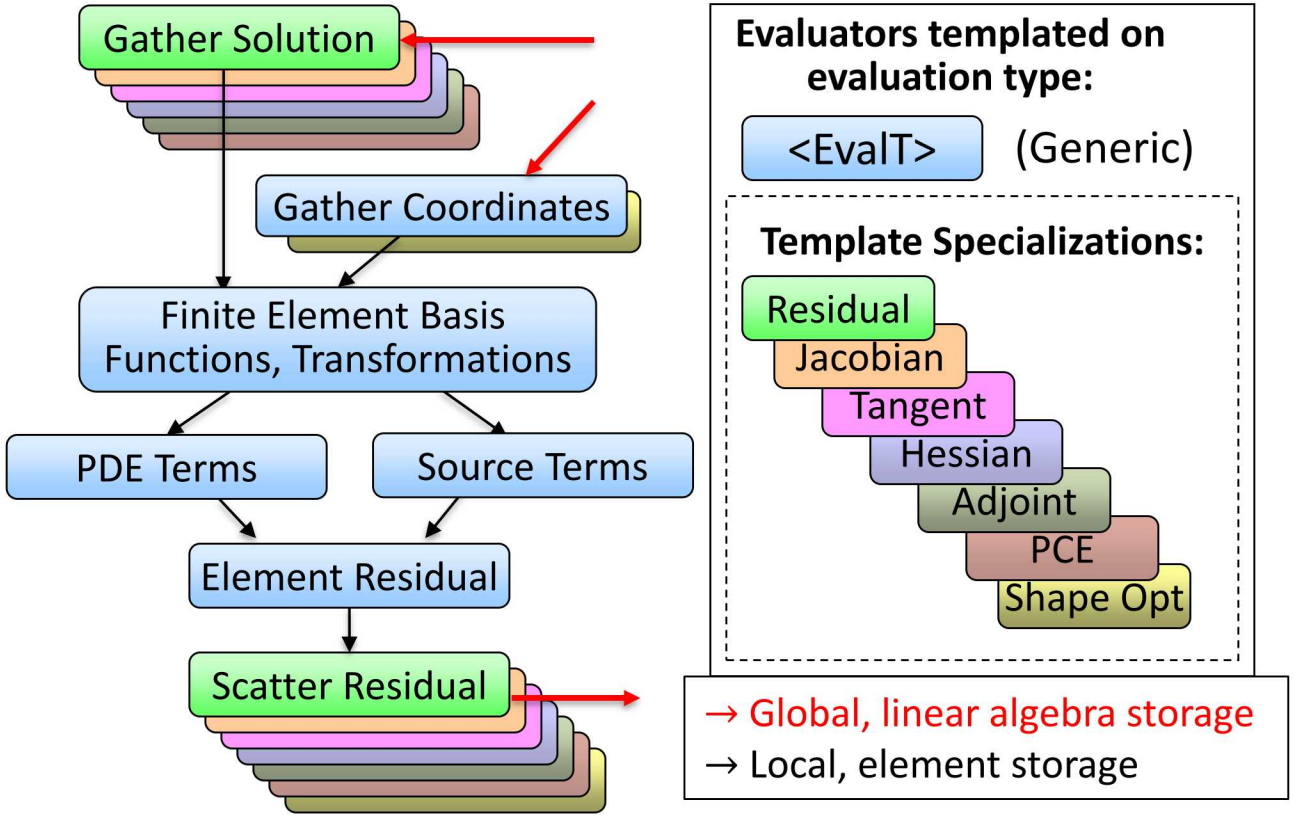

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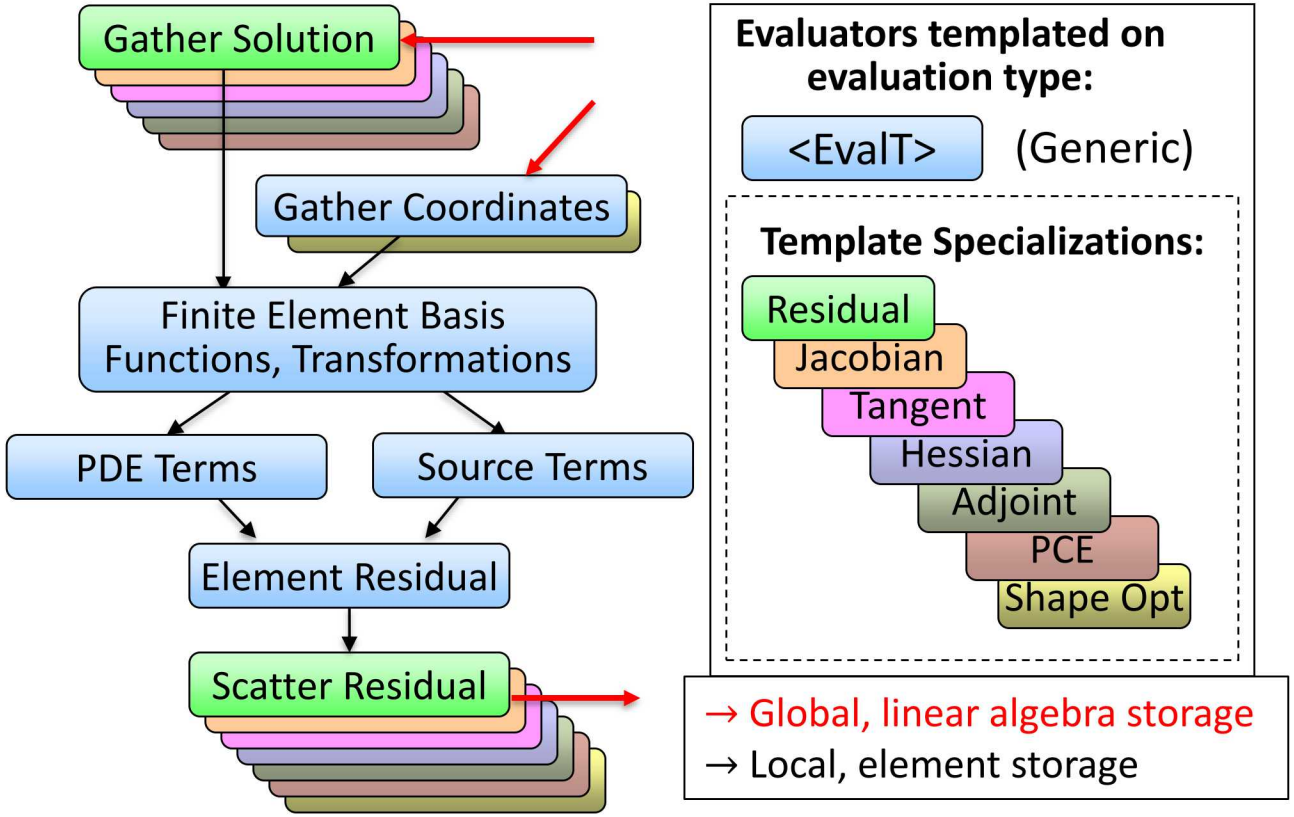

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Enables **advanced analyses** (sensitivities, optimization, …)

R. Pawlowski et. al. *Sci. Program.*, 2012.

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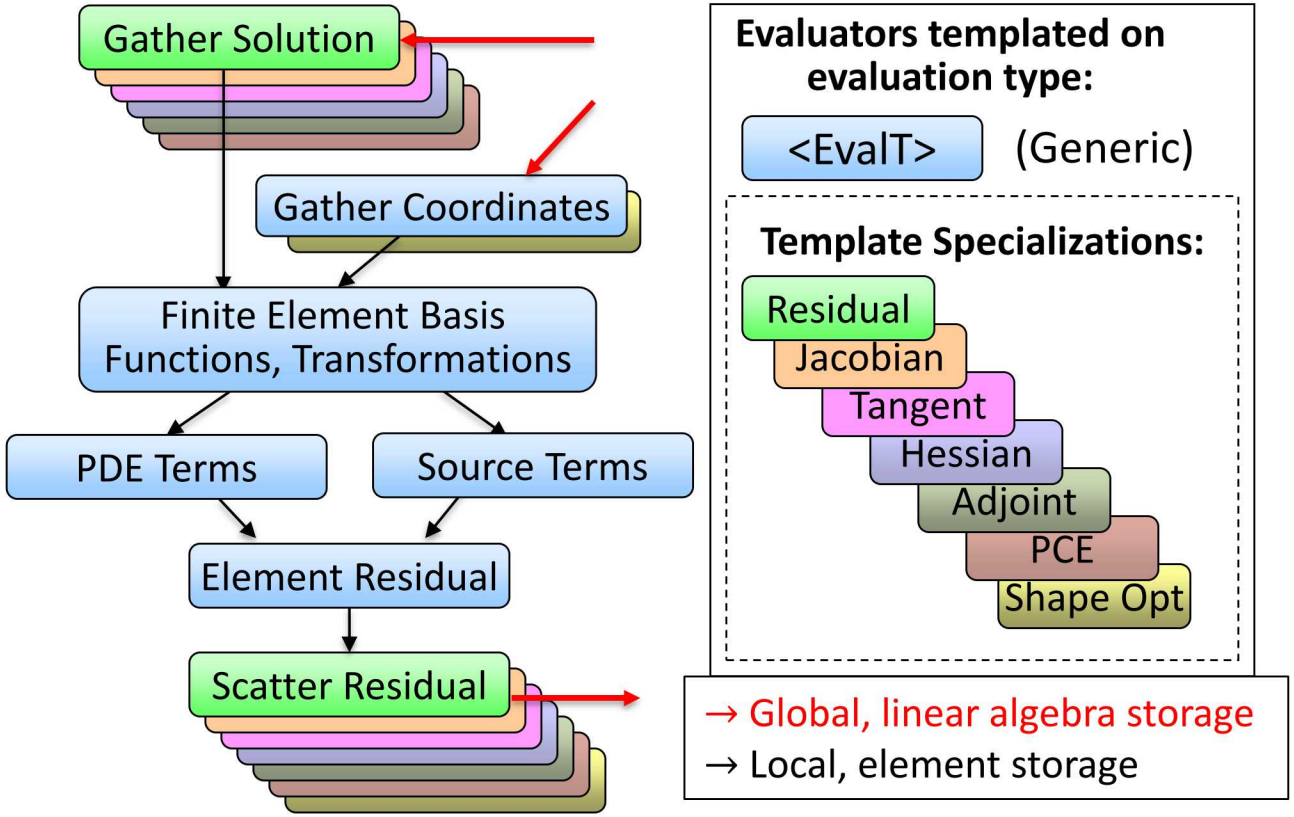

Employs **AD overloads** (Sacado, Stokhos)

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3. Graph-based finite element assembly (FEA)

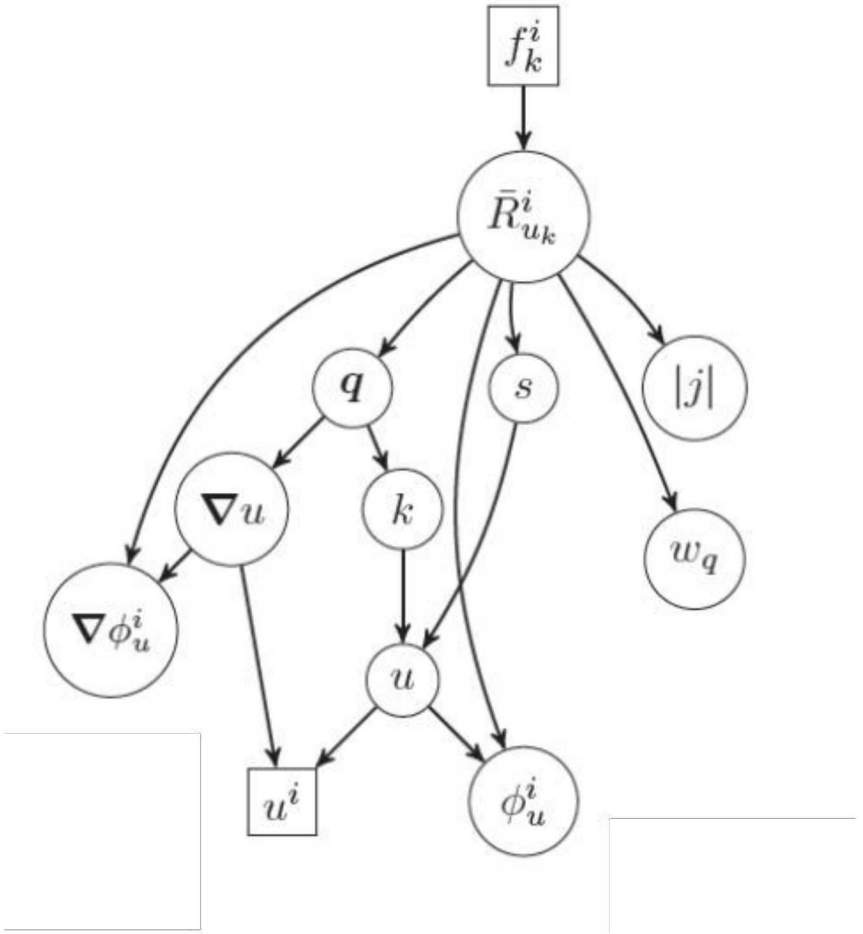
Sandia National Laboratories

Assembly of physics pieces comes down to the evaluation of a **directed acyclic graph (DAG)** of computations of field data.

$$R_u^i = \int_\Omega \left[\phi_u^i \dot{u} - \boldsymbol{\nabla} \phi_u^i \cdot \boldsymbol{q} + \phi_u^i s \right] \mathrm{d}\Omega$$

Phalanx package: Local field evaluation kernel designed for assembly of arbitrary equation sets (i.e. evaluating residuals/Jacobians).

- **Decomposes** a complex model into a graph of **simple kernels** (functors)
- A node in the graph evaluates one or more **temporary fields**
- **Runtime** DAG construction of graph
- Achieves **flexible multi-physics assembly**



R. Pawlowski, Phalanx web site, http://trilinos.sandia.gov/packages/phalanx/ 2015.

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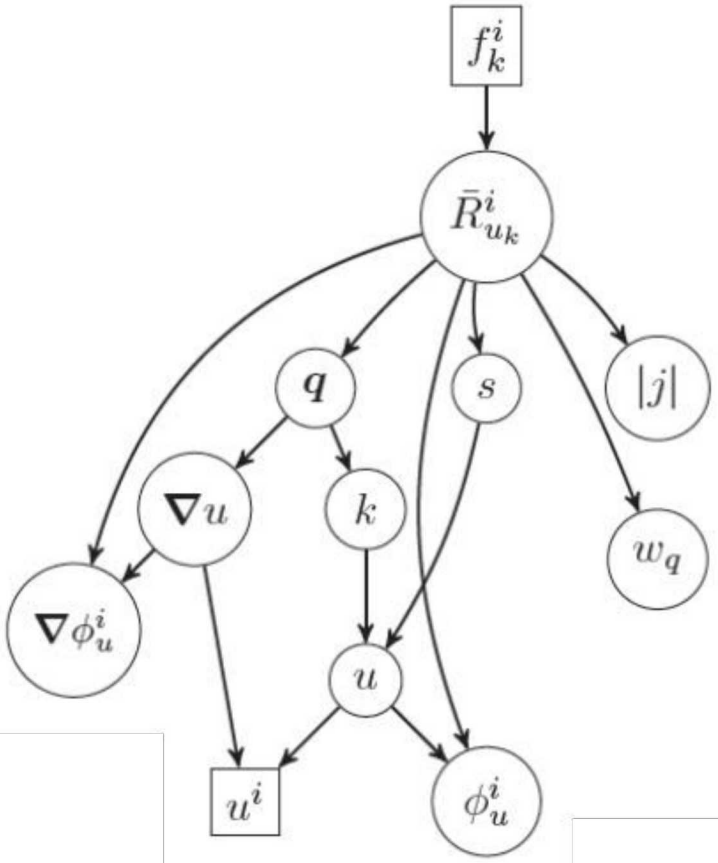


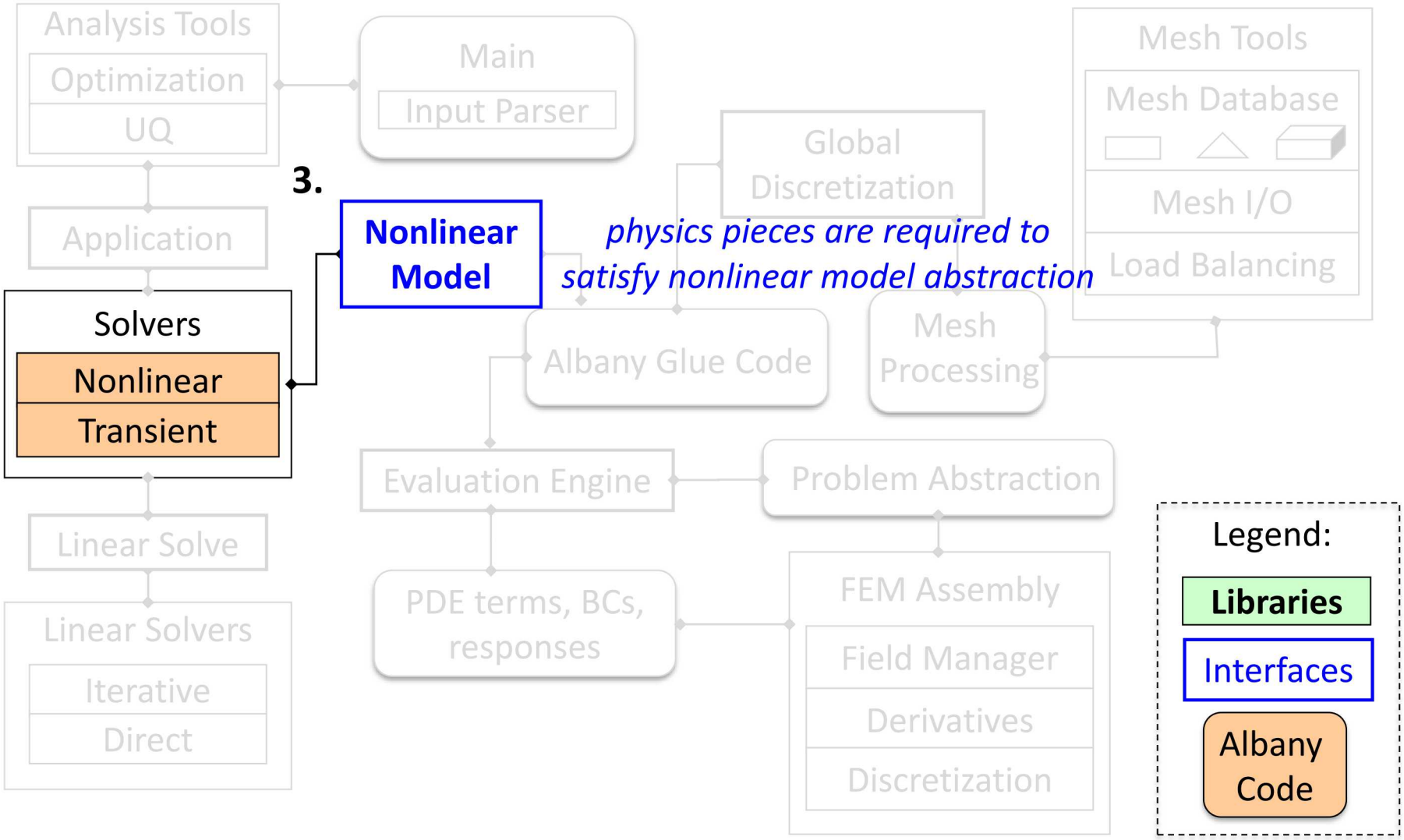
DAG-based assembly enables **flexibility**, **extensibility**, **rapid development:** to add new PDE, all you need to code is problem-specific residual R_u^i!

R. Pawlowski, Phalanx web site, http://trilinos.sandia.gov/packages/phalanx/ 2015.

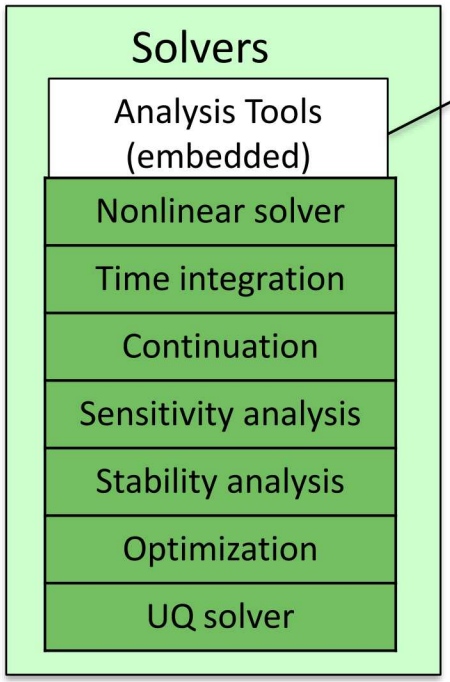
What is Albany? (under-the-hood)

Sandia National Laboratories

Albany = Component Libraries + Abstract Interfaces + "Glue Code"



Nonlinear model abstraction & libraries



"ModelEvaluator":

Given:	Computes:
x	$f(\dot{x}, \ddot{x}, x, p, t)$
$\dot{x}$	$W = \alpha \frac{df}{d\dot{x}} + \beta \frac{df}{dx} + \omega \frac{df}{d\ddot{x}}, W_{prec}$
$\ddot{x}$	$\frac{df}{dp}$
p	g
t	$\frac{dg}{dx}, \frac{dg}{dp}$

Access to Trilinos **embedded solvers** requires satisfaction of **ModelEvaluator** (nonlinear model) abstraction.

f = residual; x = solution; p = params; g = responses; t = time; W = Jacobian; W_{prec} = Preconditioner

- Interface is **general** to accommodate computation of Jacobians, user-defined preconditioners, and stochastic Galerkin expansions.
- Enables "**beyond-forward analysis**": analysts/physics experts are not burdened with analysis algorithm requirements, i.e., programming sensitivities for implicit solvers, optimization, stability, bifurcation analysis.
  - **Advanced capabilities**: optimization (ROL), homotopy continuation (LOCA), embedded UQ (Stokhos).

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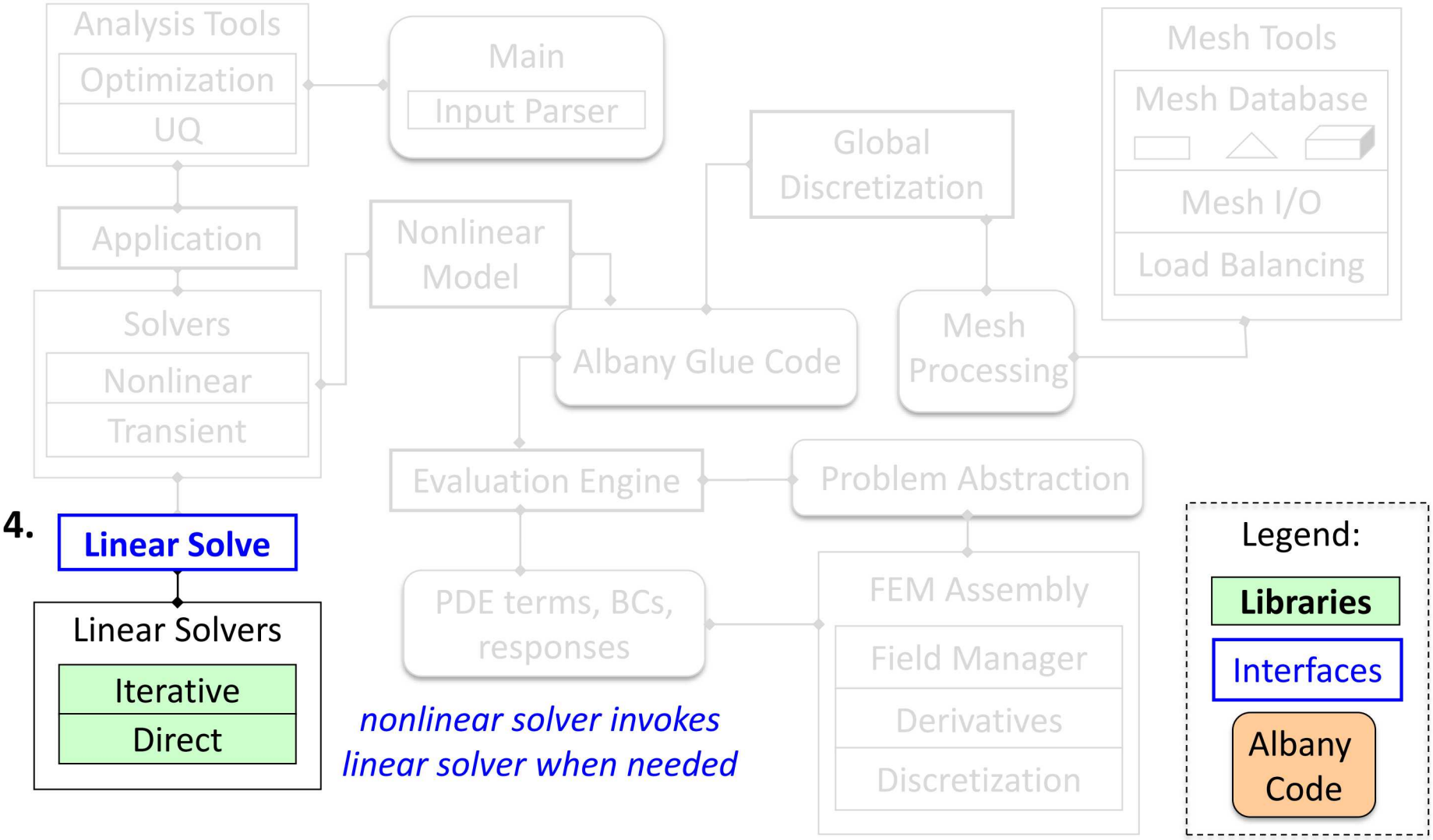
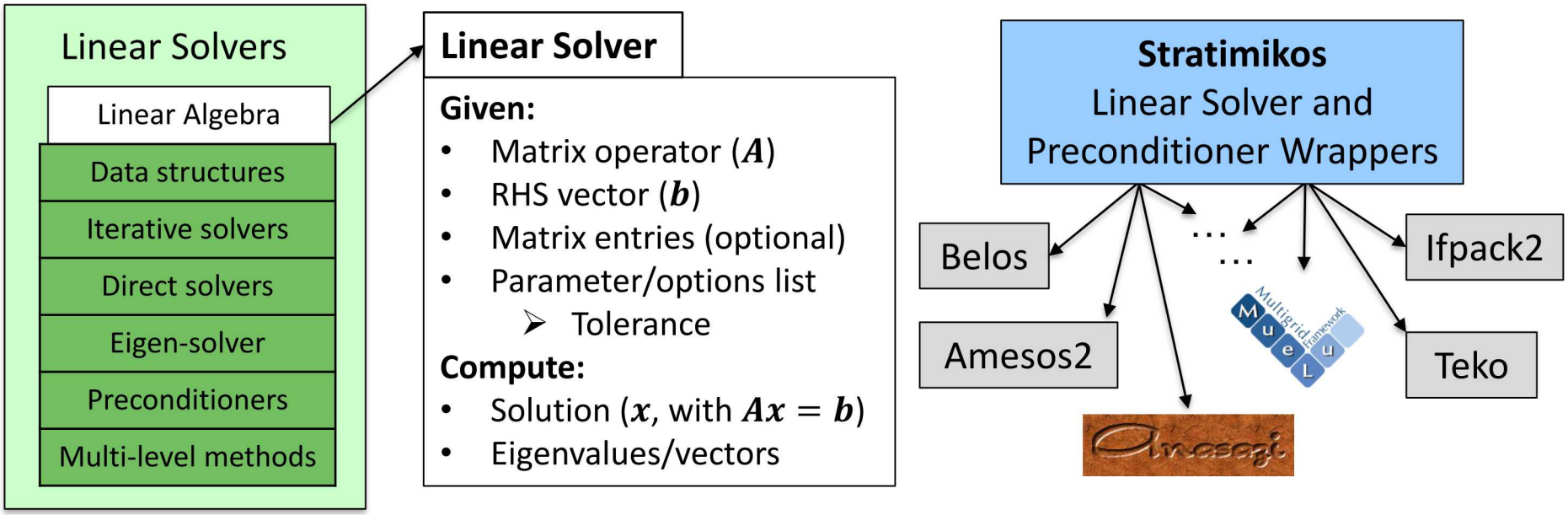


Linear solver abstraction & libraries

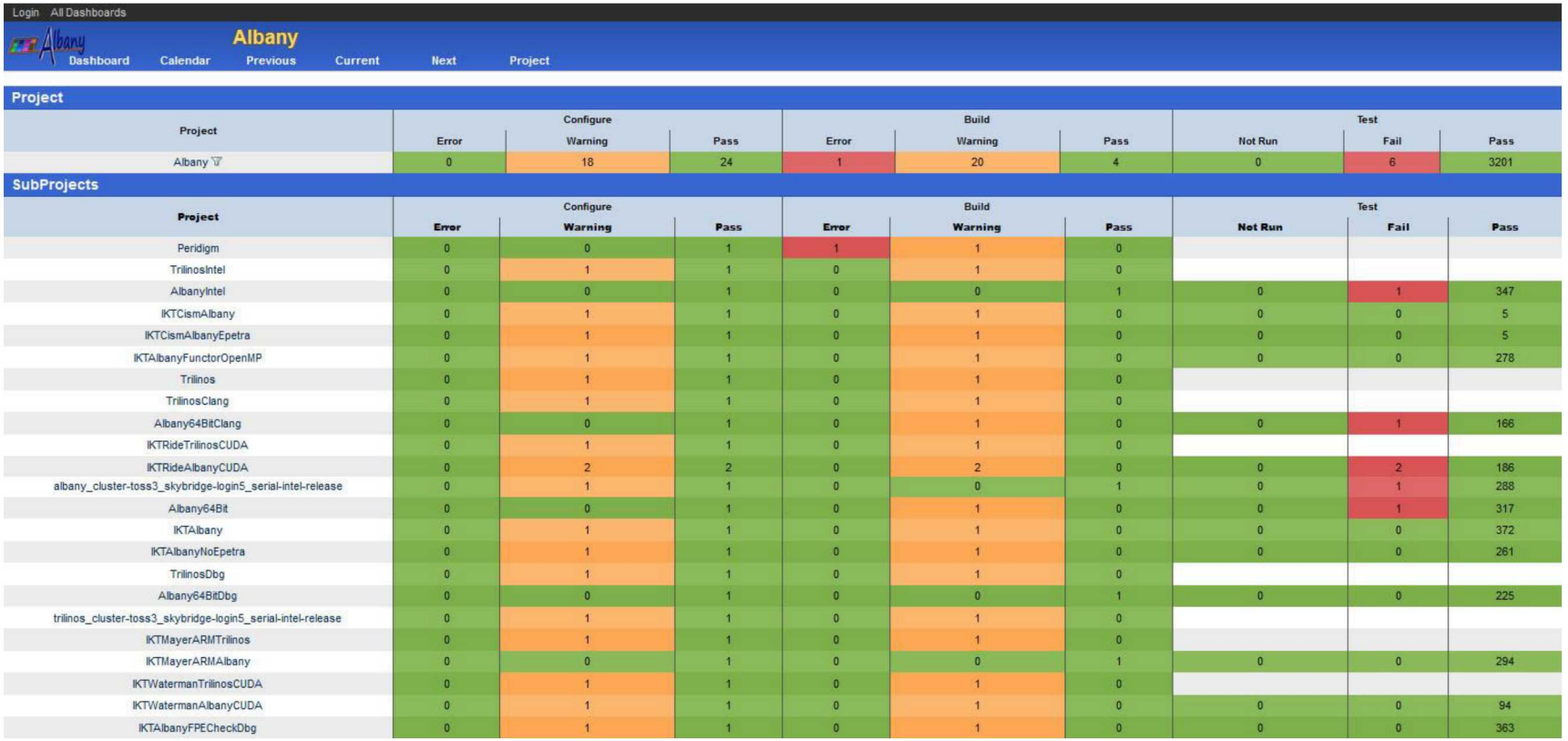


- **Linear solver abstraction** provides full access to all Trilinos linear solvers (direct and iterative), eigensolvers and preconditioners through Stratimikos interface.
- **Factory class** supports run-time solution configuration through input file options.
- **Available direct solvers**: Amesos, Amesos2 (UMFPACK, MUMPS, SuperLU, SCALAPACK, etc.).
- **Available iterative solvers**: AztecOO, Belos (CG, GMRES)
- **Available preconditioners**: Ifpack, Ifpack2 (ILU); ML, MueLu (AMG); Teko (block)
- **Eigensolvers**: Anasazi

Software quality tools & processes

Repository*	Nightly test harness	Mailing lists
Version control	Unit tests	Issue tracking
Build system	Verification tests	Web pages
Config mgmt	Code coverage	Licensing
Regression tests	Performance tests	Release process

Performance monitored via **CDash nightly testing** on a variety of architecture including GPU (P100, V100), Xeon Phi, Skylake, ARM platforms.



Login All Dashboards

Albany

Dashboard Calendar Previous Current Next Project

Project

Project	Configure			Build			Test		
	Error	Warning	Pass	Error	Warning	Pass	Not Run	Fail	Pass
Albany	0	18	24	1	20	4	0	6	3201

SubProjects

Project	Configure			Build			Test		
	Error	Warning	Pass	Error	Warning	Pass	Not Run	Fail	Pass
Peridigm	0	0	1	1	1	0			
TrilinosIntel	0	1	1	0	1	0			
AlbanyIntel	0	0	1	0	0	1	0	1	347
IKTCismAlbany	0	1	1	0	1	0	0	0	5
IKTCismAlbanyEpetra	0	1	1	0	1	0	0	0	5
IKTAlbanyFunctorOpenMP	0	1	1	0	1	0	0	0	278
Trilinos	0	1	1	0	1	0			
TrilinosClang	0	1	1	0	1	0			
Albany64BitClang	0	0	1	0	1	0	0	1	166
IKTRideTrilinosCUDA	0	1	1	0	1	0			
IKTRideAlbanyCUDA	0	2	2	0	2	0	0	2	186
albany_cluster-toss3_skybridge-login5_serial-intel-release	0	1	1	0	0	1	0	1	288
Albany64Bit	0	0	1	0	1	0	0	1	317
IKTAlbany	0	1	1	0	1	0	0	0	372
IKTAlbanyNoEpetra	0	1	1	0	1	0	0	0	261
TrilinosDbg	0	1	1	0	1	0			
Albany64BitDbg	0	0	1	0	0	1	0	0	225
trilinos_cluster-toss3_skybridge-login5_serial-intel-release	0	1	1	0	1	0			
IKTMayerARMTrilinos	0	1	1	0	1	0			
IKTMayerARMAlbany	0	0	1	0	0	1	0	0	294
IKTWatermanTrilinosCUDA	0	1	1	0	1	0			
IKTWatermanAlbanyCUDA	0	1	1	0	1	0	0	0	94
IKTAlbanyFPECheckDbg	0	1	1	0	1	0	0	0	363

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albany_cluster-toss3_skybridge-login5_serial-intel-release	0	1	1	0	0	1			
Albany64Bit	0	0	1	0	1	0			
IKTAlbany	0	1	1	0	1	0			
IKTAlbanyNoEpetra	0	1	1	0	1	0			
TrilinosDbg	0	1	1	0	1	0			
Albany64BitDbg	0	0	1	0	0	1	0	0	225
trilinos_cluster-toss3_skybridge-login5_serial-intel-release	0	1	1	0	1	0			
IKTMayerARMTrilinos	0	1	1	0	1	0			
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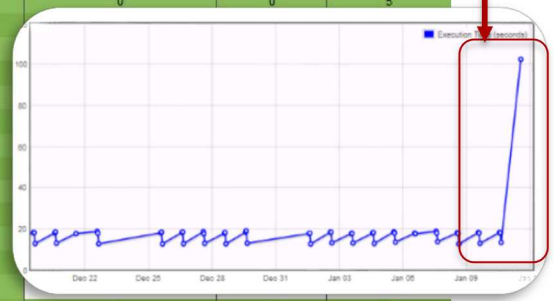
IKTWatermanTrilinosCUDA	0	1	1	0	1	0			
IKTWatermanAlbanyCUDA	0	1	1	0	1	0	0	0	94
IKTAlbanyFPECheckDbg	0	1	1	0	1	0	0	0	363

Slowdown identified by nightly CDash testing!



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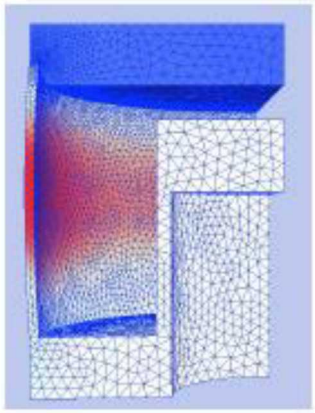
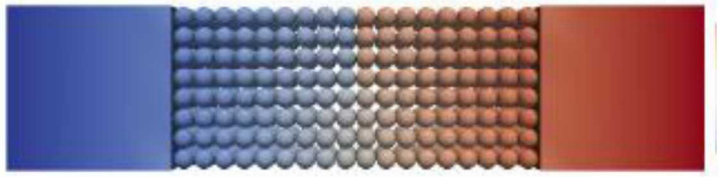
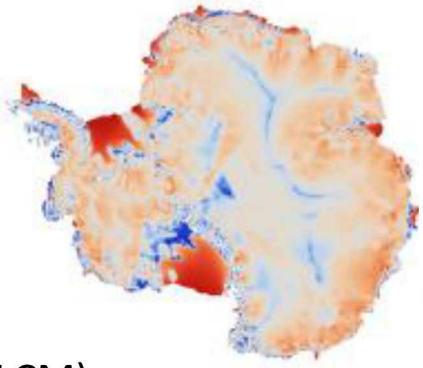
Applications hosted by Albany

Sandia National Laboratories







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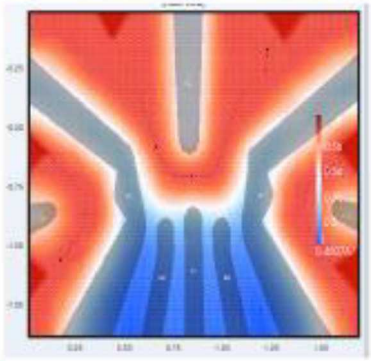
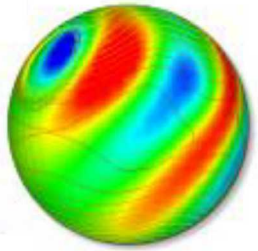
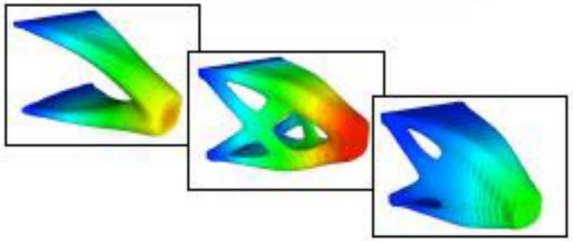
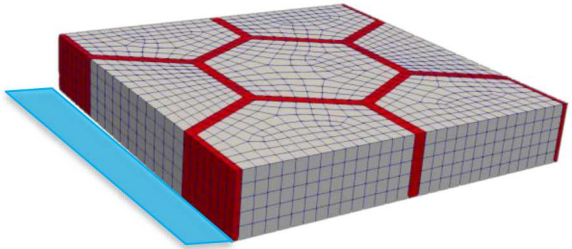




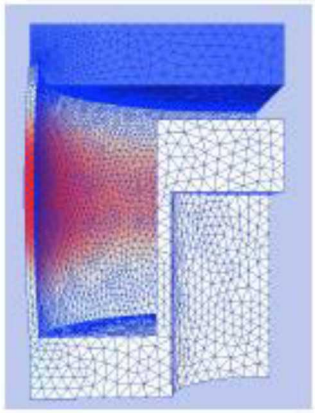


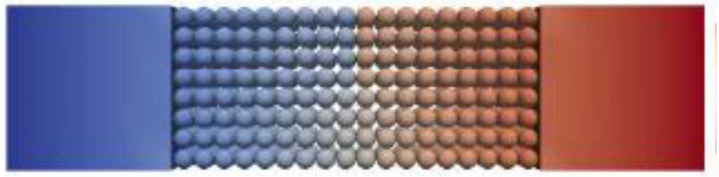


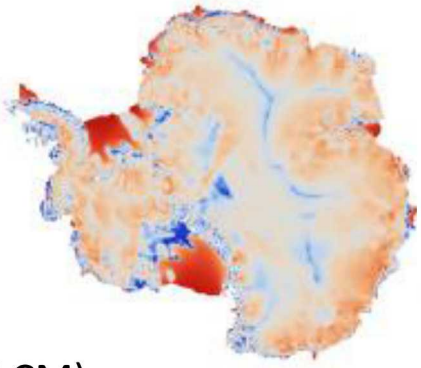
Blue: under active development

Applications hosted by Albany

Applications are "**born**" scalable, fast, robust, performance-portable, …!







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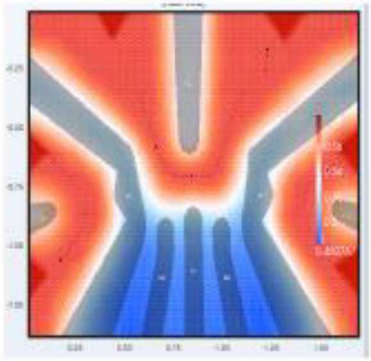

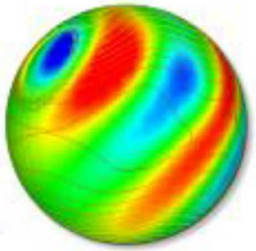

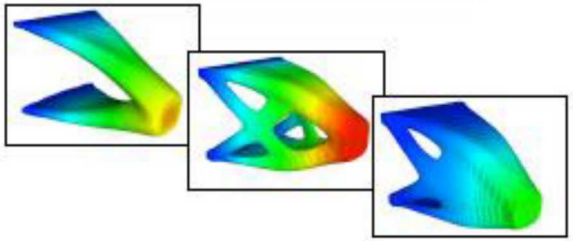

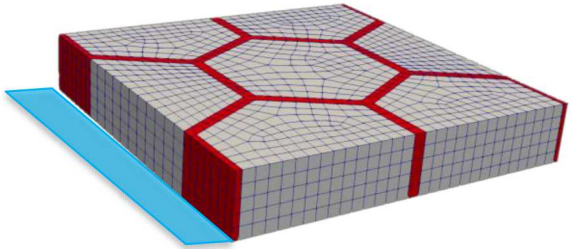

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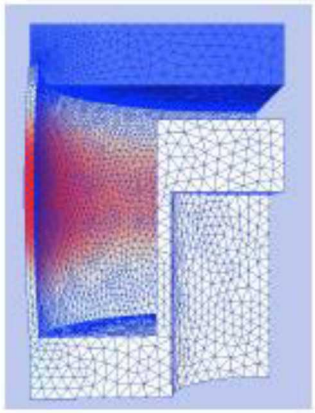

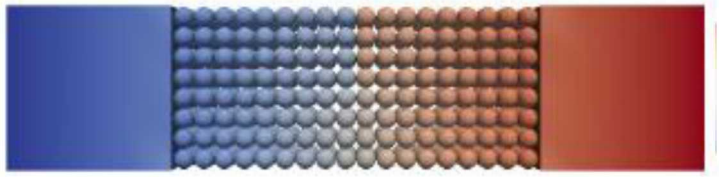

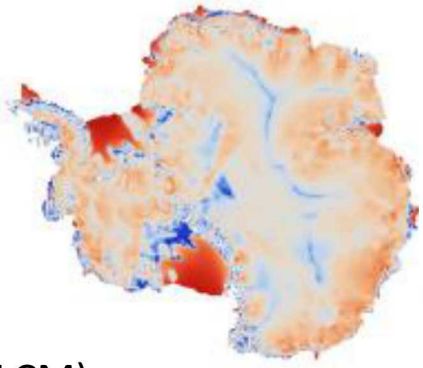

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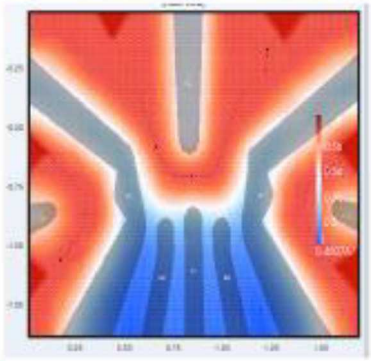

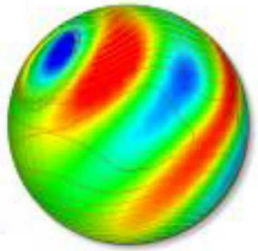

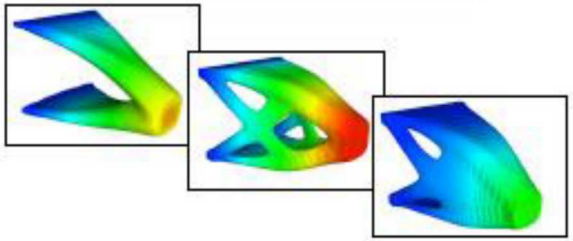

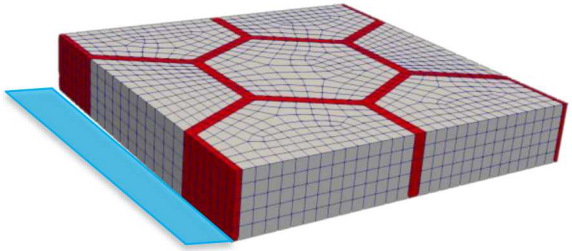

Blue: under active development

Algorithmic projects hosted by Albany

Sandia National Laboratories

Algorithms and **software** are **matured directly** on **applications.**

Algorithmic projects within Albany:

- Scalable multi-level solvers (PISCEES/ProSPect) – R. Tuminaro, I. Tezaur.
- Nonlinear solvers (FASTMath) – R. Pawlowski, M. Perego
- In-memory mesh adaptation (FASTMath) – M. Sheppard, M. Bloomfield (RPI), A. Oberai, J. Smith (USC), D. Ibanez, B. Granzow, G. Hansen
- Multi-scale coupling via Schwarz (P&EM) – A. Mota, I. Tezaur, C. Alleman, G. Phlipot (CalTech)
- Stabilized mechanics (FASTMath) – A. Bradley, J. Ostien, G. Hansen
- Adjoint-based inversion (FASTMath) – M. Perego, E. Phipps, ROL team
- Optimization-based coupling (ASCR) – M. Perego, M. D'Elia, D. Littlewood, P. Bochev
- UQ workflow (PISCEES) – J. Jakeman, I. Tezaur, M. Perego
- Embedded UQ (Equinox) – E. Phipps, J. Fike
- Performance portable FEM (PISCEES/ProSPect/ATDM) – I. Demeshko (LANL), E. Phipps, R. Pawlowski, E. Cyr, I. Tezaur, A. Bradley, J. Watkins
- Development of composite tet-10 for solid mechanics (PE&M) – J. Foulk, J. Ostien, A. Mota

Algorithmic projects hosted by Albany

Sandia National Laboratories

Algorithms and **software** are **matured directly** on **applications.**

Algorithmic projects within Albany:

- Scalable multi-level solvers (PISCEES/ProSPect) – R. Tuminaro, I. Tezaur.
- Nonlinear solvers (FASTMath) – R. Pawlowski, M. Perego
- **In-memory mesh adaptation** (FASTMath) – M. Sheppard, M. Bloomfield (RPI), A. Oberai, J. Smith (USC), D. Ibanez, B. Granzow, G. Hansen
- **Multi-scale coupling via Schwarz** (P&EM) – A. Mota, I. Tezaur, C. Alleman, G. Phlipot (CalTech)
- Stabilized mechanics (FASTMath) – A. Bradley, J. Ostien, G. Hansen
- **Adjoint-based inversion** (FASTMath) – M. Perego, E. Phipps, ROL team
- Optimization-based coupling (ASCR) – M. Perego, M. D'Elia, D. Littlewood, P. Bochev
- UQ workflow (PISCEES) – J. Jakeman, I. Tezaur, M. Perego
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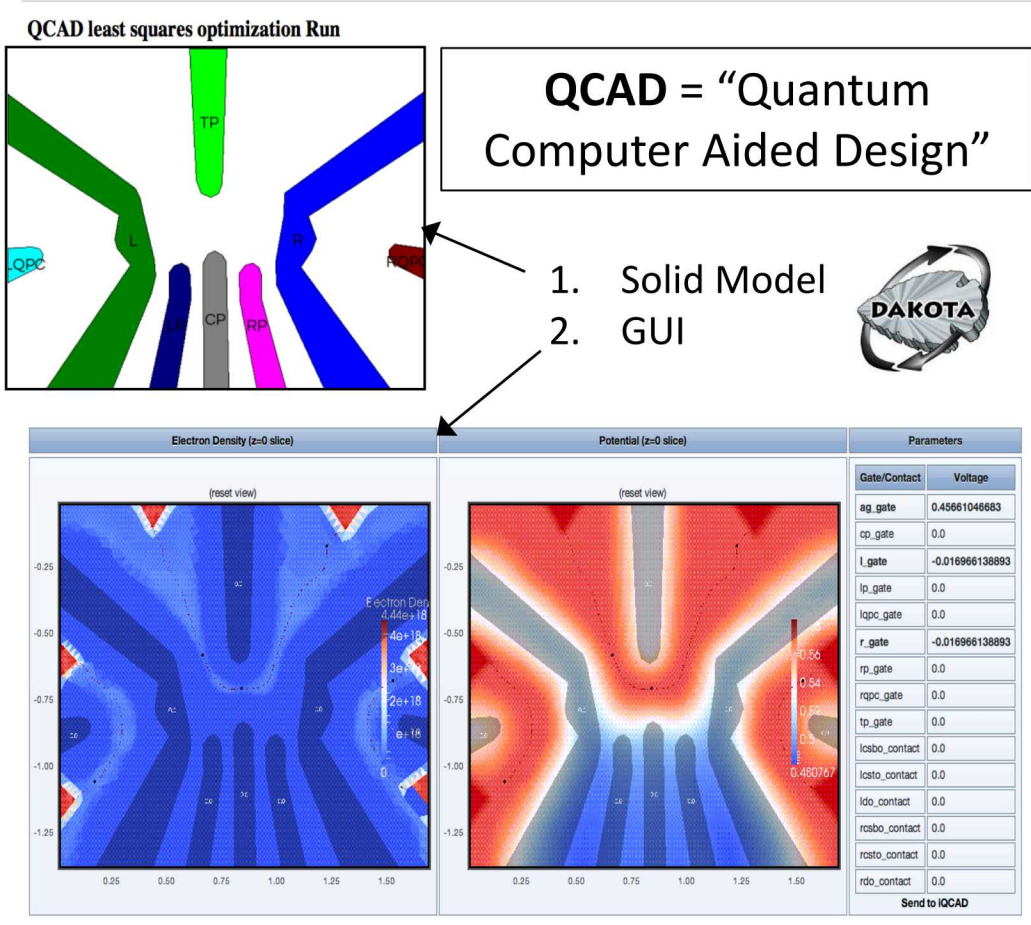
Quantum device modeling (QCAD)

Sandia National Laboratories

Albany enabled the rapid stand-up of a world-class **quantum device design tool.**

- **Application**: quantum computing
- **Objective:** simulation/optimization of semiconductor quantum double dots
  - ➢ Provide fast feedback on which device layouts are most likely to lead to **few-electron** behavior
- **Key to QCAD's success**: interfaces
  - ➢ Various **multi-physics couplings** of Poisson + Schrodinger
  - ➢ DAKOTA* for **optimization**.
- QCAD is used by experimentalist in Sandia's **world-class experimental facilities (CINT)** as design tool for quantum **device fabrication**
  - ➢ **iQCAD**: GUI for experimentalists



X. Gao, et al., J. Appl. Phys. 2013

Capacitances (in aF)

	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	0.0545326395725	3.3402953333

* https://dakota.sandia.gov

Ice sheets: Albany Land-Ice (ALI)

Sandia National Laboratories

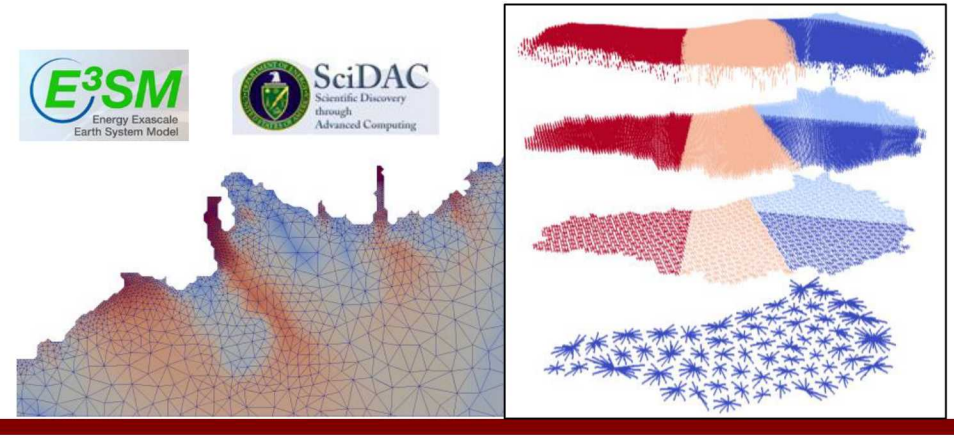
Albany enabled the **rapid development** of a production **land-ice dycore** for providing **actionable predictions** of **21st century sea-level rise** as a part of the DOE Energy Exascale Earth System Model (E3SM).

Capabilities:

- ***Unstructured grid*** finite elements.
- ***Scalable, fast*** and ***robust***
- ***Verified*** and ***validated.***
- ***Advanced analysis***: inversion, UQ.
- ***Portable*** to new/emerging architecture machines (multi-core, many-core, GPU)
- ***Multi-physics:*** velocity-temperature, velocity-thickness, velocity-hydrology.

E3SM Energy Exascale Earth System Model

SciDAC Scientific Discovery through Advanced Computing



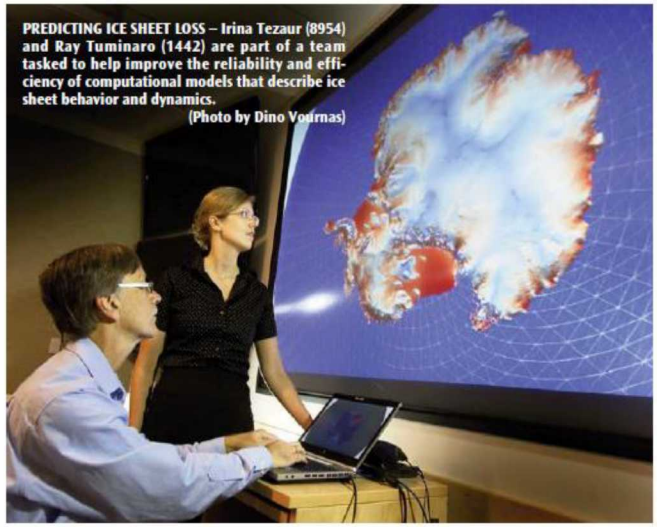
MS121: Theoretical & Computational Advancements in Ice Sheet Modeling (Tues. Feb. 26)

Ice sheet modeling of Greenland, Antarctica helps predict sea-level rise

Michael Padilla

The Greenland and Antarctic ice sheets will make a dominant contribution to 21st century sea-level rise if current climate trends continue. However, predicting the expected loss of ice sheet mass is difficult due to the complexity of modeling ice sheet behavior.

Computing (SciDAC) program. PISCEES is a multi-lab, multi-university endeavor that includes researchers from Sandia, Los Alamos, Lawrence Berkeley, and Oak Ridge national laboratories; the Massachusetts Institute of Technology; Florida State University; the University of Bristol; the University of Texas Austin; the University of South Carolina; and New York University.



PREDICTING ICE SHEET LOSS – Irina Tezaur (8954) and Ray Tuminaro (1442) are part of a team tasked to help improve the reliability and efficiency of computational models that describe ice sheet behavior and dynamics. (Photo by Dino Vournas)

Sandia's biggest contribution to PISCEES has been an analysis tool: a land-ice solver called Albany/FELIX (Finite Elements for Land Ice eXperiments). The tool is based on equations that simulate ice flow over the Greenland and Antarctic ice sheets and is being coupled to Earth models through the Accelerated Climate for Energy (ACME) project.

"One of the goals of PISCEES is to create a land-ice solver that is scalable, fast, and robust on continental scales," says computational scientist Irina Tezaur, a lead developer of Albany/FELIX. Not only did the new solver need to be reliable and efficient, but it was critical that the team develop a solver capable of running on new and emerging computers, and equipped with advanced

I. Tezaur, *et. al. GMD.* (2015).

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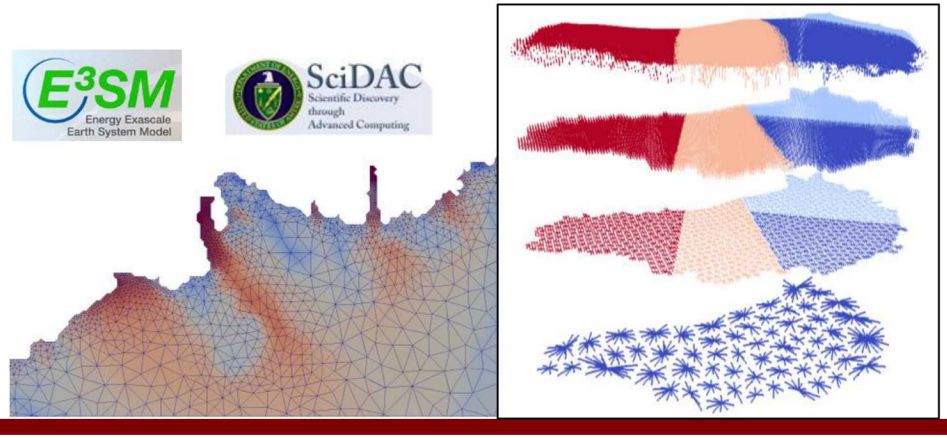

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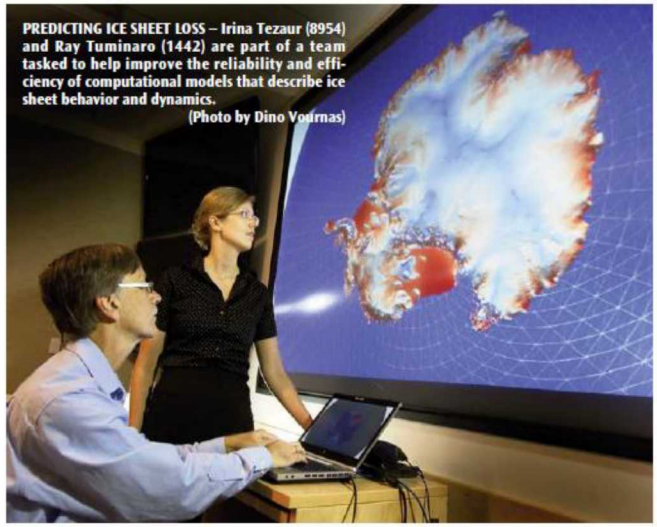

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Adjoint-based optimization/inversion

Sandia National Laboratories

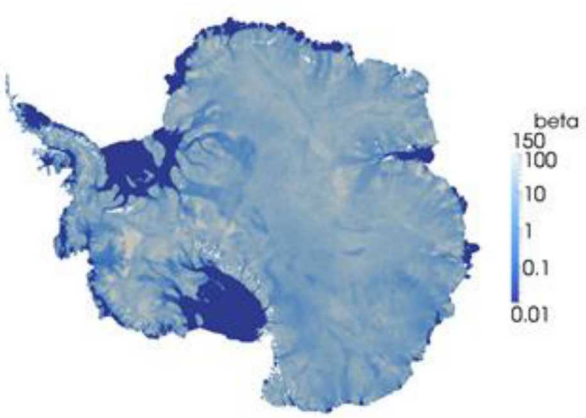
AD & TBGP in Albany enabled the efficient solution of **adjoint-based PDE-constrained optimization/inversion** problems.

Find p that minimizes	$g(u,p)$	
subject to	$f(u,p)=0$	$\leftarrow$ PDE

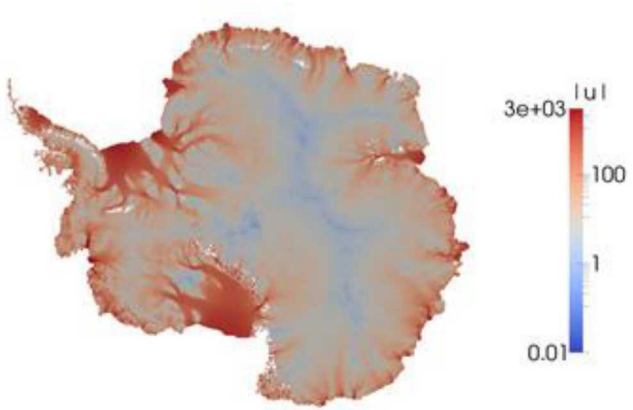
Inversion problem solved robustly for ***O*(100K) parameters**!

Application: inversion for basal friction and ice thickness in Albany Land-Ice model to initialize dynamic simulation.

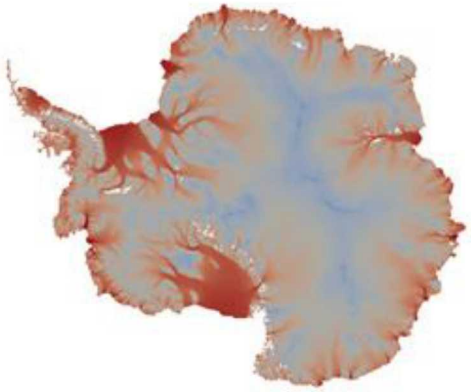
- Inversion approach **significantly reduces non-physical transients**.



β (kPa y/m) obtained through inversion



$|\boldsymbol{u}|$ (m/yr) computed with estimated β

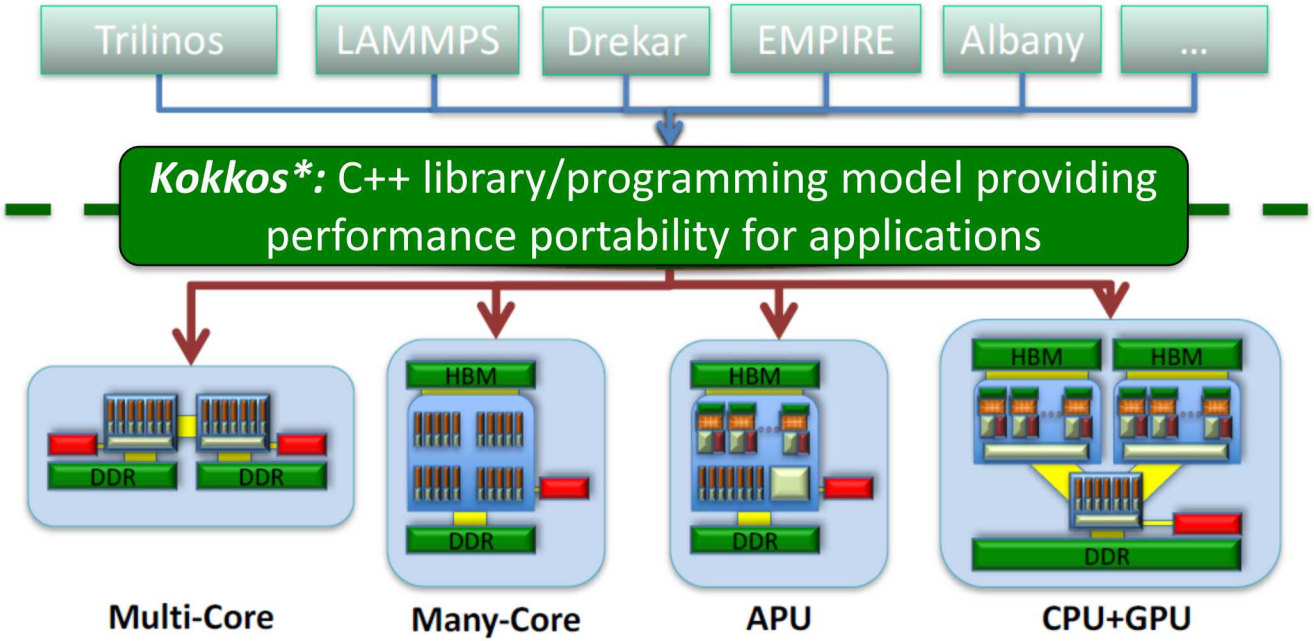


$|\boldsymbol{u}|$ (m/yr) for observed surface velocity

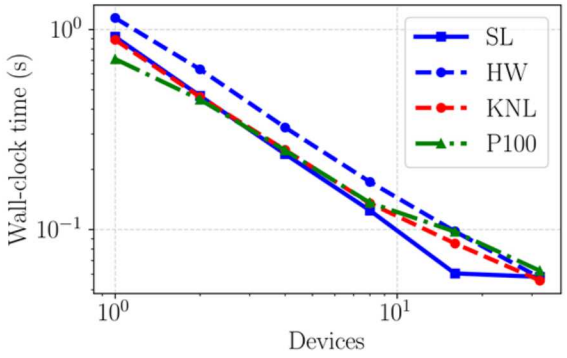
Performance-portable FEM

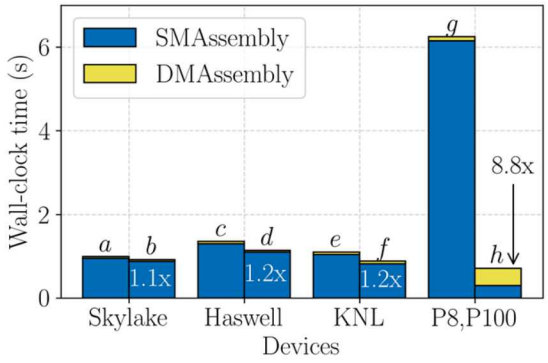
Talk by J. Watkins,
MS 121, Tues. Feb. 26

Sandia National Laboratories



- Provides ***automatic access*** to OpenMP, CUDA, etc.
- Abstracts ***data layouts*** for optimal performance





* **Kokkos github repo:** https://github.com/kokkos/Kokkos I. Demeshko *et. al.*, 2018.

Performance-portable FEM

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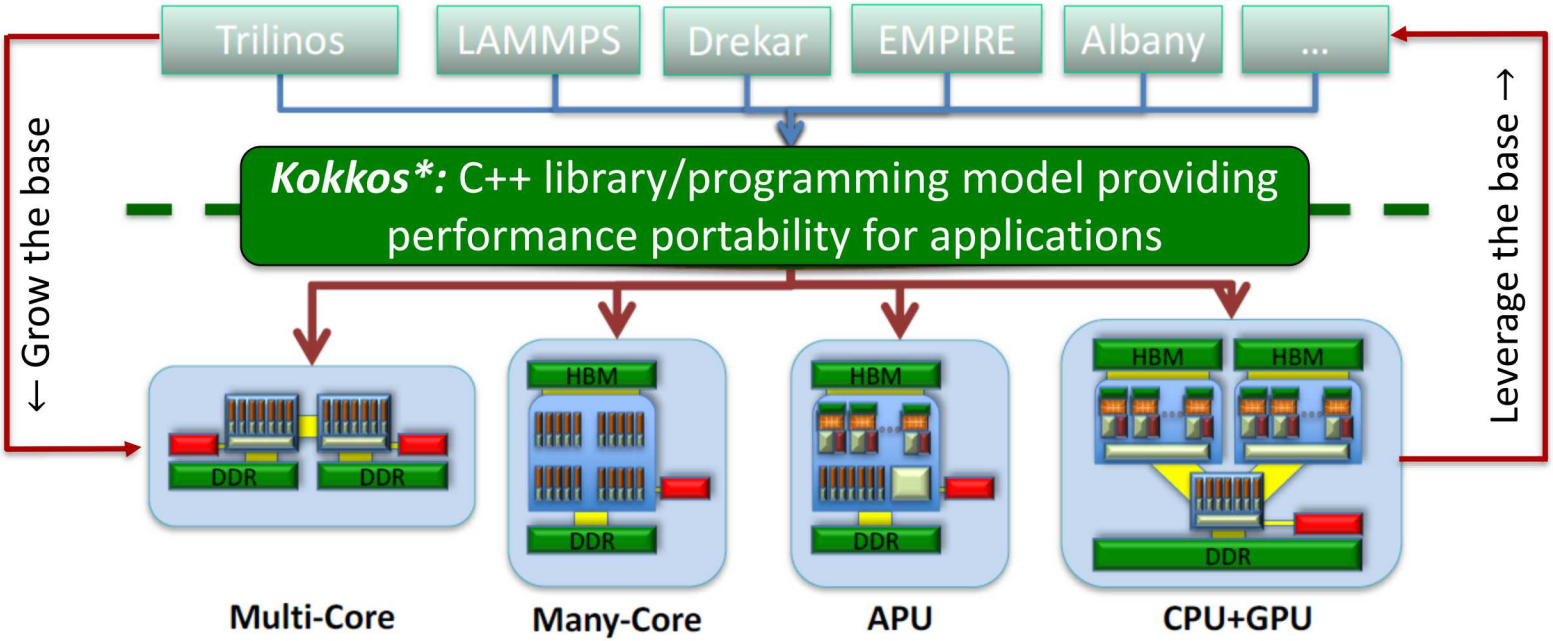
Sandia National Laboratories

Performance-portability of Albany FEA achieved using ***Kokkos;***
Albany usage has in turn led to ***Kokkos improvements***



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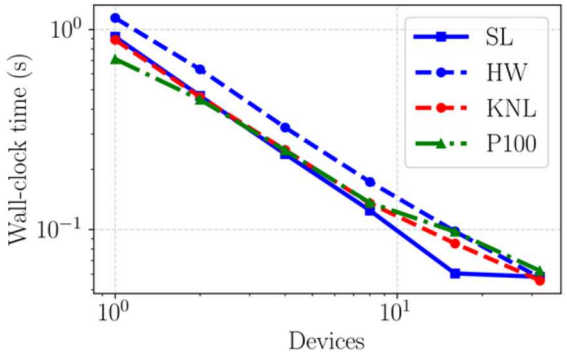

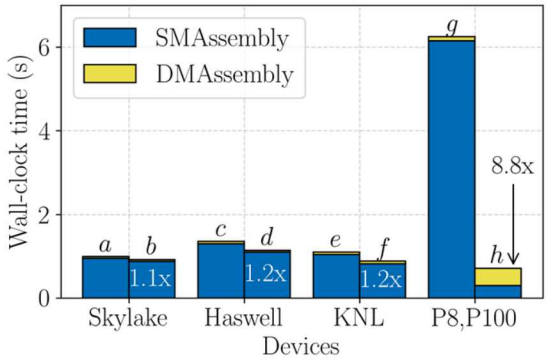

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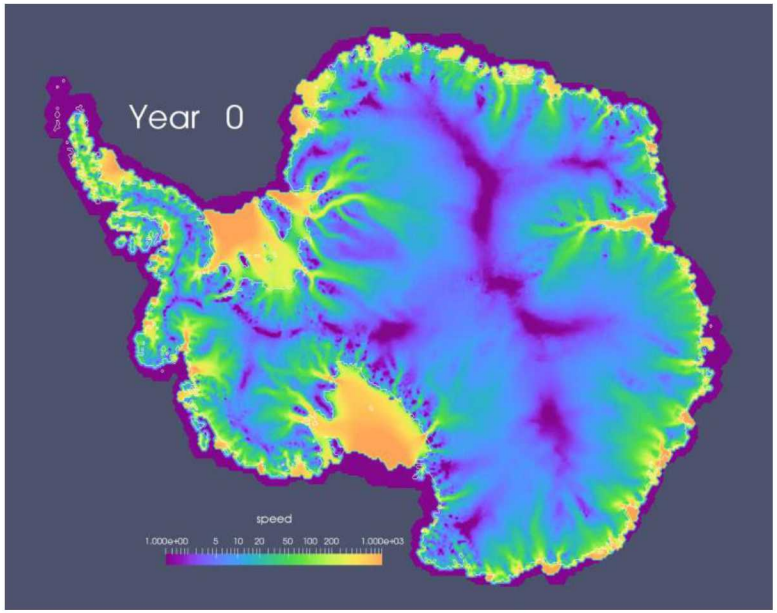
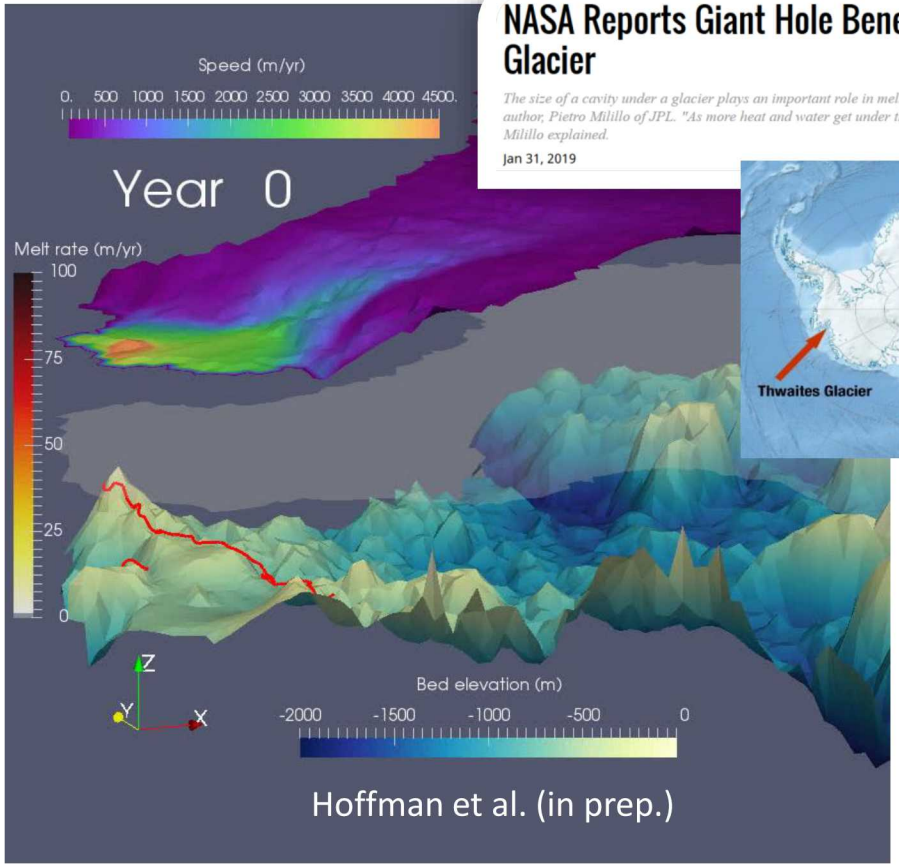




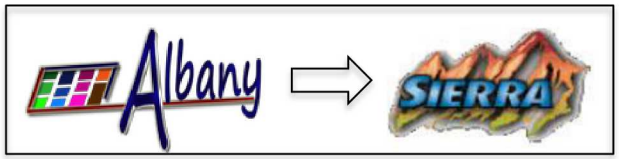
Above: ABUMIP-Antarctica experiment

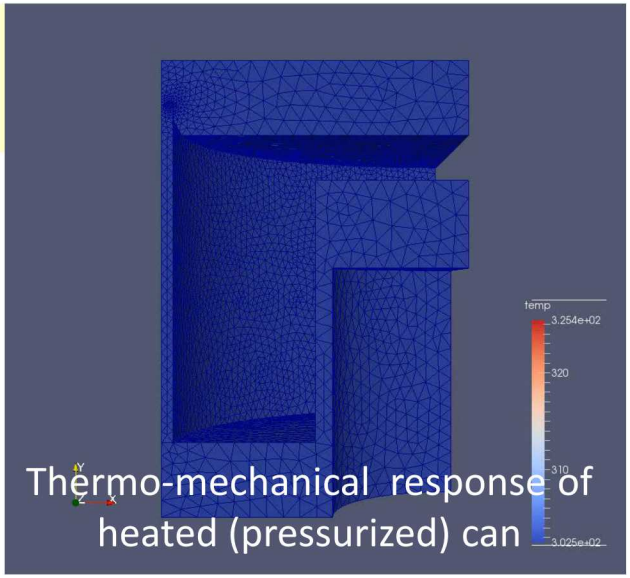
Right: Thwaites glacier retreat under parametrized submarine melting.

Laboratory for computational mechanics (LCM)

Sandia National Laboratories

The Albany LCM suite contains sophisticated **material models**, **physics** and **technologies** for solid mechanics.

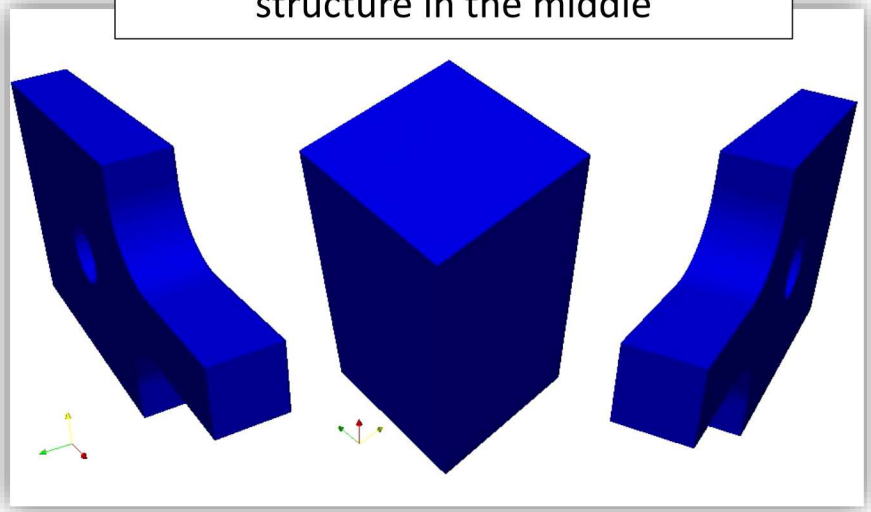




Thermo-mechanical response of heated (pressurized) can

- **Models**: elasticity, Neohookean, J_2 plasticity, crystal plasticity, creep, elasto-visco-plastic, …
- **Physics (PDEs)**: mechanics, electro-mechanics, thermo-mechanics, unsaturated poro-elasticity, thermo-poro-mechanics, …
- **Fracture** and **damage** simulation capabilities
- "**Sand-box**" for new algorithms/methods:
  - Composite 10-node tetrahedron
  - Pressure projection stabilization
  - Multi-scale coupling via Schwarz
  - In-memory mesh adaptation

Tensile specimen with micro-structure in the middle



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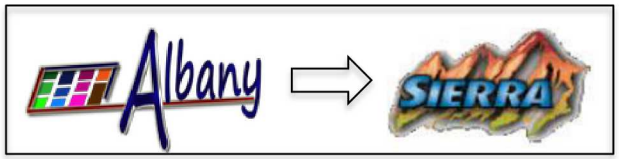

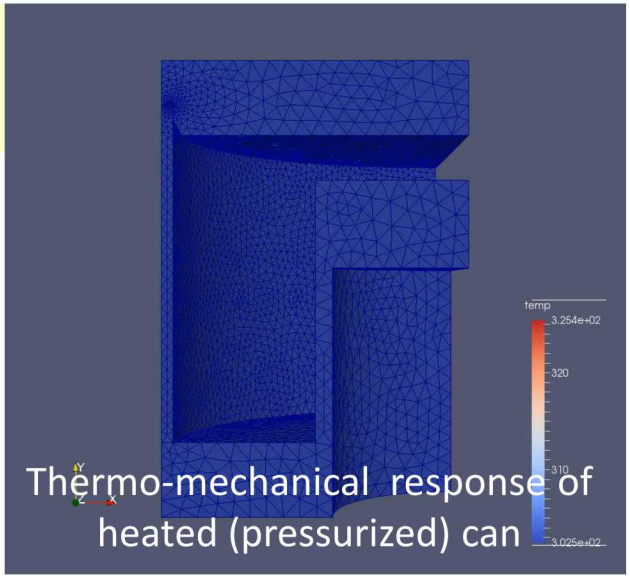

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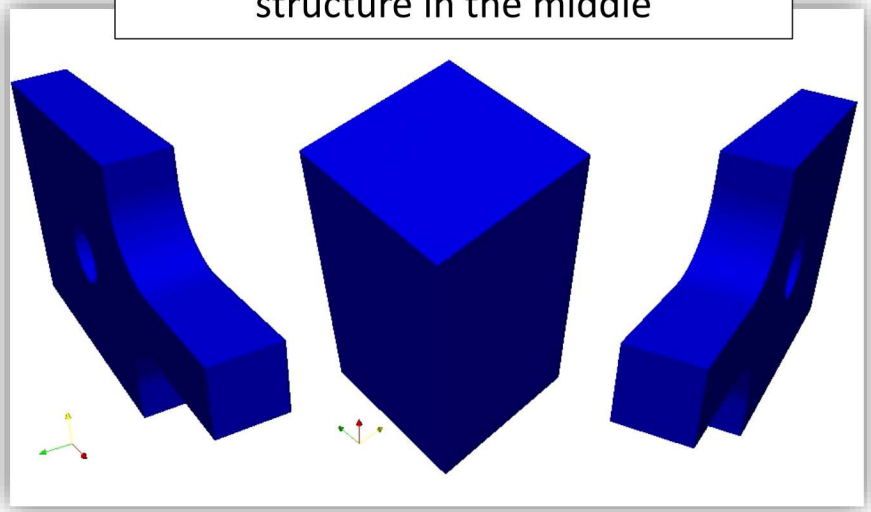
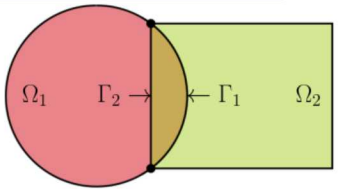
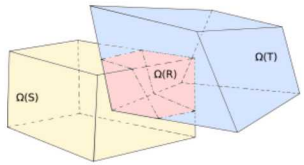


Multi-scale coupling via Schwarz

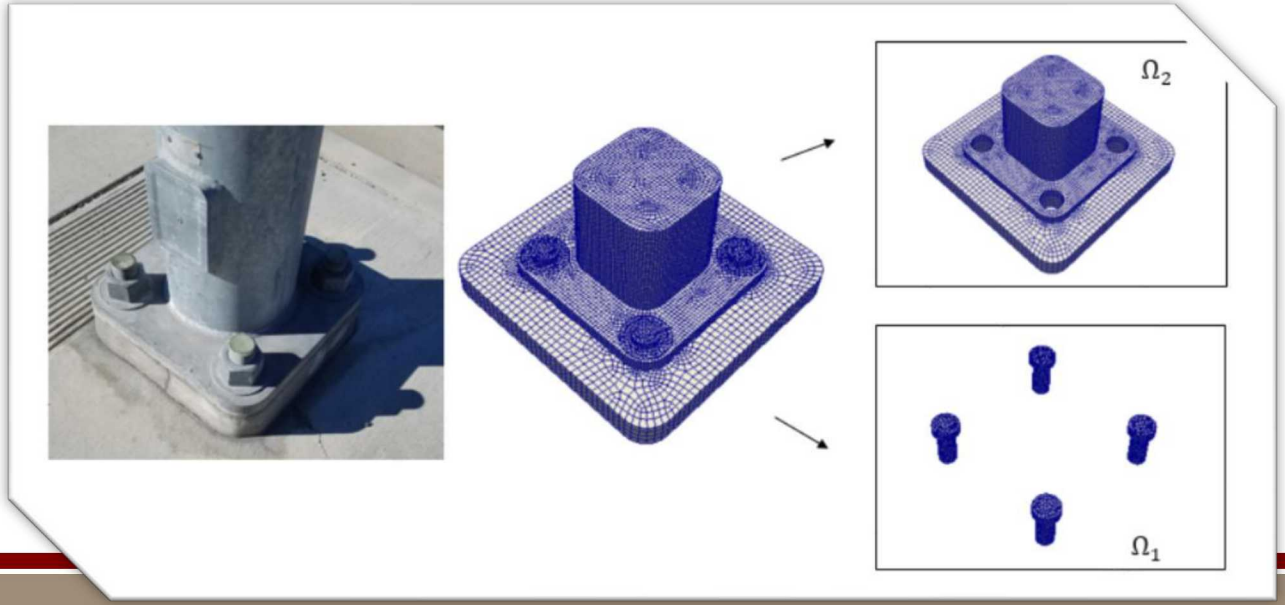
A **domain decomposition alternating-Schwarz**-based method has been developed in Albany for **concurrent multi-scale coupling** in solid mechanics.

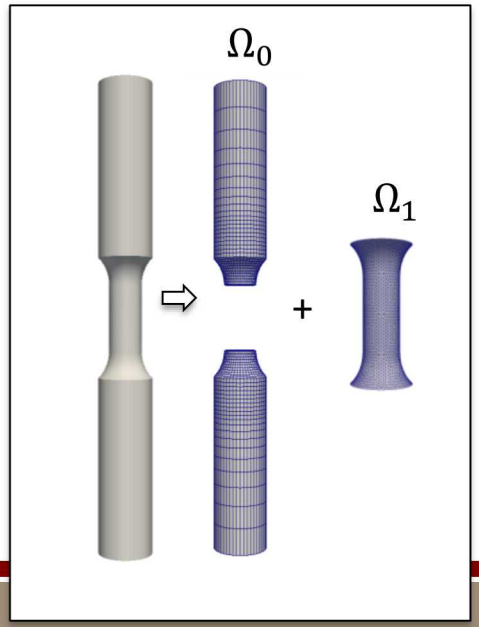
- **Crux of Method:** use solutions in simple domains to iteratively build a solution for the more complex domain.
- **Targeted application**: failure of **bolted components**.
- **"Plug-and-play" framework**: simplifies meshing complex geometries!
  - Couple regions with **different non-conformal meshes**, **element types, levels of refinement, solvers/time-integrators.**





https://github.com/ORNL-CEES/DataTransferKit





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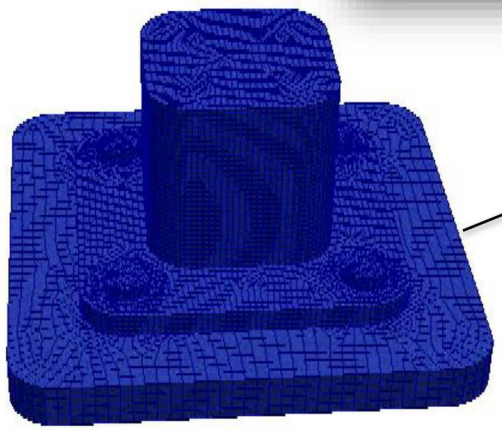
See talk by A. Mota: MS 350, Fri. Mar. 1, 10:10-10:30AM, Room 302B

Single domain



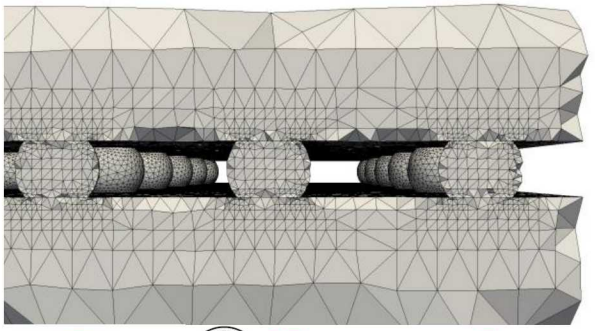
Schwarz coupling of hex (parts) + composite tet 10 (bolts) elements (J_2 material model from LCM suite)

Future work: extend method for **multi-physics** coupling

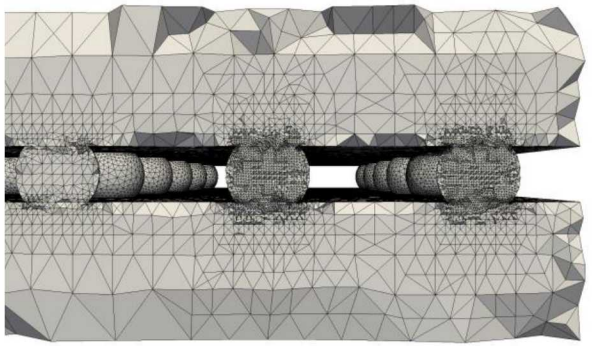
A. Mota *et. al.* "The Schwarz alternating method in solid mechanics", *CMAME.* 319 (2017), 19-51.

In-memory mesh adaptation

Collaboration with **SCOREC***: development of **mesh adaptation** capabilities in Albany to enable **multi-scale/multi-physics adaptive simulation**



SCOREC Rensselaer

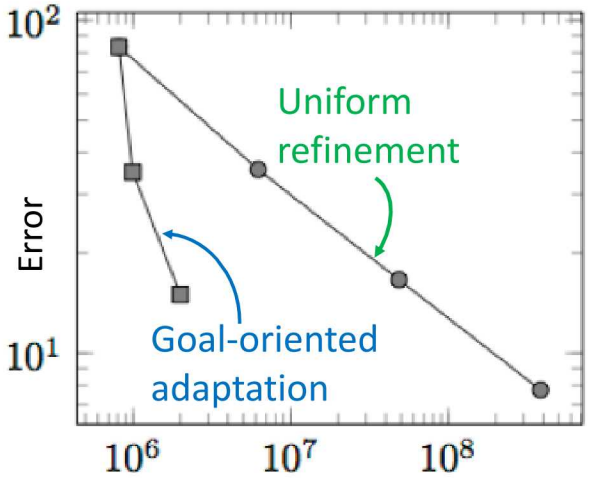


PAALS (Parallel Albany Adaptive Loop with SCOREC)

- Fully-coupled ***in-memory adaptation, solution transfer***.
- ***Parallel mesh infrastructure*** and services via ***PUMI***.
- ***Dynamic load balancing*** (ParMetis/Zoltan, ParMA).
- Automated ***parallel goal-oriented adaptive simulation***
  - Use **adjoint solution** to drive mesh adaptation
  - ~100× DoF-efficiency observed
  - Scaling out to at least 8K MPI ranks
- ***Performance portability*** to GPUs via ***Kokkos***.
- ***Applications:*** 3D manufacturing, creep/plasticity in large solder joint arrays, coupled dislocation dynamics (Albany + ParaDis), …

PUMI
Parallel Unstructured Mesh Infrastructure

Error in von Mises stress



* Scientific Computation Research Center at RPI (Mark Shephard *et al.*)

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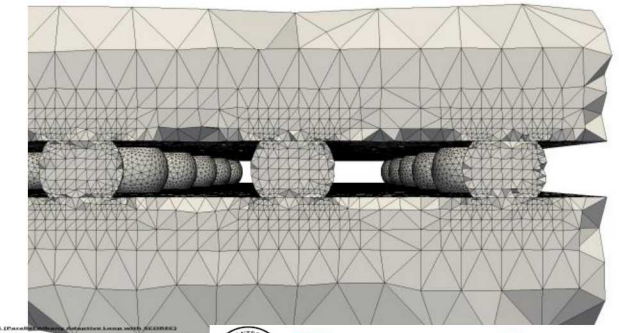
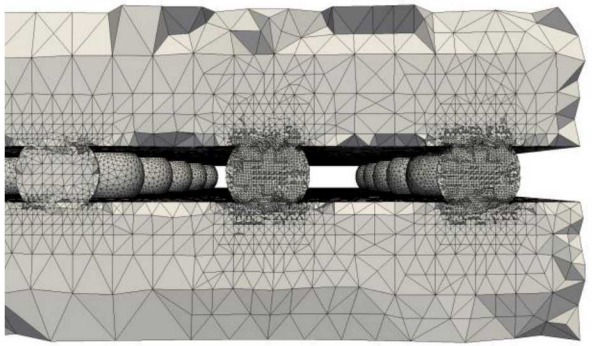


Rensselaer



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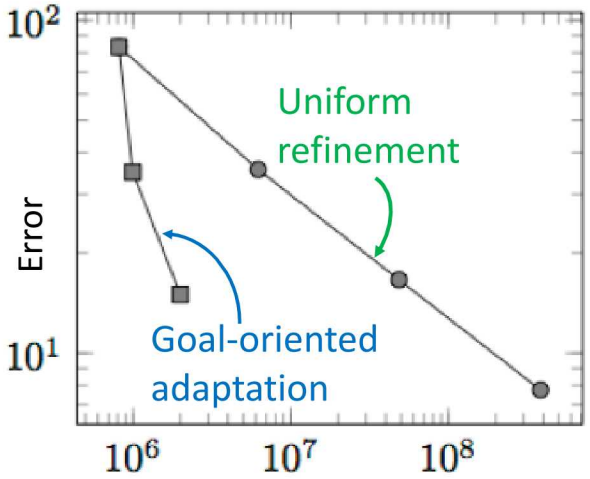
Parallel Unstructured Mesh Infrastructure

Error in von Mises stress

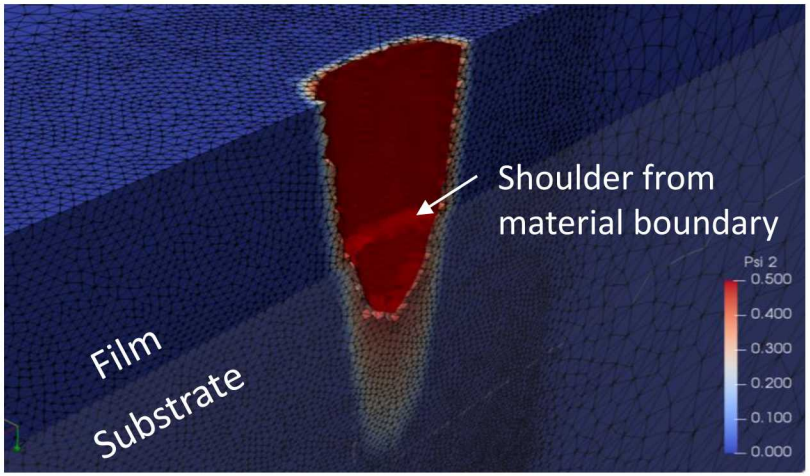


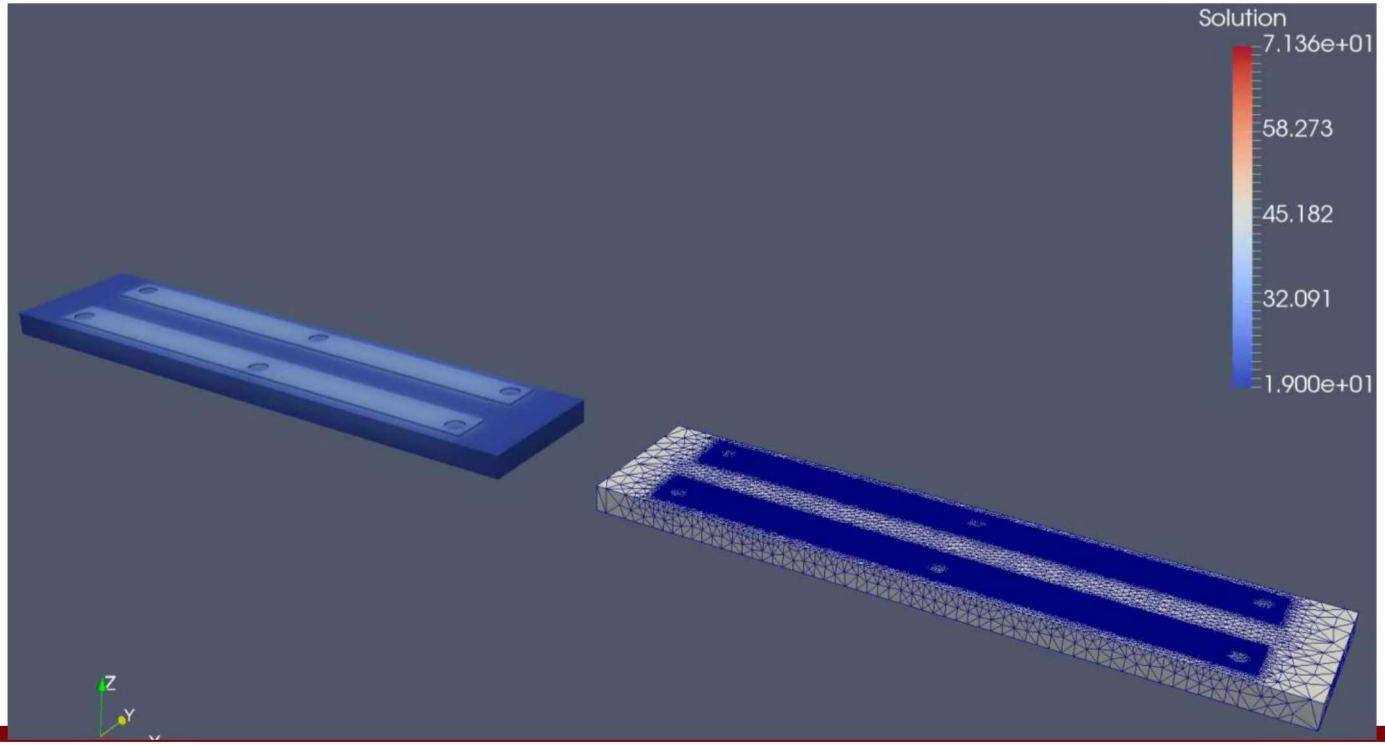
* Scientific Computation Research Center at RPI (Mark Shephard *et al.*)

3D manufacturing

- **Additive** & **subtractive** capabilities
- Employs **advanced adaptive meshing** and **evolving geometries**
- Coupling with **feedback control**

Right: simulation of subtractive manufacturing with picosecond laser*





Left: Additive manufacturing simulation showing temperature in evolving geometry

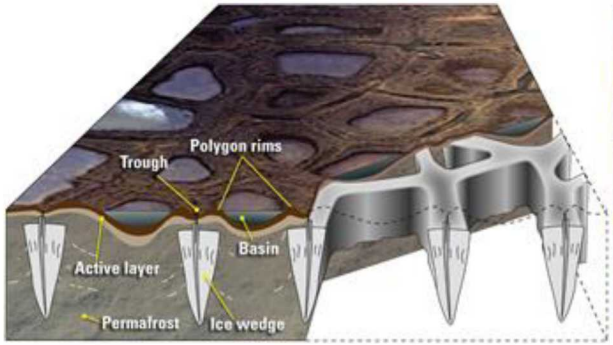
* Maniatty, et al., *Comp. Mech.*, 62:273, 2018.

Arctic Coastal Erosion (ACE)

Mechanistic modeling within Albany is **advancing state-of-the-art coastal erosion/permafrost modeling**.

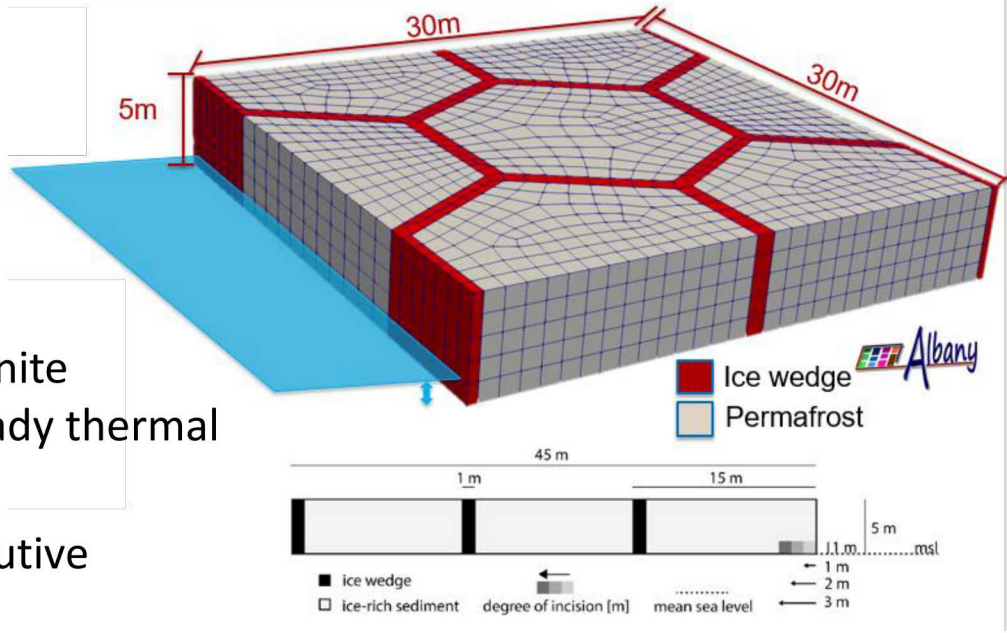
Permafrost modeling background:

- Predominant geomorphology is **ice-wedge polygons** (right).
- **State-of-the-art erosion modeling**: trend projection, empirical relation-ships, 1D steady-state heat flow, …



Albany modeling of degradation:

- **Leverages** years of LCM R&D.
- **Time-varying input variables** over the duration of a storm (water level, temperature, salinity)
- **Multi-physics FEM model of coastline**: finite deformation plasticity model + 3D unsteady thermal flow + chemical characteristics
  - **Failure modes** develop from constitutive relationships (**no empirical model**!)



Coupling with other codes

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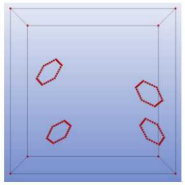
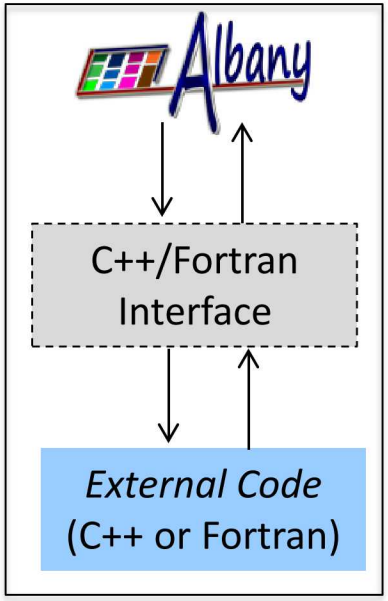
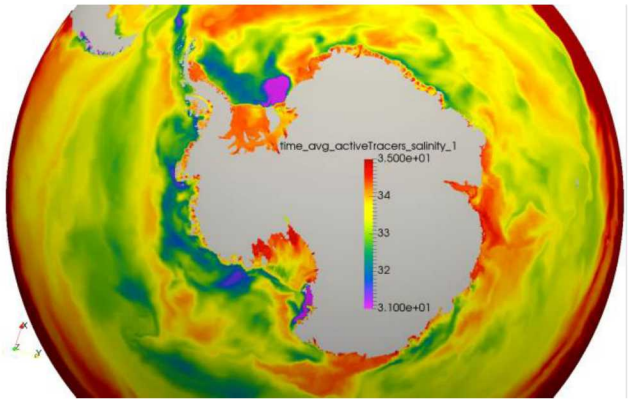
Albany has been **interfaced/coupled** with a number of other codes.

- ***Albany-Peridigm:*** local-nonlocal coupling of continuum mechanics + peridynamics
- ***Albany-ParaDis:*** coupled dislocation dynamics.
- ***Albany-PLATO***: Advanced Topology Optimization (ATO)
- ***MPAS-Albany-Land-Ice (MALI)***: ice sheets/coupling to E3SM
- ***CISM-Albany-Land-Ice (CALI)***: ice sheets/coupling to CESM
- ***Albany-PFLOTRAN (Albotran)***: coupled geomechanics problems

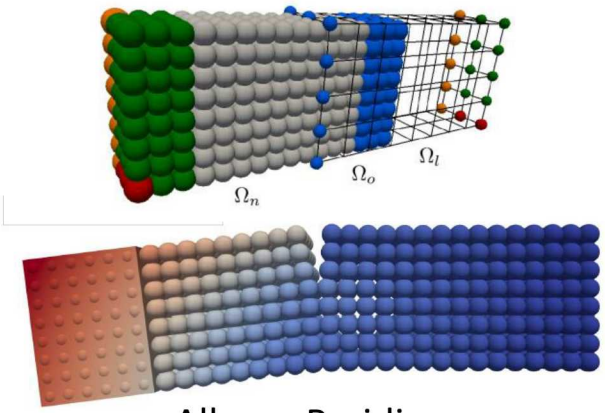


Albany-ParaDis

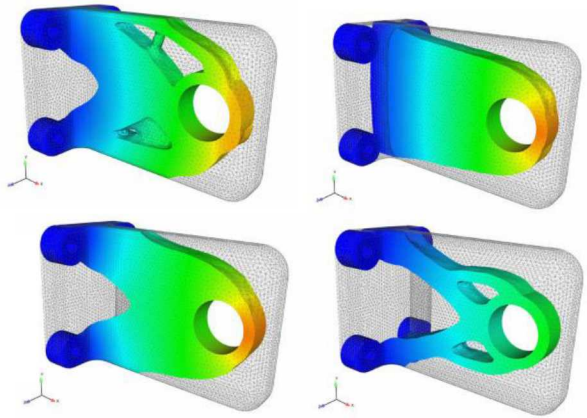




MPAS-Albany (MALI)



Albany-Peridigm



Albany-PLATO (ATO)

Work in progress

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Performance portability:

- **Code optimizations** for finite element assembly
- Performance portable **solvers** [WIP by Trilinos team]

Infrastructure work:

- Refactor of code to use **block data structures** to facilitate **multi-physics** coupling
  - "**Plug-and-play**" different PDEs within Albany
  - Ability to use **block preconditioners** (Teko*)

- Add support for **mixed finite elements**
  - Can be accomplished via incorporation of **Panzer** and **DOFManager.**

Application-driven development:

- Modeling of structural components in **hypersonic vehicles** with large mechanical and thermal loads (USC).
- Seeking funding for developing **solid-mechanics-based ice fracture/calving models** for improved ice sheet models.
- ***Much more…!***

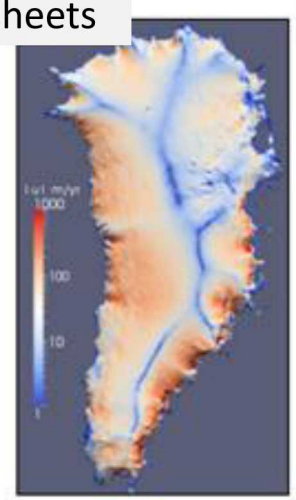
* E. Cyr *et. al.* SIAM J. Sci. Comput. 2016.

Summary

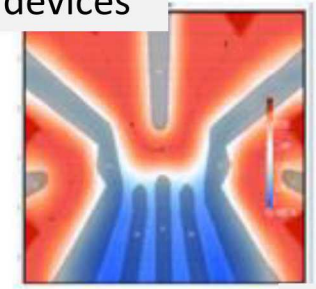
Sandia National Laboratories

Albany: open-source, parallel, C++, unstructured-grid, mostly-implicit multi-physics finite element code that demonstrates **AgileComponents** vision and can enable **rapid development** of new physics/algorithms.

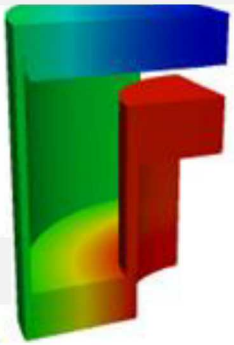
Ice sheets



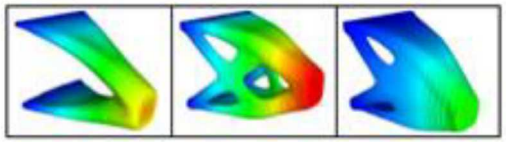
Quantum devices



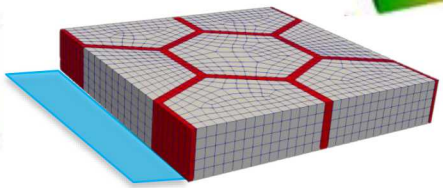
Computational mechanics



Additive manufacturing



Arctic costal erosion



Albany

Trilinos

Github: https://github.com/SNLComputation/Albany

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Albany User Meeting (AUM): every ~2 years (TBD)

Summary

Thank you! Questions?

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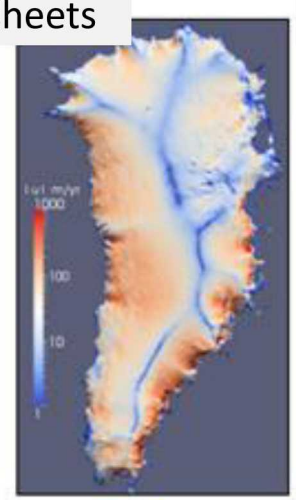
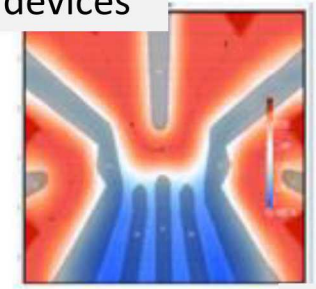
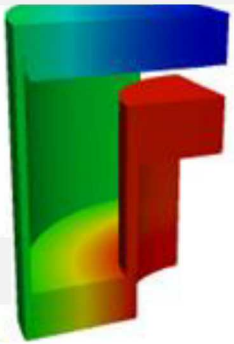


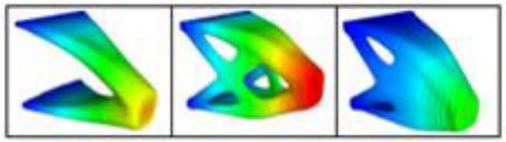
Quantum devices



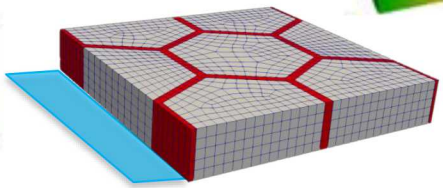
Computational mechanics



Additive manufacturing



Arctic costal erosion



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Backup Slides

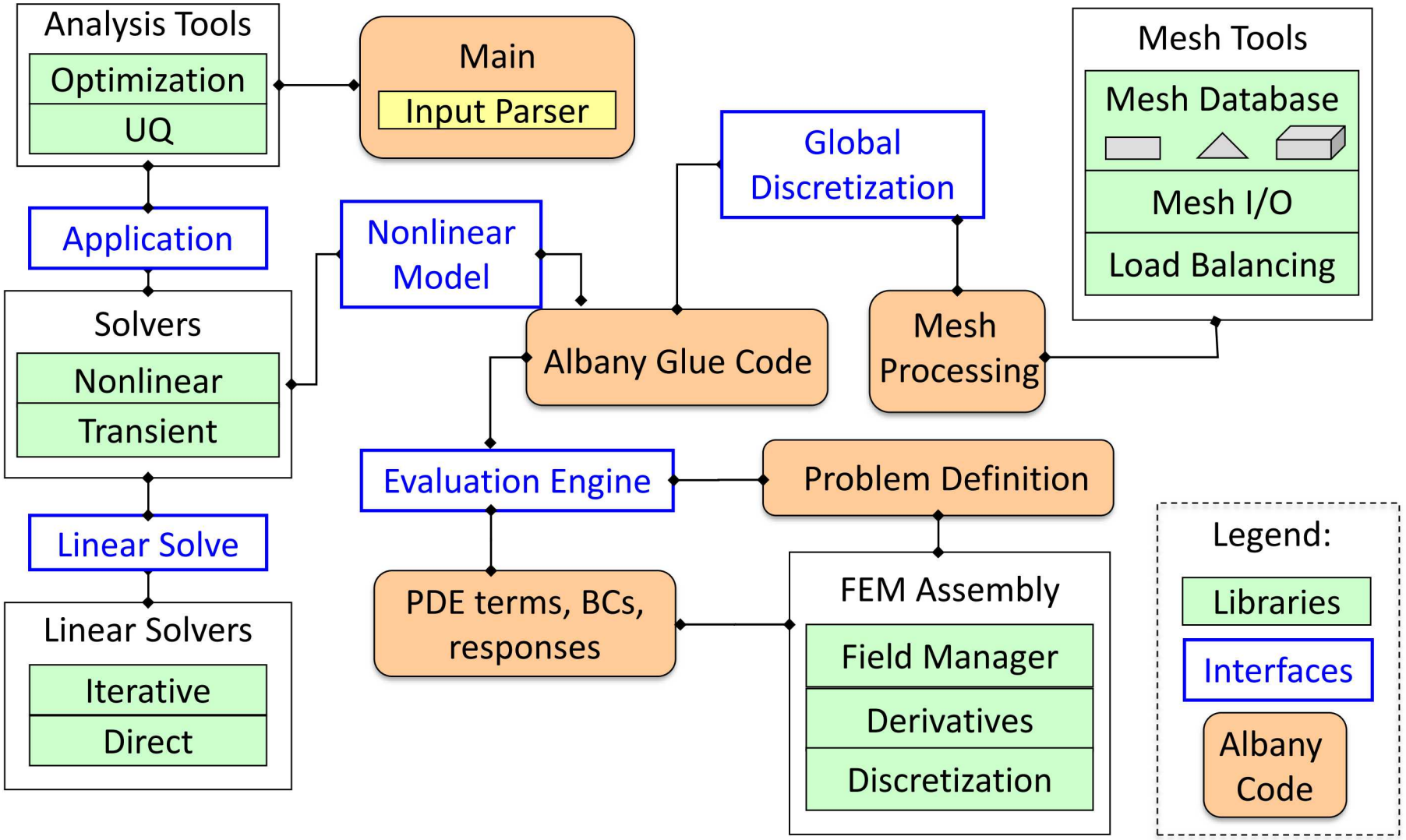
: a component-based finite element code

2008

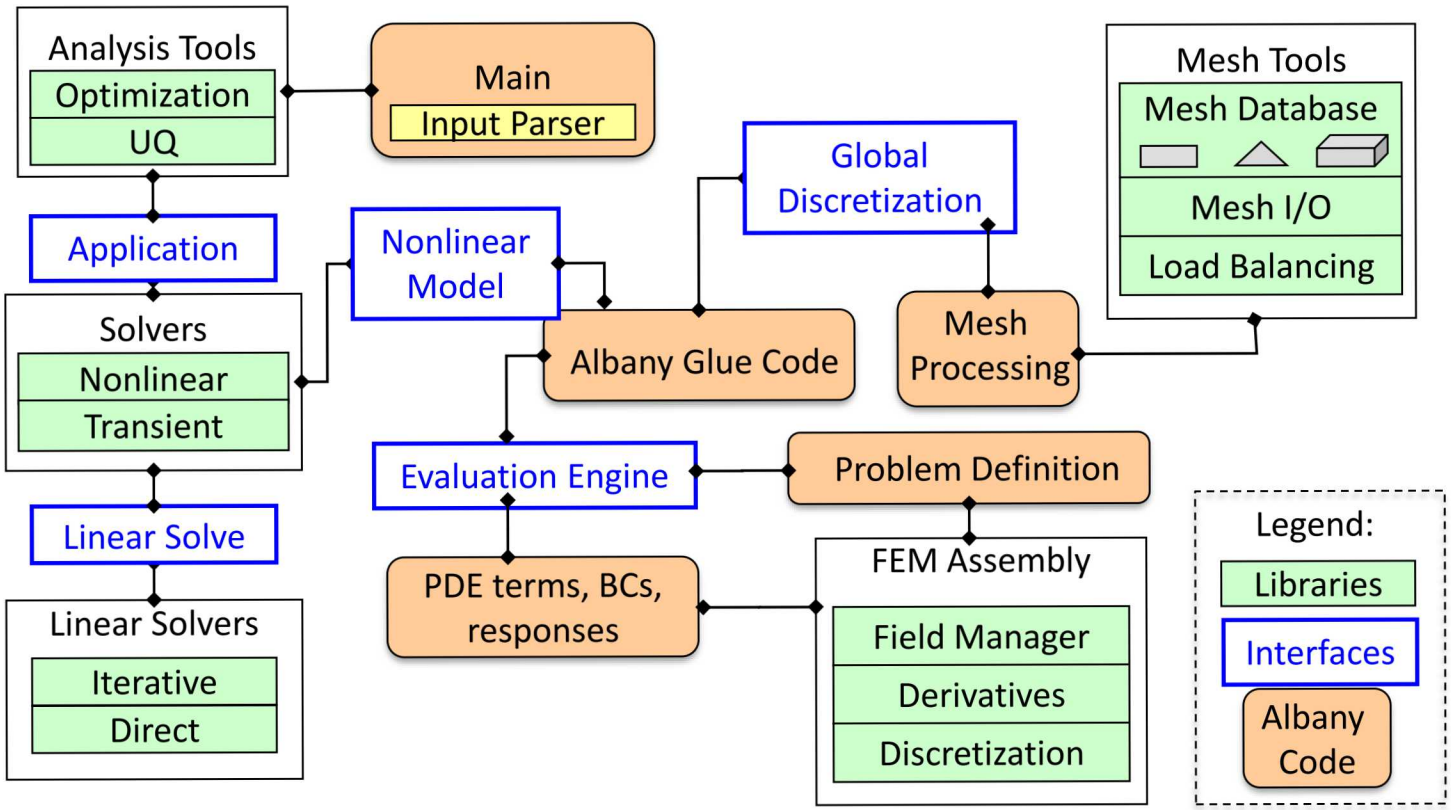
- Started by A. Salinger in 2008 as **first DemoApp** for AgileComponents code development strategy.
- During **next 10 years**, Albany became:
  - a friendly **early adopter** of cutting-edge technology from Trilinos, SCOREC, SierraToolKit, DAKOTA, FASTMath, QUEST, Kitware.
  - a model for a **Trilinos-based** and **Office of Science** application.
  - a demonstration of **transformational analysis** spanning template-based generic programming to optimization and UQ
- **11 years later**, Albany is:
  - an open-source parallel, mostly-implicit **unstructured-grid multi-physics finite element code** that demonstrates the AgileComponents vision by using, maturing, and spinning-off reusable libraries/abstract interfaces.
  - an **attractive environment** for the development of open-source application codes and research.
  - a Meso-App for maturation of **MPI+X programming model** for next generation architecture
  - the code base underlying a number of **research projects** and **applications**.

2019

Albany code design

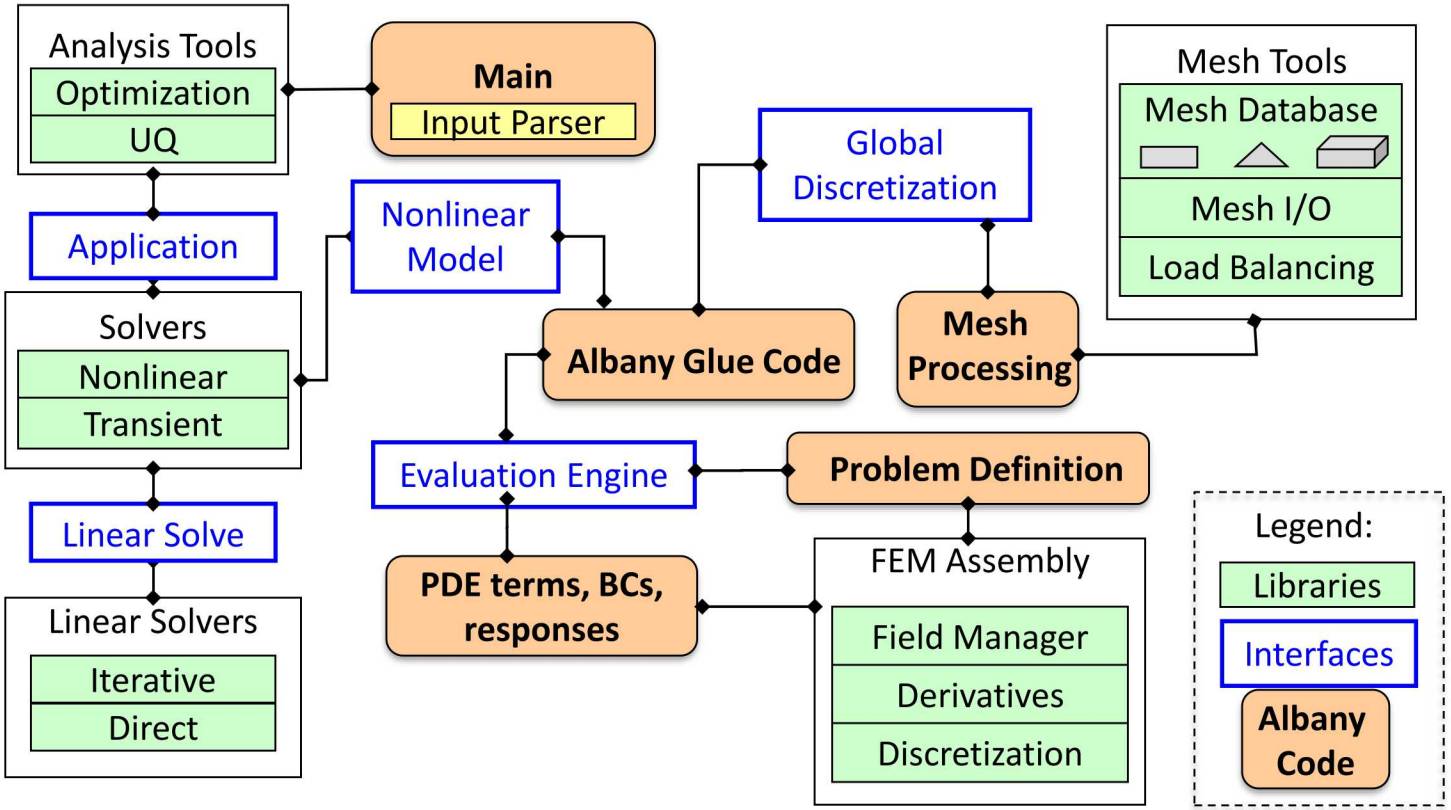


Albany code design



Albany “glue code”

“Glue Code”: driver code integrating components + providing overall capabilities



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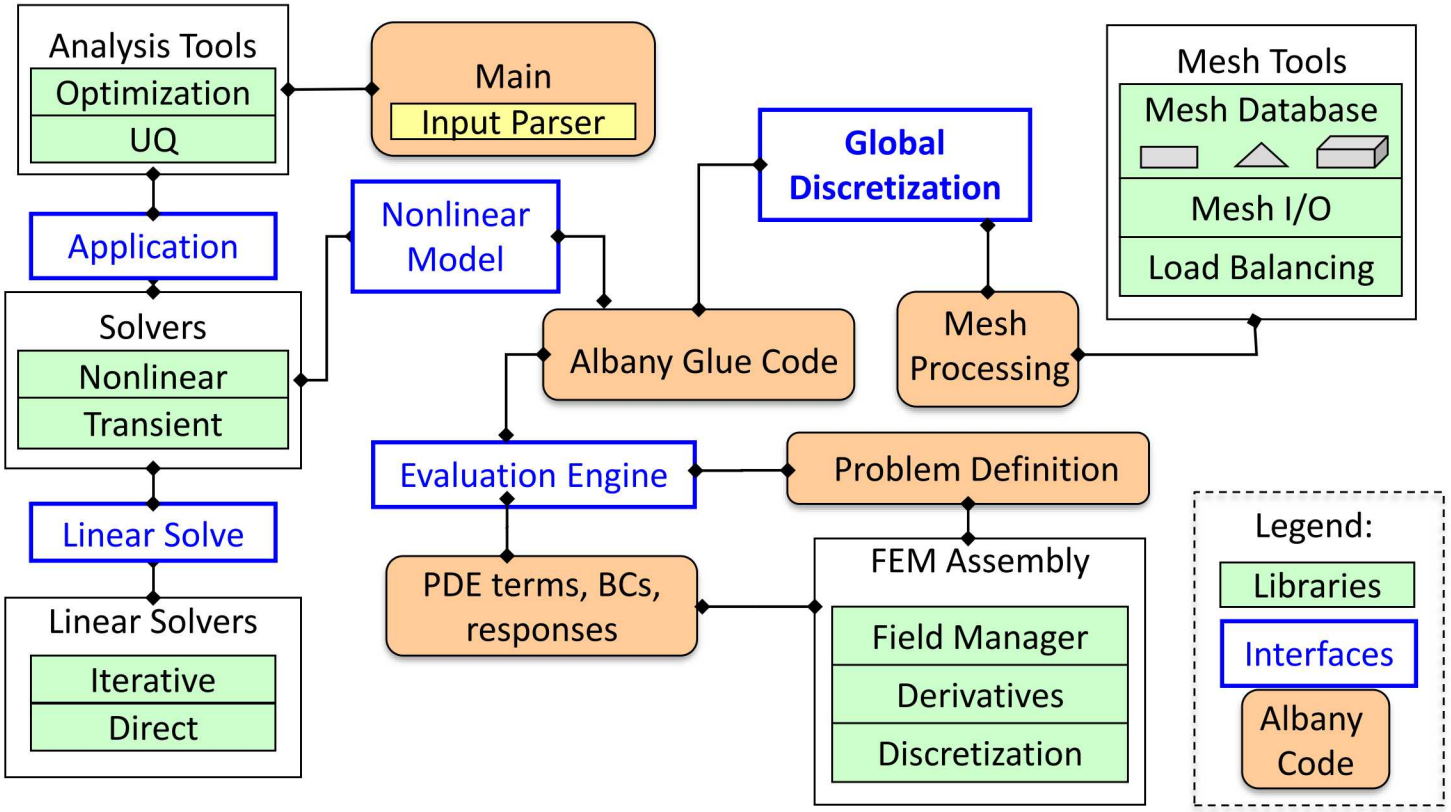

- Depends on **discretization abstraction** (serves as general interface to a mesh service)

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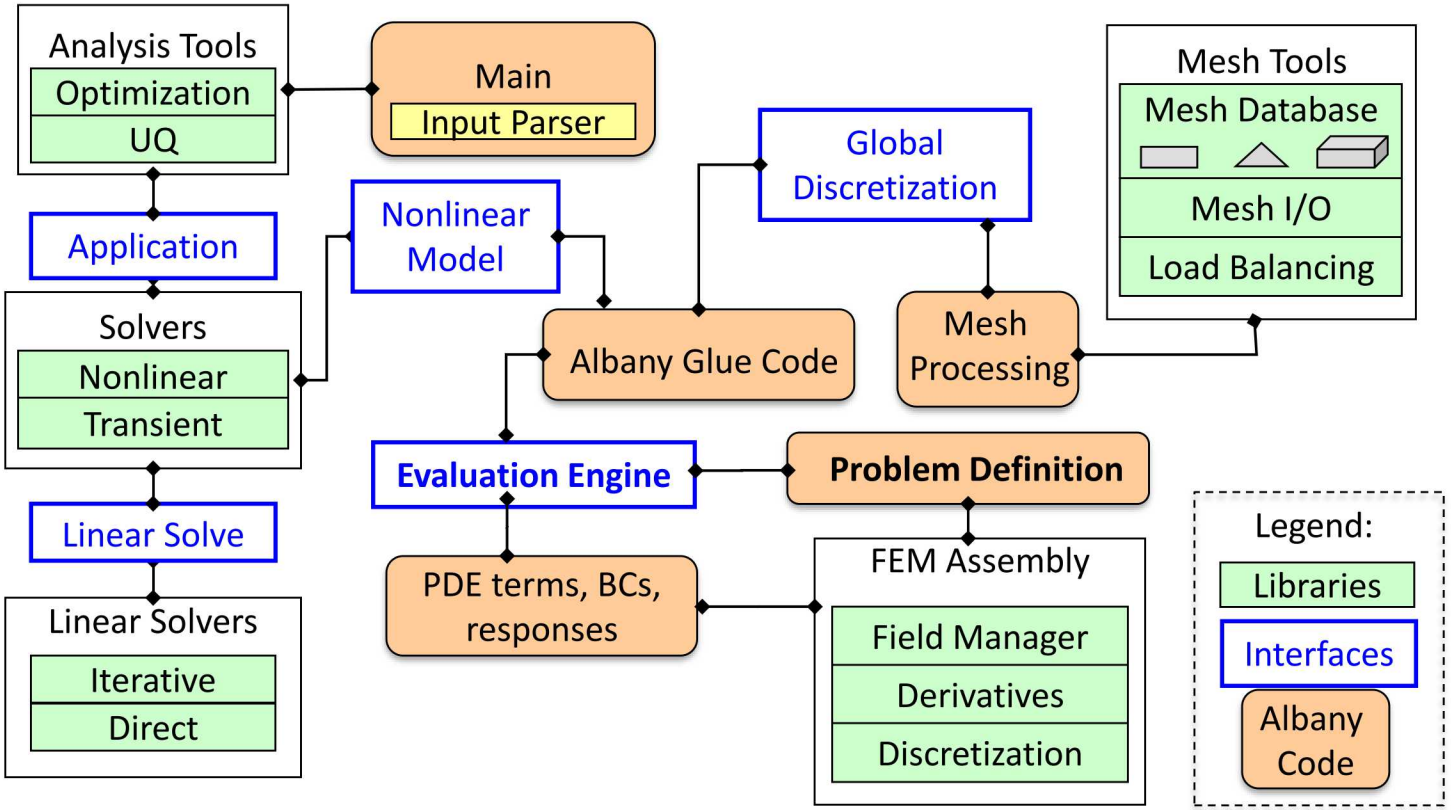
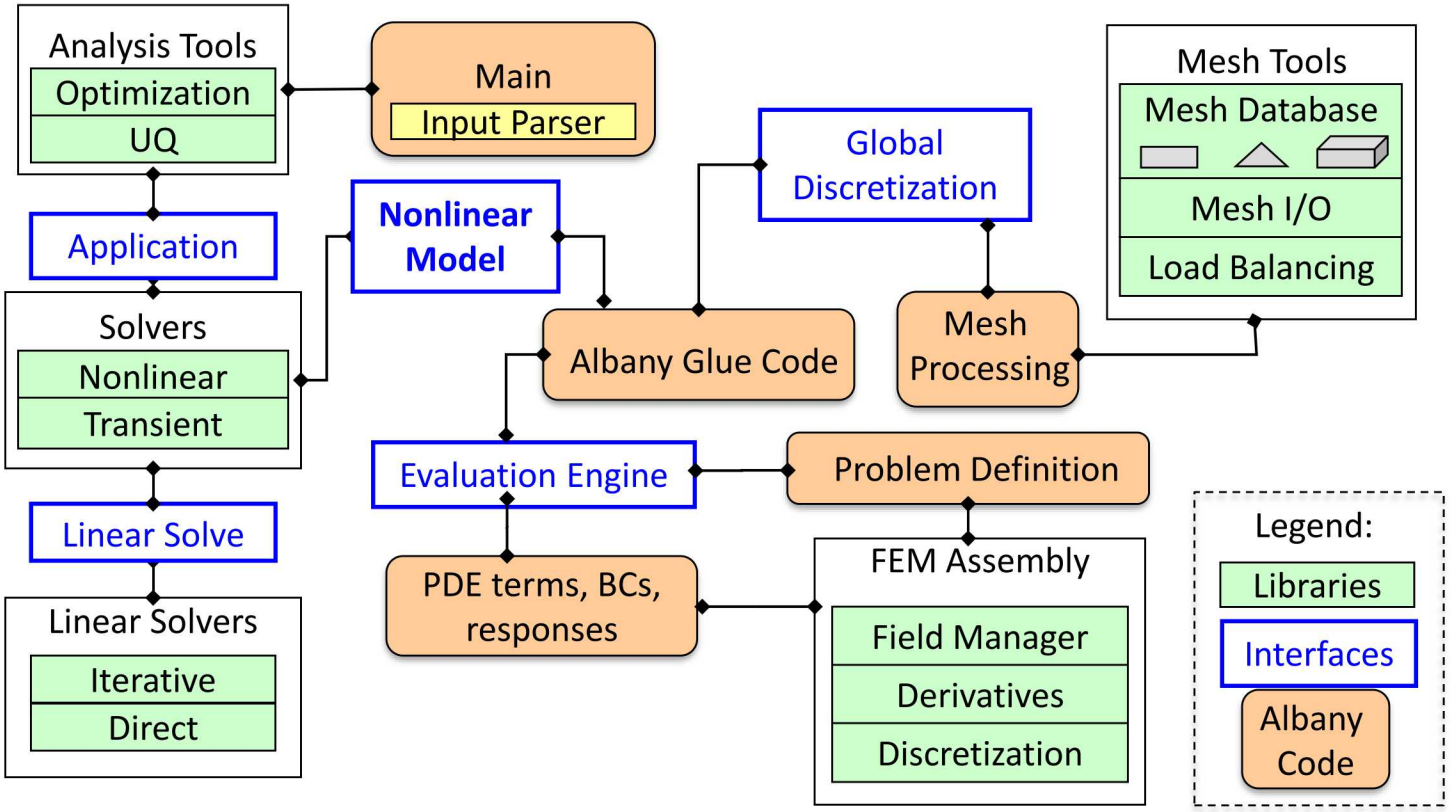
"Glue Code": driver code integrating components + providing overall capabilities



- Depends on **discretization abstraction** (serves as general interface to a mesh service)
- Employs **evaluation engine** to construct PDEs, BCs, and response calculations

Albany "glue code"

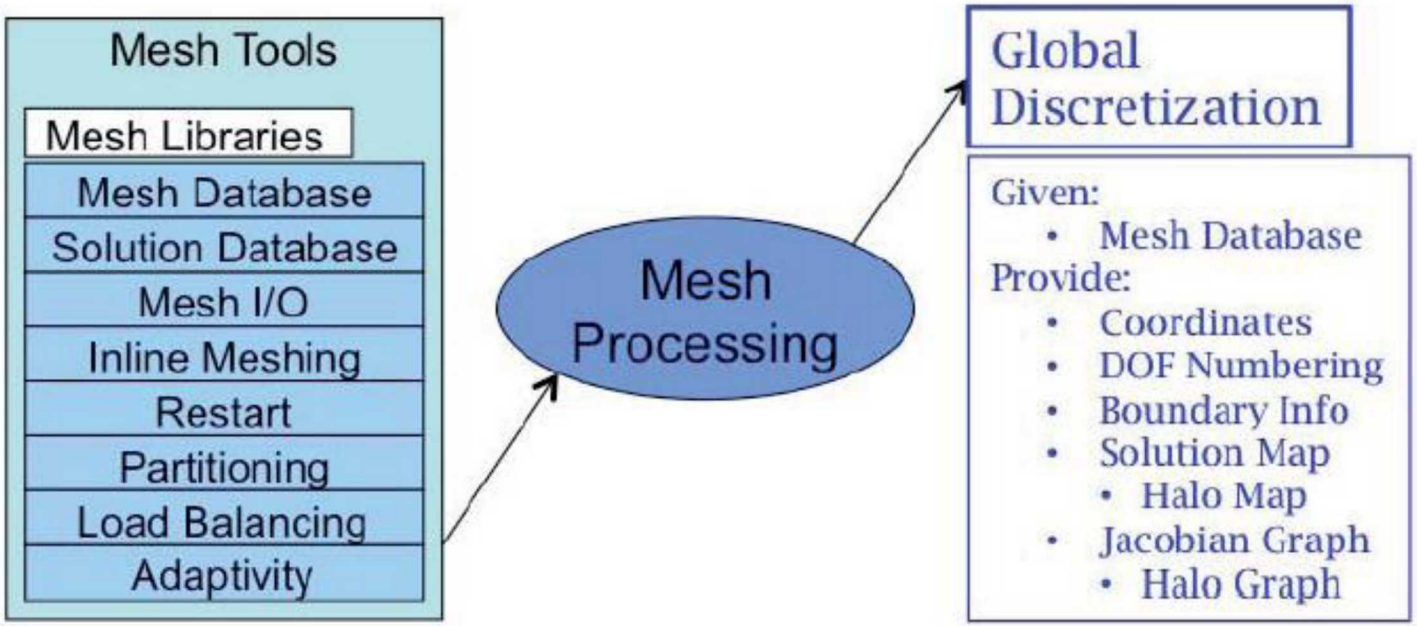
"Glue Code": driver code integrating components + providing overall capabilities



- Depends on **discretization abstraction** (serves as general interface to a mesh service)
- Employs **evaluation engine** to construct PDEs, BCs, and response calculations
- Uses physics pieces to satisfy **nonlinear model abstraction** (e.g., compute resid/Jac)

Global discretization abstraction

- **Mesh framework**: defines geometry, element topologies, connectivities, boundary info, mesh-dependent fields.
- **Global discretization abstraction**: gives the finite element assembly process access to all of the data distribution information required by the linear algebra objects.
- Mesh info is contained in in-memory mesh database accessed through abstract **global discretization interface** class.



Problem abstraction & finite element assembly

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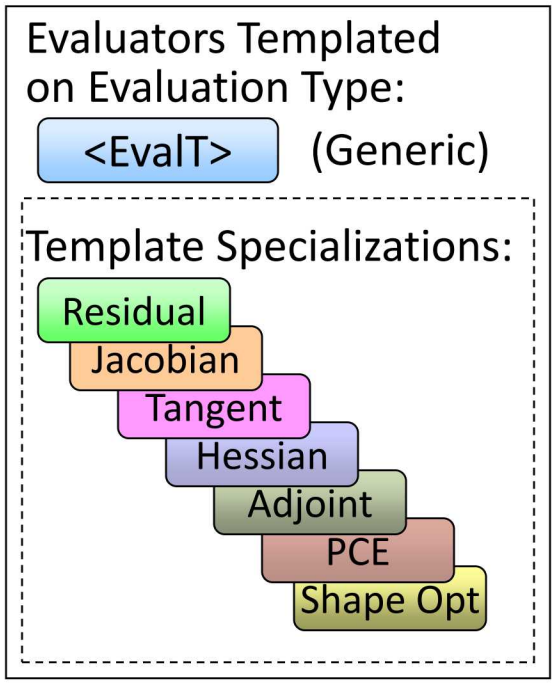
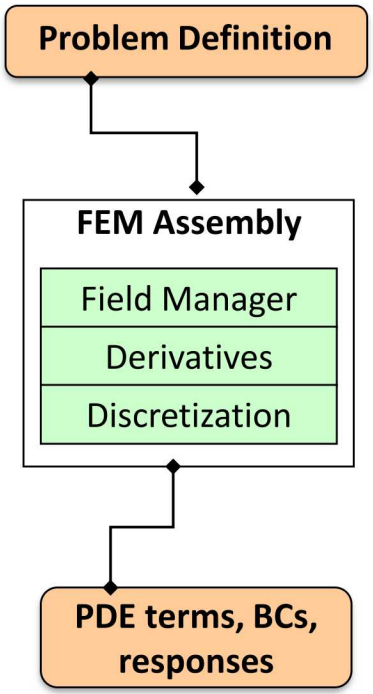
Purpose of problem abstraction & finite element assembly: given a finite element mesh, evaluate discrete finite element residual, Jacobian, and (if applicable) parameter derivatives.

3 key ingredients facilitating multi-physics implementations in Albany:

1. Template-based generic programming (TBGP)
2. Graph-based finite element assembly (FEA)
   - ➢ Handled by Phalanx package
3. Templated-based automatic differentiation
   - ➢ Handled by Sacado package





Automatic differentiation via Sacado

Automatic Differentiation (AD) provides exact derivatives w/o time/effort of deriving and hand-coding them!

- How does AD work? → **freshman calculus**!
  - Computations are composition of simple operations (+, *, sin(), etc.)
  - Derivatives computed line by line then combined via chain rule.
- Great for **multi-physics codes** (e.g., many Jacobians) and **advanced analysis** (e.g., sensitivities)
- Albany uses Trilinos package **Sacado** for AD
  - AD accomplished via **operator overloading** + **templating**: floats/double data types replaced by AD types.

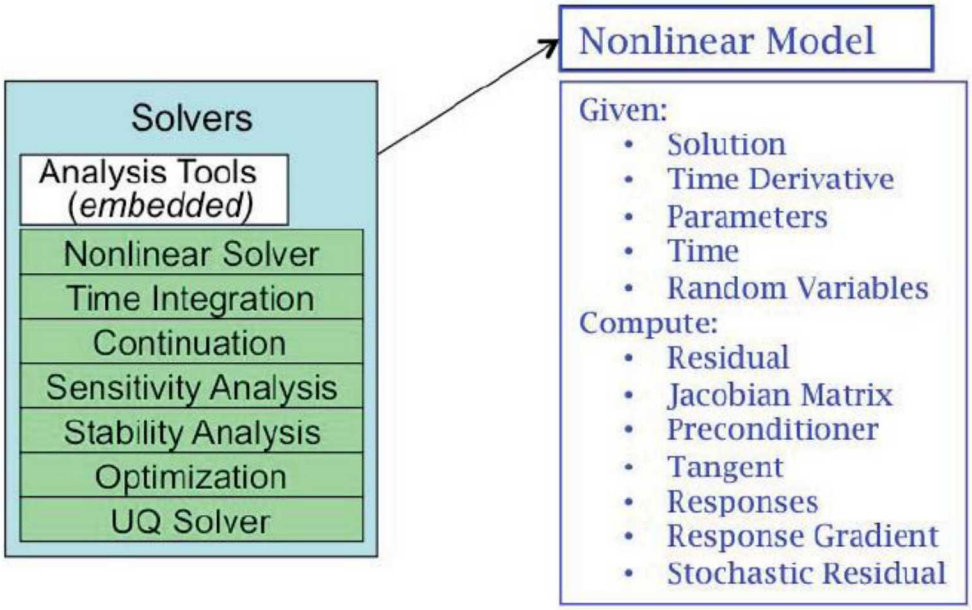
Automatic Differentiation Example:

$$y = \sin(e^x + x \log x), \quad x = 2$$

		$\frac{d}{dx}$
$x \leftarrow 2$	$\frac{dx}{dx} \leftarrow 1$	1.000
$t \leftarrow e^x$	$\frac{dt}{dx} \leftarrow t\frac{dx}{dx}$	7.389
$u \leftarrow \log x$	$\frac{du}{dx} \leftarrow \frac{1}{x}\frac{dx}{dx}$	0.500
$v \leftarrow xu$	$\frac{dv}{dx} \leftarrow u\frac{dx}{dx} + x\frac{du}{dx}$	1.301
$w \leftarrow t + v$	$\frac{dw}{dx} \leftarrow \frac{dt}{dx} + \frac{dv}{dx}$	8.690
$y \leftarrow \sin w$	$\frac{dy}{dx} \leftarrow \cos(w)\frac{dw}{dx}$	-1.188

Derivatives are ***as accurate as analytic computation*** – no finite difference truncation error!

Nonlinear model abstraction & libraries



"ModelEvaluator" Abstraction:

Given:	Computes:
x	$f(\dot{x}, \ddot{x}, x, p, t)$
$\dot{x}$	$W = \alpha \frac{df}{d\dot{x}} + \beta \frac{df}{dx} + \omega \frac{df}{d\ddot{x}}$
$\ddot{x}$	$\frac{df}{dp}$
p	g
t	$\frac{dg}{dx}$
	$\frac{df}{dp}$

- Access to the **embedded solvers** in Trilinos requires satisfaction of **ModelEvaluator** (nonlinear model) abstraction.
- Interface is **general** to accommodate computation of Jacobians, user-defined preconditioners, and stochastic Galerkin expansions.
- **Advanced capabilities**: embedded UQ (Stokhos), optimization (ROL), homotopy continuation (LOCA).

f = residual; x = solution vec;
p = parameters; g = responses;
t = time; W = Jacobian

Core building blocks of Albany

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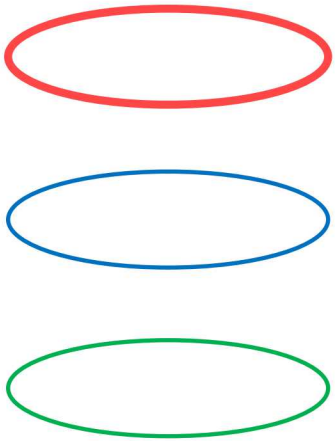
- Component-based design.
- Template-based generic programming.
- Assembly/field evaluation via Phalanx.
- Automatic differentiation.
- Discretizations/meshes, mesh adaptivity.
- Solvers, time-integration schemes.
- Performance-portable kernels.
- Software quality tools: git cmake, ctest, CDash.

Graph-based finite element assembly (FEA)

Sandia National Laboratories

Assembly of physics pieces comes down to the evaluation of a **directed acyclic graph (DAG)** of computations of field data.

Phalanx package: Local field evaluation kernel designed for assembly of arbitrary equation sets (i.e. evaluating residuals/Jacobians).

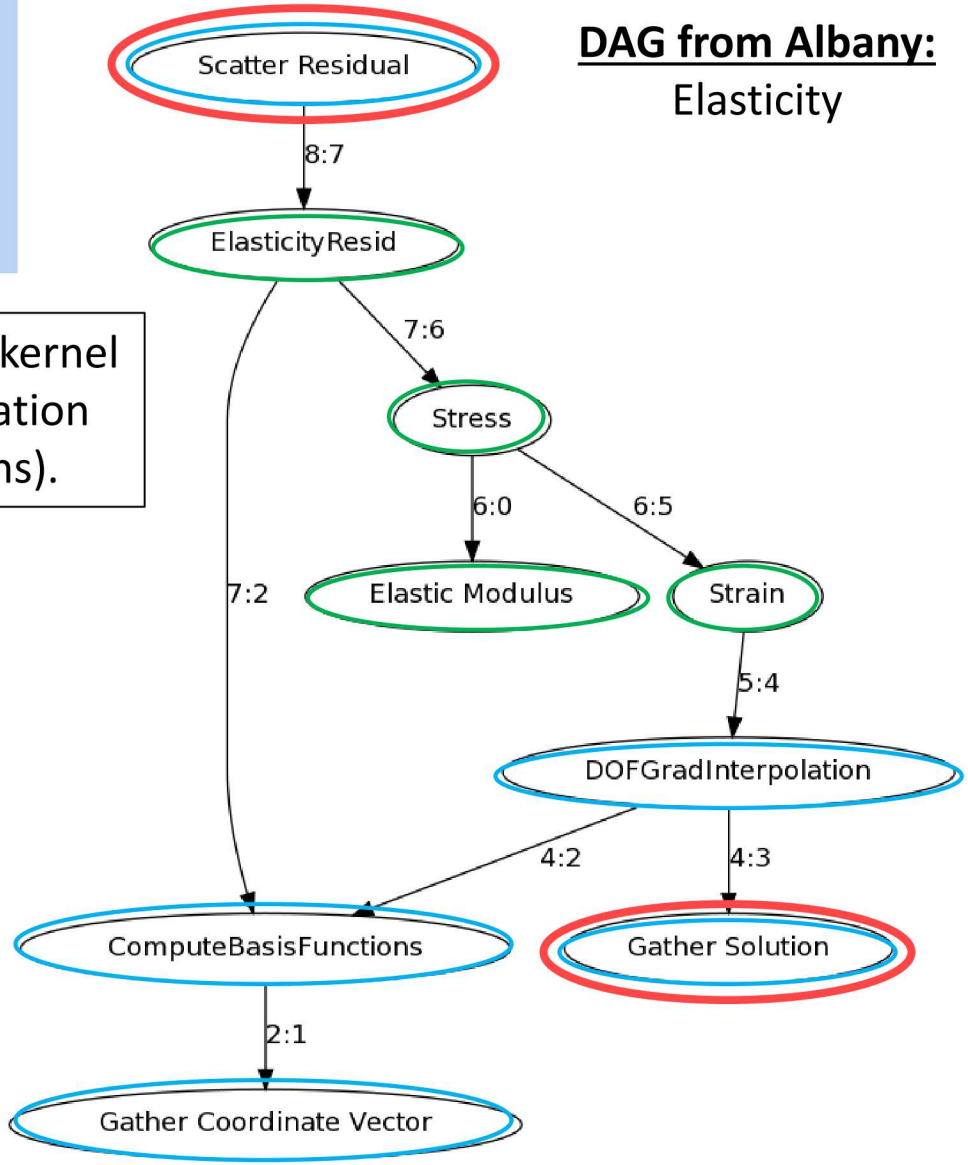


Template-specialized evaluators

Evaluator common to all FEAs

Problem-specific evaluator

DAG from Albany:
Elasticity



R. Pawlowski, Phalanx web site, http://trilinos.sandia.gov/packages/phalanx/ 2015.

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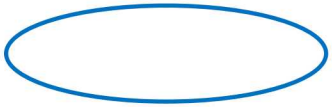
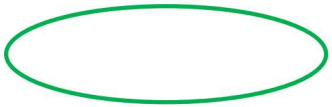
Phalanx package: Local field evaluation kernel designed for assembly of arbitrary equation sets (i.e. evaluating residuals/Jacobians).

Template-specialized evaluators



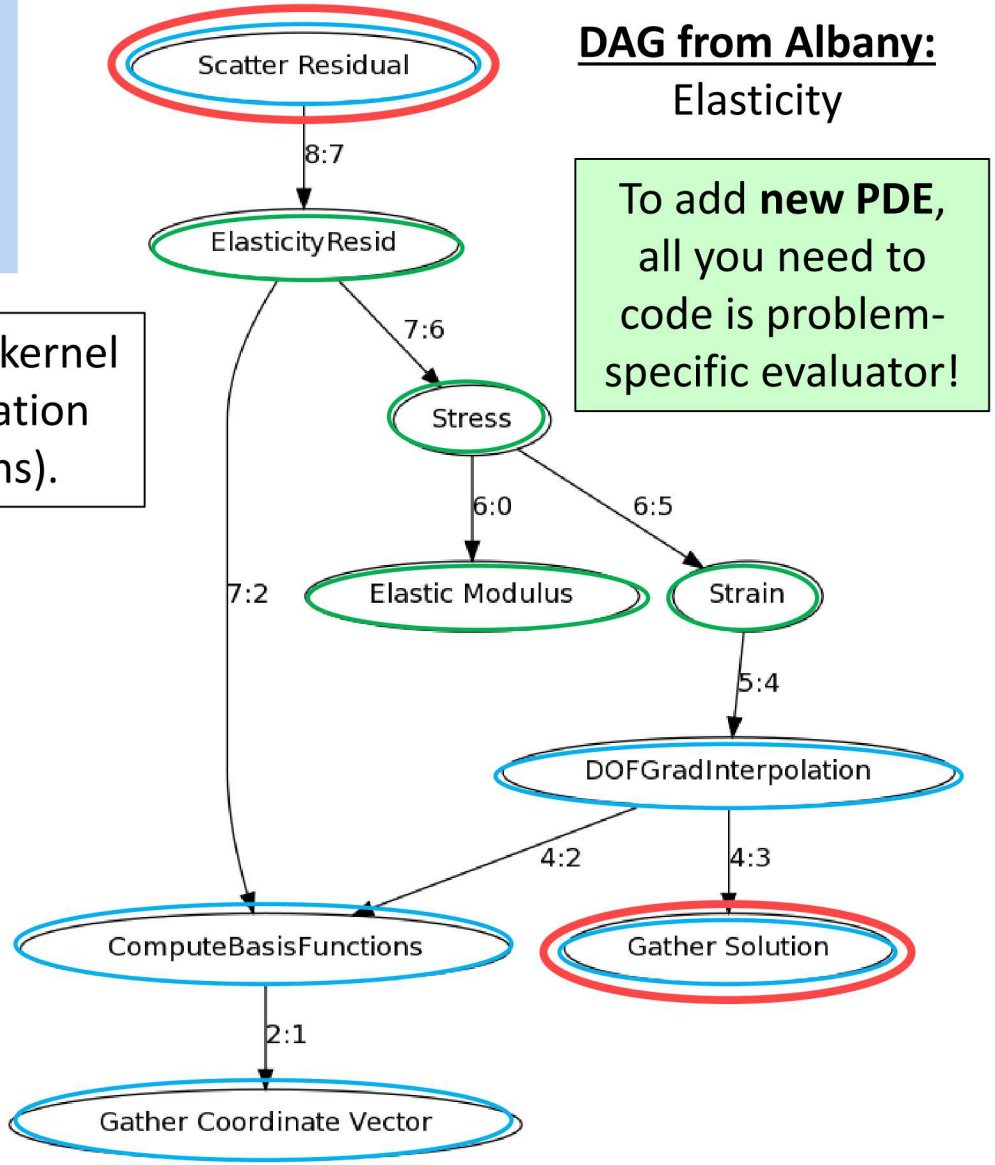
Evaluator common to all FEAs



Problem-specific evaluator

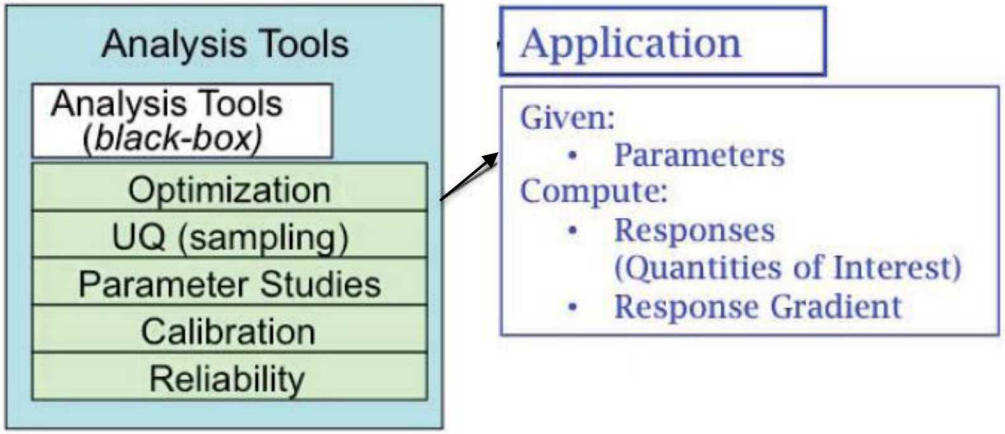
DAG from Albany:
Elasticity

To add **new PDE**, all you need to code is problem-specific evaluator!



R. Pawlowski, Phalanx web site, http://trilinos.sandia.gov/packages/phalanx/ 2015.

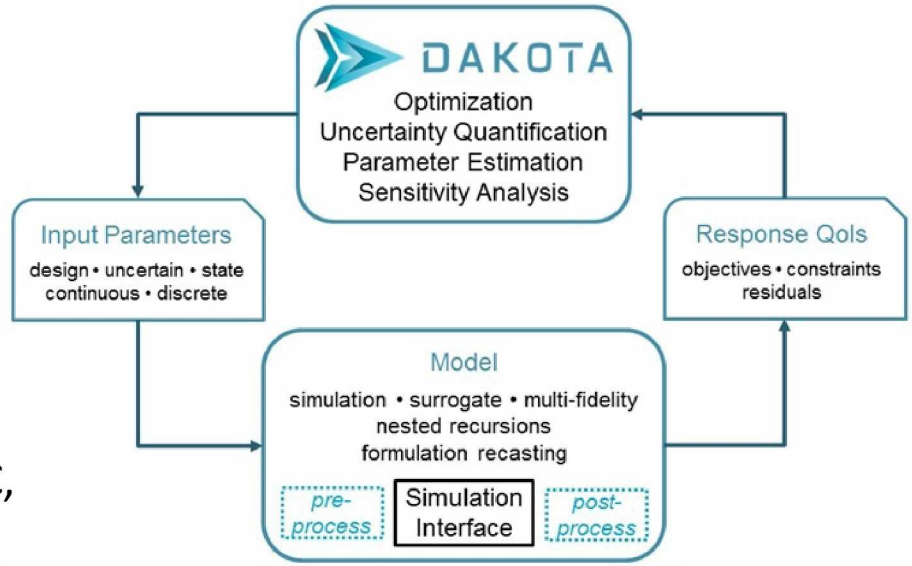
Analysis tools abstraction & libraries



"**Black box**" analysis tools at top level of software stack can perform a single forward solve, sensitivity analysis, parameter studies, bifurcation analysis, optimization, and UQ runs.

Optimization and **UQ** can be done through DAKOTA:

- **Optimization algorithms**: gradient-based local algorithms, pattern searches, and genetic algorithms, etc.
- **UQ algorithms**: Latin hypercube stochastic sampling, stochastic collocation, PCE, MCMC, etc.



Libraries/algorithms whose development was significantly aided by Albany

Sandia National Laboratories

Libraries Developed in Albany:

- Piro
- TriKota
- MiniTensor
- Razor (MOR)
- buildAgainstTrilinos

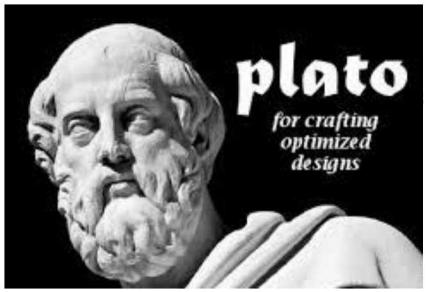
Libraries Driven by Albany:

- Stokhos Embedded UQ
- Semi-Coarsening AMG
- PAALS
- Advanced Topological Opt
- Embedded Ensembles
- CUBIT Mesh-Morpher

Libraries Matured in Albany:

- Tempus
- Phalanx
- STK
- ModelEvaluator
- Stratimikos
- TPetra
- PUMI
- ROL
- DTK
- Intrepid2/Kokkos
- DynRankView
- *And counting…*

Advanced Topology Optimization (ATO)



Coupling of Albany code and **PLATO*** engine for **optimization-based topology optimization**.

Goals:

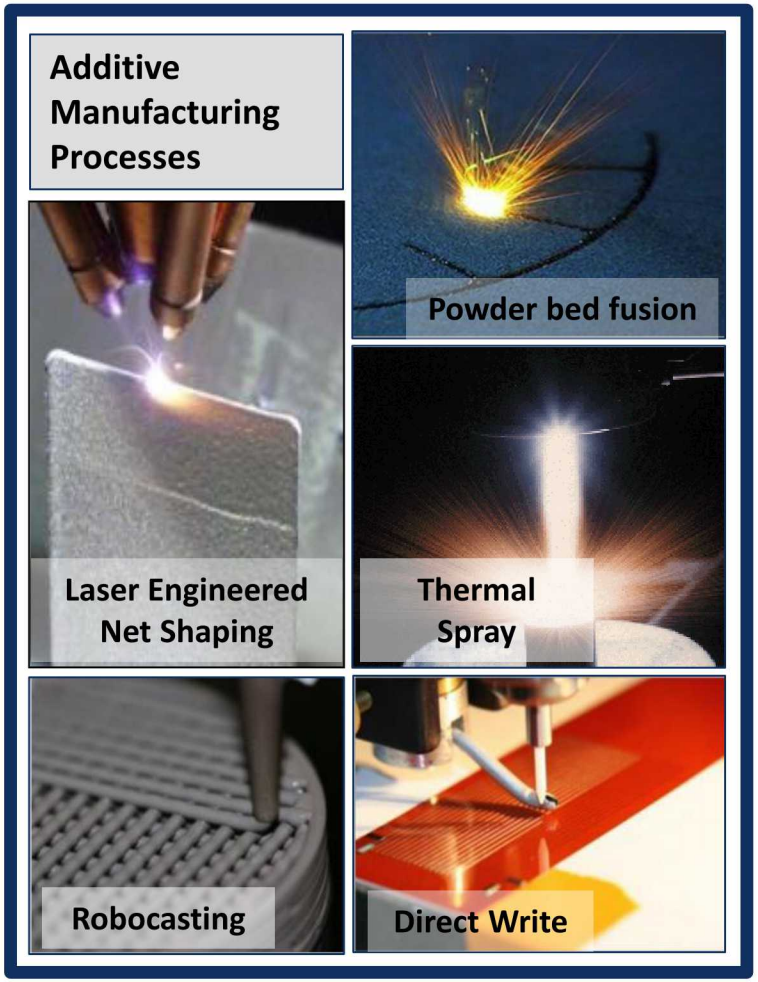
- **Qualification**: assure quality
- **Design**: effectively utilize AM

PDE-constrained optimization:

- **Physics**: elastostatics, Poisson
- **Objectives**: compliance, p-norm
- **Constraints**: volume/mass

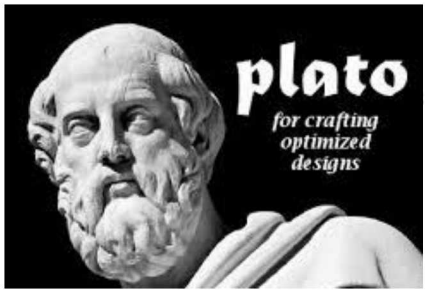
Multiple simultaneous Albany runs can inform a single design optimization by PLATO:

- Albany implements objective + gradient evaluation, optimization loop
- **New "meshless" ATO capability**: allows user to include arbitrarily many simultaneous load cases (linear thermal/electrical, mechanical)



* Topology optimization-based design environment developed by SNL.

Advanced Topology Optimization (ATO)



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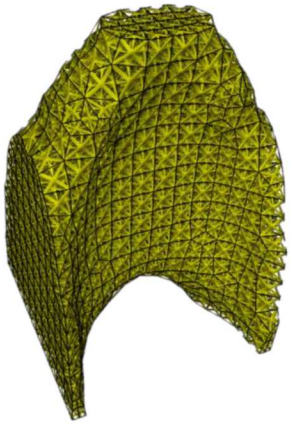

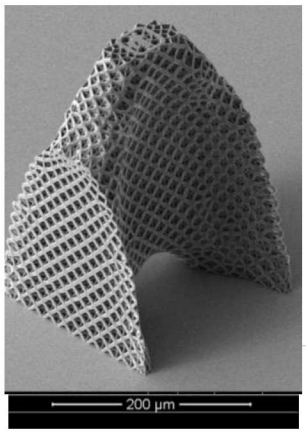

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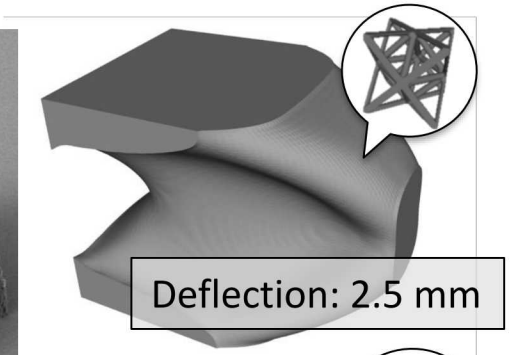
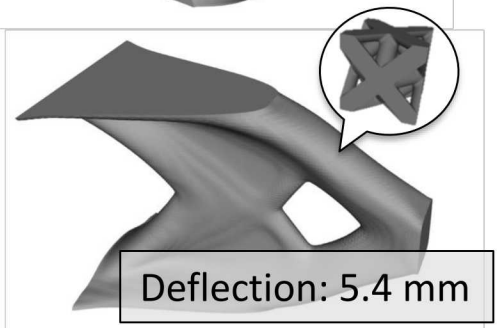
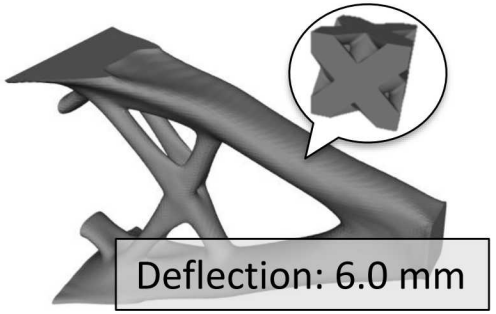
Right: cellular structures with optimized stiffness







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Albotran (Albany-PFLOTRAN)

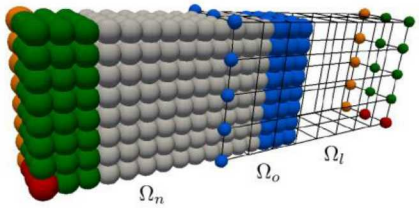
Sandia National Laboratories

Albany-Peridigm

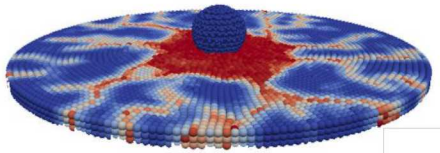
Peridigm Albany ROL

Sandia National Laboratories

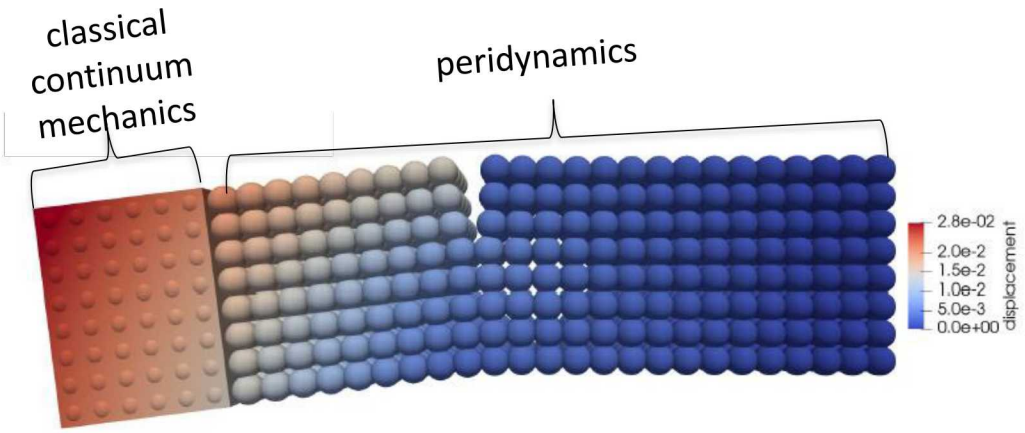
Local-nonlocal coupling for **integrated fracture modeling & multi-physics peridynamics** simulations

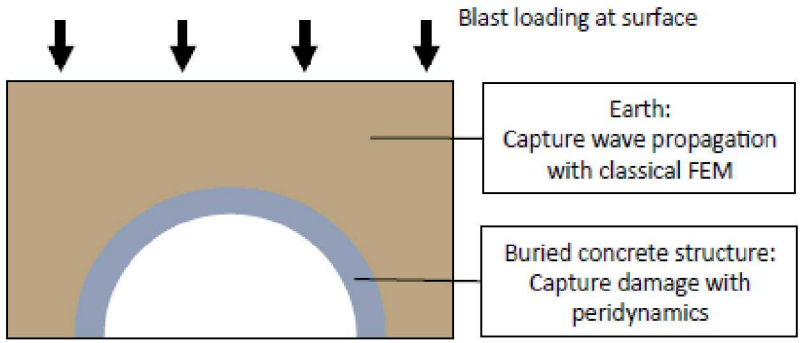


- **Peridynamics**: nonlocal extension of continuum mechanics that remains valid at discontinuities/cracks



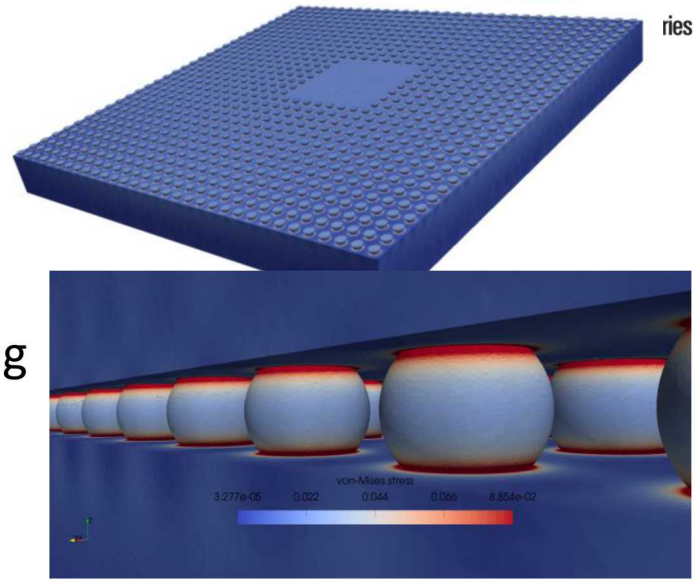
- **Peridigm** = open-source* peridynamics code
  - **Nonlocal meshfree approach** (Silling *et al.*, 2005).
- "**Best of both worlds**" by combining FEM + peridynamics: peridynamics applied in regions susceptible to material failure, easy delivery to applications via FEM.
- **Optimization-based** local-to-nonlocal **coupling** using ROL (D'Elia *et al.* 2016).





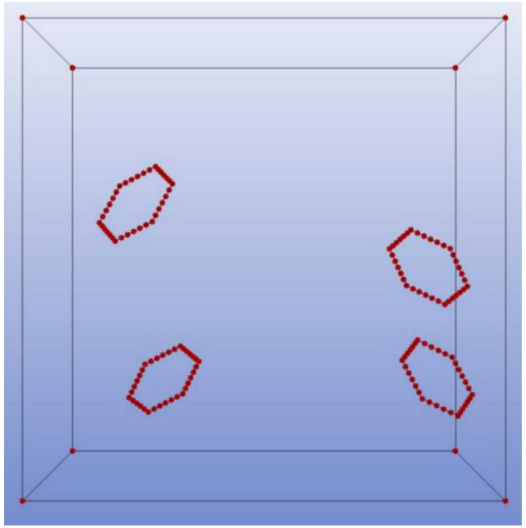
* **Peridigm github repo**: https://github.com/peridigm/peridigm.

Mesh adaptation applications



Creep/Plasticity in Large Solder Joint Arrays*

- Strategic reliability process in semiconductor manufacturing
- Automated workflows with locally refined meshing
- Novel materials models
- Scaling out to 16K processors, 1B+ elements



Coupled Dislocation Dynamics

- Integrates Albany and ParaDis
- Computes dislocation dynamics (DD) in complex geometry
- Allows intersection of dislocations with free surfaces
- ***Left***: prismatic dislocation loops in finite domain

* Li, et al. *Comp. Mech.*, 62:323, 2018. Bloomfield, et al. *Eng. with* Comp., 33: 509, 2017.