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Building a PDE Code from Components, Including Shape Optimization and Embedded UQ

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intro..

Agile Components is a strategic effort at Sandia to maximize our impact as computational scientists. The central idea is for all projects to **both leverage and contribute to** a common base of knowledge and software. This builds the foundation for impacting future projects.

Agile Components implementation plan:

- Develop a full range of independent yet interoperable software components, both: ☑ Capabilities ☑ Interfaces
- Adopt high standards for **Software Quality** tools and procedures
- Develop prototype applications that mature and demonstrate capabilities and interoperability, and drive development

Agile Components stretch goals:

- Rapid development of PDE codes for new applications
    - New codes can developed in 2 FTEs
- PDE code born with transformational analysis capabilities
    - Shape Optimization, Embedded UQ, Sensitivity Analysis, Optimization

Agile Components: A full range of independent-yet-interoperable software libraries and software quality tools

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
- Mulit-Core
- Accelerators

Composite Physics
- MultiPhysics Coupling
- Solution Control
- System Models
- System UQ

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

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

PostProcessing
- Visualization
- Verification
- Feature Extraction
- Model Reduction

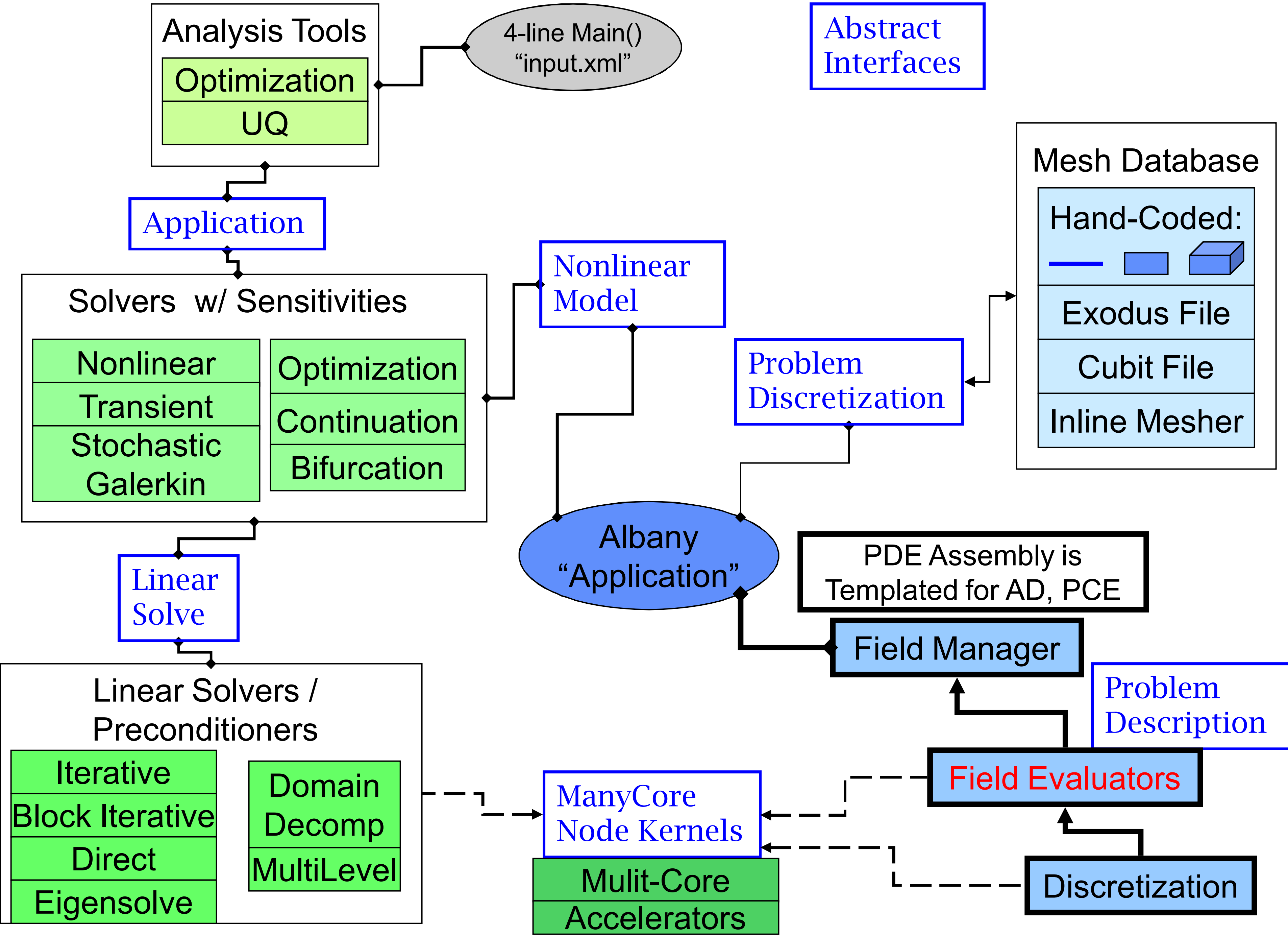
Mesh Database
- Mesh Database
- Geometry Database
- Solution Database
- Modification Journal
- Checkpoint/Restart

Utilities
- Input File Parser
- Parameter List
- Memory Management
- I/O Management
- Communicators
- Runtime Compiler
- MultiCore Parallelization Tools

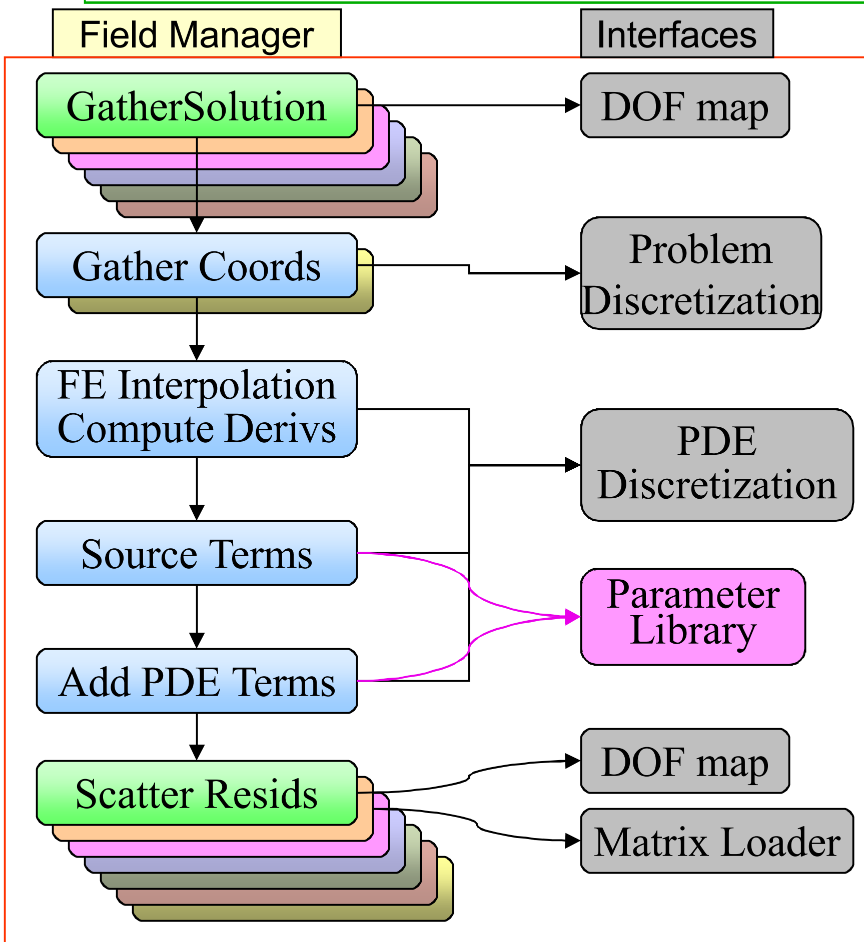
Software Quality
- Version Control
- Regression Testing
- Build System
- Backups
- Verification Tests
- Mailing Lists
- Unit Testing
- Bug Tracking
- Performance Testing
- Code Coverage
- Porting
- Web Pages
- Release Process

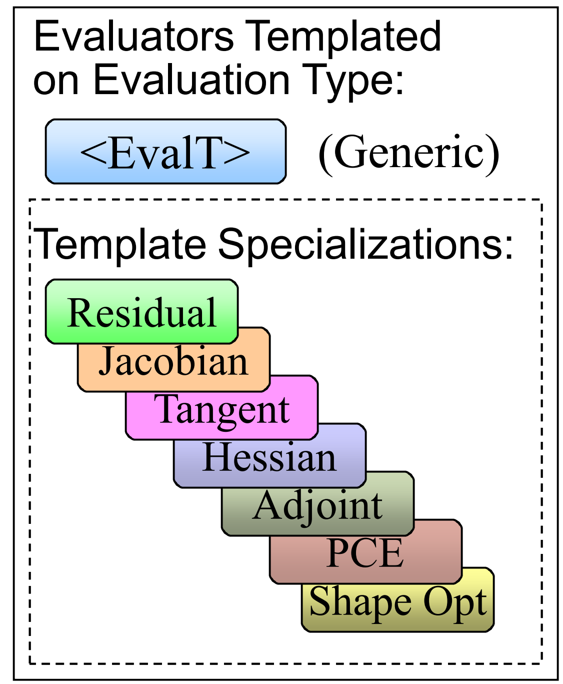
part 2..

Albany is an *Agile Components* demonstration application that has been used to drive development of the vision, and measure progress towards the stretch goals. Albany has interfaces to most of the algorithms delivered through Trilinos, Dakota, Cubit, and SierraToolkit libraries. The code design differs from a monolithic framework in that well-defined **abstract interfaces** keep a clear separation of concerns.


Analysis Tools
Optimization
UQ
4-line Main()
"input.xml"
Abstract Interfaces
Mesh Database
Hand-Coded:
Exodus File
Cubit File
Inline Mesher
Application
Nonlinear Model
Solvers w/ Sensitivities
Nonlinear
Transient
Stochastic Galerkin
Optimization
Continuation
Bifurcation
Problem Discretization
Albany "Application"
PDE Assembly is Templated for AD, PCE
Linear Solve
Field Manager
Problem Description
Linear Solvers / Preconditioners
Iterative
Block Iterative
Direct
Eigensolve
Domain Decomp
MultiLevel
ManyCore Node Kernels
Mulit-Core
Accelerators
Field Evaluators
Discretization

The stretch goals to (A) rapidly development of new physics and (B) use transformational analysis capabilities are reachable in large part by use of templated field evaluators. When data types for Automatic Differentiation and Polynomial Chaos Expansions are appropriately seeded, and passed through the PDE residual evaluation, analytic Jacobians, Tangents, and Stochastic Expansions are automatically generated.





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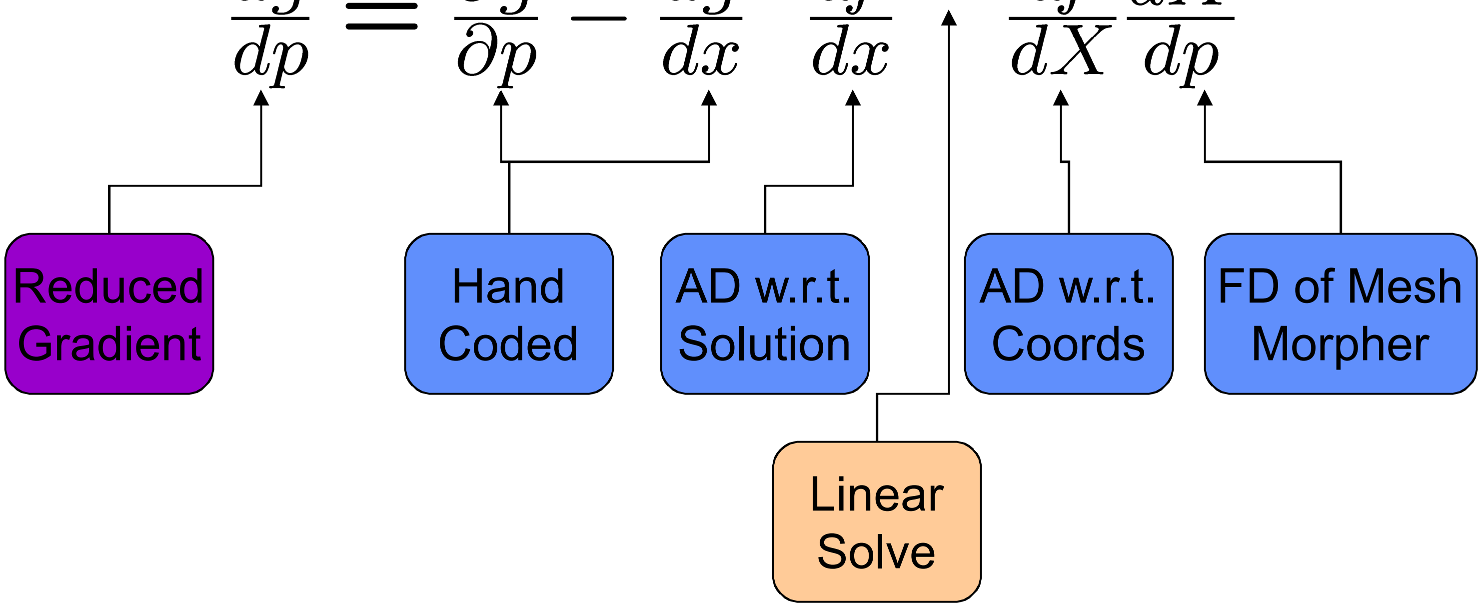
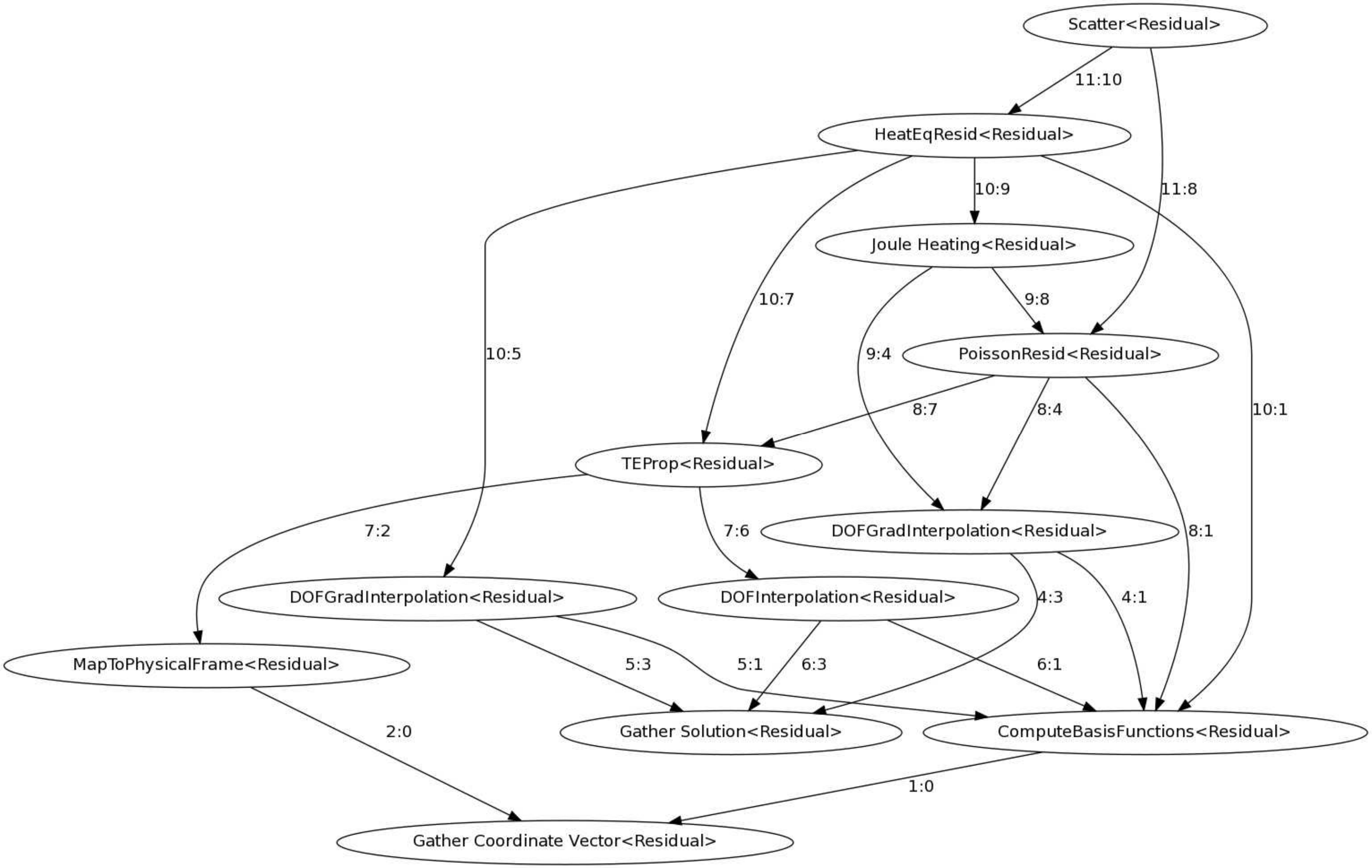
Shape optimization is a special case where derivatives with respect to the coordinate vector X are required. The reduced gradient which is needed for gradient-based optimization algorithms, is assembled using a variety of differentiation methods.

$$\frac{dg}{dp} = \frac{\partial g}{\partial p} - \frac{dg}{dx}^{T} \frac{df}{dx}^{-1} \frac{df}{dX} \frac{dX}{dp}$$



This fig can go with part2 or part3, or cut

Field Manager with Field Evaluators For Sliding ElectroMagnetic Contact Application



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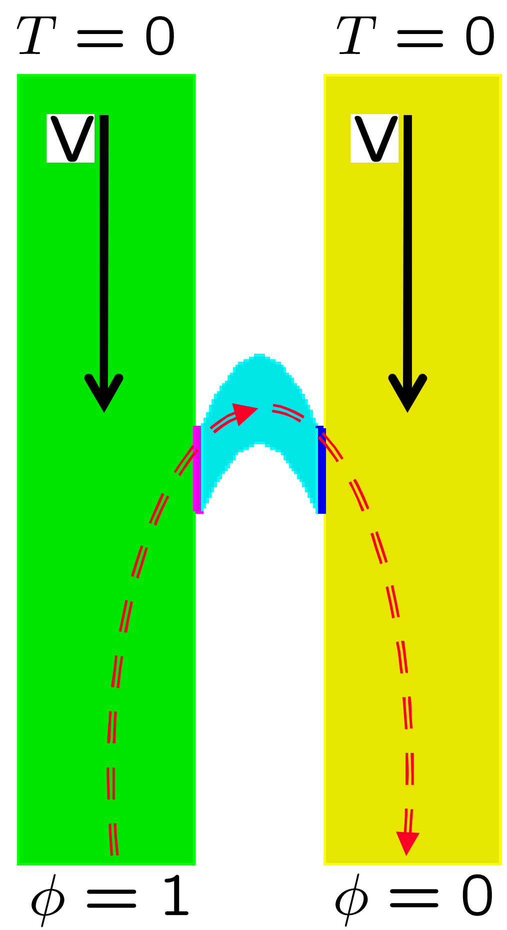
part 3..

Sliding ElectroMagnetic Contact Demonstration: In this application, a slider (blue) is propelled between two conductors (green and yellow) when a current is passed through it (red dashed line). The design optimization problem is to find the shape of the slider that minimizes the temperature increase.

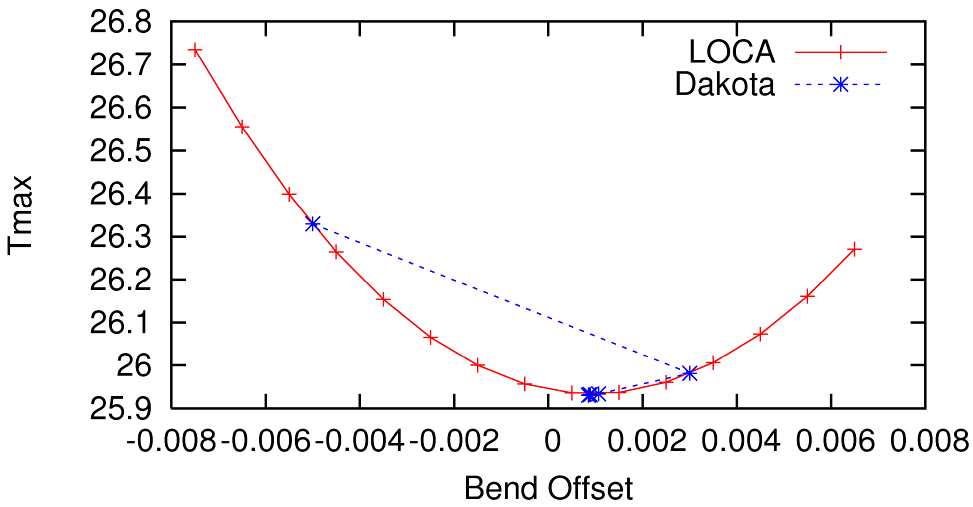
The shape is parameterized by 3 parabolas in the Cubit mesh generator. A set of MeshMorphing algorithms are under development, which reprocess the coordinate positions as a function of geometry changes.

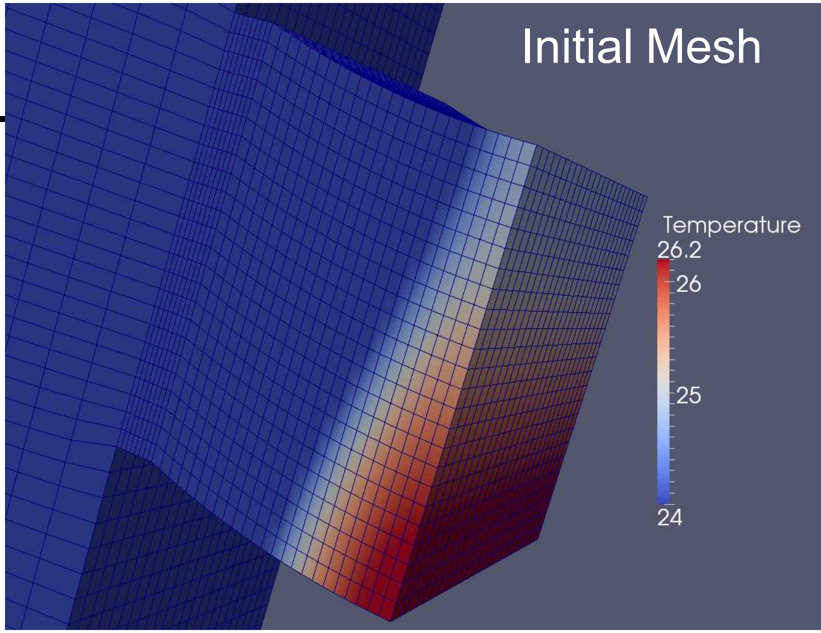
The current is simulated by a potential equation with a proscribed voltage drop. The heat equation captures conduction, convection, and a nonlinear joule heating term. Since the electrical permittivity is inversely dependent on the temperature, the two PDEs are coupled and nonlinear. The properties, such as σ_0, vary by material. A quasi-steady approximation is used.

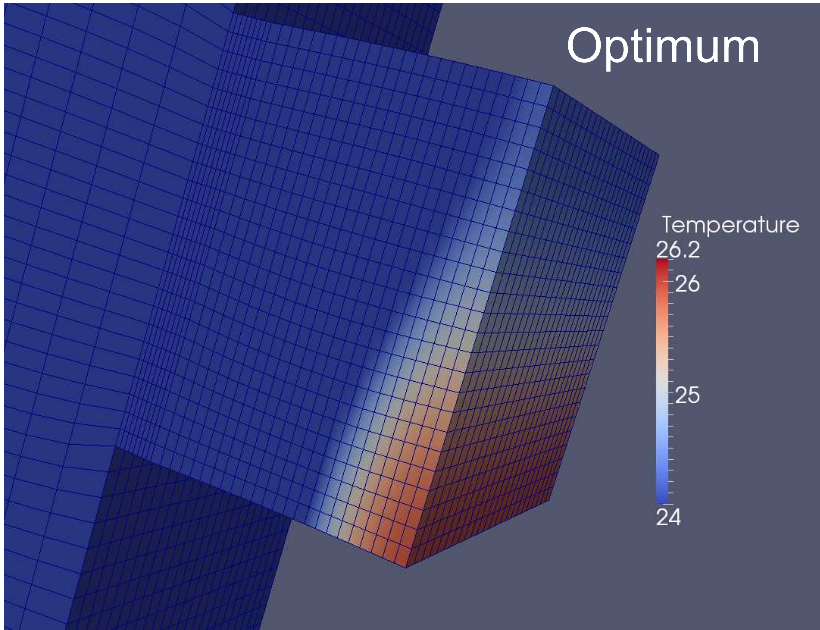
$$
\begin{aligned}
-\nabla \cdot \sigma \nabla \phi &= 0 \\
-\nabla \cdot \kappa \nabla T - \mathsf{v} \cdot \nabla T &= \sigma (\nabla \phi)^2 \\
\sigma(T) &= \sigma_0 / [1 + \beta (T - T_0)]
\end{aligned}
$$



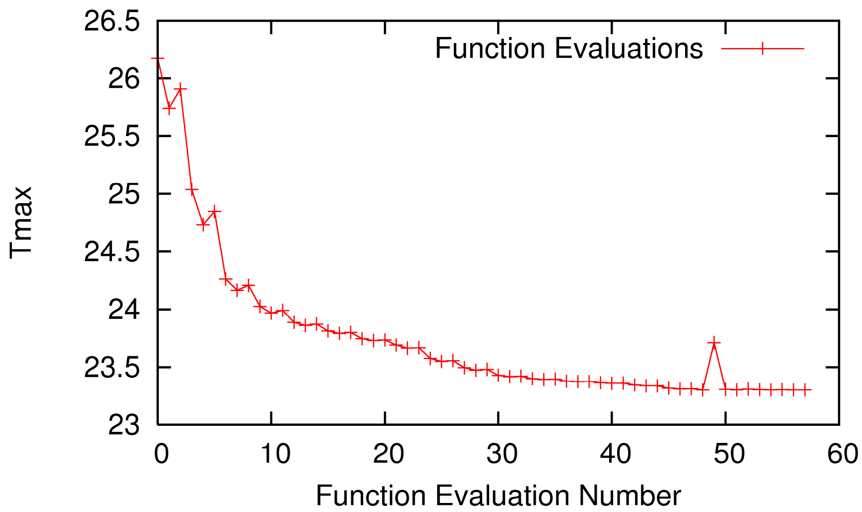
A 1-parameter design problem is solved with a gradient-based optimization algorithm in Dakota, which is verified through a LOCA continuation run.

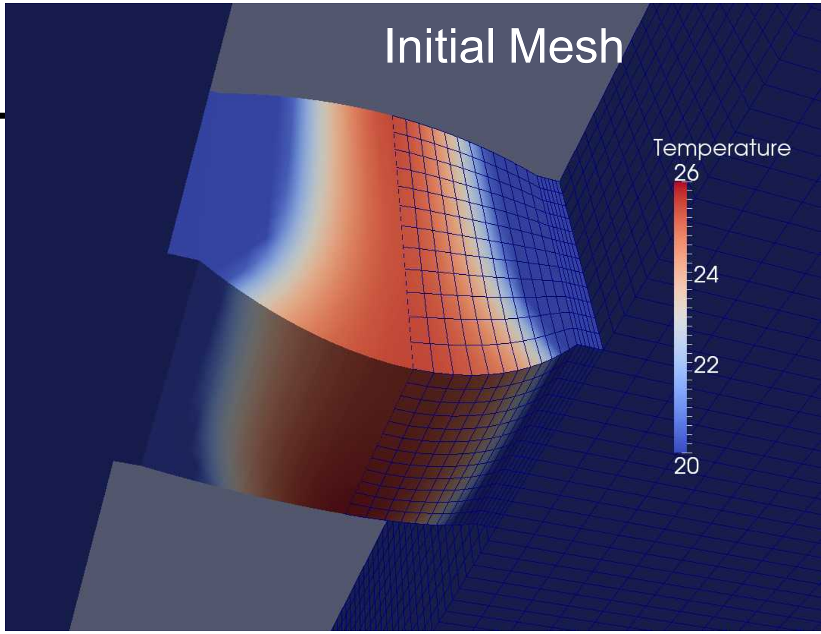


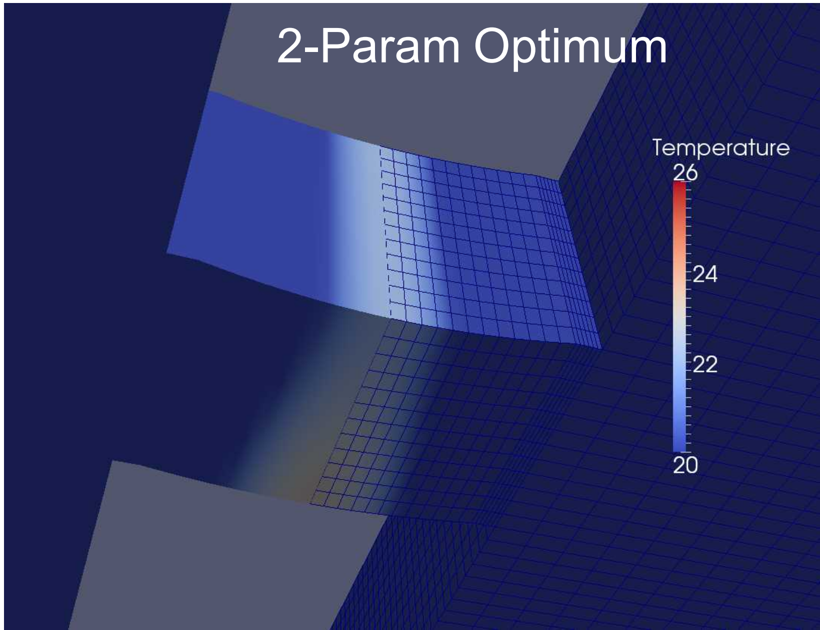




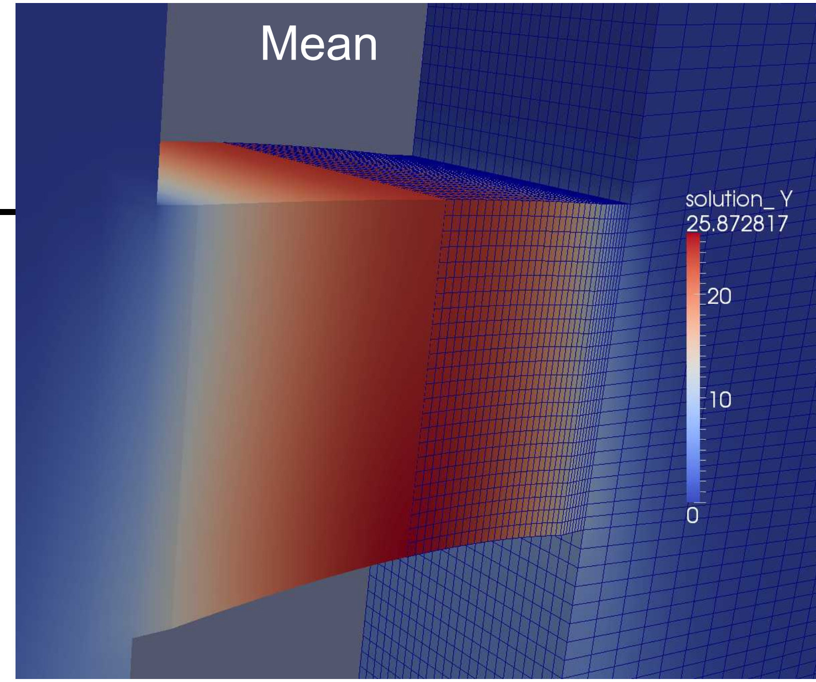
Three parabolic deflections (leading edge, trailing edge, and z-bulge), when subject to a volume constraint on the slider, result in a 2-parameter design optimization. The optimization run results in a significant decrease of T_{max}







Embedded UQ capability: A UQ Study was performed for the 3D model. PCE expansions are automatically propagated through the PDEs. The full stochastic nonlinear system is solved with Newton's Methods. No application-specific code development was required.

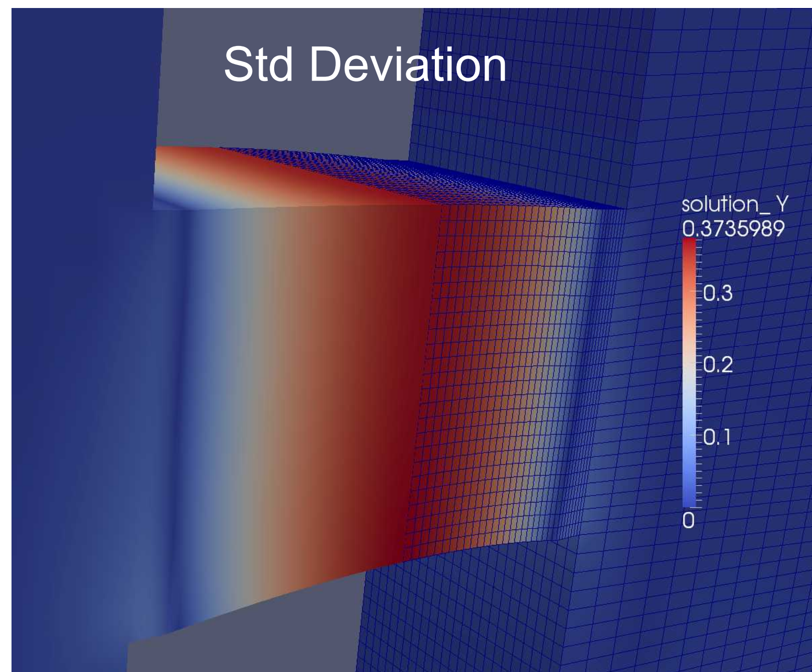


The base electrical conductivity in the thin gap regions is gien the following distribution:

$$\sigma_0^g = [35.0P_0(\xi) + 15.0P_1(\xi)]$$

leading to a polynomial expansion in Tmax

$$37P_0(\xi) + 0.61P_1(\xi) - 0.17P_2(\xi) + 0.04P_3(\xi)$$



Conclusions: The Agile Components strategy is to assemble a comprehensive set of independent-yet-interoperable software libraries, abstract interfaces, and software quality procedures. With this infrastructure and knowledge base, new PDE codes can be rapidly written from scratch. By writing a templated PDE assembly, one can just write the residual equations and a whole host of information automatically. This provides the quantities needed for transformational analysis algorithms.

As a demonstration, we created a simulator for a 3D coupled nonlinear model: sliding electromagnetic contact. With just adding a few evaluators for the PDE terms, all the infrastructure was in place to perform Shape Optimization and embedded UQ.

Acknowledgements: The *Agile Components* strategy relies on the collected efforts of the Trilinos, Dakota, SierraToolkit, and Cubit teams. We'd like to thank the developers, managers, and funding sources for these assemblies of projects. In particular, the ASC and ASCR programs at DOE.

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