Embedded Algorithms through Template-based Generic Programming

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Outline

- Embedded algorithms
- Template-based generic programming
- Incorporating approach into complex codes
- Computational demonstrations
- Ongoing and future work

What does *embedded* mean?

- We used to call this *intrusive*
- Generally anything that requires more of a simulation code than just running it
  - i.e., not black-box or non-intrusive
- Why do this?
  - By asking for more, improvements can be made
    - Increased efficiency, scalability, robustness
    - Greater understanding through deeper analysis

Examples of embedded algorithms

- **Model problem**

$$f(\dot{x}, x, p) = 0, \quad \dot{x}, x \in \mathbb{R}^n, \quad p \in \mathbb{R}^m, \quad f : \mathbb{R}^{2n+m} \to \mathbb{R}^n$$

- **Direct to steady-state, implicit time-stepping, linear stability analysis**

$$\left(\alpha \frac{\partial f}{\partial \dot{x}} + \beta \frac{\partial f}{\partial x} \right) \Delta x = -f$$

- **Steady-state parameter continuation**

$$f(x^{(n)}, p^{(n)}) = 0$$

$$g(x^{(n)}, p^{(n)}) = v_x^T (x^{(n)} - x^{(n-1)}) + v_p^T (p^{(n)} - p^{(n-1)}) - \Delta s_n = 0$$

$$\longrightarrow \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial p} \\ v_x^T & v_p^T \end{bmatrix} \begin{bmatrix} \Delta x^{(n)} \\ \Delta p^{(n)} \end{bmatrix} = - \begin{bmatrix} f \\ g \end{bmatrix}$$

- **Bifurcation analysis**

$$\begin{aligned} f(x, p) &= 0, \\ \sigma(x, p) &= 0, \end{aligned} \quad \sigma = -u^T J v, \quad \frac{\partial \sigma}{\partial x} = -u^T \frac{\partial}{\partial x}(Jv), \quad \frac{\partial \sigma}{\partial p} = -u^T \frac{\partial}{\partial p}(Jv),$$

$$\begin{bmatrix} J & a \\ b^T & 0 \end{bmatrix} \begin{bmatrix} v \\ s_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \begin{bmatrix} J^T & b \\ a^T & 0 \end{bmatrix} \begin{bmatrix} u \\ s_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Examples of embedded algorithms

- **Steady-state sensitivity analysis**

$$f(x^*, p) = 0, \quad s^* = g(x^*, p) \implies$$
$$\frac{ds^*}{dp} = -\frac{\partial g}{\partial x}(x^*, p)\left(\frac{\partial f}{\partial x}(x^*, p)\right)^{-1}\frac{\partial f}{\partial p}(x^*, p)) + \frac{\partial g}{\partial p}(x^*, p)$$

- **Transient sensitivity analysis**

$$f(\dot{x}, x, p) = 0,$$
$$\frac{\partial f}{\partial \dot{x}}\frac{\partial \dot{x}}{\partial p} + \frac{\partial f}{\partial x}\frac{\partial x}{\partial p} + \frac{\partial f}{\partial p} = 0$$

Stochastic Galerkin UQ Methods

- **Steady-state stochastic problem (for simplicity):**

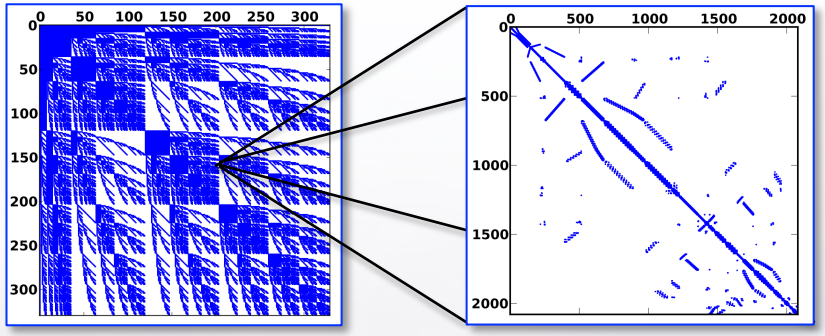
$$\text{Find } u(\xi) \text{ such that } f(u,\xi) = 0,\ \xi : \Omega \to \Gamma \subset R^M, \text{ density } \rho$$

- **Stochastic Galerkin method (Ghanem and many, many others…):**

$$\hat{u}(\xi) = \sum_{i=0}^{P} u_i \psi_i(\xi) \to F_i(u_0, \ldots, u_P) = \frac{1}{\langle \psi_i^2 \rangle} \int_\Gamma f(\hat{u}(y), y)\psi_i(y)\rho(y)dy = 0, \quad i = 0, \ldots, P$$

- **Method generates new coupled spatial-stochastic nonlinear problem (intrusive)**

$$0 = F(U) = \begin{bmatrix} F_0 \\ F_1 \\ \vdots \\ F_P \end{bmatrix}, \quad U = \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_P \end{bmatrix} \quad \frac{\partial F}{\partial U} :$$



Stochastic sparsity Spatial sparsity

- **Advantages:**
  - Many fewer stochastic degrees-of-freedom for comparable level of accuracy
- **Challenges:**
  - Computing SG residual and Jacobian entries in large-scale, production simulation codes
  - Solving resulting systems of equations efficiently

Challenges of embedded algorithms

- Many kinds of quantities required
  - State and parameter derivatives
  - Various forms of second derivatives
  - Polynomial chaos expansions
  - …
- Incorporating these directly requires significant effort
  - Time consuming, error prone
  - Gets in the way of physics/model development
- Requires code developers to understand requirements of algorithmic approaches
  - Limits embedded algorithm R&D on complex problems

A solution

- Need a framework that
  - Allows simulation code developers to focus on complex physics development
  - Doesn't make them worry about advanced analysis
  - Allows derivatives and other quantities to be easily extracted
  - Is extensible to future embedded algorithm requirements
- Template-based generic programming
  - Code developers write physics code templated on scalar type
  - Operator overloading libraries provide tools to propagate needed embedded quantities
  - Libraries connect these quantities to embedded solver/ analysis tools
- Foundation for this approach lies with Automatic Differentiation (AD)

What is Automatic Differentiation (AD)?

- Technique to compute analytic derivatives without hand-coding the derivative computation
- How does it work -- freshman calculus
  - Computations are composition of simple operations (+, *, sin(), etc…) with known derivatives
  - Derivatives computed line-by-line, combined via chain rule
- Derivatives accurate as original computation
  - No finite-difference truncation errors
- Provides analytic derivatives without the time and effort of hand-coding them

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

	x	$\frac{d}{dx}$
$x \leftarrow 2$	2.000	1.000
$t \leftarrow e^x$	7.389	7.389
$u \leftarrow \log x$	0.301	0.500
$v \leftarrow xu$	0.602	1.301
$w \leftarrow t + v$	7.991	8.690
$y \leftarrow \sin w$	0.991	-1.188

Sacado: AD Tools for C++ Codes

- Several modes of Automatic Differentiation (AD)
  - Forward (Jacobians, Jacobian-vector products, …)
  - Reverse (Gradients, Jacobian-transpose-vector products, …)
  - Taylor (High-order univariate Taylor series)
  - Modes can be nested for various forms of higher derivatives
- Sacado uses operator overloading-based approach for C++ codes
  - Sacado provides C++ data type for each AD mode
  - Replace scalar type (e.g., double) with AD type in your code
  - Mathematical operations replaced by overloaded versions provided by Sacado
  - Sacado uses expression templates to reduce overhead

Templating for AD

- Sacado AD types are designed for utmost efficiency of overloaded operators
  - Small, simple, highly optimized AD classes for each AD mode
  - Higher order modes are implemented by nesting lower order AD classes
  - Many AD types to incorporate into your code
- Templating to automate process of incorporating sacado AD
  - Replace scalar type with template parameter
  - Instantiate this template code on each AD data type
  - Use metaprogramming techniques to manage templates

Data type	Calculation
double	$f(x)$
DFad<double>	$f_x V$
Rad<double>	$f_x^T W$
DFad< DFad< double> >	$(f_x V_1)_x V_2$
Rad< DFad<double> >	$(f_x^T W)_x V$

Simple Sacado Example

```
#include "Sacado.hpp"

// The function to differentiate
template <typename ScalarT>
ScalarT func(const ScalarT& a, const ScalarT& b, const ScalarT& c) {
  ScalarT r = c*std::log(b+1.)/std::sin(a);

  return r;
}

int main(int argc, char **argv) {
  double a = std::atan(1.0);                          // pi/4
  double b = 2.0;
  double c = 3.0;
  int num_deriv = 2;                                  // Number of independent variables

  // Fad objects
  Sacado::Fad::DFad<double> afad(num_deriv, 0, a); // First (0) indep. var
  Sacado::Fad::DFad<double> bfad(num_deriv, 1, b); // Second (1) indep. var
  Sacado::Fad::DFad<double> cfad(c);               // Passive variable
  Sacado::Fad::DFad<double> rfad;                  // Result

  // Compute function
  double r = func(a, b, c);

  // Compute function and derivative with AD
  rfad = func(afad, bfad, cfad);

  // Extract value and derivatives
  double r_ad = rfad.val();     // r
  double drda_ad = rfad.dx(0);  // dr/da
  double drdb_ad = rfad.dx(1);  // dr/db
```

AD to TBGP

- **Benefits of templating**
  - Developers only develop, maintain, test one templated code base
  - Developers don't have to worry about what the scalar type really is
  - Easy to incorporate new scalar types
- **Templates provide a deep interface into code**
  - Can use this interface for more than derivatives
  - Any calculation that can be implemented in an operation-by-operation fashion will work
    - i.e., any calculation who's data can be encoded in an object that looks like a scalar where operations on that scalar can be written in closed form
- **We call this extension Template-Based Generic Programming (TBGP)**
  - Extended precision
  - Floating point counts
  - Logical sparsity
  - Uncertainty propagation
    - Intrusive stochastic Galerkin/polynomial chaos
    - Simultaneous ensemble propagation

Intrusive polynomial chaos through TBGP

$$f(u,\xi)=0, \quad \hat{u}(\xi)=\sum_{i=0}^{P} u_i\psi_i(\xi)$$

$$\rightarrow F_i(u_0,\ldots,u_P)=\frac{1}{\langle\psi_i^2\rangle}\int_\Gamma f(\hat{u}(y),y)\psi_i(y)\rho(y)dy=0, \quad i=0,\ldots,P$$

- **By orthogonality of the basis polynomials**

$$(\psi_i,\psi_j)=\langle\psi_i\psi_j\rangle=\int_\Gamma \psi_i(y)\psi_j(y)\rho(y)dy=\langle\psi_i^2\rangle\delta_{ij}$$

- **The F_i are just the first $P+1$ coefficients of the polynomial chaos expansion**

$$f(\hat{u}(y),y)=\sum_{i=0}^{\infty} F_i\psi_i(y)$$

- **Basic idea is to compute such a truncated polynomial chaos expansion for each intermediate operation in the calculation of $f(u,y)$**

$$\text{Given } a(y)=\sum_{i=0}^{P} a_i\psi_i(y),\ b=\sum_{i=0}^{P} b_i\psi_i(y),\ \text{find } c(y)=\sum_{i=0}^{P} c_i\psi_i(y)$$

$$\text{such that } \int_\Gamma (c(y)-\phi(a(y),b(y)))\psi_i(y)\rho(y)dy=0, \quad i=0,\ldots,P$$

Projections of intermediate operations

- **Addition/subtraction**

$$c = a \pm b \Rightarrow c_i = a_i \pm b_i$$

- **Multiplication**

$$c = a \times b \Rightarrow \sum_i c_i \psi_i = \sum_i \sum_j a_i b_j \psi_i \psi_j \rightarrow c_k = \sum_i \sum_j a_i b_j \frac{\langle \psi_i \psi_j \psi_k \rangle}{\langle \psi_k^2 \rangle}$$

- **Division**

$$c = a/b \Rightarrow \sum_i \sum_j c_i b_j \psi_i \psi_j = \sum_i a_i \psi_i \rightarrow \sum_i \sum_j c_i b_j \langle \psi_i \psi_j \psi_k \rangle = a_k \langle \psi_k^2 \rangle$$

- **Several approaches for transcendental operations**
  - **Taylor series and line integration (Fortran UQ Toolkit by Najm, Debusschere, Ghanem, Knio)**
  - **Tensor product and sparse-grid quadrature (Pecos/Dakota)**
  - **New work by Kevin Long on using the AGM method**

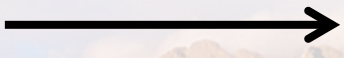
Intrusive PCE Data Types

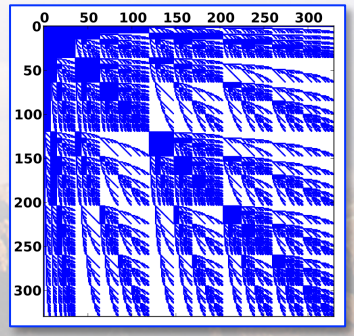
- By creating a new data type storing PC coefficients, and overloaded operators using these formulas, we can "automatically" propagate PC expansions (these live in Stokhos package)

`OrthogPoly<double>:` $x(\xi) = \sum_{i=0}^{P} x_i \psi_i(\xi) \longrightarrow f(x(\xi)) \approx \sum_{i=0}^{P} f_i \psi_i(\xi)$

- Nesting with traditional AD types enables PC expansions of derivatives

`DFad< OrthogPoly<double> >:` $x(\xi) = \sum_{i=0}^{P} x_i \psi_i(\xi) \longrightarrow \frac{\partial f}{\partial x}(x(\xi)) \approx \sum_{i=0}^{P} J_i \psi_i(\xi)$

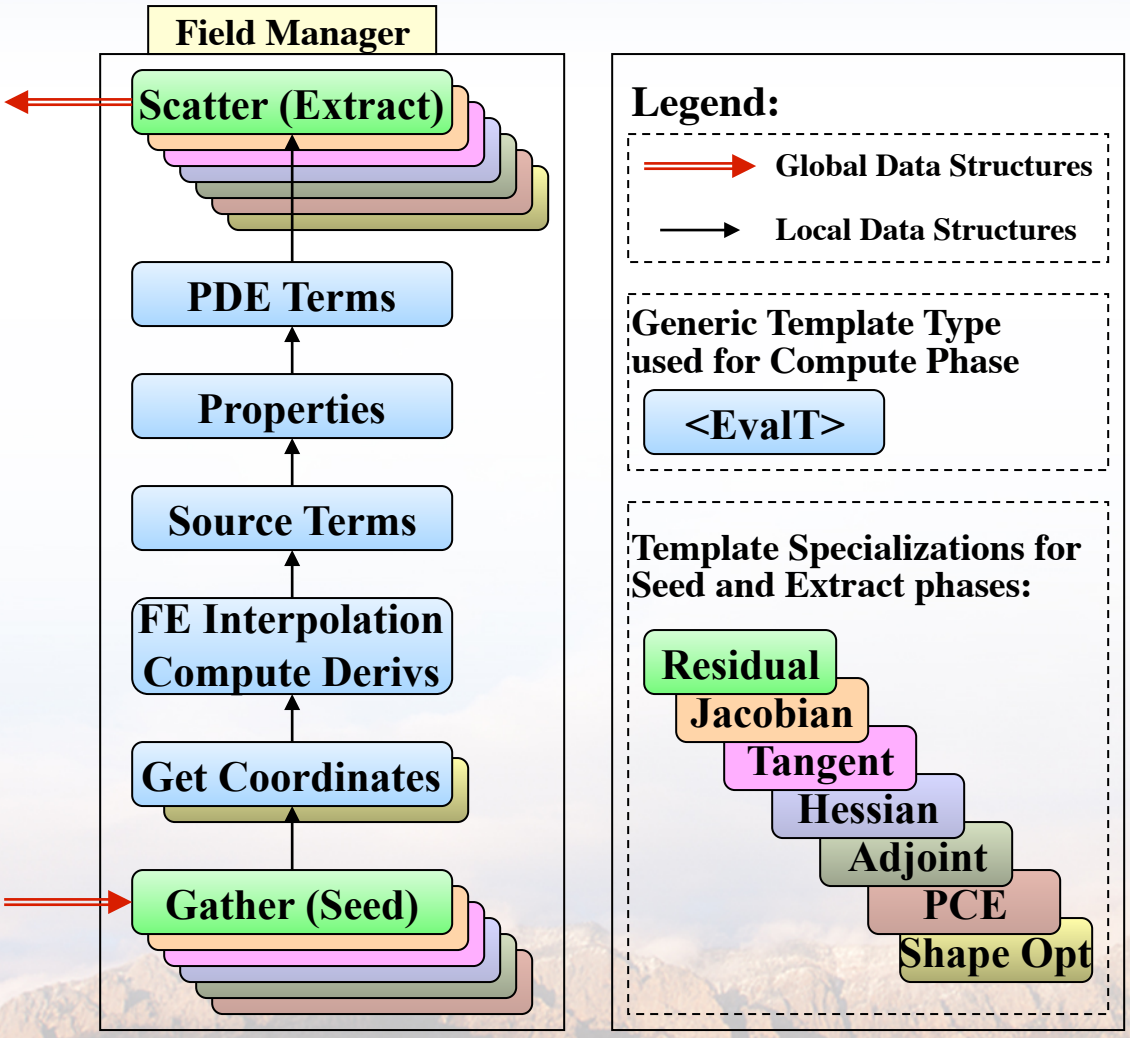




Applying TBGP to PDEs

- Sacado overloaded operators are designed for small, dense operations
  - Avoids performance issues of sparse arrays
  - Eliminates need for row/column compression
  - Avoids issues with MPI
- PDEs don't generate small dense computations
  - But discretizations do generate sparse combinations of small, dense computations
- Apply Sacado at PDE "element-fill" level
  - Template element-fill routines
  - Manually gather/scatter data to/from global data structures
    - Highly dependent on AD type used
    - Make it appear templated through template specialization

Templated Element Fill



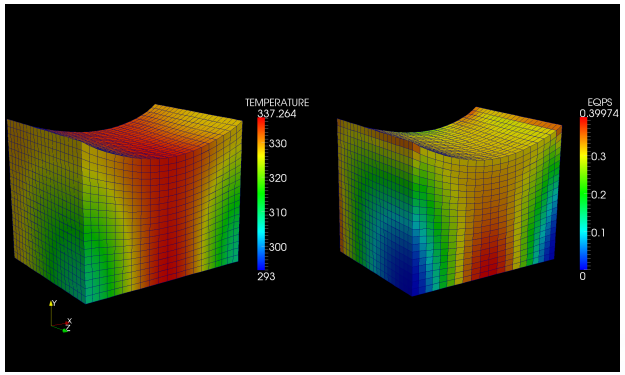
Trilinos Tools for PDEs Supporting TBGP

- **Intrepid: Tools for discretizations of PDEs**
  - Basis functions, quadrature rules, …
  - All Intrepid classes/functions templated on scalar type
    - Derivatives w.r.t. DOFs
    - Derivatives w.r.t. coordinates
- **Phalanx: Local field evaluation kernels**
  - Organize consistent evaluation of "terms" in PDEs
  - Explicitly manages fields/evaluators for different scalar types
- **Shards**
  - Templated multi-dimensional array
- **Stokhos**
  - PCE classes, overloaded operators
  - Simultaneous ensemble propagation classes, overloaded operators
  - Tools and data structures for forming, solving embedded SG systems
- **Sacado**
  - Parameter library – tools to manage model parameters
  - Template manager – tools to manage instantiations of a template class on multiple scalar types
  - MPL – simple implementation of some metaprogramming constructs

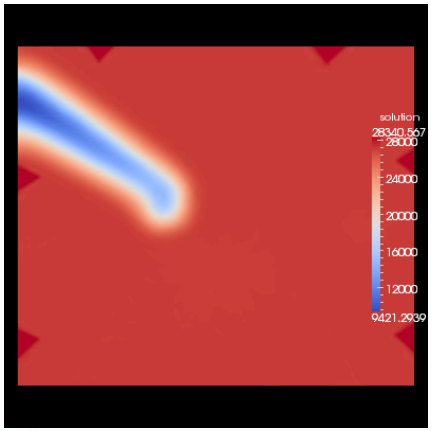
- These ideas provide tools to implement calculations needed for embedded analysis algorithms
  - Tools to implement ModelEvaluator OutArgs
  - Connect to high level nonlinear analysis algorithms
- Examples of how to put these ideas together
  - Trilinos/packages/FEApp – simple 1D finite element code demonstrating TBGP
  - Albany – real PDE code
- These ideas really do work for complex physics

Rapid Physics Development

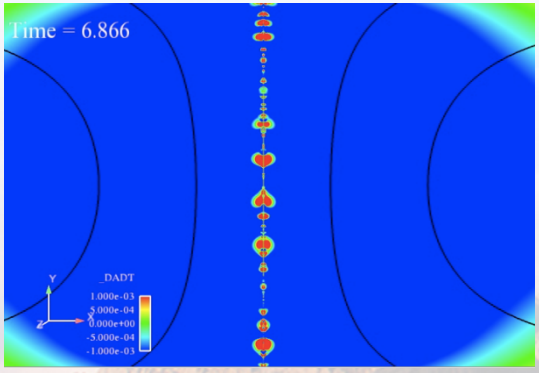
Albany/LCM – Thermo-Elasto-Plasticity
– J. Ostein et al



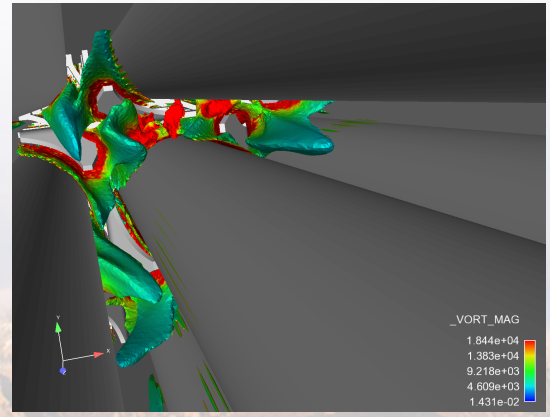
Albany/QCAD – Quantum Device Modeling
– R. Muller et al



Charon/MHD – Magnetic Island Coalescence
– Shadid, Pawlowski, Cyr



Drekar/CASL – Thermal-Hydraulics
– Pawlowski, Shadid, Smith, Cyr



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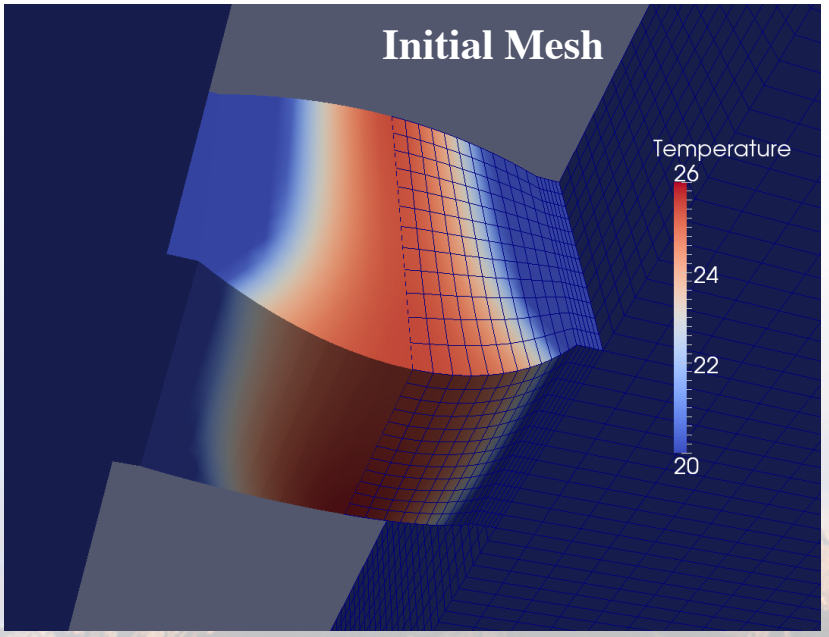
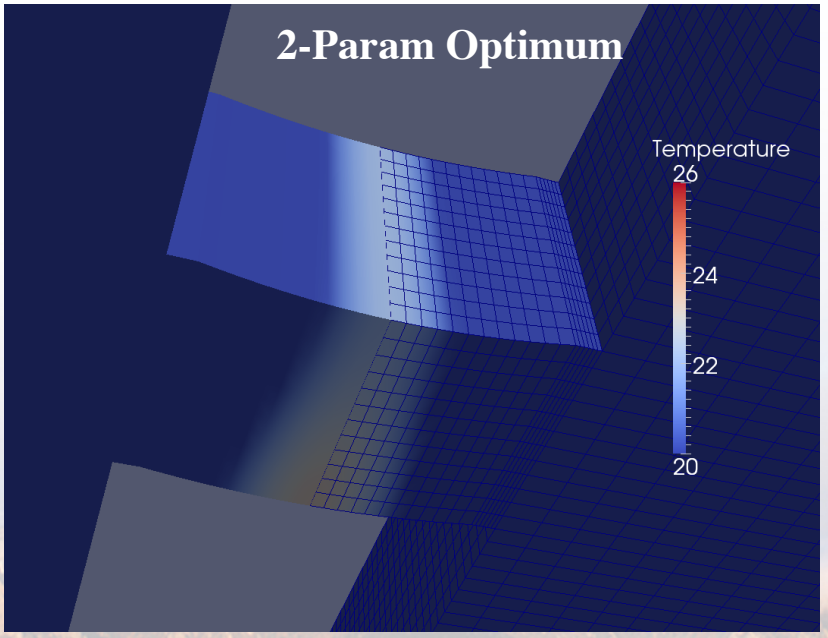
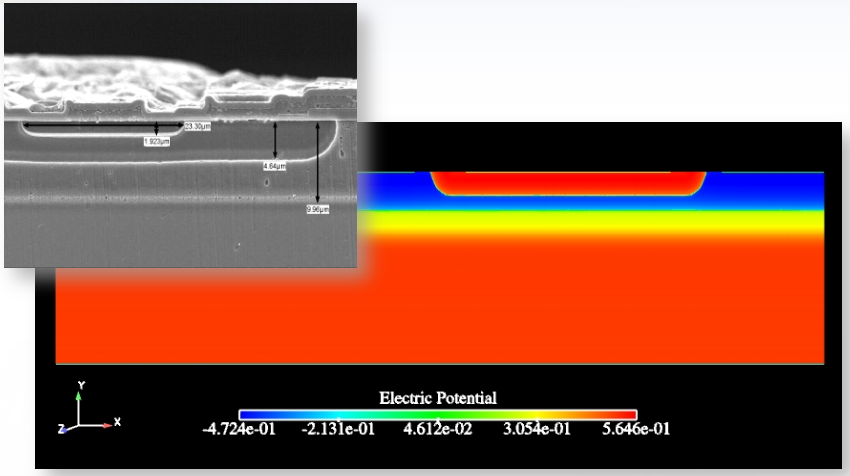
Partially Embedded Optimization

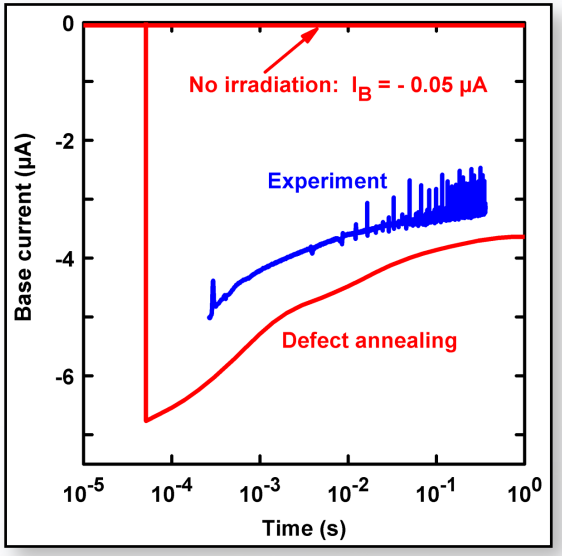
- Shape optimization of a sliding electromagnetic contact
  - Salinger et al
  - Coupled electrostatics, heat conduction
  - Minimize increase in temperature
  - Analytic derivatives w.r.t. mesh coordinates
  - Finite differences of mesh coordinates w.r.t. shape parameters (FD around Cubit)
  - Dakota gradient-based optimization





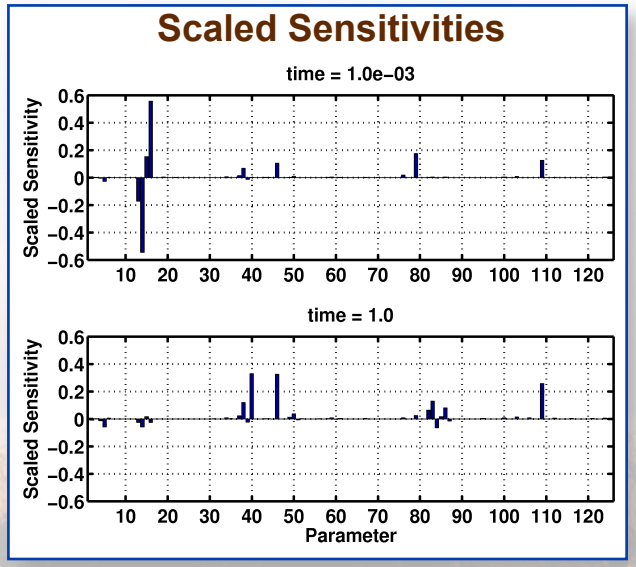
Transient Sensitivities of Radiation Damage in Semiconductor Devices





Comparison to FD:

- ✓ Sensitivities at all time points
- ✓ More accurate
- ✓ More robust
- ✓ 14x faster!



CHARON

QASPR
QUALIFICATION ALTERNATIVES TO SPR

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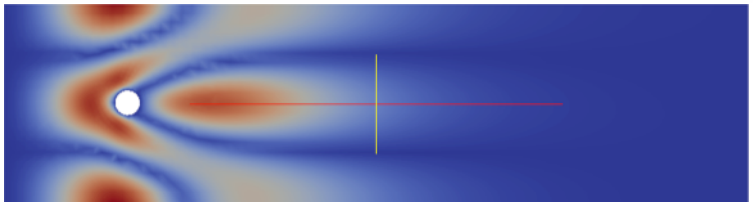
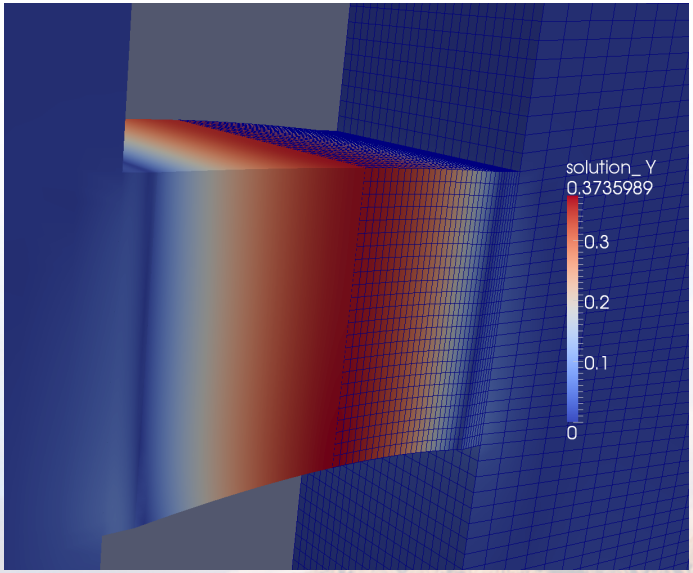
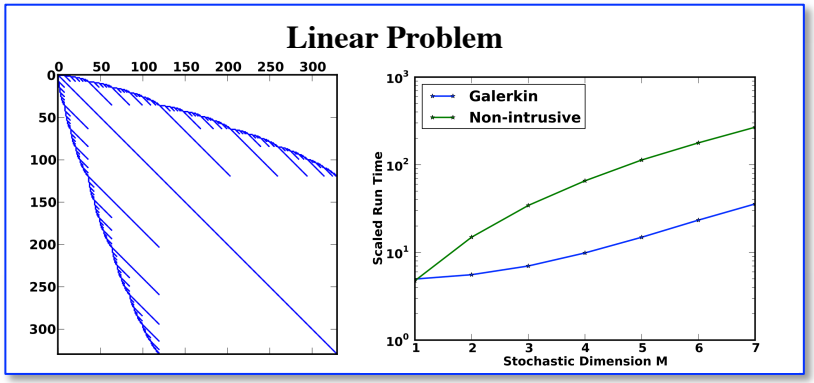
Embedded UQ R&D in Albany

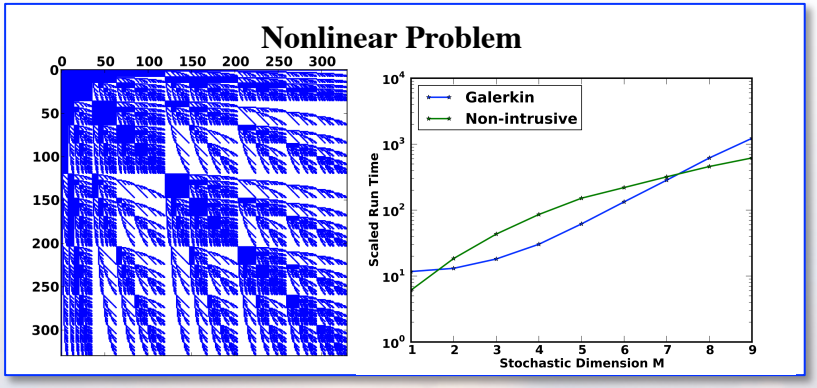
Navier-Stokes



Thermal-Electrostatics







Enabling embedded UQ R&D on complex problems

Simultaneous propagation leads to greater performance

Set of N hypothetical chemical species:

$$2X_j \rightleftharpoons X_{j-1} + X_{j+1}, \quad j = 2, \ldots, N-1$$

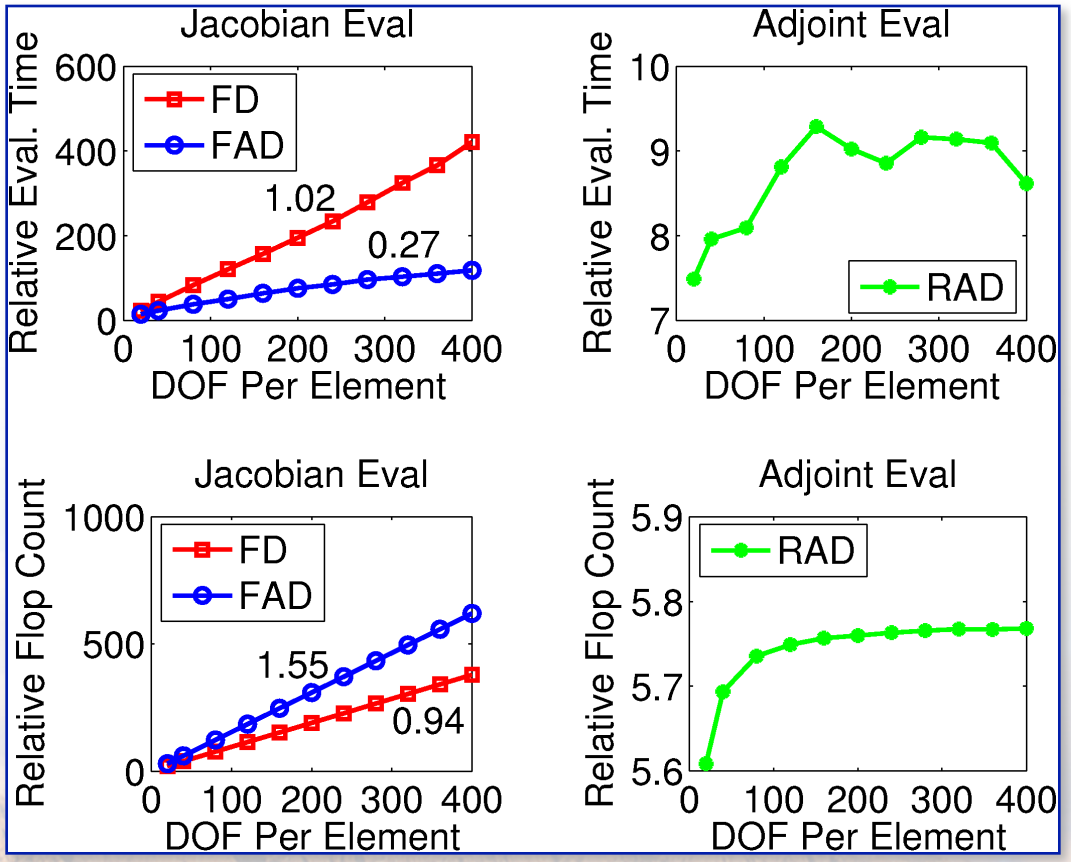
Steady-state mass transfer equations:

$$\mathbf{u} \cdot \nabla Y_j + \nabla^2 Y_j = \dot{\omega}_j, \quad j = 1, \ldots, N-1$$

$$\sum_{j=1}^{N} Y_j = 1$$

- Sacado AD C++ operator overloading library (Trilinos)
- Charon implicit finite element code

Scalability of the element-level derivative computation



DOF per element = 4*N

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Simultaneous propagation of UQ sample points

- "Non-intrusive" polynomial chaos
- Simultaneous calculation of residuals & Jacobians
  - Sacado overloaded operators
- Simultaneous solution of block diagonal linear systems
  - Reuse preconditioner
  - Krylov basis recycling (Belos)
- Simple stochastic PDE
  - Albany implicit PDE code (Salinger et al)

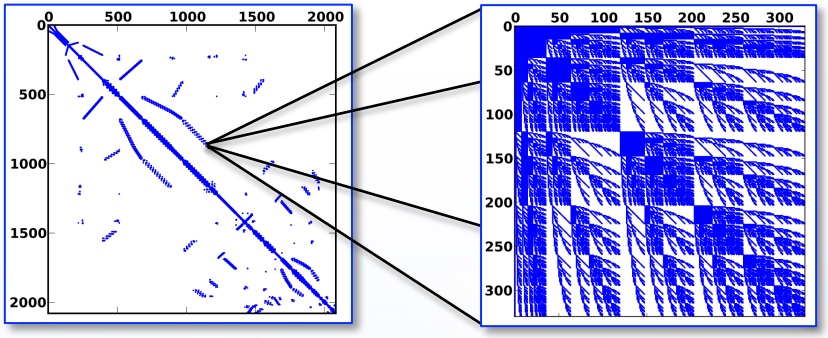
	Non-Intrusive		Embedded		Speed-Up		
# of uncertain parameters	Solve Time	Residual + Jacobian Time	Solve Time	Residual + Jacobian Time	Solve	Residual + Jacobian	Total
2	18	41	11	20	1.6	2	1.9
4	100	200	54	44	1.9	4.5	3.1
6	267	546	146	106	1.8	5.2	3.2
8	495	1094	315	245	1.6	4.5	2.8

Ongoing and Future Work

- Incorporating Sacado types in Tpetra
  - Indirect serialization appears to be a challenge
- Incorporating Sacado types in Kokkos MDArray
  - Expression templates?
  - Dynamic memory allocation?
  - Threading within overloaded operators?
- Rearranging embedded UQ algorithms for emerging multicore architectures

Exploit large stochastic blocks for multicore shared-memory parallelism

- Rearrange for an outer-spatial, inner-stochastic, ordering
  - Obtain very large, nearly dense blocks
  - Use sparse outer layout for distributed memory parallelism
  - Use dense inner blocks for on-node shared memory parallelism



Spatial sparsity Stochastic sparsity

- Requires heterogeneous multicore parallelism in complete forward uncertainty propagation calculation
  - Application fill
  - Iterative solver matrix-vector productions
  - Preconditioning

- FY12-14 SNL LDRD

Concluding Remarks

- Enable embedded algorithms through
  - Application code templating
  - Operator overloading
- Numerous advantages
  - Single templated code base to develop, test, maintain
  - Developers for the most part don't need to worry about embedded algorithms
  - Provides hooks for current and future embedded algorithms
- Main disadvantage is dealing with templates
  - Templates are becoming ubiquitous in Trilinos
  - Template metaprogramming ideas are becoming much more common
  - C++ Template Metaprogramming by D. Abrahams and A. Gurtovoy
  - Some recent work by Argonne OpenAD group to automatically transform code to use Sacado
    - But doesn't work with templates!

Multicore and AD-based SG propagation through application code

- **Quadrature approach for an arbitrary intermediate operation:**

$$a(y) = \sum_{i=0}^{P} a_i \psi_i(y), \quad b(y) = \sum_{i=0}^{P} b_i \psi_i(y), \quad c(y) = \sum_{i=0}^{P} c_i \psi_i(y),$$

$$c = \phi(a,b) \implies c_i = \frac{1}{\langle \psi_i^2 \rangle} \int_{\Gamma} \phi(a(y), b(y)) \psi_i(y) \rho(y) dy \approx \sum_{j=0}^{Q} w_j \phi(a(y_j), b(y_j)) \psi_i(y_j)$$

- **2 dense mat-vecs, for-loop, and dense mat-vec:**

$$\Psi = [\psi_i(y_j)] \in \mathbb{R}^{(P+1)\times(Q+1)}, \quad \bar{a} = [a_i] \in \mathbb{R}^{P+1}, \quad \bar{b} = [b_i] \in \mathbb{R}^{P+1}, \quad \bar{c} = [c_i] \in \mathbb{R}^{P+1},$$

$$A = [a(y_j)] \in \mathbb{R}^{Q+1}, \quad B = [b(y_j)] \in \mathbb{R}^{Q+1},$$

$$\implies A = \Psi^T \bar{a}, \quad B = \Psi^T \bar{b}, \quad \Phi = [w_j \phi(A_j, B_j)] \in \mathbb{R}^{Q+1}, \quad \bar{c} = \Psi \Phi$$

- **Each scalar operation is replaced by dense matrix-vector products and easily parallelized for loops**
  - **Great opportunity for multicore parallelization**

- **Challenge: Designing overloaded operators that function effectively on GPUs**