Embedded Stochastic Galerkin Projection and Solver Methods via Template-based Generic Programming

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Goal: Understand costs vs. benefits of intrusive methods

Embedded Stochastic Galerkin UQ Methods

- Steady-state stochastic problem:

$$\text{Find } u(\xi) \text{ such that } f(u,\xi) = 0 \text{ a.e., } \xi : \Omega \to \Gamma \subset \mathbb{R}^M, \text{ density } \rho,\ \langle\cdot\rangle \equiv \int_\Gamma \cdot\, \rho(y)dy$$

- Stochastic Galerkin (SG) method, a.k.a., Intrusive Polynomial Chaos (PC):

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

- Basis polynomials are *usually* tensor products of 1-D orthogonal polynomials of total degree at most N (assumes independence):

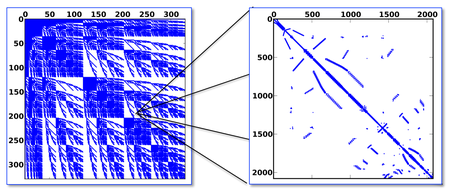
$$\psi_i(y) = \psi_{i_1}^1(y_1)\dots\psi_{i_M}^M(y_M),\quad i_1+\dots+i_M \le N,\quad i = 0,\dots,P,\quad P = \frac{(M+N)!}{M!N!} - 1$$

- Method generates new coupled spatial-stochastic nonlinear problem:

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

$$\left(\frac{\partial F}{\partial U}\right)_{i,j} = \frac{\partial F_i}{\partial u_j} = \frac{1}{\langle\psi_i^2\rangle}\int_\Gamma \frac{\partial f}{\partial u}(\hat{u}(y),y)\psi_i(y)\psi_j(y)\rho(y)dy \approx \sum_{k=0}^{P} J_k\frac{\langle\psi_i\psi_j\psi_k\rangle}{\langle\psi_i^2\rangle},$$

$$\frac{\partial f}{\partial u}(\hat{u}(y),y) \approx \sum_{k=0}^{P} J_k\psi_k(y),\ J_k = \frac{1}{\langle\psi_k^2\rangle}\int_\Gamma \frac{\partial f}{\partial u}(\hat{u}(y),y)\psi_k(y)\rho(y)dy$$



Stochastic sparsity — Spatial sparsity

Challenges: Computing SG residual/Jacobian coefficients and solving resulting SG systems

Stokhos: Trilinos Tools for Embedded SG Methods

- Eric Phipps, Ramakrishna Tipireddy (USC), Chris Miller (Maryland), Habib Najm (SNL), Bert Debusschere (SNL), Omar Knio (Johns Hopkins)
- Overloaded operators for TBGP-based embedded PC propagation (see below)
  - –Sacado: Trilinos AD tools for C++ applications
  - –Hooks to UQToolkit of Najm *et al* for Taylor, integration-based approaches
  - –Hooks to Burkardt sparse grid quadrature libraries through DAKOTA/PECOS
- Tools for forming/solving SG linear/nonlinear systems
  - –Block product vectors, multi-vectors, and matrices
  - –"Matrix free" block SG operator

$$\frac{\partial F_i}{\partial u_j} \approx \sum_{k=0}^{P} J_k\frac{\langle\psi_i\psi_j\psi_k\rangle}{\langle\psi_i^2\rangle} \implies \left(\frac{\partial F}{\partial U}V\right)_i = \sum_{j=0}^{P}\sum_{k=0}^{P} J_k v_j\frac{\langle\psi_i\psi_j\psi_k\rangle}{\langle\psi_i^2\rangle}$$

  - –Distributed memory parallelism (MPI) over spatial and stochastic degrees-of-freedom
  - –Hooks to Trilinos parallel, iterative linear solvers & preconditioners
  - –Customized SG block solver, preconditioning methods (see below)
- Nonlinear SG application code interface
  - –Interface to nonlinear solver, time integrator, optimizer, …

Enables study of intrusive methods in complex simulation codes

Embedded PC Propagation through Template-Based Generic Programming

- Foundation in automatic differentiation (AD) techniques
  - –AD relies on known derivative formulas for all intrinsic operations plus chain rule:

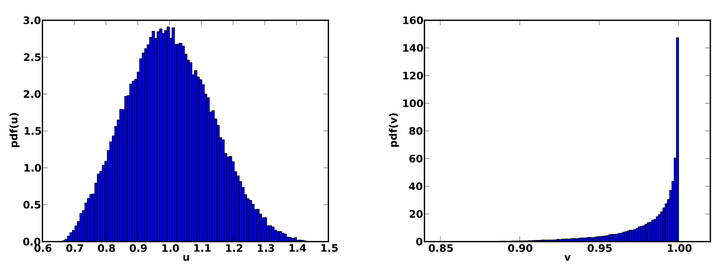
$$c = a * b \implies dc = da * b + a * db$$

  - –Principle applies to all kinds of calculations:
    - Jacobians, directional derivatives, Hessians, adjoints, Taylor series, …
    - Sparsity patterns, extended precision, flop counts, bounding intervals, …
  - –Similar approach possible for SG expansion, e.g.,

$$a = \sum_{i=0}^{P} a_i\psi_i,\ b = \sum_{j=0}^{P} b_j\psi_j,\ c = ab \approx \sum_{k=0}^{P} c_k\psi_k,\ c_k = \sum_{i,j=0}^{P} a_i b_j\frac{\langle\psi_i\psi_j\psi_k\rangle}{\langle\psi_k^2\rangle}$$

  - –Transcendental operations more difficult (see Debusschere *et al*, 2004)
    - Taylor series (simple but not robust), line integration (robust but expensive)
    - Sparse grid quadrature (simple and robust)
- Implement in C++ codes through classing, operator overloading, and templating
  - –Sacado: Trilinos AD tools for C++ applications
  - –Pawlowski, *et al*, 2011

```
#include "Stokhos_Sacado.hpp"

// The function to compute the polynomial chaos expansion of, written as a template function
template <class ScalarType>
inline ScalarType simple_function(const ScalarType& u) {
  return 1.0/(std::pow(std::log(u),2.0) + 1.0);
}

// Typename of PC expansion type
typedef Sacado::PCE::OrthogPoly<double, Stokhos::StandardStorage<int,double> > pce_type;

int main(int argc, char **argv) {

    // Basis of dimension 3, order 5
    const int d = 3; const int p = 5;
    Teuchos::Array< Teuchos::RCP<const Stokhos::OneDOrthogPolyBasis<int,double> > > bases(d);
    for (int i=0; i<d; i++) {
      bases[i] = Teuchos::rcp(new Stokhos::LegendreBasis<int,double>(p));
    }
    Teuchos::RCP<const Stokhos::CompletePolynomialBasis<int,double> > basis =
      Teuchos::rcp(new Stokhos::CompletePolynomialBasis<int,double>(bases));

    // Quadrature method
    Teuchos::RCP<const Stokhos::Quadrature<int,double> > quad =
      Teuchos::rcp(new Stokhos::TensorProductQuadrature<int,double>(basis));

    // Triple product tensor
    Teuchos::RCP<Stokhos::Sparse3Tensor<int,double> > Cijk =
      basis->computeTripleProductTensor(basis->size());

    // Expansion method
    Teuchos::RCP<Stokhos::QuadOrthogPolyExpansion<int,double> > expn =
      Teuchos::rcp(new Stokhos::QuadOrthogPolyExpansion<int,double>(
                                        basis, Cijk, quad));

    // Polynomial expansions
    pce_type u(expn);
    u.term(0,0) = 1.0;
    for (int i=0; i<d; i++) {
      u.term(i,1) = 0.4 / d; u.term(i,2) = 0.06 / d; u.term(i,3) = 0.002 / d;
    }

    // Compute PCE expansion of function
    pce_type v = simple_function(u);
```



Simplifies incorporation of SG methods in complex code

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4. **R.P. Pawlowski, E.T. Phipps, and A.G. Salinger, S.J. Owen, C. Seifert and M.L. Staten, "Applying template-based generic programming to the simulation and analysis of partial differential equations," submitted to Journal of Scientific Programming, 2011**
5. **R. Tipireddy, E.T. Phipps, and R.G. Ghanem, "A comparison of solution methods for stochastic partial differential equations," submitted to International Journal of Computer Mathematics, 2011.**
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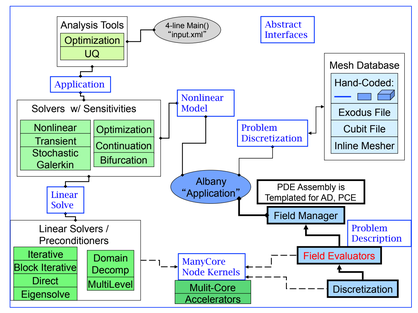
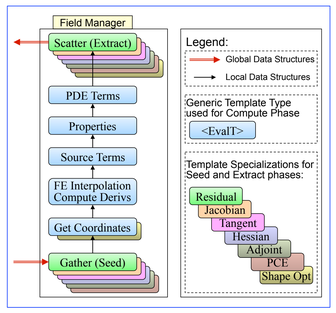
Albany Agile Components Demonstration Application

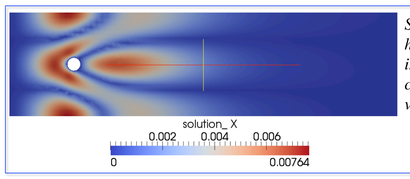
(Salinger – PI)

- Brings together numerous Trilinos tools in fully functional application code
  - –Finite element discretizations of 1, 2, and 3D PDEs on unstructured meshes
- Fully integrates template-based generic programming approach
  - –Templated finite element residual calculation
  - –Analytic derivatives, sensitivities with Sacado
  - –Intrusive polynomial chaos expansions with Stokhos
  - –Pawlowski, *et al*, 2011





- Rapid development of complex physics
  - –Incompressible Navier-Stokes (Salinger)
  - –Neutronics (Phipps)
  - –Linear and nonlinear elasticity (Ostien)
  - –Quantum device modeling (Muller)



Standard deviation of horizontal fluid velocity for incompressible flow around a cylinder with uncertain viscosity field

Rapid development of complex physics supporting advanced analysis

New Block Preconditioning Methods for SG Discretizations

$$\bar{P}X = B \implies X = \bar{P}^{-1}B$$

- Traditional mean-based preconditioning (e.g., Elman *et al*, 2010)

$$P_0 \approx J_0,\quad \bar{P} = I \otimes P_0 \implies x_i = (\bar{P}^{-1}B)_i = P_0^{-1}b_i,\quad i = 0,\dots,P$$

- Kronecker-product precondtioner (Ullman, 2010)

$$\bar{P} = G\otimes P_0,\quad G = \sum_{k=0}^{P}\frac{\mathrm{tr}(J_k^T J_0)}{\mathrm{tr}(J_0^T J_0)}G_k,\quad G_k(i,j) = \frac{\langle\psi_i\psi_j\psi_k\rangle}{\langle\psi_i^2\rangle},\quad i,j,k = 0,\dots,P$$

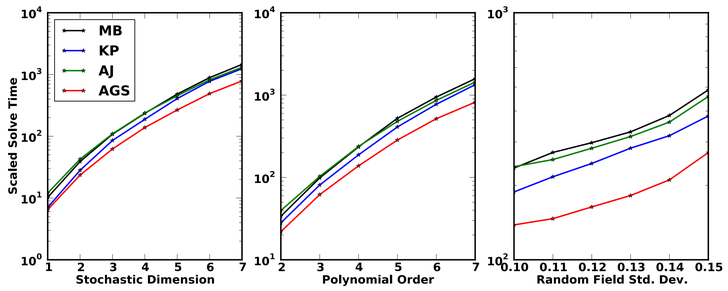
- Approximate Jacobi (Tipireddy *et al*, 2011)

$$x_i^{(l+1)} = P_0^{-1}\left(b_i - \sum_{j=0}^{P}\sum_{k=1}^{P} J_k x_j^{(l)}\frac{\langle\psi_i\psi_j\psi_k\rangle}{\langle\psi_i^2\rangle}\right),\quad i = 0,\dots,P,\quad l = 1,2$$

- Approximate Gauss-Seidel (Tipereddy *et al*, 2011)

$$x_i^{(l+1)} = P_0^{-1}\left(b_i - \sum_{j=0}^{l}\sum_{k=1}^{P} J_k x_j^{(l+1)}\frac{\langle\psi_i\psi_j\psi_k\rangle}{\langle\psi_i^2\rangle} - \sum_{j=l+1}^{P}\sum_{k=1}^{P} J_k x_j^{(l)}\frac{\langle\psi_i\psi_j\psi_k\rangle}{\langle\psi_i^2\rangle}\right),$$
$$i = 0,\dots,P,\quad l = 1$$

- 2-D linear diffusion equation with uniform random field (exponential covariance) diffusion coefficient:



Simple ideas, but significant improvement over existing approaches

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