Stokhos: Trilinos Tools for Embedded Stochastic-Galerkin Uncertainty Quantification Methods

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Models of Uncertainty

- Predictive simulation means making a rigorous statement about the world based on computational simulation
  - Must understand uncertainty in simulation input data and its effects on simulations
- Two broad classes of uncertainty
  - Aleatory or irreducible uncertainty: "inherent randomness"
    - Probabilistic representations (random variables, stochastic processes)
  - Epistemic or reducible uncertainty: "lack of knowledge"
    - Set/knowledge representations (intervals, fuzzy sets, evidence theory)
    - Probabilistic representations (Bayesian point of view)
- Two basic sources of uncertainty
  - Finite-dimensional simulation parameters
    - Represented through random variables/vectors with given distributions
  - Infinite-dimensional correlated random fields/stochastic processes
    - Realizations often smoothly varying in time/space; allows representation with small number of random variables/vectors (e.g., Karhunen-Loeve representation)
- Assume a finite dimensional representation given by random variables/vectors with known probability distributions
  - Generating such models is a research area in its own right

Stochastic Galerkin Uncertainty Quantification Methods
(More Commonly Known as Polynomial Chaos Methods)

- Deterministic, steady-state problem (possibly after spatial discretization):

  Find $u(p)$ such that $F(u;p) = 0$, $p \in \Gamma \subset \mathrm{R}^M$

- Stochastic problem:

  Find $u(\xi)$ such that $F(u;\xi) = 0$, $\xi : \Omega \rightarrow \Gamma$, density ρ

- Let Z be a finite-dimensional subspace of $L^2_\rho(\Gamma)$ with basis $\{\psi_i : i = 0, \ldots, N_{PC}\}$ orthogonal with respect to inner product

$$\langle fg \rangle \equiv \int_\Gamma f(y)g(y)\rho(y)dy$$

- Stochastic Galerkin method (Ghanem, …):

$$\hat{u}(\xi) = \sum_{i=0}^{N_{PC}} u_i \psi_i(\xi) \in Z \rightarrow F_i(u_0, \ldots, u_{N_{PC}}) = \int_\Gamma F(\hat{u}(y); y)\psi_i(y)\rho(y)dy = 0, \quad i = 0, \ldots, N_{PC}$$

- Typically Z is the complete polynomial space of total degree P, basis polynomials are tensor products of 1-D polynomials orthogonal with respect to 1-D density of each random parameter
  - Assumes independence of random parameters
  - Gaussian random variables -- Hermite polynomials
  - Uniform random variables -- Legendre polynomials, …
- Exponential convergence in P when solution is sufficiently smooth

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Stochastic Galerkin Nonlinear System

- Method generates new coupled spatial-stochastic nonlinear problem

$$0 = \bar{F}(\bar{u}) = \begin{bmatrix} F_0 \\ F_1 \\ \vdots \\ F_{N_{PC}} \end{bmatrix}, \quad \bar{u} = \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_{N_{PC}} \end{bmatrix}$$

- Dimension grows rapidly with degree or dimension

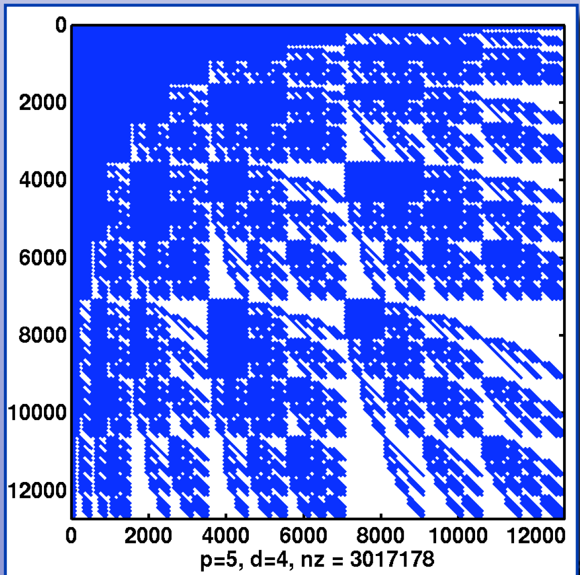
$$N_{PC} = \frac{(M+P)!}{M!P!}$$

Stochastic dimension M	Polynomial degree P	Number of terms N_{PC}
5	3	56
	5	252
10	3	286
	5	3003
20	3	1,771
	5	~53,000
100	3	~177,000
	5	~96,000,000

- System Jacobian:

$$\hat{J}(\xi) = \sum_{k=0}^{N_{PC}} J_k \psi_k(\xi) \rightarrow J_k = \frac{1}{\langle \psi_k^2 \rangle} \int_\Gamma \frac{\partial F}{\partial u}(\hat{u}(y); y) \psi_k(y) \rho(y) dy$$

$$\frac{\partial F_i}{\partial u_j} \approx \sum_{k=0}^{N_{PC}} J_k \langle \psi_i \psi_j \psi_k \rangle$$



Implementing SG Methods in Nonlinear Applications is Challenging

- Code transformation from deterministic code to SG code
  - Need tools/libraries to automate computation of SG residual and Jacobian entries

$$F(u;p) = 0 \rightarrow \bar{F}(\bar{u}) = \begin{bmatrix} F_0 \\ F_1 \\ \vdots \\ F_{N_{PC}} \end{bmatrix} = 0$$

- Data structures & interfaces for forming block SG systems
  - Linear, nonlinear, transient, optimization, stability, …

- Solver algorithms for block SG systems
  - Exploit new dimensions of parallelism
  - "Jacobian-free" methods are key

$$\frac{\partial F_i}{\partial u_j} \approx \sum_{k=0}^{N_{PC}} J_k \langle \psi_i \psi_j \psi_k \rangle \implies \left(\frac{\partial \bar{F}}{\partial \bar{u}} \bar{v} \right)_i = \sum_{j,k=0}^{N_{PC}} J_k v_j \langle \psi_i \psi_j \psi_k \rangle$$

- Trilinos provides powerful capabilities here

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SG Code Transformation Through Automatic Differentiation (AD)

- Trilinos package Sacado provides AD capabilities to C++ codes
  - AD data types & overloaded operators
  - Replace scalar type in application with Sacado AD data types

- AD relies on known derivative formulas for all intrinsic operations plus chain rule

- AD infrastructure provides deep interface into application code
  - Access to scalar-level computations in application

- Similar approach can be used for any computation that can be done in an operation by operation manner
  - Assume inductively that SG expansions for two intermediate variables *a* and *b* have been computed, and we wish to compute a third *c* = φ*(a,b)*

Given $\hat{a}(\xi) = \sum_{i=0}^{N_{PC}} a_i \psi_i(\xi)$, $\hat{b}(\xi) = \sum_{i=0}^{N_{PC}} b_i \psi_i(\xi)$, Find $\hat{c}(\xi) = \sum_{i=0}^{N_{PC}} c_i \psi_i(\xi)$ such that

$$\int_\Gamma (\hat{c}(y) - \varphi(\hat{a}(y), \hat{b}(y)))\psi_i(y)\rho(y)dy = 0, \quad i = 0, \ldots N_{PC}$$

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SG 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
  - Implemented in Fortran library by Najm, Debusschere, Ghanem, Knio

- These ideas allow the implementation of Sacado “AD” types for intrusive stochastic Galerkin methods
  - Easy transition once code is setup to use AD

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Other Trilinos Tools Useful for SG Methods

- Epetra -- MPI-based vector/matrix data structures & operator interfaces
  - Used by application codes to form FE residuals, Jacobians
- Thyra -- Abstract vector, operator, and nonlinear interfaces
  - Product vectors for representing block SG solution/residual vectors

$$\bar{F}(\bar{u}) = \begin{bmatrix} F_0 \\ F_1 \\ \vdots \\ F_P \end{bmatrix}, \quad \bar{u} = \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_P \end{bmatrix} \qquad (\bar{J}\bar{v})_i = \sum_{j,k=0}^{P} \langle \psi_i \psi_j \psi_k \rangle J_k v_j$$

  - Operators implementing SG matrix-vector-product in "matrix-free" fashion
  - Nonlinear interface transforming deterministic Thyra interface into SG
- AztecOO, Belos, Ifpack, ML -- Linear solvers and preconditioners
  - Advanced linear solver techniques optimized for block SG structure
- Zoltan, Isorropia -- Graph partitioning & reordering
  - Partitioning, reordering of block SG linear system
- NOX, LOCA, Rythmos -- Nonlinear solver & time integration algorithms
  - Use nonlinear Thyra SG interface to solve steady & transient SG problems

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Trilinos Package Stokhos

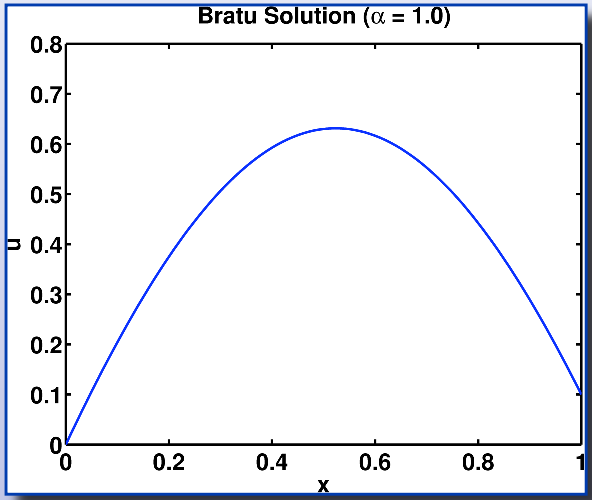
- These ideas form the basis for a new Trilinos package called Stokhos
  - Collaborative effort among the SG/PCE community to develop tools for large-scale codes
- Initial thoughts are Stokhos will provide (or push development of)
  - SG vector/operator interfaces
  - Nonlinear SG application interface
  - Solver/preconditioner algorithms
  - Intrusive propagation methods
- Currently it only has
  - General facilities for intrusive propagation
  - Wrappers around UQLib library of Najm, Debusschere, Ghanem & Knio
  - Sacado wraps these for AD SG/PCE
    - Sacado::PCE::OrthogPoly<double>
- Sacado::FEApp
  - Example 1D finite element code demonstrating AD
  - Initial implementation of SG interfaces using Epetra & EpetraExt

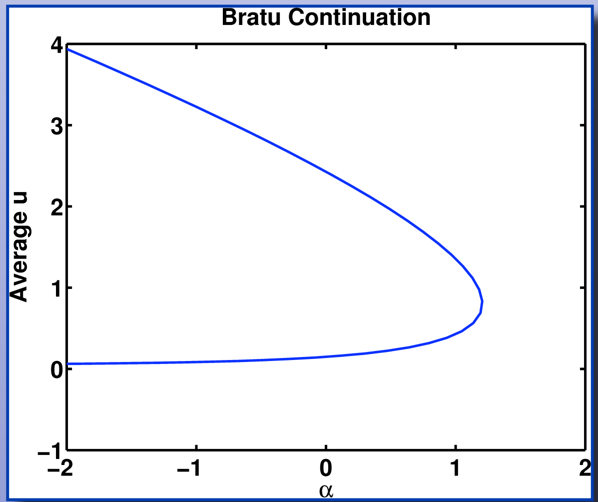
Sacado::FEApp Demonstration of Intrusive SG using Stokhos & Sacado

- 1-D Bratu problem:

$$\frac{\partial^2 u}{\partial x^2} + e^{(\alpha_1 + \cdots + \alpha_M)/M} e^u = 0, \quad 0 \le x \le 1$$

- Linear finite element discretization, 100 elements
- Uniform random variables for nonlinear factor over [-1, 1] using Legendre polynomials
- SG residual/Jacobian entries computed through Sacado
- "Jacobian free" linear solver method using Ifpack RILU(0) of mean block for preconditioner
- Solution mean used as quantity of interest





Intrusive SG Compared to Non-Intrusive Polynomial Chaos (NIPC)

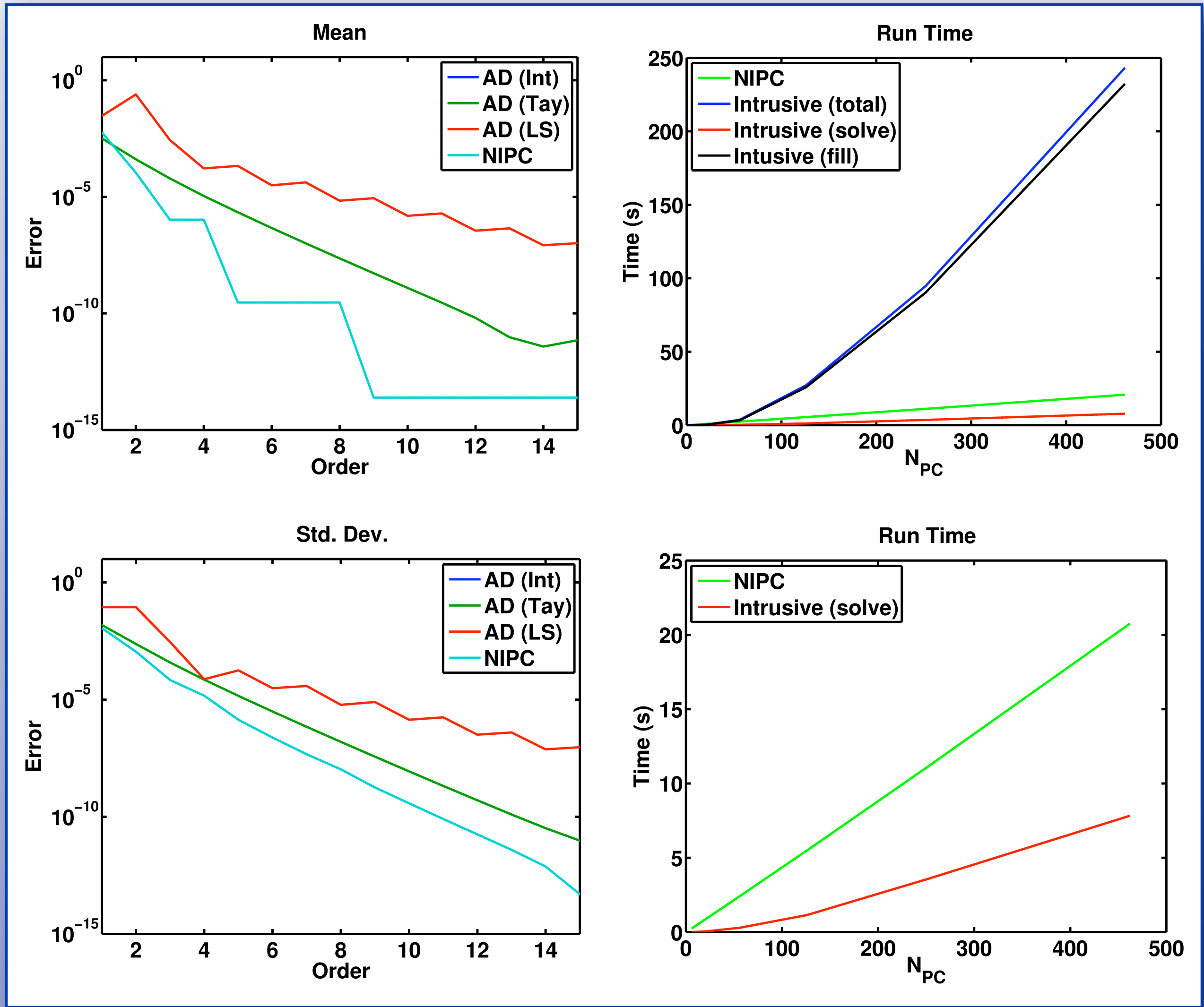
Non-Intrusive Polynomial Chaos
- Dakota
- Sparse-grid quadrature

$$\hat{u}(\xi) = \sum_{i=0}^{N_{PC}} u_i \psi_i(\xi)$$

$$u_i = \frac{1}{\langle \psi_i^2 \rangle} \int_\Gamma u(y)\psi_i(y)\rho(y)dy$$

$$\approx \frac{1}{\langle \psi_i^2 \rangle} \sum_{k=0}^{N_Q} w_k u_k \psi_i(y_k)$$

$$F(u_k; y_k) = 0, \quad k = 0, \dots, N_Q$$



Results Motivate Quadrature Approach for Element-Based Codes

$$F(u;p) = \sum_{j=0}^{N_E} Q_j^T f_j(P_k u; p)$$

- Evaluate via quadrature for globally assembled residual

$$F_i = \int_\Gamma F(\hat{u}(y); y)\psi_i(y)\rho(y)dy \approx \sum_{k=0}^{N_Q} w_k F(\hat{u}(y_k); y_k)\psi_i(y_k)$$

  – Requires parallel quadrature routines but only interface to global residual

- Apply quadrature for each element residual then assemble

$$F_i = \sum_{j=0}^{N_E} Q_j^T \int_\Gamma f_j(P_j\hat{u}(y); y)\psi_i(y)\rho(y)dy \approx \sum_{j=0}^{N_E} Q_j^T \left(\sum_{k=0}^{N_Q} w_k f_j(P_j\hat{u}(y_k); y_k)\psi_i(y_k) \right)$$

  – Requires only serial quadrature routines but needs element-level interface
  – Boundary conditions add complexity

- Jacobian decomposes similarly

- Speed of quadrature residual/Jacobian fills + benefits of intrusive solve

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What We're Working on

- SG residual/Jacobian fills
  - Sparse quadrature (Dakota)
  - Can the AD approach be improved?
- Linear solver/preconditioner methods for block SG linear systems
  - Multi-level, incomplete factorization methods?
- Stokhos software tools
  - Trilinos/Dakota integration
  - Thyra interfaces
  - Coordination with Najm, *et al* on UQLib development
- Demonstration/investigation in real apps
  - Charon, Albany
- Release Stokhos with Trilinos 10

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