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"
  - Epistemic or reducible uncertainty: "lack of knowledge"
- Two basic sources of uncertainty
  - Finite-dimensional simulation parameters
  - Infinite-dimensional correlated random fields/stochastic processes
- 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

(AKA Polynomial Chaos, Spectral Galerkin, Stochastic Finite Elements)

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

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

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

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

- Stochastic Galerkin method (Ghanem, …):

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

- *Typically* basis polynomials are tensor products of 1-D orthogonal polynomials of total degree *N*
  - Assumes independence of random parameters
  - Named polynomials for common densities (Hermite, Legendre, …)
  - Polynomials can be generated numerically for any density (Gautschi)

- Exponential convergence in *N* when solution is sufficiently smooth

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Stochastic Galerkin Nonlinear System

- Method generates new coupled spatial-stochastic nonlinear problem

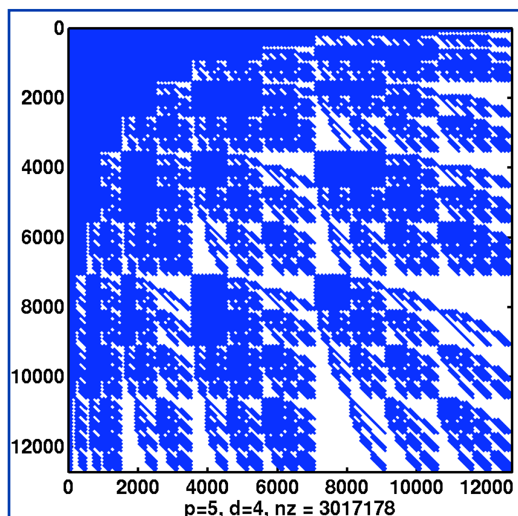
$$0 = F(U) = \begin{bmatrix} F_0 \\ F_1 \\ \vdots \\ F_P \end{bmatrix}, \quad U = \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_P \end{bmatrix}$$

- Dimension grows rapidly with degree or dimension

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

Stochastic dimension M	Polynomial degree N	Number of terms P
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

- Block system Jacobian:



Trilinos Package Stokhos

- Tools for generating SG residual and Jacobian entries
  - Automatic differentiation with Sacado

$$F_i = \int_\Gamma f(\hat{u}(y), y)\psi_i(y)\rho(y)dy, \quad \langle \cdot \rangle = \int_\Gamma \cdot\, \rho(y)dy$$

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

- Nonlinear SG application code interface through EpetraExt::ModelEvaluator
  - New In/Out Args for SG expansions (x_sg, xdot_sg, f_sg, W_sg, …)
  - ModelEvaluator that implements calculation of SG in/out args via quadrature
  - ModelEvaluator adaptor translating SG expansion to block nonlinear problems using EpetraExt::BlockVector, etc… (f_sg --> block f)

- Epetra operators for solving block SG linear systems
  - Jacobian-free operator with mean-based preconditioning, and fully assembled Jacobian

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

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Generating SG Residual/Jacobian Entries Through Automatic Differentiation (AD)

- Trilinos package Sacado provides AD capabilities to C++ codes
  - AD relies on known derivative formulas for all intrinsic operations plus chain rule
  - AD data types & overloaded operators
  - Replace scalar type in application with Sacado AD data types

- Similar approach can be used to apply SG projections in an operation by operation manner

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

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

  - Simple formulas for addition, subtraction, multiplication, division
  - Transcendental operations are more difficult
    - Taylor series and time integration (Fortran UQ Toolkit by Najm, Debusschere, Ghanem, Knio)
    - Tensor product and sparse-grid quadrature (Dakota)

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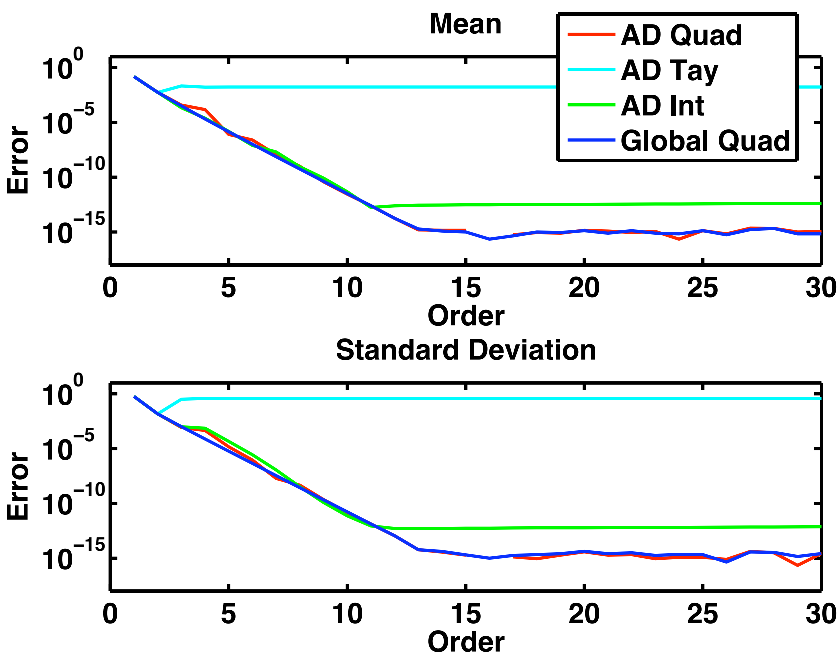
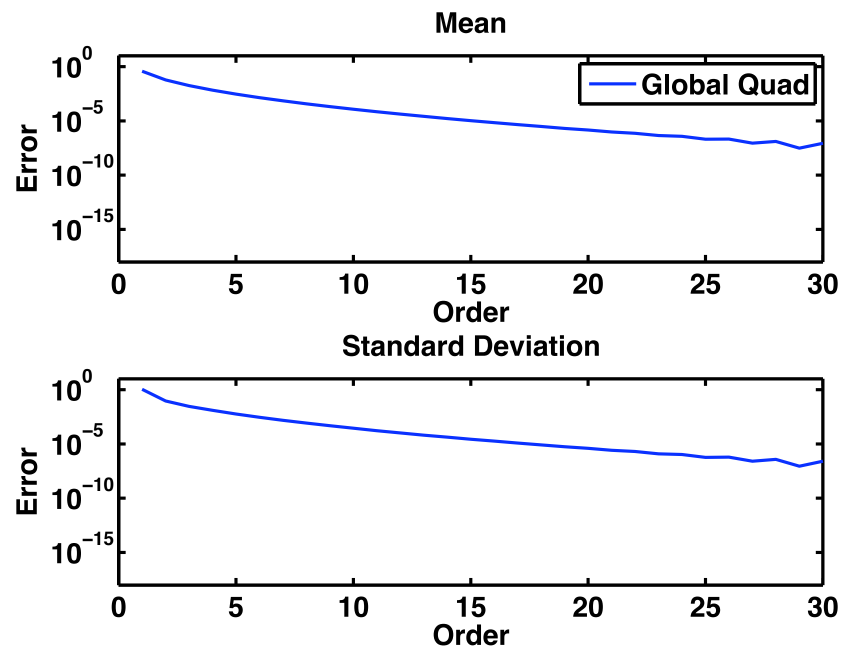
AD Approach Generally Works Well

$$u = \log\left(\frac{1}{1+(e^x)^2}\right)$$

Uniform U(-1,1) x



Gaussian N(0,1) x



All 3 AD approaches fail

- AD approach is usually accurate
- Truncation error *can* cause catastrophic failure

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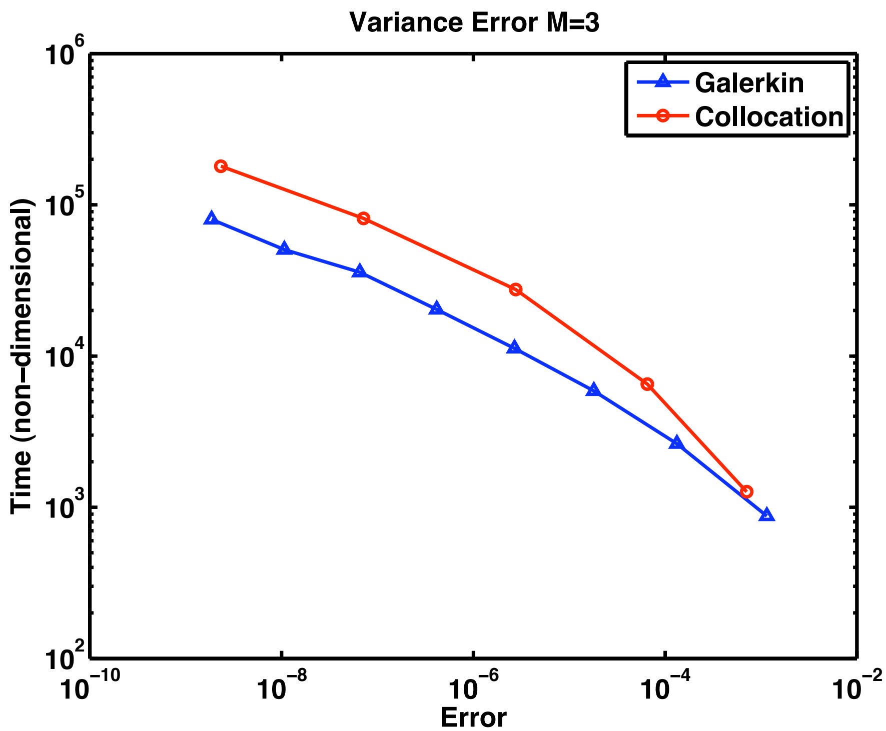
2-D Linear Diffusion Problem

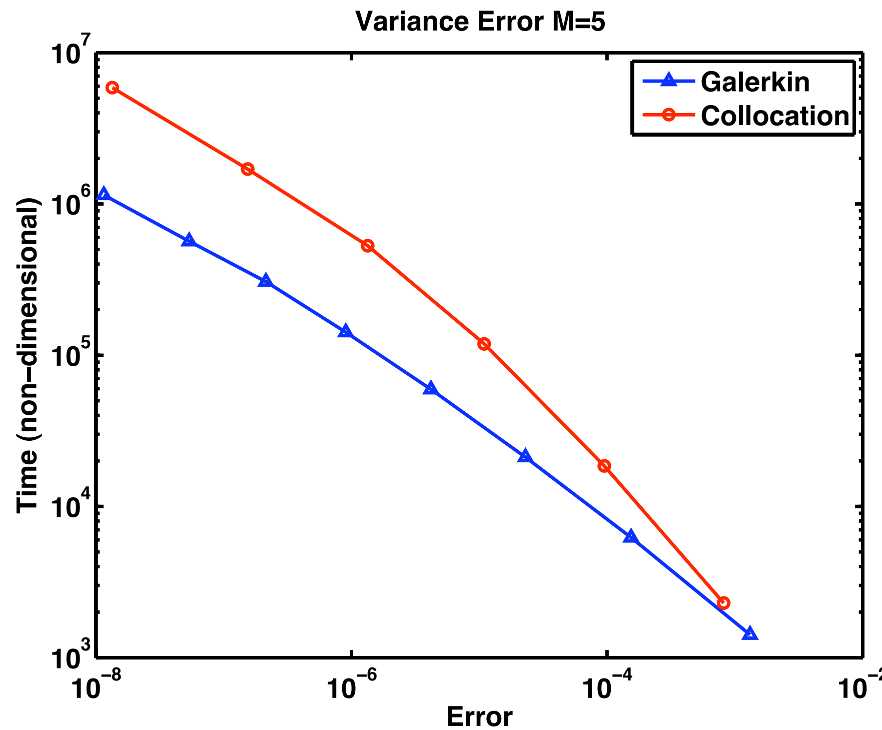
(Chris Miller – 2009 CSRI Summer Student & Ray Tuminaro)

$$-\nabla \cdot (a(x,\xi)\nabla u) = 1$$

$$a(x,\xi) = \mu + \sigma \sum_{k=1}^{M} \sqrt{\lambda_k} f_k(x)\xi_k$$

- 2-D finite difference discretization
- ML multi-level mean preconditioner
- Exponential covariance kernel
- Truncated Gaussian random variables (Rys polynomials)

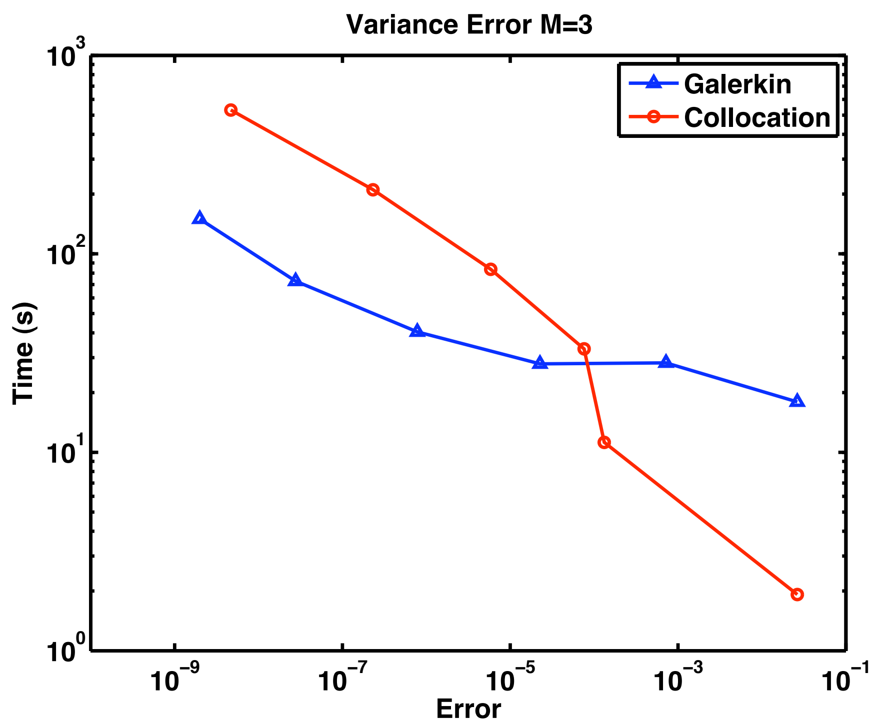


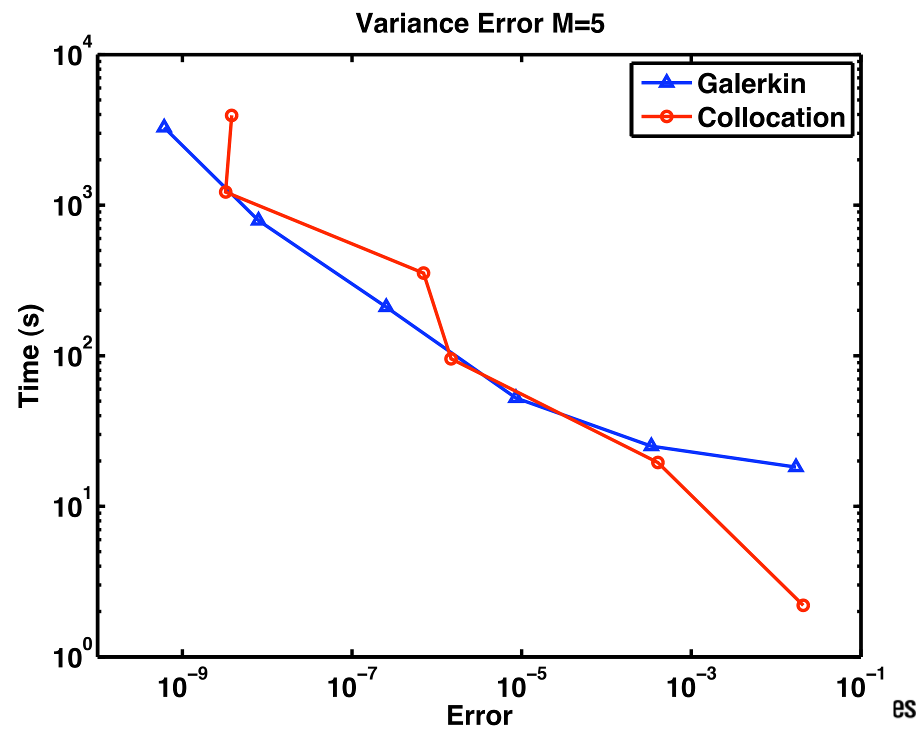


2-D Nonlinear Diffusion Problem

$$\nabla^2 u + \frac{\alpha_1 + \cdots + \alpha_M}{M} u^2 = 0$$

- New Albany code (Salinger *et al*)
- 2-D finite element discretization
- RILU mean preconditioner
- Uniform random variables (Legendre polynomials)





Summary of Stokhos Capabilities

- Stokhos provides a complete set of tools for stochastic Galerkin UQ problems
  - Sacado overloaded operators for generating SG residual/Jacobian entries via AD
  - Nonlinear application code interface for SG nonlinear problems (EpetraExt)
  - Operators and preconditioners for SG linear systems (Epetra)

- Optional third-party libraries
  - Fortran UQ toolkit for Taylor/time integration approaches for SG expansion
  - Dakota for sparse-grid quadrature (brought in through TriKota)

- Demonstration provided by Sacado's FEApp

- Stokhos is fully functional, but still primarily a research tool
  - Dakota provides robust UQ capabilities

What We're Working on

- Software
  - Building Stokhos capabilities from PECOS
  - Thyra interfaces

- Algorithmic
  - Linear solver/preconditioner methods for block SG linear systems
  - Reducing high linear solve cost for nonlinear problems
  - Stochastic Galerkin methods for multi-physics systems

- Continuing investigation in target applications
  - Charon, Albany

- Finishing the release
  - Internal for Trilinos 10
  - External once copyright is completed (3 months and counting!)