Intrusive Stochastic Galerkin Methods for Uncertainty Quantification of Nonlinear Stochastic PDEs

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Intrusive Stochastic Galerkin Uncertainty Quantification Methods

- **Steady-state stochastic problem:**

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

- **Stochastic Galerkin method, specifically, (Generalized) Polynomial Chaos:**

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

- **Method generates new coupled spatial-stochastic nonlinear problem:**

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

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

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

Stokhos: Trilinos Tools for Intrusive Stochastic Galerkin UQ Methods

- Eric Phipps, Chris Miller, Habib Najm, Bert Debusschere, Omar Knio

- AD overloaded operators for automatic SG propagation
  - Sacado: Trilinos AD tools for C++ applications

- Tools for solving SG linear systems
  - Hooks to Trilinos parallel iterative linear solvers & preconditioners
  - Jacobian-free (Ghanem) or fully assembled SG matrix-vector product
  - Mean-based preconditioning (so far)

- Nonlinear SG application code interface
  - Interface to nonlinear solver, time integrator, optimizer

- Enabling study of intrusive methods in complex simulation codes

http://trilinos.sandia.gov

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

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

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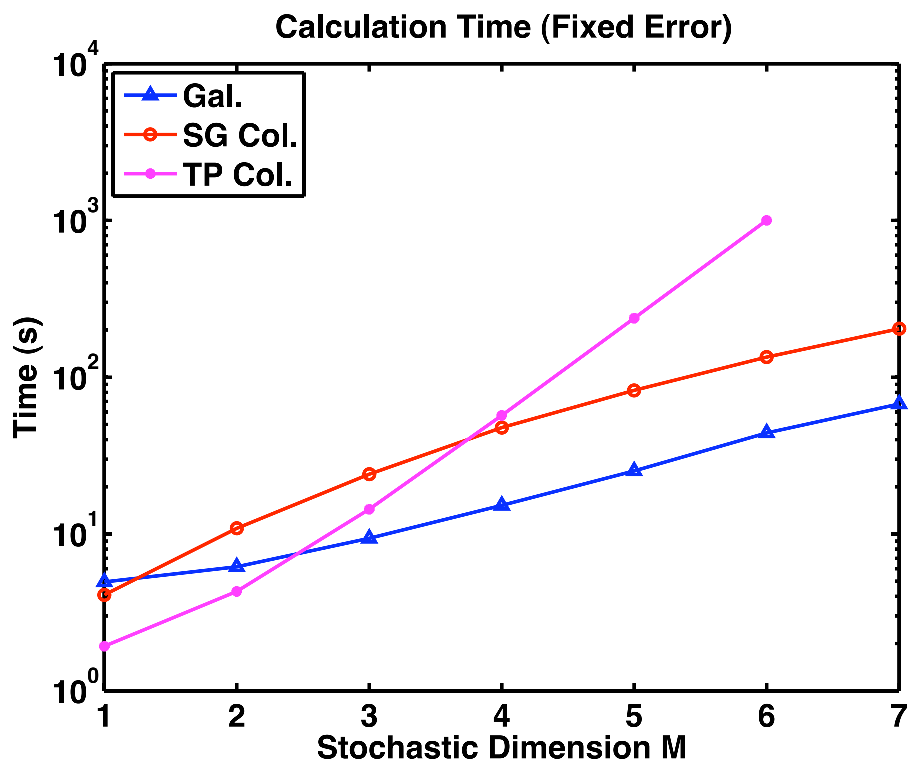
Comparing Linear and Nonlinear PDEs

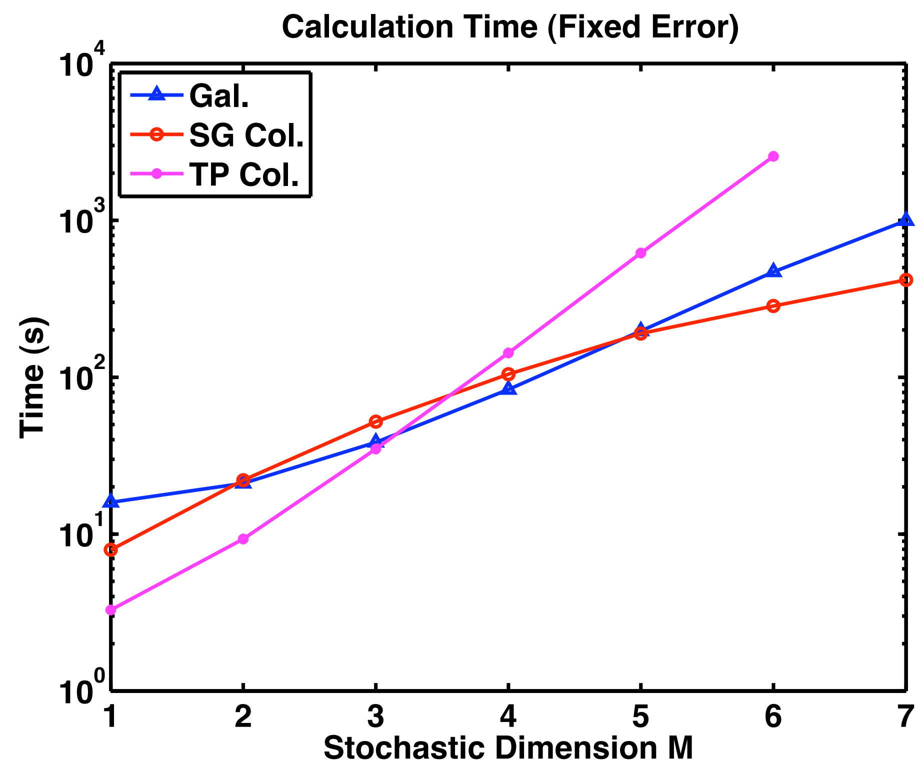
$$-\nabla \cdot (a(x,\xi)\nabla u) = 1,\ x \in [0,1]\times[0,1]$$

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

$$-\nabla \cdot (a(x,\xi)\nabla u) = \alpha u^2,\ x \in [0,1]\times[0,1]$$

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





DAKOTA tensor product (Gauss-Legendre) and sparse grid stochastic collocation (Gauss-Patterson, Burkardt/Eldred)

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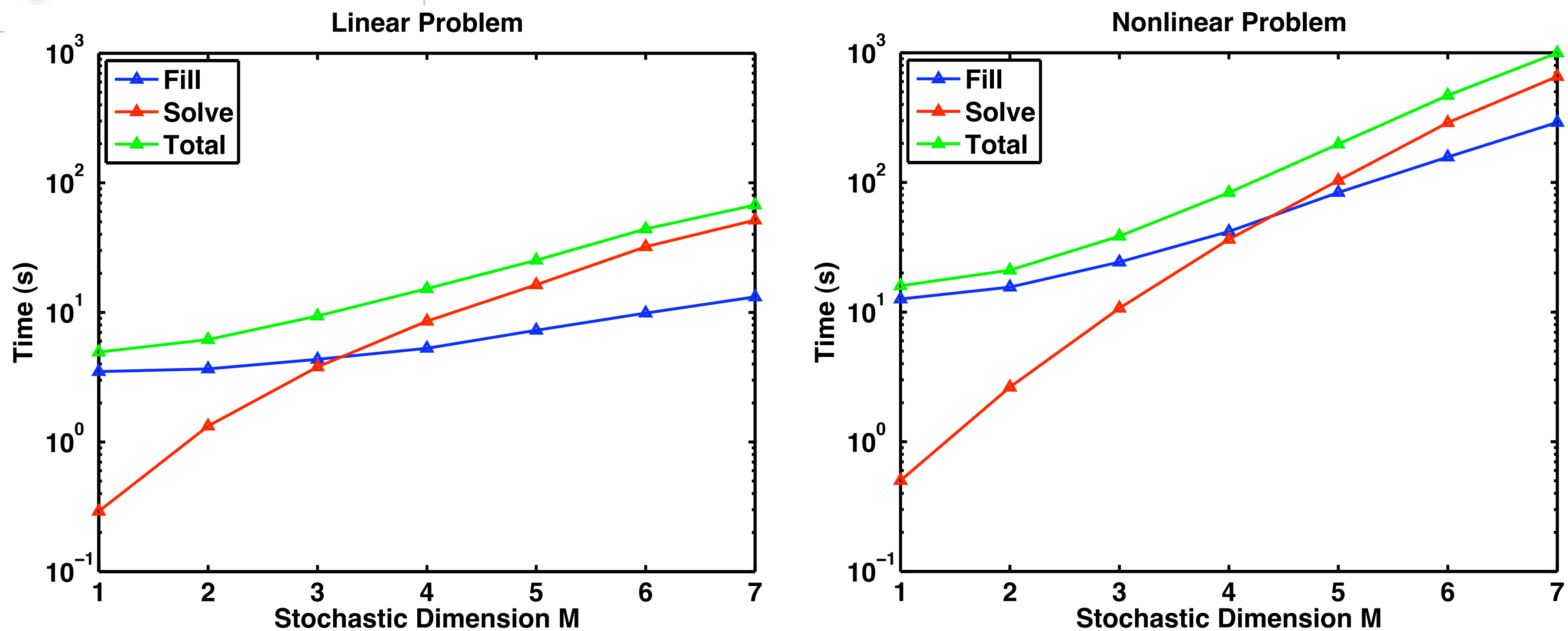
Analysis of Intrusive SG Computational Cost



- **Increased cost due to two sources**
  - **Filling nonlinear SG residual and Jacobian**
  - **Linear solve for each Newton iteration**
    Matrix-vector product scales as $O(P^2)$ versus $O(MP)$

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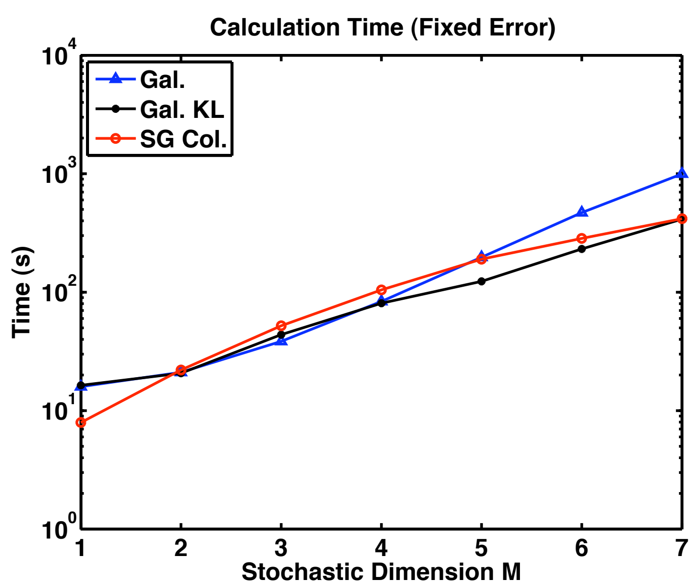
KL Expansion of SG Jacobian Operator

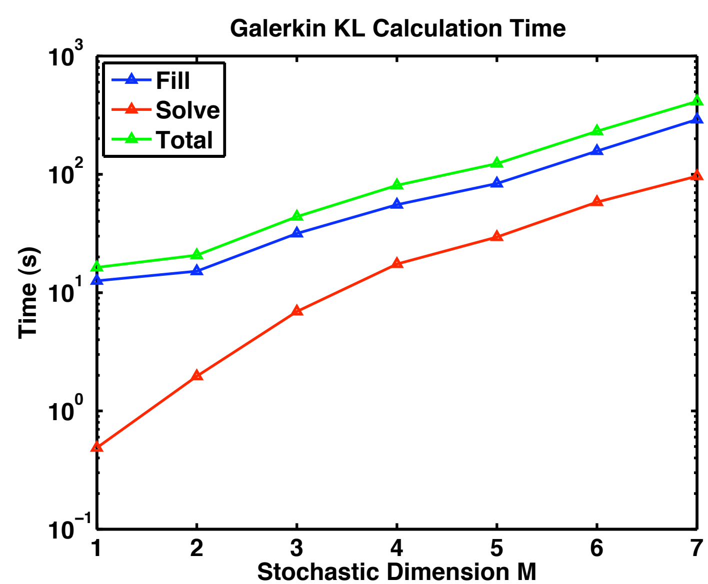
- **SG Jacobian operator can be approximated by a truncated KL expansion:**

$$\frac{\partial f}{\partial u}(\hat{u}(\xi),\xi) \approx \sum_{k=0}^{P} J_k \psi_k(\xi) \approx J_0 + \sum_{j=1}^{\bar{M}} \sqrt{\lambda_j} B_j \eta_j$$

$$\eta_j = \frac{1}{\sqrt{\lambda_j}} \sum_{k=1}^{P} \mathrm{vec}(B_j)^T \mathrm{vec}(J_k)\psi_k(\xi), \quad (ZZ^T)\mathrm{vec}(B_j) = \lambda_j \mathrm{vec}(B_j), \quad Z = [\mathrm{vec}(J_1)\ldots\mathrm{vec}(J_P)]$$

- **Reduces matrix-vector product cost to** $\sim O(\bar{M}P)$





Concluding Remarks

- **Intrusive approach seems to work well for linear problems**
  - **Need to do larger (stochastic) problems**
  - **Parallelization of linear solve is necessary for scalability to larger problems (using GMRES)**

- **KL approach appears to significantly reduce solver cost for nonlinear problems**
  - **Need to understand "stochastic dimension" of Jacobian**

- **Cost of residual/Jacobian fills for nonlinear problems is a significant bottleneck for Galerkin approach**

- **Tools/techniques publicly available through Stokhos/ Trilinos**
  - **http://trilinos.sandia.gov**