Stochastic Dimension Reduction of Multiphysics Systems through Measure Transformation

Eric Phipps (etphipp@sandia.gov),
John Red-Horse, Tim Wildey
Sandia National Laboratories,

Paul Constantine – Colorado School of Mines,
Roger Ghanem – University of Southern California, and
Maarten Arnst – University of Liège, Belgium

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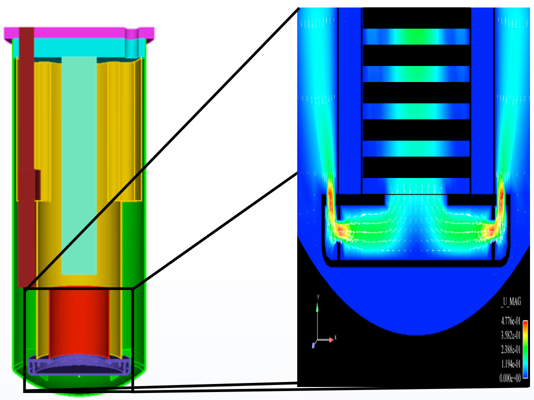
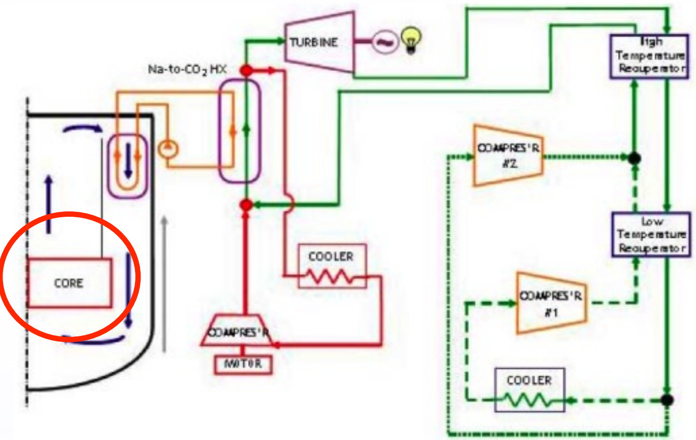
Uncertainty Quantification for Complex Coupled Systems

Network Nuclear Power Plant Model



High-fidelity Multi-physics Component Model (Core)



Low-fidelity Network Plant Model

Graphics courtesy: Rod Schmidt, BRISC project

$$\mathcal{L}_1(u_1(x), v_2) = 0, \quad v_2 = \mathcal{G}_2(u_2)$$
$$\mathcal{L}_2(v_1, u_2(x)) = 0, \quad v_1 = \mathcal{G}_1(u_1)$$

Finite Dimensional Coupled Network Systems

- Network system after discretization:

$$
\begin{aligned}
f_1(u_1, v_2) = 0, \quad & u_1 \in \mathbb{R}^{n_1}, \quad v_2 = g_2(u_2) \in \mathbb{R}^{m_2}, \quad f_1 : \mathbb{R}^{n_1+m_2} \rightarrow \mathbb{R}^{n_1} \\
f_2(v_1, u_2) = 0, \quad & u_2 \in \mathbb{R}^{n_2}, \quad v_1 = g_1(u_1) \in \mathbb{R}^{m_1}, \quad f_2 : \mathbb{R}^{m_1+n_2} \rightarrow \mathbb{R}^{n_2}
\end{aligned}
$$

$$
1 \sim m_1, m_2 \ll n_1, n_2
$$

- Variety of solution methods
  - Successive substitution (Picard, Gauss-Seidel)
  - Newton's method (Full, inexact, JFNK)
  - Nonlinear elimination:

$$
\begin{aligned}
v_1 - g_1(u_1(v_2)) = 0 \ \text{ s.t. } \ f_1(u_1, v_2) = 0 \\
v_2 - g_2(u_2(v_1)) = 0 \ \text{ s.t. } \ f_2(v_1, u_2) = 0
\end{aligned}
$$

$$
\begin{bmatrix} 1 & -dg_1/dv_2 \\ -dg_2/dv_1 & 1 \end{bmatrix} \begin{bmatrix} \Delta v_1 \\ \Delta v_2 \end{bmatrix} = - \begin{bmatrix} v_1 - g_1(u_1(v_1)) \\ v_2 - g_2(u_2(v_2)) \end{bmatrix}
$$

$$
\frac{dg_1}{dv_2} = -\frac{\partial g_1}{\partial u_1} \left(\frac{\partial f_1}{\partial u_1} \right)^{-1} \frac{\partial f_1}{\partial v_2}, \quad \frac{dg_2}{dv_1} = -\frac{\partial g_2}{\partial u_2} \left(\frac{\partial f_2}{\partial u_2} \right)^{-1} \frac{\partial f_2}{\partial v_1}
$$

Polynomial Chaos Uncertainty Propagation Framework

- Steady-state spatially finite-dimensional stochastic problem:

$$\textbf{Find } u(\xi) \textbf{ such that } f(u,\xi) = 0 \textbf{ a.e., } \xi : \Omega \to \Gamma \subset \mathbb{R}^s\textbf{, density } \rho$$

- Polynomial chaos approximation:

$$Z = \text{span}\{\Psi_i : i = 0, \dots, P\} \subset L^2_\rho(\Gamma) \to u(\xi) \approx \hat{u}(\xi) = \sum_{i=0}^{P} u_i \Psi_i(\xi)$$

- Orthogonal polynomial basis of total order at most N:

$$\langle \Psi_i \Psi_j \rangle \equiv \int_\Gamma \Psi_i(x)\Psi_j(x)\rho(x)dx = \delta_{ij}, \quad i,j = 0,\dots,P, \quad P+1 = \binom{N+s}{s}$$

- Intrusive stochastic Galerkin (SG):

$$0 = F_i(u_0,\dots,u_P) = \langle f(\hat{u}(\xi),\xi)\Psi_i(\xi)\rangle = \int_\Gamma f(\hat{u}(x),x)\Psi_i(x)\rho(x)dx = 0,\ i = 0,\dots,P$$

- Non-intrusive polynomial chaos (NIPC)/spectral projection (NISP):

$$u_i = \langle u(\xi)\Psi_i(\xi)\rangle \approx \sum_{k=0}^{Q} w_k u^k \Psi_i(\xi^k),\ f(u^k,\xi^k) = 0,\ i = 0,\dots,P,\ k = 0,\dots,Q$$

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Stochastic Coupled Network Systems

- Introduce random variables: $\xi = (\xi_1, \xi_2), \quad |\xi_1| = s_1, \quad |\xi_2| = s_2, \quad |\xi| = s = s_1 + s_2$

$$h_1(v_1, v_2, \xi) = v_1(\xi) - g_1(u_1(v_2(\xi), \xi_1), \xi_1) = 0 \quad s.t. \quad f_1(u_1(\xi), v_2(\xi), \xi_1) = 0$$
$$h_2(v_1, v_2, \xi) = v_2(\xi) - g_2(u_2(v_1(\xi), \xi_2), \xi_2) = 0 \quad s.t. \quad f_2(v_1(\xi), u_2(\xi), \xi_2) = 0$$

- Stochastic Galerkin network equations:

$$\begin{aligned} \hat{v}_1(\xi) &= \sum_{i=0}^{P} v_{1,i}\Psi_i(\xi) \\ \hat{v}_2(\xi) &= \sum_{i=0}^{P} v_{2,i}\Psi_i(\xi) \end{aligned} \quad \text{s.t.} \quad \left.\begin{aligned} H_{1,i} &\equiv \langle h_1(\hat{v}_1(\xi), \hat{v}_2(\xi), \xi)\Psi_i(\xi)\rangle = 0 \\ H_{2,i} &\equiv \langle h_2(\hat{v}_1(\xi), \hat{v}_2(\xi), \xi)\Psi_i(\xi)\rangle = 0 \end{aligned}\right\}, \quad i = 0, \ldots, P$$

- Stochastic Galerkin residual equations evaluated via NISP approach:

$$\hat{g}_1(\xi) = \sum_{i=0}^{P} g_{1,i}\Psi_i(\xi) \;\; g_{1,i} = \sum_{k=0}^{Q} w_k g_1(u_1^k, \xi_1^k)\Psi_i(\xi^k) \;\; s.t. \;\; f_1(u_1^k, \hat{v}_2(\xi^k), \xi_1^k) = 0, \;\; k = 0, \ldots, Q$$
$$\hat{g}_2(\xi) = \sum_{i=0}^{P} g_{2,i}\Psi_i(\xi) \;\; g_{2,i} = \sum_{k=0}^{Q} w_k g_2(u_2^k, \xi_2^k)\Psi_i(\xi^k) \;\; s.t. \;\; f_2(\hat{v}_1(\xi^k), u_2^k, \xi_2^k) = 0, \;\; k = 0, \ldots, Q,$$
$$H_{1,i} = v_{1,i} - g_{1,i}, \quad i = 0, \ldots, P$$
$$H_{2,i} = v_{2,i} - g_{2,i}, \quad i = 0, \ldots, P$$

- Results in SG analog of deterministic network system
  - Allows similar nonlinear elimination approach

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Curse of Dimensionality

- At each iteration of the nonlinear elimination method, we will have approximations to the coefficients

$$\hat{v}_1(\xi) = \sum_{k=0}^{P} v_{1,k}\Psi_k(\xi), \quad \hat{v}_2(\xi) = \sum_{k=0}^{P} v_{2,k}\Psi_k(\xi)$$

- Task is to then evaluate the coefficients

$$\hat{g}_1(\xi) = \sum_{k=0}^{P} g_{1,k}\Psi_k(\xi), \quad \hat{g}_2(\xi) = \sum_{k=0}^{P} g_{2,k}\Psi_k(\xi)$$

- where

$$g_1 = g_1(u_1(v_2(\xi)), \xi_1), \quad g_2 = g_2(u_2(v_1(\xi)), \xi_2)$$

- Requires solving sub-problems of larger stochastic dimensionality, e.g.,

$$\text{Solve } \; f_1(u_1^k, \hat{v}_2(\xi^k), \xi_1^k) = 0 \; \text{ for } \; \{u_1^k\} \; \text{ given } \; \{v_2^k\}, \quad k = 0, \ldots, Q$$

The Key is Measure Transformation

- Use coupling terms to define new random variables

$$\hat{g}_1(\xi_1, \xi_2) = \sum_{k=0}^{P} g_{1,k} \Psi_k(\xi_1, \xi_2) \longrightarrow \tilde{g}_1(\eta) = \sum_{k=0}^{P_1'} \tilde{g}_{1,k} \Phi_k(\eta), \quad \eta = (\hat{v}_2(\xi_1, \xi_2), \xi_1)$$

  - Fewer basis terms in expansion
  - Less work to compute unknown coefficients

- Must generate orthogonal polynomials & quadrature rules for new joint measure
  - Components are dependent
  - We don't have the joint measure

- What we can compute is expectation through transformation of measure

$$\int f(\eta) d\eta = \int f(\eta(\xi)) d\xi \approx \sum_{k=0}^{Q} w_k f(\eta(\xi^k)) = \sum_{k=0}^{Q} w_k f(\eta^k)$$

- Can numerically approximate integrals with respect to unknown measure
  - Compute inner products → generate new orthonormal bases via Gram-Schmidt
  - Define quadrature rules for new basis that preserve discrete orthogonality

Constructing a Reduced Basis

(Constantine et al, IJNME, 2014)

- Given PCE $\hat{v}(\xi) = \sum_{k=0}^{P} v_k \Psi_k(\xi)$ with $m = |v| < s$, and quadrature rule

$$\{(w_j, \xi^j) : w_j \geq 0,\ j = 0, \ldots, Q\},$$

- Construct a new basis $\{\Phi_k(\eta) :\ k = 0, \ldots, P'\}$ with $\eta(\xi) = \hat{v}(\xi)$ and $P' < P$

$$\text{such that } \sum_{j=0}^{Q} w_j \Phi_{k_1}(\eta(\xi^j)) \Phi_{k_2}(\eta(\xi^j)) = \delta_{k_1 k_2},\ 0 \leq k_1, k_2 \leq P'.$$

- Given polynomial order N', define the matrix of m-variate monomials

with total order at most N': $V \in \mathbb{R}^{(Q+1)\times(P'+1)}$,

$$V_{jl} = (\eta_1(\xi^j))^{l_1} \cdots (\eta_m(\xi^j))^{l_m} \text{ s.t. } l_1 + \cdots + l_m \leq N', P' + 1 = \binom{N'+m}{m}.$$

- Compute weighted QR factorization (e.g., weighted, modified Gram-Schmidt):

$$V = ZB \ \ s.t.\ \ Z^T W Z = I,\ \ Z \in \mathbb{R}^{(Q+1)\times(P'+1)},\ \ W = \mathrm{diag}(\{w_k\}) \in \mathbb{R}^{(Q+1)\times(Q+1)}$$

- Entries of Z are new basis functions evaluated at quadrature points:

$$\Phi_k(\eta(\xi^j)) = Z_{jk},\ \ j = 0, \ldots, Q,\ k = 0, \ldots, P'.$$

Constructing a Reduced Quadrature (1)

- Using measure transformation, original quadrature rule $\{(w_j, \eta^j = \eta(\xi^j)\}_{j=0}^{Q}$, enables computing projections onto new basis.
  - However this does not reduce computational work.
- Idea: Find a new set of weights $\{\tilde{w}^k\}_{j=0}^{Q}$ with as many as zero as possible
  - Drop quadrature points with zero weight to reduce cost
- Constraint: Quadrature rule must preserve discrete orthogonality

$$\sum_{j=0}^{Q} \tilde{w}_j \Phi_{k_1}(\eta^j)\,\Phi_{k_2}(\eta^j) = \sum_{j=0}^{Q} \tilde{w}_j Z_{jk_1} Z_{jk_2} = \delta_{k_1 k_2} \implies Z^T \tilde{W} Z = I$$

- Define

$$A \in \mathbb{R}^{(Q+1)\times(P'+1)^2} \quad s.t. \quad A_{jk} = Z_{jk_1} Z_{jk_2}, \quad k = (k_1, k_2)$$

- Constraint is equivalent to

$$A^T \tilde{w} = A^T w, \quad \text{where} \quad w = [w_0, \ldots, w_Q]^T, \quad \tilde{w} = [\tilde{w}_0, \ldots, \tilde{w}_Q]^T.$$

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Constructing a Reduced Quadrature (2)

- Elements of *A* are polynomials of degree at most *2N'*, so *A* is rank deficient
  - Find a full rank set of columns *Y* via (weighted) column-pivoted QR

$$A\Pi = YS, \quad Y^T W Y = I, \quad \text{Find largest } R \text{ such that } |S(R,R)| > \text{TOL}$$

- Compute new weights by solving

$$\begin{array}{cc} \min\limits_{\tilde{w}} & 0^T \tilde{w} \\ \text{s.t.} & Y_R^T \tilde{w} = Y_R^T w, \\ & \tilde{w} \geq 0 \end{array}$$

- By using the simplex method, obtain a solution $\tilde{w}_*$ with exactly *R* nonzero weights
  - Solve for weights by finding feasible point using any suitable linear program solver, e.g., Clp

- Resulting discrete orthogonality $I - Z^T \tilde{W}_* Z$ controlled by TOL.

Putting the Pieces Together

- Define $\mathcal{J} = \left\{ j \in \{0, \ldots, Q\} \ : \ \tilde{w}_j \neq 0 \right\}, \ \ |\mathcal{J}| = R$

- Given a mapping $h = h(\eta(\xi))$, with $\eta(\xi) = \hat{v}(\xi)$, we wish to compute
$$\hat{h}(\xi) = \sum_{k=0}^{P} h_k \Psi_k(\xi)$$

- First compute $\tilde{h}(\eta) = \sum_{k=0}^{P'} \tilde{h}_k \Phi_k(\eta)$ with $\tilde{h}_k = \sum_{j \in \mathcal{J}} \tilde{w}_j h(\eta^j) \Phi_k(\eta^j)$

- Then $h_k = \sum_{j=0}^{Q} w_j h(\eta(\xi^j)) \Psi_k(\xi^j) \approx \sum_{j=0}^{Q} w_j \tilde{h}(\eta(\xi^j)) \Psi_k(\xi^j), \ \ k = 0, \ldots, P.$

Simple Composite Function Example

$$y_1(x) = x_1, \quad y_2(x) = \frac{1}{10 + \sum_{i=1}^{4} \frac{x_i}{i}}, \quad h(y) = \exp\left(y_1 + y_2\right),$$

Tensor-product Gauss-Legendre quadrature, QR tolerance = 10^{-12}

N	$P+1$	$Q+1$	$P'+1$	R	$\lVert\hat{h}^{(10)} - \hat{h}^{(N)}\rVert_\infty$	$\lVert\hat{h}^{(10)} - \tilde{h}^{(N)}\rVert_\infty$	$\lVert\mathrm{vec}(I - Z^T\tilde{W}Z)\rVert_\infty$
1	5	16	3	5	2.93E-02	2.93E-02	2.22E-16
2	15	81	6	12	3.58E-03	3.58E-03	2.10E-14
3	35	256	10	22	3.55E-04	3.55E-04	1.46E-12
4	70	625	15	47	2.94E-05	2.94E-05	1.37E-12
5	126	1296	21	101	2.09E-06	2.09E-06	1.83E-12
6	210	2401	28	188	1.30E-07	1.30E-07	2.55E-12
7	330	4096	36	346	7.18E-09	7.18E-09	3.81E-12
8	495	6561	45	587	3.58E-10	3.57E-10	6.10E-12
9	715	10000	55	941	1.62E-11	1.63E-11	2.62E-12
10	1001	14641	66	1425	0.00E+00	1.63E-12	2.70E-12

QR tolerance = 10^{-6}

N	$P+1$	$Q+1$	$P'+1$	R	$\lVert\hat{h}^{(10)} - \hat{h}^{(N)}\rVert_\infty$	$\lVert\hat{h}^{(10)} - \tilde{h}^{(N)}\rVert_\infty$	$\lVert\mathrm{vec}(I - Z^T\tilde{W}Z)\rVert_\infty$
1	5	16	3	5	2.93E-02	2.93E-02	2.22E-16
2	15	81	6	12	3.58E-03	3.58E-03	2.10E-14
3	35	256	10	22	3.55E-04	3.55E-04	1.46E-12
4	70	625	15	35	2.94E-05	2.94E-05	1.90E-11
5	126	1296	21	50	2.09E-06	1.83E-06	2.28E-06
6	210	2401	28	70	1.30E-07	1.22E-07	4.02E-08
7	330	4096	36	92	7.18E-09	4.24E-07	1.11E-06
8	495	6561	45	158	3.58E-10	4.23E-06	1.12E-03
9	715	10000	55	252	1.62E-11	3.86E-06	4.87E-06
10	1001	14641	66	475	0.00E+00	1.30E-05	3.85E-02

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Applying Dimension Reduction to Network Systems (1)

- Recall stochastic network system:

$$\begin{aligned} h_1(v_1, v_2, \xi) &= v_1(\xi) - g_1(u_1(v_2(\xi), \xi_1), \xi_1) = 0 \quad s.t. \quad f_1(u_1(\xi), v_2(\xi), \xi_1) = 0 \\ h_2(v_1, v_2, \xi) &= v_2(\xi) - g_2(u_2(v_1(\xi), \xi_2), \xi_2) = 0 \quad s.t. \quad f_2(v_1(\xi), u_2(\xi), \xi_2) = 0 \end{aligned}$$

- And it's stochastic Galerkin discretization:

$$\begin{aligned} \hat{v}_1(\xi) &= \sum_{i=0}^{P} v_{1,i}\Psi_i(\xi) \\ \hat{v}_2(\xi) &= \sum_{i=0}^{P} v_{2,i}\Psi_i(\xi) \end{aligned} \quad \text{s.t.} \quad \left. \begin{aligned} H_{1,i} &\equiv \langle h_1(\hat{v}_1(\xi), \hat{v}_2(\xi), \xi)\Psi_i(\xi)\rangle = 0 \\ H_{2,i} &\equiv \langle h_2(\hat{v}_1(\xi), \hat{v}_2(\xi), \xi)\Psi_i(\xi)\rangle = 0 \end{aligned} \right\}, \quad i = 0, \dots, P$$

- Stochastic Galerkin residual equations evaluated via NISP approximation for each component:

$$\begin{aligned} &\hat{g}_1(\xi) = \sum_{i=0}^{P} g_{1,i}\Psi_i(\xi) \quad g_{1,i} = \sum_{k=0}^{Q} w_k g_1(u_1^k, \xi_1^k)\Psi_i(\xi^k) \quad s.t. \quad f_1(u_1^k, \hat{v}_2(\xi^k), \xi_1^k) = 0, \quad k = 0, \dots, Q \\ &\hat{g}_2(\xi) = \sum_{i=0}^{P} g_{2,i}\Psi_i(\xi) \quad g_{2,i} = \sum_{k=0}^{Q} w_k g_2(u_2^k, \xi_2^k)\Psi_i(\xi^k) \quad s.t. \quad f_2(\hat{v}_1(\xi^k), u_2^k, \xi_2^k) = 0, \quad k = 0, \dots, Q, \\ &H_{1,i} = v_{1,i} - g_{1,i}, \quad i = 0, \dots, P \\ &H_{2,i} = v_{2,i} - g_{2,i}, \quad i = 0, \dots, P \end{aligned}$$

- Requires O(2*Q) internal solves

Applying Dimension Reduction to Network Systems (2)

- At each step of nonlinear iteration, build reduced basis and quadrature for each component separately:

$$\eta_1(\xi) = (v_2(\xi), \xi_1)$$
$$\eta_2(\xi) = (v_1(\xi), \xi_2)$$

- Build PCE for each component using reduced random variables

$$\tilde{g}_1(\eta) = \sum_{i=0}^{P_1'} \tilde{g}_{1,i}\Phi_{1,i}(\eta_1) \quad \tilde{g}_{1,i} = \sum_{k\in\mathcal{J}_1} \tilde{w}_{1,k} g_1(u_1^k, \xi_1^k)\Phi_{1,i}(\eta_1^k) \quad s.t. \quad f_1(u_1^k, \hat{v}_2(\xi^k), \xi_1^k) = 0, \quad k \in \mathcal{J}_1$$

$$\tilde{g}_2(\eta) = \sum_{i=0}^{P_2'} \tilde{g}_{2,i}\Phi_{2,i}(\eta_2) \quad \tilde{g}_{2,i} = \sum_{k\in\mathcal{J}_2} \tilde{w}_{1,k} g_2(u_2^k, \xi_2^k)\Phi_{2,i}(\eta_2^k) \quad s.t. \quad f_2(\hat{v}_1(\xi^k), u_2^k, \xi_2^k) = 0, \quad k \in \mathcal{J}_2$$

- Project back to original PCE basis

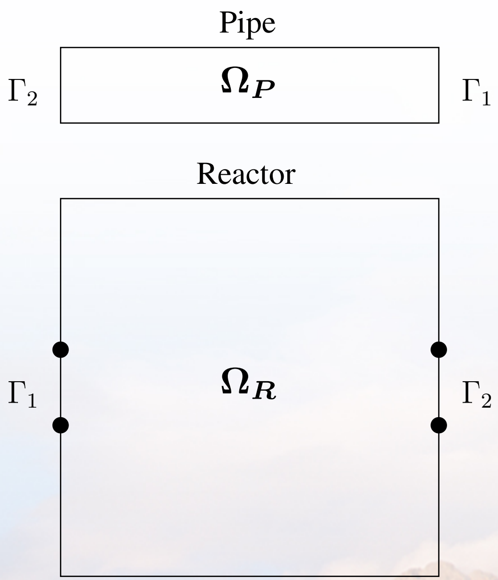
$$\hat{g}_1(\xi) = \sum_{i=0}^{P} g_{1,i}\Psi_i(\xi) \quad g_{1,i} = \sum_{k=0}^{Q} w_k g_1(u_1^k, \xi_1^k)\Psi_i(\xi^k) \approx \sum_{k=0}^{Q} w_k \tilde{g}_1(\eta_1(\xi^k))\Psi_i(\xi^k)$$

$$\hat{g}_2(\xi) = \sum_{i=0}^{P} g_{2,i}\Psi_i(\xi) \quad g_{2,i} = \sum_{k=0}^{Q} w_k g_2(u_2^k, \xi_2^k)\Psi_i(\xi^k) \approx \sum_{k=0}^{Q} w_k \tilde{g}_2(\eta_2(\xi^k))\Psi_i(\xi^k)$$

- Similar procedure for derivatives needed by nonlinear elimination method

Application to Network-Coupled PDE Problem

- Incompressible fluid flow/heat transfer in a coupled pipe-reactor with temperature source
  - Implemented within Albany code (Salinger et al)
  - https://github.com/gahansen/Albany



$$\left.\begin{aligned} -\nu\Delta u + u\cdot\nabla u + \nabla p &= \beta(T - T_{\text{ref}})g \\ -\kappa\Delta T + u\cdot\nabla T + T_s &= 0 \end{aligned}\right\}, \quad x \in \Omega_P \cup \Omega_R,$$

$$\left.\begin{aligned} \bar{T}_P &= \bar{T}_R \\ \kappa\nabla\bar{T}_P\cdot n_1 &= \kappa\nabla\bar{T}_R\cdot n_1 \end{aligned}\right\}, \quad x \in \Gamma_1,$$

$$\left.\begin{aligned} \bar{T}_R &= \bar{T}_P \\ \kappa\nabla\bar{T}_R\cdot n_2 &= \kappa\nabla\bar{T}_P\cdot n_2 \end{aligned}\right\}, \quad x \in \Gamma_2.$$

Discrete 2x2 Network Coupled System

- PDEs discretized via 1st order, stabilized FEM
  - SUPG, PSPG stabilization
  - Pipe: 40x4 cells, reactor 40x40 cells

- Pipe thermal diffusivity uncertain random field with exponential covariance
  - Discretized with KL-expansion in s terms

$$Cov_\kappa(x, y, x', y') = \sigma \exp\left(-\frac{|x - x'|}{L_x} - \frac{|y - y'|}{L_y}\right)$$

$$\kappa(\xi) = \mu + \sum_{i=0}^{s} \kappa_i(x)\xi_i, \quad \xi_i = U(-1, 1).$$

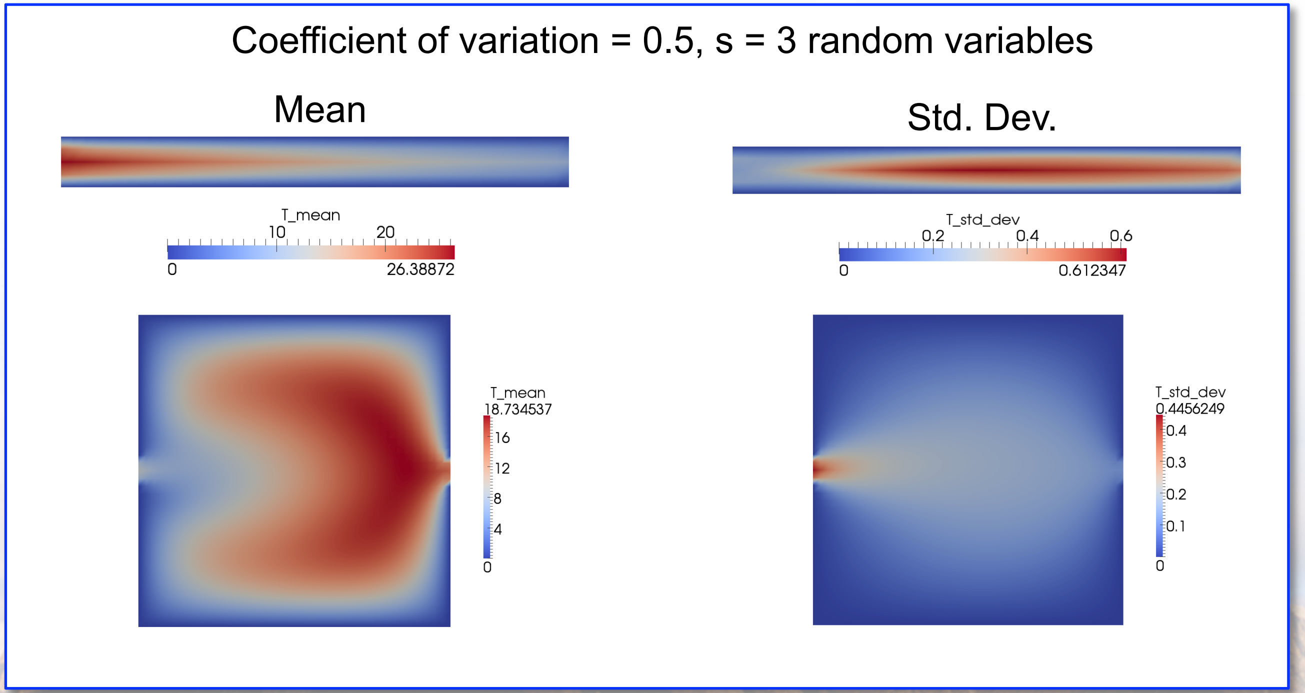
- 2x2 network coupled system
  - Neumann-to-Dirichlet maps

$$\begin{array}{ccc} g_1(u_1) - g_2(u_2) = 0 & & f_1(u_1, v_1, v_2, \xi) = 0 \\ g_3(u_2) - g_4(u_1) = 0 & & f_2(u_2, v_1, v_2) = 0 \\ g_1(u_1) = \bar{T}_P|_{\Gamma_1}, \;\; g_2(u_2) = \bar{T}_R|_{\Gamma_1} & s.t. & v_1 = \kappa \nabla \bar{T} \cdot n_1|_{\Gamma_1} \\ g_3(u_2) = \bar{T}_R|_{\Gamma_2}, \;\; g_4(u_1) = \bar{T}_P|_{\Gamma_2} & & v_2 = \kappa \nabla \bar{T} \cdot n_2|_{\Gamma_2} \end{array}$$

Stochastic Network System

- Outer network system
  - Stokhos instrusive stochastic Galerkin package (part of Trilinos)
  - Standard Newton iteration
  - GMRES linear solver, approximate Gauss-Seidel stochastic preconditioner, LU factorization of mean matrix
- Inner PDE solves
  - Non-intrusive polynomial chaos at supplied quadrature points (tensor-product Gauss-Legendre)
  - Standard Newton iteration for each sample
  - GMRES linear solver, incomplete ILU preconditioner
  - Distributed memory parallelism (MPI), 8 processors

http://trilinos.sandia.gov



Performance

Polynomial order *N* = *N'* = 3

					Time (sec)			Reduced Time(sec)		
s	$P+1$	$Q+1$	$P'+1$	R	Pipe	Reactor	Total	Pipe	Reactor	Total
2	10	16	10	16	4	62	67	4	53	58
3	20	64	10	40	17	246	263	17	120	137
4	35	256	10	41	82	1052	1134	73	129	202
5	56	1024	10	35	353	4051	4405	341	116	458

Reactor time for reduced approach roughly constant with regards to number of uncertain variables in pipe

Concluding Remarks

- UQ problems for multi-physics systems quickly become intractable
  - Adding more components/physics increases stochastic dimensionality in all components
- Ideas studied here appear to help mitigate this
  - UQ cost in each sub-problem approximately constant
  - Rigorous error analysis is needed
- Building method on tensor-product quadrature (to ensure positive weights) limits scalability
- Ideas extend to e.g., sparse grids, but with challenges
  - Non-positive weights lead to non-positive-definite inner product
  - Can be mitigated by formulating basis reduction on PC coefficients instead of quadrature values
    - Inner products become standard dot-products on PC coefficients
  - Modify reduced quadrature linear program by removing positivity constraint
    - Enables other solution approaches, e.g., column-pivoted QR
  - Requires sparse grid to preserve discrete orthogonality
    - Can this be extended to Smolyak PCE approaches?
- So far only investigated "segregated solve" type methods
  - Can this be incorporated into full Newton or JFNK methods?

References

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Auxiliary Slides

Embedded Stochastic Galerkin UQ Methods

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

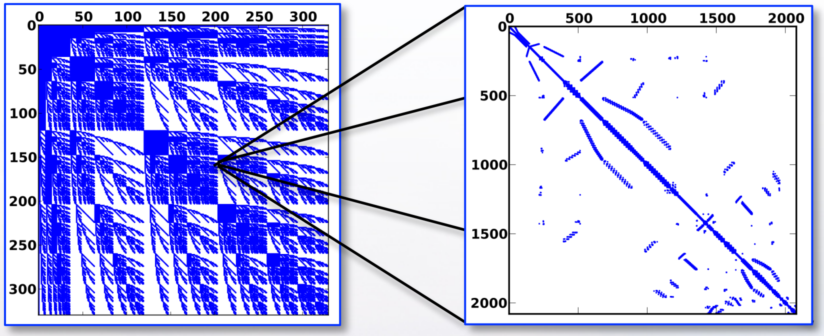
$$\text{Find } u(\xi) \text{ such that } f(u,\xi)=0,\ \xi:\Omega\rightarrow\Gamma\subset R^M,\ \text{density } \rho$$

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

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

  - Multivariate orthogonal basis of total order at most N – (generalized polynomial chaos)
- **Method generates new coupled spatial-stochastic nonlinear problem (intrusive)**

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



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, particularly for nonlinear problems

Stokhos: Trilinos tools for embedded stochastic Galerkin UQ methods

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

- Tools for describing SG discretization
  - Stochastic bases, quadrature rules, etc…
- C++ operator overloading library for automatically evaluating SG residuals and Jacobians
  - Replace low-level scalar type with orthogonal polynomial expansions
  - Leverages Trilinos Sacado automatic differentiation library

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

- Tools forming and solving SG linear systems
  - SG matrix operators
  - Stochastic preconditioners
  - Hooks to Trilinos parallel solvers and preconditioners
- Provides tools for investigating embedded UQ methods in large-scale applications

Trilinos

http://trilinos.sandia.gov