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Stochastic Dimension Reduction of Multiphysics Systems through Measure Transformation

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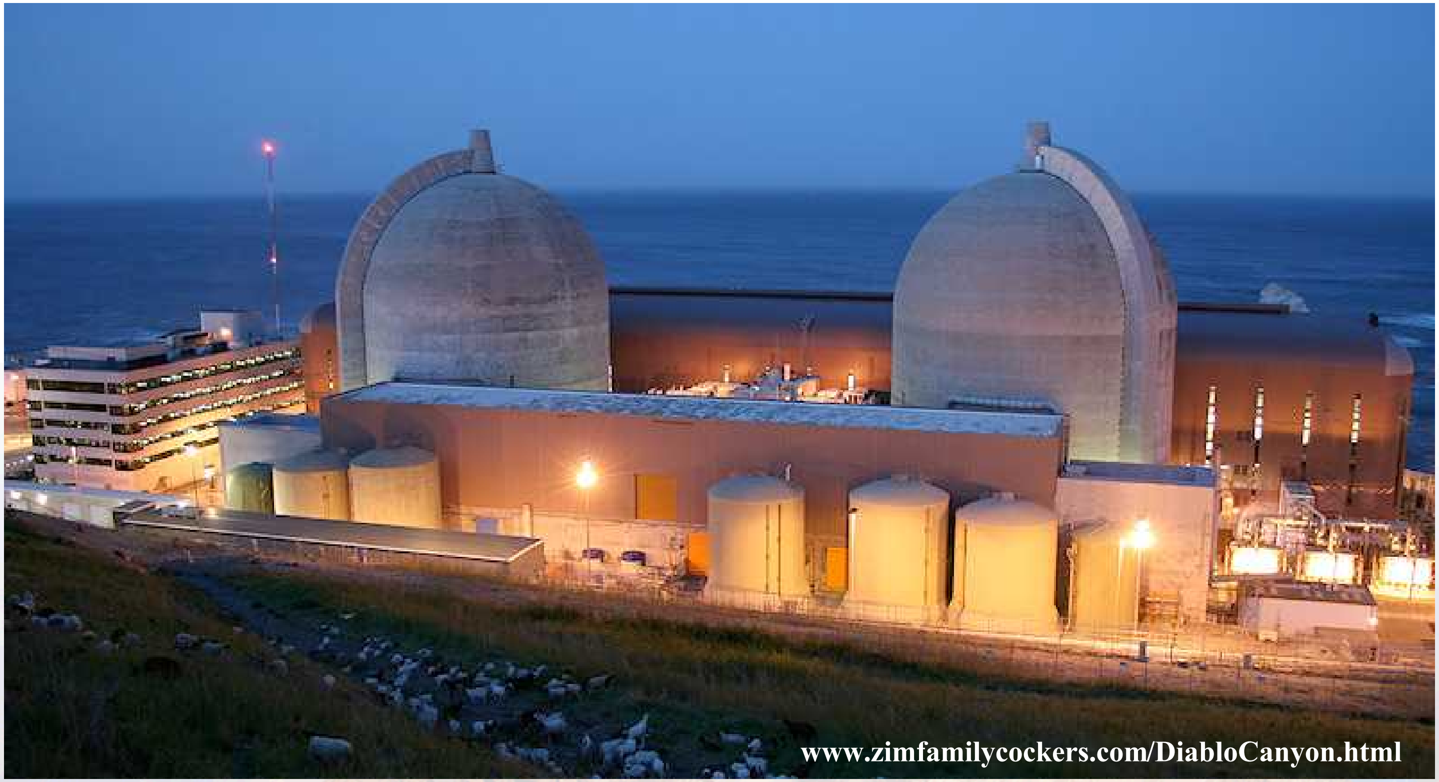
Uncertainty Quantification for Complex Coupled Systems

- Address *some* of the mathematical and computational challenges in predictive simulation of complex coupled systems such as…



Challenges for UQ of Complex Coupled Systems

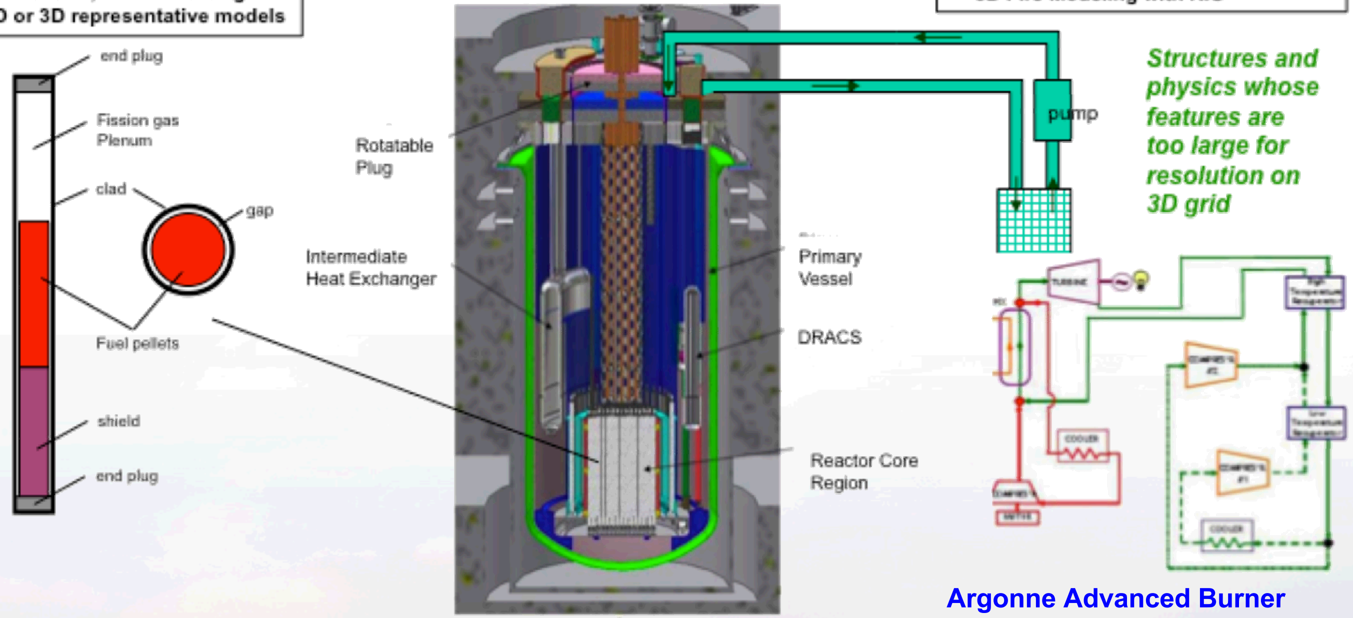
Structures and physics whose features are too small for resolution on 3D grid

Fuel-pins and control rods
- 0.5 - 10 mm-scale features
- conduction, fission heating …
- 2D or 3D representative models

"Meso-scale" resolved by 3D grid

In-vessel Reactor Components
- 10 cm to 10 m scale geomtry
- Neutronics, Turb flow & heat transfer, thermal-mechanics, conduction, …
- 3D Modeling Framework

Balance of Plant Reactor System Components (& Containment)
- 1 - 50 m scale
- Pipes, pumps, valves, heat exchangers, turbines, rooms,
- 0D MELCOR models
- 3D Fire Modeling with RIO



Structures and physics whose features are too large for resolution on 3D grid

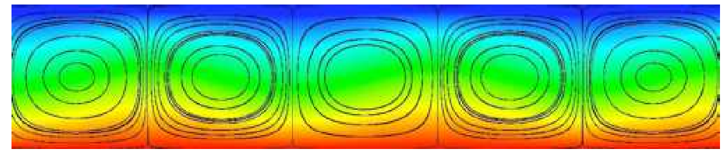
Argonne Advanced Burner Reactor Preconceptual Design

- Predictive simulation must capture critical couplings
- Coupling physics often necessitates reduction in model **fidelity**
- Reducing fidelity introduces additional uncertainty (component & interface)
- Strong coupling adds new dimensions of uncertainty to all components
- Cost of uncertainty quantification grows dramatically **with stochastic dimension**

Coupled Nonlinear Systems

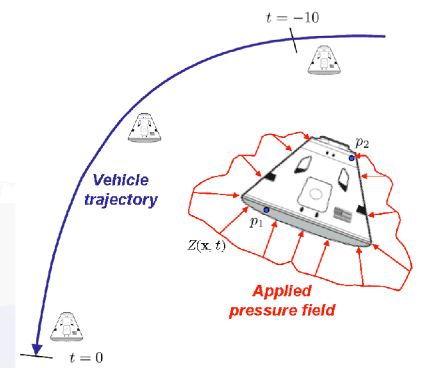
- Shared-domain multi-physics coupling
  - Equations coupled at each point in domain

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



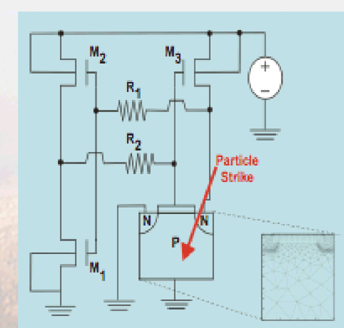
- Interfacial multi-physics coupling
  - Equations are coupled through boundaries

$$\mathcal{L}_1(u_1(x), v_2(x_2)) = 0, \quad v_2(x_2) = \mathcal{G}_2(u_2(x_2)), \quad x_2 \in \Gamma_2$$
$$\mathcal{L}_2(v_1(x_1), u_2(x)) = 0, \quad v_1(x_1) = \mathcal{G}_1(u_1(x_1)), \quad x_1 \in \Gamma_1$$



- Network coupling
  - Equations are coupled through a set of scalars

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



Finite Dimensional Coupled Network Systems

- Network system after discretization:

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

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

- 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:

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

- 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):

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

Stochastic Coupled Network Systems

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

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

- Introduce polynomial chaos approximation for all variables:

$$\hat{u}_i(\xi) = \sum_{j=0}^{P} u_{i,j} \Psi_j(\xi), \quad \hat{v}_i(\xi) = \sum_{j=0}^{P} v_{i,j} \Psi_j(\xi)$$

- Stochastic Galerkin network equations:

$$\left.\begin{array}{l} \langle f_1(\hat{u}_1(\xi), \hat{v}_2(\xi), \xi_1)\Psi_i(\xi)\rangle = 0 \\ \langle f_2(\hat{v}_1(\xi), \hat{u}_2(\xi), \xi_2)\Psi_i(\xi)\rangle = 0 \end{array}\right\}, \quad i = 0, \dots, P$$

$$\left.\begin{array}{l} H_{1,i} \equiv \langle h_1(\hat{v}_1(\xi), \hat{v}_2(\xi), \xi)\Psi_i(\xi)\rangle = 0 \\ H_{2,i} \equiv \langle h_2(\hat{v}_1(\xi), \hat{v}_2(\xi), \xi)\Psi_i(\xi)\rangle = 0 \end{array}\right\}, \quad i = 0, \dots, P$$

$$u_{i,j} = \sum_{k=0}^{Q} w_k u_i^k \Psi_j(\xi^k) \quad s.t. \quad \left.\begin{array}{l} f_1(u_1^k, \hat{v}_2(\xi^k), \xi_1^k) = 0 \\ f_2(\hat{v}_1(\xi^k), u_2^k, \xi_2^k) = 0 \end{array}\right\}, \quad k = 0, \dots, Q$$

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

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.,

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

The Key is Measure Transformation

- Use coupling terms to define new random variables

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

- 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

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

- Looked at several ways to leverage this for multi-physics
  - Single coupling variable: Lanczos
  - Multiple coupling variables Gram-Schmidt QR + linear programming

Constructing a Reduced Basis

- **Given PCE** $\hat{v}(\xi) = \sum_{k=0}^{P} v_k \Psi_k(\xi)$, quadrature rule $\{(w^j, \xi^j) \,:\, j = 0, \dots, Q\}$

  and mapping $h = h(v)$, $|v| = m < s$,

- **Construct** $\hat{h}(\xi) = \sum_{k=0}^{P} h_k \Psi_k(\xi) \approx \sum_{k=0}^{P'} \tilde{h}_k \Phi_k(\eta(\xi))$, $\eta(\xi) = \hat{v}(\xi)$, $P' = \binom{N'+m}{m}$

- Define

$$\mathcal{L} = \{(l_1, \dots, l_m) \in \mathbb{N}^m \,:\, l_1 + \cdots + l_m \le N'\}, \quad |\mathcal{L}| = P' + 1$$

$$V \in \mathbb{R}^{(Q+1)\times(P'+1)}, \quad V_{jl} = \hat{v}_1^{l_1}(\xi^j) \cdots \hat{v}_m^{l_m}(\xi^j), \quad W = \mathrm{diag}(\{w^k\}) \in \mathbb{R}^{(Q+1)\times(Q+1)}$$

- Compute weighted QR factorization (e.g., MGS):

$$V = ZB \;\; s.t. \;\; Z^T W Z = I, \quad Z \in \mathbb{R}^{(Q+1)\times(P'+1)}, \quad Z_{jk} = \Phi_k(\hat{v}(\xi^j))$$

- *Z* defines our new basis

Constructing a Reduced Quadrature

- Goal: Find a new set of weights $\{u^j\}_{j=0}^{Q}$ with as many as zero as possible

- Requirement: Quadrature rule must integrate products of basis functions exactly:

$$\sum_{j=0}^{Q} \Phi_{k_1}(\hat{v}(\xi^j))\,\Phi_{k_2}(\hat{v}(\xi^j))\,u^j = \sum_{j=0}^{Q} Z_{jk_1} Z_{jk_2} u_j = \delta_{k_1 k_2}$$

- Define

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

- A is rank deficient, find a full rank set of columns via column-pivoted QR

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

- Compute new weights by solving

$$\begin{aligned} \min_u \quad & 0^T u \\ \text{s.t.} \quad & Y_R^T u = Y_R^T w, \\ & u \geq 0 \end{aligned}$$

- Really just need a feasible point via simplex method

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Putting the Pieces Together

- Define

$$\mathcal{J} = \left\{ j \in \{0,\dots,Q\} \ : \ u_j \neq 0 \right\}, \quad |\mathcal{J}| = R$$

- Compute

$$\tilde{h}(\hat{v}(\xi)) = \sum_{k=0}^{P'} \tilde{h}_k \Phi_k(\hat{v}(\xi))$$

$$\tilde{h}_k = \sum_{j \in \mathcal{J}} u_j h(\hat{v}(\xi^j)) \Phi_k(\hat{v}(\xi^j)) = \sum_{j \in \mathcal{J}} u_j h(\hat{v}(\xi^j)) Z_{jk}, \quad k = 0,\dots,P'$$

- Then

$$h(\xi) = \sum_{k=0}^{P} h_k \Psi_k(\xi), \quad h_k = \sum_{j=0}^{Q} w_j \tilde{h}(\hat{v}(\xi^j)) \Psi_k(\xi^j), \quad k = 0,\dots,P$$

- Solve for weights using any suitable linear program solver, e.g., Clp
- Similar procedure for derivatives needed by nonlinear elimination method

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}

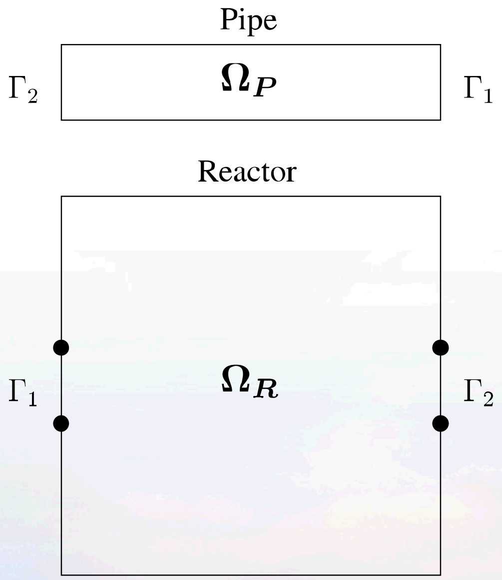
N	P + 1	Q + 1	P′ + 1	R	$\|\hat{h}^{(10)} - \hat{h}^{(N)}\|_\infty$	$\|\hat{h}^{(10)} - \tilde{h}^{(N)}\|_\infty$	$\|\mathrm{vec}(I - Z^T U Z)\|_\infty$
1	5	16	3	5	2.93E-02	2.93E-02	2.22E-16
2	15	81	6	12	3.58E-03	3.58E-03	2.10E-14
3	35	256	10	22	3.55E-04	3.55E-04	1.46E-12
4	70	625	15	47	2.94E-05	2.94E-05	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	$\|\hat{h}^{(10)} - \hat{h}^{(N)}\|_\infty$	$\|\hat{h}^{(10)} - \tilde{h}^{(N)}\|_\infty$	$\|\mathrm{vec}(I - Z^T U Z)\|_\infty$
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

Application to Network-Coupled PDE Problem

- Incompressible fluid flow/heat transfer in a coupled pipe-reactor with temperature source



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

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

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

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

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

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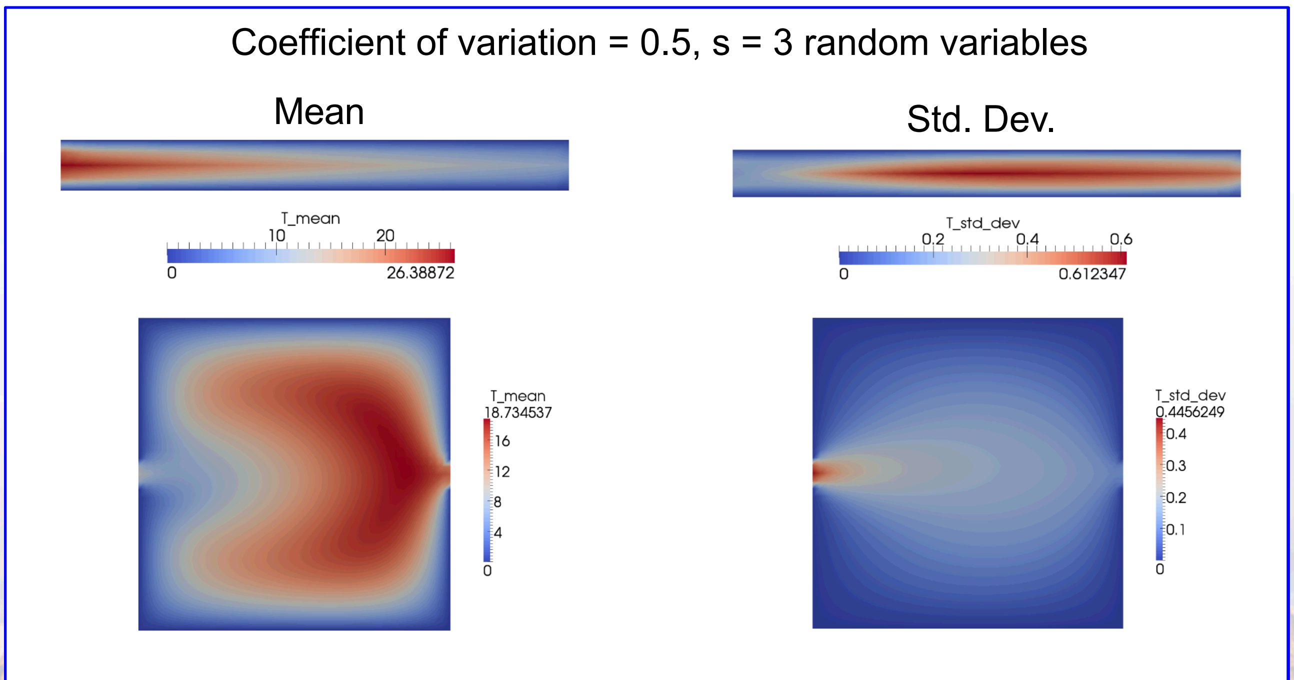
Stochastic Network System

- 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

					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

Concluding Remarks

- UQ problems for multi-physics systems quickly become intractable
  - Adding more components/physics increases stochastic dimensionality in all components
- Ideas studied here help mitigate this
  - UQ cost in each sub-problem approximately constant
- Building method on tensor-product quadrature limits scalability
- Ideas extend to 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
  - Requires sparse grid to preserve discrete orthogonality
    - Fine for Gaussian abscissas with linear growth, but not anything else
- So far only investigated “segregated solve” type methods
  - Can this be incorporated into full Newton or JFNK methods?
    - Probably, nonlinear elimination is just a nonlinear Schur complement

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Auxiliary Slides

Embedded Stochastic Galerkin UQ Methods

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

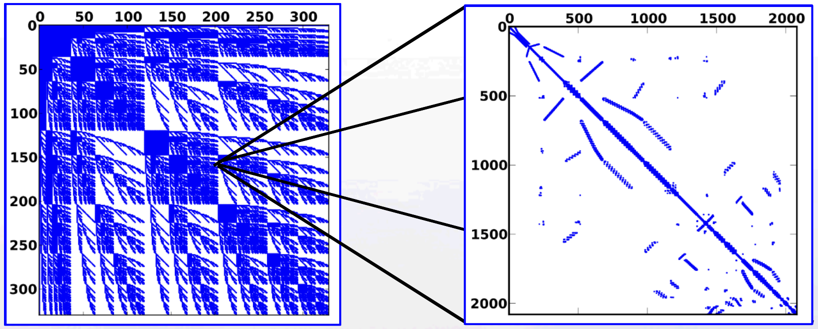
$$\text{Find } u(\xi) \text{ such that } f(u,\xi)=0,\ \xi:\Omega\rightarrow\Gamma\subset R^M,\ \text{density } \rho$$

- **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)**

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



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

http://trilinos.sandia.gov

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

- 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