Hybrid Uncertainty Quantification Methods for Reactive Transport

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What do we mean by hybrid uncertainty quantification?

Purely Intrusive approach

Uncertain inputs → Model → Uncertainty information
Stochastic simulation (UQ embedded in the model)

Non-intrusive approach

Uncertain inputs → UQ Engine → Model
Many deterministic simulations

hybrid approach for multi-physics
• decompose the system into components with each having its own UQ
• create algorithms to use these modules to propagate global uncertainties
• in this project, we consider decomposition along physics boundaries

Uncertain inputs → M1 → M2 → M3
Uncertain inputs → M4 → M5
M2 → Intrusive modules → M1
M3 → Intrusive modules → M5

Wrapped by mini-UQ engines (sampling)
Why Hybrid UQ?

- current model development practice
  - “plug-and-play” gives flexibility
  - operator splitting widely used
  - well-defined module interfaces
  - extensive use of open source or commercial codes as modules

- Likely scenario in multi-physics models if UQ is embedded
  - Intrusive UQ may be readily available for some modules
  - Only non-intrusive UQ may be available for other modules
  - With time, advanced UQ may be available for some modules
  - Also, new uncertain parameters may be added from time to time
  - Thus, it is reasonable to consider UQ at module level
  - Yet, **global** uncertainties/sensitivities must be propagated
  - Is “plug-and-play” feasible with embedded UQ? If so, how?
    - The objective of this project is to explore this.
Consider a 1D reaction-diffusion equation (D and K are second order random variables (rv))

\[
\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - KC
\]

\[0 \leq x \leq 1; 0 \leq t \leq T; u(0,t) = u(1,t) = 0; u(x,0) = f(x)\]

**Operator splitting**

\[C^{n+1/2} = F_T(C^n, D)\]
\[C^{n+1} = F_R(C^{n+1/2}, K)\]

**Suppose we have the following scenario:**

- intrusive polynomial chaos is available for the diffusion equation
- only non-intrusive methods are available for the reaction equation
- this scenario may be realistic, especially for multi-species systems
  - the reaction system may have an analytic solution
  - the reaction equation may benefit from a fast ODE solver
  - in some cases, one module may be open source or commercial code
Goal: build a global uncertainty propagation algorithm via “gluing” an intrusive and a sampling module

Objective: design a forward “global” uncertainty propagation algorithm
- which permits 2 different UQ methods in the two modules, and
- which permits each module to be developed independently of the other
- given that the base uncertainty format is polynomial chaos coefficients
- Thus, at each time time, the following are performed by each module
  (which can be captured by a generic software layer):

Intrusive module:
- convert from base to local format
- run local module
- analyze results
- convert from local to base format

Non-intrusive module:
- convert from base to local format
- create appropriate sampling schemes
- run samples
- analyze results
- convert from local to base format
Polynomial Chaos for the Diffusion Equation

- Expand independent and dependent variables in PCE

\[
D = \sum_{i=0}^{P} D_i \Psi_i(\xi); \quad C = \sum_{i=0}^{P} D_i \Psi_i(\xi)
\]

- Substitute into the transport equation

\[
\frac{\partial}{\partial t} \left( \sum_{i=0}^{P} C_i \Psi_i(\xi) \right) = \sum_{i=0}^{P} D_i \Psi_i(\xi) \frac{\partial^2}{\partial x^2} \left( \sum_{j=0}^{P} C_j \Psi_j(\xi) \right)
\]

- Project onto each of the P+1 polynomial bases

\[
\frac{\partial C_k}{\partial t} = \frac{1}{<\Psi_k>^2} \sum_{j=0}^{P} \left[ \sum_{i=0}^{P} D_i e_{ijk} \right] \frac{\partial^2 C_j}{\partial x^2}; \quad e_{ijk} = <\Psi_i \Psi_j \Psi_k>, k=0, \ldots, P
\]

- apply initial/boundary conditions and then solve the equations

- Q: how to propagate global uncertainties locally?
Goal: plug the stand-alone PCE-based diffusion module into the overall global uncertainty propagation algorithm.

Idea: for linear diffusion equations, the global uncertainty stream can be broken up into pieces that can be handled naturally.

An example, to break up the 2\textsuperscript{nd} order PCE for 2 variables (D, K).

<table>
<thead>
<tr>
<th>D order</th>
<th>K order</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
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<tr>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>0</td>
<td>2</td>
</tr>
</tbody>
</table>

Intuitively, the global matrix can be decomposed into subproblems.
Non-intrusive Method for the Reaction Equation

- $C^{n+1/2}$ coming into the reaction module is a 2-rv PC expansion
- This needs to be converted to initial conditions for reaction
- How is this transformation done?
  - reconstruct the Legendre polynomials (2-parameter)
  - create a sample (2-parameter) for the reaction equation (size N)
  - evaluate the Legendre polynomials at the sample points
- Now we have N initial conditions for the N sample points
- Next, run the reaction solver on each sample point
- How to convert from the sample outputs back to the PC format?
  - the outputs will be fed into a Legendre regression analyzer
  - use either projection or least-squares approach
  - the results will be the PC coefficients
  - beware of scaling issues
- Sampling and transformation can be handled by a software API
Response Surfaces for different diffusion ranges

D=[0.0001,0.001], K=[0.1, 0.5]

D=[0.001,0.01], K=[0.1, 0.5]
Numerical Results (D = [0.001, 0.01]; k = [0.1, 0.5])

- Purpose: investigate whether the hybrid method gives accurate answers
- Observations: convergence of hybrid at p=3, pure intrusive at p=2
- Hybrid gives more accurate answers due to the use of analytic reaction
- In practical cases, hybrid may be needed out of necessity
Another Test Problem: multi-species reactive transport

Sequential Reactions

\[
\begin{align*}
A_1 + C_1 & \Rightarrow y_1 C_2 \\
A_2 + C_2 & \Rightarrow y_2 C_3 \\
\vdots \\
A_i + C_i & \Rightarrow y_i C_{i+1} \\
\vdots \\
A_n + C_n & \Rightarrow y_n C_{n+1}
\end{align*}
\]

\(A_i\) is a reactant participating in reaction \(i\)
\(C_i\) is product of reaction \(i-1\)
\(y_i\) is the yield coefficient of reaction \(i\)
\(k_i\) is the reaction rate constant in reaction \(i\)

Reactive Transport

\[
\begin{align*}
\frac{\partial c_1}{\partial t} &= L(c_i) - k_1 c_1 \\
\frac{\partial c_2}{\partial t} &= L(c_2) - k_2 c_2 + y_1 k_1 c_1 \\
\vdots \\
\frac{\partial c_i}{\partial t} &= L(c_i) - k_i c_i + y_{i-1} k_{i-1} c_{i-1} \\
\vdots \\
\frac{\partial c_n}{\partial t} &= L(c_n) - k_n c_n + y_{n-1} k_{n-1} c_{n-1}
\end{align*}
\]

Uncertain Parameters
- diffusion, velocity (2 rv’s in \(L\))
- reaction rates (4 rv’s, \(n=4\))

Example reactions in subsurface flow: TCE \(\rightarrow\) DCE \(\rightarrow\) VC \(\rightarrow\) ETH
Stochastic Transport System

Let \( c(x,t) \) be species concentration defined on a bounded domain \( \Omega \times [0,T] \). Let \( \mathcal{Y} = \left\{ c \in H^1_0(\Omega) : c = c_d \text{ on } \Gamma_d \right\} \) and nonhomogeneous boundary \( \Gamma_d \)

Consider now \( \alpha, \nu^x, \) and \( \nu^y \) are functions of random event \( \theta \) of an abstract probability space \( (\Theta, \Sigma, P) \):

\[
\alpha = \alpha(\theta), \quad \nu^x = \nu^x(\theta), \quad \nu^y = \nu^y(\theta)
\]

Find

\[
c(x,\theta,t) \in \mathcal{Y} \otimes L_2(\Theta, P)
\]

such that it satisfies almost surely the stochastic problem:

\[
\begin{aligned}
\frac{\partial c(x,\theta,t)}{\partial t} &= \frac{\alpha(\theta)\nu^x}{R} \frac{\partial^2 c(x,\theta,t)}{\partial x^2} + \frac{\alpha(\theta)\nu^y}{R} \frac{\partial^2 c(x,\theta,t)}{\partial y^2} \\
&\quad - \frac{\nu^x(\theta)}{R} \frac{\partial c(x,\theta,t)}{\partial x} - \frac{\nu^y(\theta)}{R} \frac{\partial c(x,\theta,t)}{\partial y} \\
c(x,\theta,t) &= c_d(x,\theta) 
\end{aligned}
\]

\( \alpha : \) dispersivity; \( \nu^x, \nu^y : \) velocity in \( x, y \) direction; \( R : \) retardation factor
Stochastic Variational Form for the Transport System

Find \( c(x, \theta, t) \in \mathcal{V} \otimes L_2(\Theta, P) \) such that

\[
A(c, w) = \mathbb{E}[a(c, w)] \quad \forall w(x, \theta) \in \mathcal{V} \otimes L_2(\Theta, P)
\]

where

\[
A(c, w) = \int_{\Theta} w(x, \theta) \left[ \int_{\Omega} \frac{\partial c(x, \theta, t)}{\partial t} dx \right] dP(\theta)
\]

\[
+ \frac{1}{R} \int_{\Theta} \alpha(\theta) v^x(\theta) \left( \int_{\Omega} \frac{\partial w(x, \theta)}{\partial x} \frac{\partial c(x, \theta, t)}{\partial x} dx \right) dP(\theta)
\]

\[
+ \frac{1}{R} \int_{\Theta} \alpha(\theta) v^y(\theta) \left( \int_{\Omega} \frac{\partial w(x, \theta)}{\partial y} \frac{\partial c(x, \theta, t)}{\partial y} dx \right) dP(\theta)
\]

\[
- \frac{1}{R} \int_{\Theta} v^x(\theta) \left( \int_{\Omega} w(x, \theta) \frac{\partial c(x, \theta, t)}{\partial x} dx \right) dP(\theta)
\]

\[
- \frac{1}{R} \int_{\Theta} v^y(\theta) \left( \int_{\Omega} w(x, \theta) \frac{\partial c(x, \theta, t)}{\partial y} dx \right) dP(\theta)
\]
Stochastic Discretization

Let $\mathcal{N}$ be the set of nodes of the finite-element mesh not lying on $\Gamma_d$ and $\Phi_i(x)$ be the corresponding shape function. Let $\alpha, \nu^x, \nu^y$ be independent second-order random variables in

$$\mathcal{W}^P \equiv \text{span} \{\Psi_0, \ldots, \Psi_P\} \subset \mathcal{W} \equiv L_2(\Theta, P)$$

Using $(P+1)$-term polynomial chaos expansion, one obtains

$$\alpha(\xi, \theta) = \sum_{i=0}^{P} \alpha_i \Psi_i(\xi(\theta))$$

$$\nu^x(\xi, \theta) = \sum_{i=0}^{P} \nu^x_i \Psi_i(\xi(\theta)) \quad \nu^y(\xi, \theta) = \sum_{i=0}^{P} \nu^y_i \Psi_i(\xi(\theta))$$

$$\alpha_i = \frac{\langle \alpha(\xi), \Psi_i \rangle}{\langle \Psi_i^2 \rangle} \quad \nu^x_i = \frac{\langle \nu^x(\xi), \Psi_i \rangle}{\langle \Psi_i^2 \rangle} \quad \nu^y_i = \frac{\langle \nu^y(\xi), \Psi_i \rangle}{\langle \Psi_i^2 \rangle}$$

$$c^h(x, \xi, t) = \sum_{i \in \mathcal{N}} \left( \sum_{k=0}^{P} c_{i,k}(t) \Psi_k(\xi) \right) \Phi_i(x) \in \left( \mathcal{W}^h \otimes \mathcal{W}^P \right)$$
Stochastic Discretization and Galerkin Projection

Find $u_{i,k}$, $i \in \mathcal{N}$, $0 \leq k \leq P$ for $\forall w_{j,k} j \in \mathcal{N}$, $0 \leq k \leq P$ such that

$$0 = \sum_{i \in \mathcal{N}} \sum_{k=0}^{P} \left[ \int_{\Omega} \frac{\partial \Phi_i(x, \theta, t)}{\partial t} \Phi_j(x, \theta) \, dx \right] u_{i,k} w_{j,k} + \frac{1}{R} \left\{ \sum_{i,j \in \mathcal{N}} \right.$$

$$+ \left[ \sum_{k,l,m,s=0}^{P} \alpha_s \nu_k^x \langle \Psi_k \Psi_l \Psi_m \Psi_s \rangle \left( \int_{\Omega} \frac{\partial \Phi_i(x, \theta, t)}{\partial x} \frac{\partial \Phi_j(x, \theta)}{\partial x} \, dx \right) u_{i,l} w_{j,m} \right.$$

$$+ \left. \sum_{k,l,m,s=0}^{P} \alpha_s \nu_k^y \langle \Psi_k \Psi_l \Psi_m \Psi_s \rangle \left( \int_{\Omega} \frac{\partial \Phi_i(x, \theta, t)}{\partial y} \frac{\partial \Phi_j(x, \theta)}{\partial y} \, dx \right) u_{i,l} w_{j,m} \right.$$

$$- \left. \sum_{k,l,m=0}^{P} \nu_k^x \langle \Psi_k \Psi_l \Psi_m \rangle \left( \int_{\Omega} \frac{\partial \Phi_i(x, \theta, t)}{\partial x} \Phi_j(x, \theta) \, dx \right) u_{i,l} w_{j,m} \right.$$

$$- \left. \sum_{k,l,m=0}^{P} \nu_k^y \langle \Psi_k \Psi_l \Psi_m \rangle \left( \int_{\Omega} \frac{\partial \Phi_i(x, \theta, t)}{\partial y} \Phi_j(x, \theta) \, dx \right) u_{i,l} w_{j,m} \right\}$$
Hybrid UQ for multi-species reactive transport

- Operator splitting
  - 2D transport using finite element (4 equations, decoupled)
  - Multi-species reaction (coupled, use analytic solution)

- Test problem
  - Transport (PCE): dispersivity and velocity varies +/- 20%
  - Reaction (non-intrusive): +/-20% in reaction rates

- At each time step
  - Partition the incoming global states into subproblems
  - Perform transport solves
  - Re-package solution into global states
  - Generate initial conditions for each reaction solve
  - Perform reaction solves (sampling)
  - Reconstruct reaction solutions into global states
    - Latin hypercube (least squares)
    - Sparse grid (projection)
Numerical Results on 4-species reactive transport (means)

- PCE order = 2 (same for p=3)
  - Note: absolute differences are small (~5e-4 relative to 1.5e-2)
Numerical Results on 4-species reactive transport (std dev)

- PCE order = 2 (same for p=3)
  
Note: absolute differences are small (~1e-4 relative to 5e-2)
Scalability analysis of Hybrid UQ methods

- Transport: species coupled, PCE decoupled, multiple rhs systems
- Reaction: each sample instantiation independent from the others
- However, there are all-to-all communications
Summary and future work

- Hybrid uncertainty quantification is appealing
  - accommodate embedded (intrusive) UQ methods
  - compatible with modern-day “plug-and-play” philosophy
  - facilitate progressive integration of advance UQ methods
  - sometimes out of necessity, e.g.
    - different time step requirement for each module
    - accommodate commercial/open source modules
  - may increase parallelism

- Still there are many challenges
  - high dimensional uncertain parameter space
  - highly nonlinear parameter to output mapping
  - errors in propagating uncertainties
  - load balancing/fault tolerance on HPC