Uncertainty quantification using stochastic finite element method; application to heat distribution in the nuclear reactor core.

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Salient Question: Uncertainty Calculations in High Dimensional System

• How to approximate the stochastic distribution of functions over very large uncertain spaces?

\[ 0 = F(x, p) : R^n \times R^q \rightarrow R^n \Rightarrow x = x(p) \]

\[ p = p(\omega) \sim D(\mu(\omega)) \Rightarrow E_\omega \left[ G(x(p)) \right] = ? \]

• Example: F can be the equations of TH+Neutronics, p the physical parameters. (p \sim 1000 \ldots 10000 \ldots 100000).

• G can be:
  – Max output temperature, max centerline temperature.
  – A characteristic function \( G = \chi[a \leq T \leq b] \) which computes the probability of the max T to be in a given range.
High dimensional Approximation… The curse of dimensionality

- But computing the correct average is strongly connected to approximating the function G.
- In a high dimensional problem, this is subject to the “curse of dimensionality” – the fact that the sample density is decreasing exponentially with the dimension of the problem.
- Classical solutions:
  - Sampling: global but slow.
  - Sensitivity analysis fast but local and hard to adjust. What if the precision in assessment is insufficient? Higher-order? Hard to develop and implement.
- Can we create a method that efficiently uses the advantages of both methods, and is adjustable?
- We think so: using adapted stochastic finite element method (PCE), fitted with derivative information, and used as a control variate.
Example: Distribution and transport of heat in ABR reactor core

- There are two aspects of heat exchange in the reactor core: thermal hydraulics, and neutron interaction.
- Basic element of thermo-hydraulic model is a cylindrical pin surrounded by flowing coolant. Reactor core contains a hexagonal assembly of pins.
- Finite volumes description of temperature distribution includes:
  - a partition of the core into horizontal layers of volume elements;
  - a heat flux equilibrium equation producing temperature $T$ in each element;
  - temperature dependencies of the material properties $R$ of each element.
Choose a single output $J(T)$ to characterize the performance of the model. For example: (maximal, average) temperature of coolant.

Evaluation of the model:

- For current values of thermodynamical parameters, compute thermal fluxes $F$ over all types of interfaces (pin-pin, pin-coolant, coolant-coolant, coolant-outflow). Temperature gradient is estimated by a finite difference, all fluxes are linear in $T$.

- For a given nuclear reaction source term, assemble the conservation law $0 = \sum_{\partial \Omega} F - \int_\Omega q'' dV$ into the form $\Delta T = \sum_{\Omega} q'' dV$.

- Repeat the iterations $R := R(T), T := T(R)$ until convergence of the output.
Example: Equations

\[ 0 = -\nabla \cdot \mathbf{K} \nabla T - \rho c_p \bar{u} \nabla T + q'''' \]

When discretized we obtain

\[ \Phi = h(T_j - T_{\text{surface}}) = c_p \frac{T_{\text{surface}} - T_l}{D/2} \]

\[ \int q'''' dV = \sum_j 2 \frac{h c_p}{hD + 2c_p} T_j - \sum_j 2 \frac{h c_p}{hD + 2c_p} T_l + \sum_{I, I+} K \frac{1}{H_{I \rightarrow I+,+}} \int_{\partial \Omega} ndST_{I,+} + \ldots \]

\[ \ldots - \sum_{I, I+} K \frac{1}{H_{I \rightarrow I+,+}} \int_{\partial \Omega} ndST_{I} \]

\[ 0 = \sum_j K \frac{1}{H_{J \rightarrow J}} \int_{\partial \Omega} ndST_{j} + \sum_{J+J-} K \frac{1}{H_{J \rightarrow J+J-}} \int_{\partial \Omega} ndST_{J+,J-} - \sum_j K \frac{1}{H_{J \rightarrow J}} \int_{\partial \Omega} ndST_{j} + \ldots \]

\[ - \sum_{J+J-} K \frac{1}{H_{J \rightarrow J+J-}} \int_{\partial \Omega} ndST_{l} + \frac{1}{2} \sum_j \rho c_p \int \bar{u} ndST_{j} + \frac{1}{2} \sum_{J+J-} \rho c_p \int \bar{u} ndST_{J+,J-} + \ldots \]

\[ + \frac{1}{2} \sum_j \rho c_p \int \bar{u} ndST_{l} + \frac{1}{2} \sum_{J+J-} \rho c_p \int \bar{u} ndST_{l} + \sum_j 2 \frac{h c_p}{hD + 2c_p} T_{j*} - \sum_j 2 \frac{h c_p}{hD + 2c_p} T_{l} \]
Fig. 1.1-11 Deviations of Values from Other Assessments from the Recommended Values for the Heat Capacity at Constant Pressure of Liquid Sodium
Uncertainty in fluid flow core

- The parameters\material properties $R$ of the model include heat capacity $c_p$, heat conductivity $K$ for the coolant and fuel; convective heat transfer coefficient $h$.
- A fixed-point iteration procedure $R:=R(T)$, $T:=T(R)$ is used to couple the dependence of the temperature distribution on the material parameters, and the dependence of the material parameters on temperature.
- Uncertainty in the performance $J(T)$ of the nuclear reactor is attributed to the uncertainty in the values of parameters $R$.

Note: the available temperature-dependencies are built as a best fit to experimental data + uncertainties, but this results in an uncertainty band, even if the data warrants finer representation, such as no/little oscillation. 

with uncertainty estimated at 0.1% at 300 K, 3% at 1000 K, 8% at 2000 K.
**Representation of temperature-dependent uncertainty**

- Assume a temperature-dependent structure for the uncertainty:

  \[ R = \left( \sum_i r^{(i)} T^i \right) \cdot (1 + \alpha^{(0)} C^{(0)}(T) + \alpha^{(1)} C^{(1)}(T) + \alpha^{(2)} C^{(2)}(T)) + \ldots) \]

  \[ h = \left( \sum_i r^{(i)} T^i \right) \cdot (1 + \alpha^{(0)} C^{(0)}(Pe(T)) + \alpha^{(1)} C^{(1)}(Pe(T)) + \alpha^{(2)} C^{(2)}(Pe(T))) + \ldots) \]

  in the Chebyshev polynomial basis

- With no oscillations in uncertainty, use 2nd order expansion, resulting in 3 uncertainty parameters per thermo-dynamical property.

\[ R = \sum_i (r^{(i)} + \alpha^{(i)}) T^i \]
**Representation of temperature-dependent uncertainty.**

- Find the validity region for the uncertainty coefficients \{\alpha\} by random sampling. Start with a large uniform sample of values, reject the points that violate the uncertainty condition \[ \frac{\Delta R}{R} \leq \xi\%(T) \]

\[ c_p \approx 1.6582 - 8.470 \cdot 10^{-4} T + 4.4541 \cdot 10^{-7} T^2 - 2992.6 T^{-2} \]

with uncertainty \( \frac{\Delta c_p}{c_p} \) estimated at 0.1% at 300 K, 3% at 1000 K, 8% at 2000 K.

- In the multiplicative uncertainty model,

- In the new representation the parameters become but the validity region is not necessarily rectangular

\[ \{\alpha_{C_1}^{(i)}\}, \{\alpha_{C_2}^{(i)}\}, \ldots, \{\alpha_{C_n}^{(i)}\} \]
Stochastic finite element method

- A surrogate model is an explicit approximation in some basis $\Psi(\alpha)$.

- Stochastic Finite Element Method (SFEM):
  - Choose a set of multi-variable orthogonal polynomials $\Psi$. Use some subset $\{\Psi_q\}$ to approximate the output function: $J \approx \hat{J} = \sum_q x_q \Psi_q$
  - The coefficients $P$ in the definition of each polynomial are chosen to satisfy the orthogonality condition in some measure $\pi$:
    $$\int_\Omega \Psi_p \Psi_q d\pi = 0 \quad p \neq q$$
  - For Gaussian probability measure, the basis is a set of Hermite polynomials:
  - The coefficients $x_q$ are found by collocation.
SFEM: Derivative-based Regression

- Collocation procedure: evaluate the basis polynomials at the sample points in the parameter space, run full model to compute the outputs $S$ at the sample points, assemble the collocation system $\Psi x = S$:

\[
\begin{pmatrix}
\Psi(S_1) \\
\Psi(S_2) \\
\vdots \\
\Psi(S_m)
\end{pmatrix} x =
\begin{pmatrix}
J(S_1) \\
J(S_2) \\
\vdots \\
J(S_m)
\end{pmatrix}
\]

- Issue: we would like to use high-order polynomials. The number of sample points required to assemble $\Psi$ grows rapidly.

- Suggestions:
  - For each sample point, include derivative information.
  - Use an incomplete basis.
Using Derivatives

\[
\begin{pmatrix}
\Psi(S_1) \\
\frac{\partial}{\partial \alpha} \Psi(S_1) \\
\Psi(S_2) \\
\frac{\partial}{\partial \alpha} \Psi(S_2) \\
\vdots \\
\Psi(S_n) \\
\frac{\partial}{\partial \alpha} \Psi(S_n)
\end{pmatrix}
\begin{pmatrix}
\frac{\partial}{\partial \alpha} J(S_1) \\
\frac{\partial}{\partial \alpha} J(S_2) \\
\vdots \\
\frac{\partial}{\partial \alpha} J(S_n)
\end{pmatrix}
= x
\begin{pmatrix}
J(S_1) \\
J(S_2) \\
\vdots \\
J(S_n)
\end{pmatrix}
\]

- The only interaction with the physics code is only by the right hand side.
- If we implement the adjoint wisely, we can get NP times more information for not even on extra function evaluation cost !!!
How to choose basis/ how to sample

- SFEM setup choices:
  - “Full” basis vs. “truncated” basis.
  - “Tall” $\Psi$ with over-sampling vs. “square” matrix $\Psi$ with a minimal number of sample points

- Goal-oriented basis: polynomials of high degree are only included for “important” variables. Importance is defined as sensitivity of the output function to a particular parameter.

- Goal-oriented sample set: mostly an open question, especially when derivative is also involved. Sample points may be chosen: in the directions of highest sensitivity of the output function; for the best condition of $\Psi$; for optimal approximation error; for the best condition of $\Lambda$. 
Approximating the output of the model

- For a moderate number of parameters (3-15), a good choice is “tall” matrix, “truncated” basis.

- Possible definitions of “importance” of a parameter $r^{(i)}$:
  - Derivative (at some “typical” temperature distribution): $\left| \frac{\partial J}{\partial r^{(i)}} \right|$
  - Derivative adjusted by parameter variance: $\left| \frac{\partial J}{\partial r^{(i)}} \right| \sigma_i$

- We start with a full basis of order 3, separate the variables, by “importance”, into groups I, II and III of sizes $n_I > n_{II} >> n_{III}$. We allow polynomials that include variables from group III to have degree 3; allow the polynomials that include variables from group II have degree 2; only keep polynomials of degree 1 in the variables from group I.
Computing derivatives using adjoints

- The dependencies can be studied directly, by random sampling.

- The derivative $\nabla_\alpha J$ can be used for sensitivity analysis.

- Derivative using the adjoint method:
  - Start with an algebraic form of the flux equilibrium equation:
    \[ F(T, \alpha) = 0 \]
  - Assemble a system for the adjoint variable $\lambda$:
  - Evaluate the expression:
    \[ \nabla_\alpha J = -\lambda^T \nabla_\alpha F \]
Consider the finite volumes equation in the form $F(T_n(\alpha), R(T_{n-1}, \alpha)) = 0$

$F(T_n, R(T_{n-1})) = \Lambda(R) \cdot T_n - B = 0$

$T_n \approx T_{n-1}$

Differentiate to obtain

$$\left( \frac{\partial F}{\partial T_n} + \frac{\partial F}{\partial R} \cdot \frac{\partial R}{\partial T_n} \right) \cdot \frac{dT_{n-1}}{d\alpha} + \frac{\partial F}{\partial R} \cdot \frac{\partial R}{\partial \alpha} = 0$$

We need two partial derivatives:

$$\frac{\partial F}{\partial T_n} = \Lambda$$

$$\frac{\partial F}{\partial R} = \frac{\partial \Lambda}{\partial R} \cdot T_n$$

We have assembled the adjoint variable:

$$\frac{dT_n}{d\alpha} = \left( \frac{\partial F}{\partial T_n} + \frac{\partial F}{\partial R} \cdot \frac{\partial R}{\partial T_n} \right)^{-1} \cdot \frac{\partial F}{\partial R} \cdot \frac{\partial R}{\partial \alpha} = -\lambda^T \cdot \frac{\partial F}{\partial R} \cdot \frac{\partial R}{\partial \alpha}$$
**Adjoints**

The required components of the derivatives arrays

\[
\frac{\partial \Lambda}{\partial R^{(i,j)}}, \frac{\partial R^{(i,j)}_i}{\partial \alpha_k}, \frac{\partial R^{(i,j)}_j}{\partial \alpha_k}, \frac{\partial R^{(i,j)}_j}{\partial T^{(i)}}
\]

for the volume cells \(I,J\) and parameter components \(R, \alpha\) are defined and stored during the last step of the iteration \(R_n := R(T_{n-1}), T_n := T(R_n)\).

Finally, the derivative is expressed as:

\[
\frac{dJ}{d\alpha} = \frac{\partial J}{\partial T_n} \cdot \frac{dT_n}{d\alpha}
\]

\[
\frac{dJ}{d\alpha} = \frac{\partial J}{\partial T_n} \cdot \left(\Lambda + \frac{\partial \Lambda}{\partial R} \cdot T_n \cdot \frac{\partial R}{\partial T_n}\right)^{-1} \cdot \frac{\partial \Lambda}{\partial R} \cdot T_n \cdot \frac{\partial R}{\partial \alpha}\bigg|_{T_n=T_{n-1}=T}
\]

Note: in Matlab, computing all derivatives for a single output typically produces an overhead of 10-40%.
Performance of SFEM model

- Size of the finite volume model: 7 pins, 20 horizontal layers.

- The output function is a measure of temperature in the outflow layer:

\[ J(T) = \frac{1}{\text{const}} \cdot \|T_{\text{outflow}}\|_p \]

\[ \tilde{J} = J_0 + \sum_i \frac{\partial J}{\partial a_i} a_i \]
“Preconditioning” with SFEM for assessment,

- We can compute our expectation using a control variate technique.

\[
E_\omega \left[ J(x(p)) \right] = E_\omega \left[ J(x(p)) - \hat{J}(x(p)) + E_\omega \left[ \hat{J}(x(p)) \right] \right]
\]

\[
\text{Var} \left[ J(x(p)) - \hat{J}(x(p)) \right] \ll \text{Var} \left[ J(x(p)) \right]
\]

- If the approximation is good, then we need far fewer samples to compute our estimate
### Performance of SFEM model

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<th>Variance</th>
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<th># points</th>
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### Performance of SFEM model

6 parameters: Range | Variance | Error variance | # points
---|---|---|---
**Cp-coolant, K-fuel**
- Random sampling
  - Range: 953.8098
  - Variance: 1.2900
  - Error variance: 0.0008
- Linear model
  - Range: 953.7528
  - Variance: 1.3527
  - Error variance: 0.0008
- SFEM, full
  - Range: 953.8031
  - Variance: 1.2942
  - Error variance: 1.6105e-5
  - # points: 26
- SFEM, truncated
  - Range: 953.8020
  - Variance: 1.2942
  - Error variance: 1.6113e-5
  - # points: 10
## Performance of SFEM model

9 parameters:

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### Performance of SFEM model

- **12 parameters:** Range | Variance | Error variance | # points
- **Cp-coolant, K-fuel, K-coolant, h**
  - Random sampling
    - 953.8162 | 1.2902 | |
    - 957.5340 | |
  - Linear model
    - 953.7482 | 1.3679 | 0.0012 |
    - 957.5786 | |
  - SFEM, full
    - 953.8040 | 1.2941 | 1.5786e-5 | 72
    - 957.5280 | |
  - SFEM, truncated
    - 953.8033 | 1.2941 | 1.5762e-5 | 11
    - 957.5273 | |
Max temp For 12 parameters:
Mean Square Error
Control variate error versus effort.
Conclusion

- We have defined a SFEM method for high-order approximation of the response of a multiphysics system.
- The method uses derivatives to fit the SFEM polynomial, a first, to our knowledge.
- For a simplified ABR model this results in 2 orders of magnitude improvement in variance over the linear model when both are used as a control variate. The absolute value of the improvement is small in this case, but we expect it to grow with more parameters.
- The method has several challenges: basis pruning, sample choice which will be studied in further work.