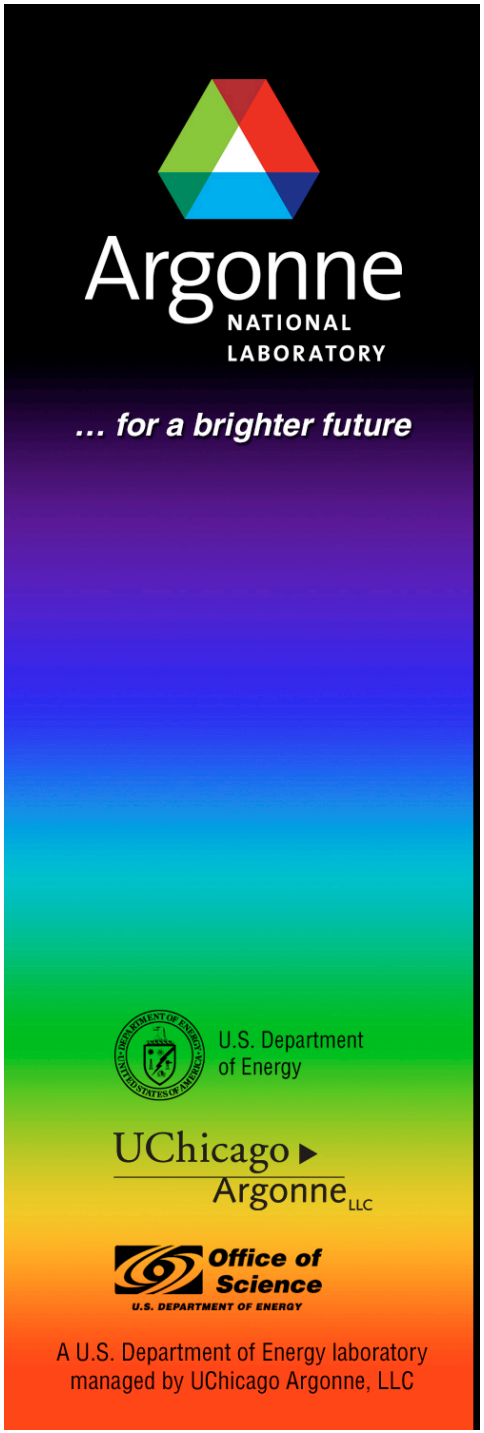

Uncertainty quantification using stochastic finite element method; application to heat distribution in the nuclear reactor core.

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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 ~ 1000 … 10000 … 100000).
- G can be:
  - Max output temperature, max centerline temperature.
  - A characteristic function $G = \chi[a \le T \le b]$ which computes the probability of the max T to be in a given range.

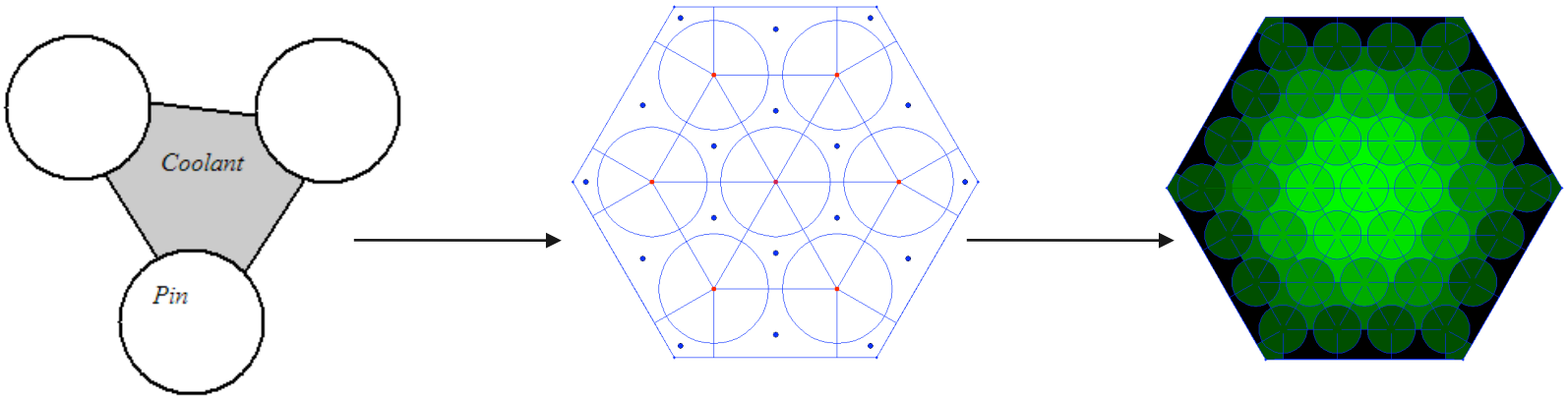
High dimensional Approximation… The curse of dimensionality

- 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.

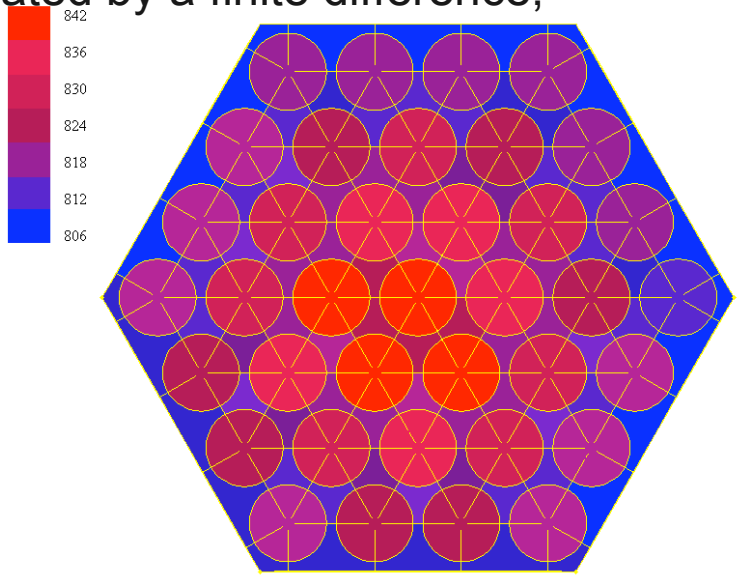


Example: Distribution and transport of heat in the reactor core

- 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 $\Lambda T = \sum q'''dV$.
- Repeat the iterations *R:=R(T) , T:=T(R)* until convergence of the output.



Example: Equations

$$0 = -\nabla \cdot K\nabla T - \rho c_p \vec{u}\nabla T + q'''$$

Interface

- When discretized we obtain

$$\Phi = h(T_J - T_{surface}) = c_p \frac{T_{surface} - T_I}{D/2}$$

Fuel

$$\int_\Omega q'''dV = \sum_J 2\frac{hc_p}{hD + 2c_p}T_J - \sum_J 2\frac{hc_p}{hD + 2c_p}T_I + \sum_{I-,I+} K\frac{1}{H_{I\to I-.+}}\int_{\partial\Omega} ndST_{I-,+} + \ldots$$

$$\ldots - \sum_{I-,I+} K\frac{1}{H_{I\to I-.+}}\int_{\partial\Omega} ndST_I$$

Fluid

$$0 = \sum_J K\frac{1}{H_{I\to J}}\int_{\partial\Omega} ndST_J + \sum_{J+,J-} K\frac{1}{H_{I\to J}}\int_{\partial\Omega} ndST_{J+,J-} - \sum_J K\frac{1}{H_{I\to J}}\int_{\partial\Omega} ndST_I + \ldots$$

$$- \sum_{J+,J-} K\frac{1}{H_{I\to J}}\int_{\partial\Omega} ndST_I + \frac{1}{2}\sum_J \rho c_p \int_{\partial\Omega} \vec{u}ndST_J + \frac{1}{2}\sum_{J+,J-} \rho c_p \int_{\partial\Omega} \vec{u}ndST_{J+,J-} + \ldots$$

$$+ \frac{1}{2}\sum_J \rho c_p \int_{\partial\Omega} \vec{u}ndST_I + \frac{1}{2}\sum_{J+,J-} \rho c_p \int_{\partial\Omega} \vec{u}ndST_I + \sum_{J^*} 2\frac{hc_p}{hD + 2c_p}T_{J^*} - \sum_{J^*} 2\frac{hc_p}{hD + 2c_p}T_I$$

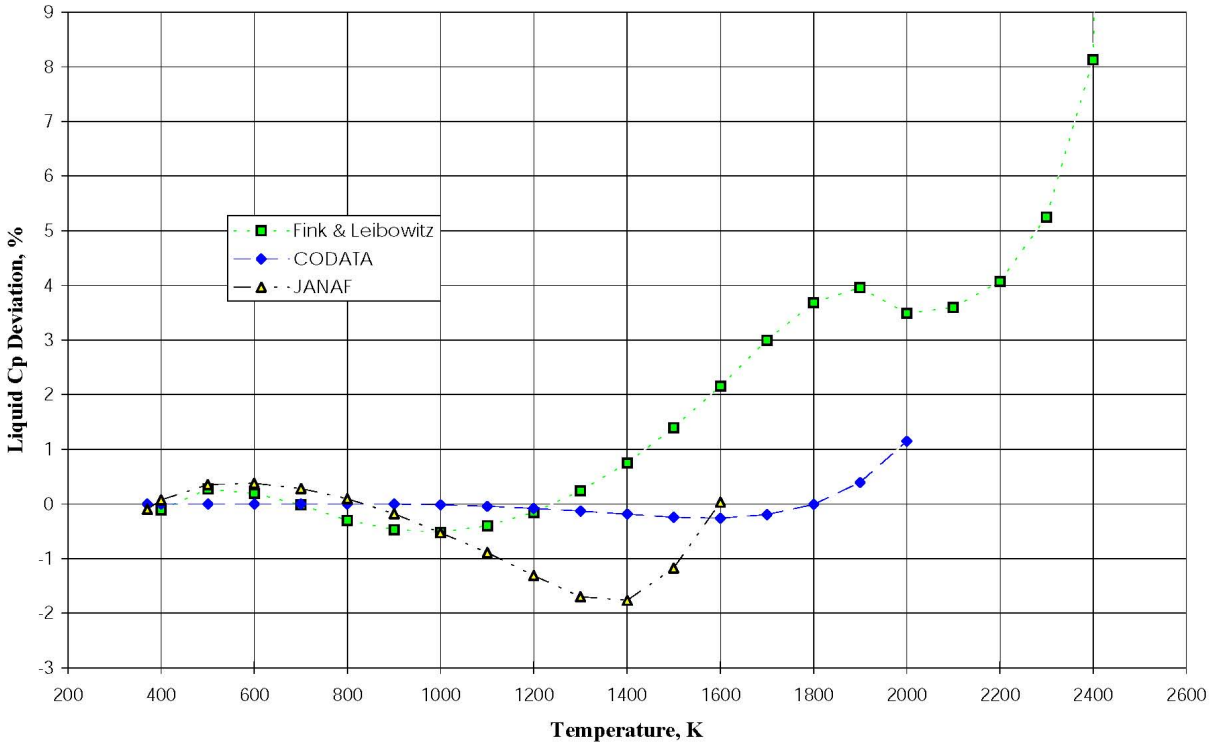


Fig. 1.1-11 Deviations of Values from Other Assessments from the Recomended Values for the Heat Capacity at Constant Pressure of Liquid Sodium

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:

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

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

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 {α} by random sampling. Start with a large uniform sample of values, reject the points that violate the uncertainty condition $\Delta R / R \le \xi\%(T)$

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

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

$$\{\alpha_{C_1}^{(i)}\}\{\alpha_{C_2}^{(i)}\}\ldots\{\alpha_{Cn}^{(i)}\}$$

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 Ψ. Use some subset $\{\Psi_q\}$ to approximate the output function: $J \approx \widehat{J} = \sum_q x_q \Psi_q$

- The coefficients *P* in the definition of each polynomial are chosen to satisfy the orthogonality condition in some measure π:

$$\int_\Omega \Psi_p \Psi_q d\pi = 0 \quad p \neq q$$

- For Gaussian probability measure,

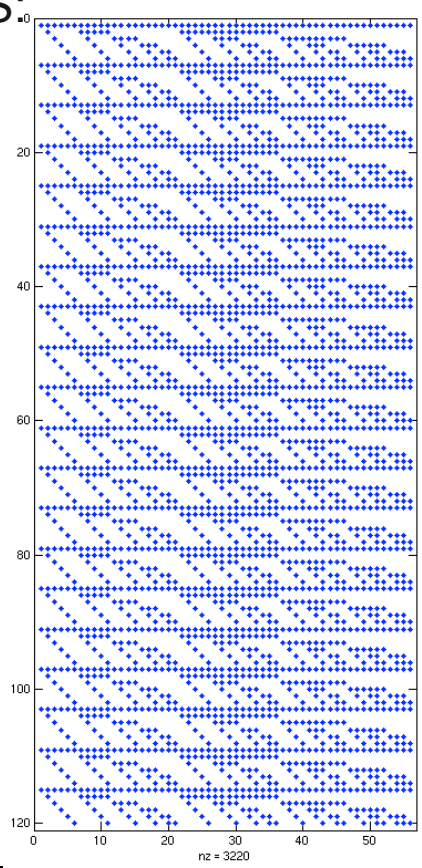
the basis is a set of Hermite polynomials:

- 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 Ψx=S:

$$\begin{pmatrix} \Psi(S_1) \\ \Psi(S_2) \\ \vdots \\ \Psi(S_m) \end{pmatrix} X = \begin{pmatrix} J(S_1) \\ J(S_{2)} \\ \vdots \\ J(S_m) \end{pmatrix}$$

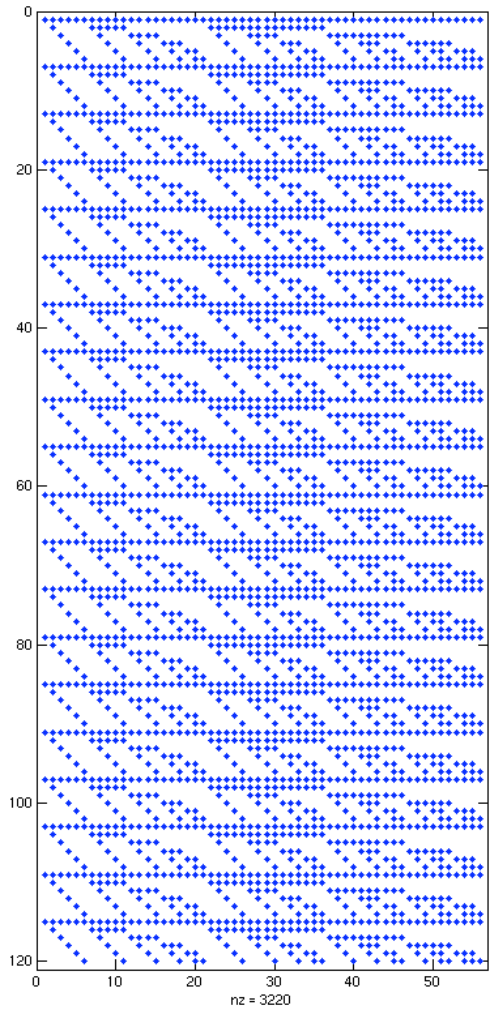


- Issue: we would like to use high-order polynomials. The number of sample points required to assemble Ψ grows rapidly.

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

Using Derivatives

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



- 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" Ψ with over-sampling vs. "square" matrix Ψ 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 Ψ; for optimal approximation error; for the best condition of Λ.

Approximating the output of the model

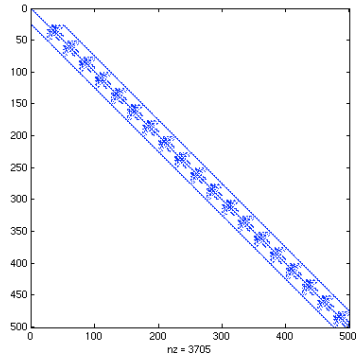
- For a moderate number of parameters (3-15), a good choice is “tall” matrix, “truncated” basis.

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

- 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.

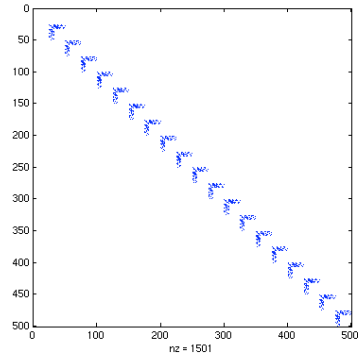
Computing derivatives using adjoints

- 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: $F(T,\alpha)=0$ with
  - Assemble a system for the adjoint variable λ:



  - Evaluate the expression:

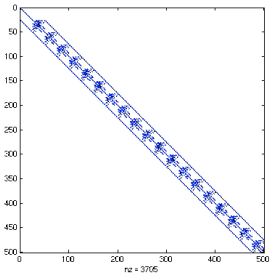
$$\nabla_\alpha J = -\lambda^T \nabla_\alpha F$$

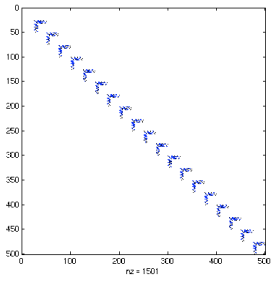
Adjoints.

- Consider the finite volumes equation in the form $F(T_n(\alpha), R(T_{n-1}, \alpha)) = 0$

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

$$T_n \approx T_{n-1}$$





- 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: $\frac{\partial F}{\partial T_n} = \mathbf{\Lambda}$

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

- 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

$$\frac{\partial \Lambda}{\partial R^{(I,J)}{}_j}, \quad \frac{\partial R^{(I,J)}{}_j}{\partial \alpha_k}, \quad \frac{\partial R^{(I)}{}_j}{\partial \alpha_k}, \quad \frac{\partial R^{(I,J)}{}_j}{\partial T^{(I)}}$$

  for the volume cells I,J and parameter components R_j, α_k 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: $\frac{dJ}{d\alpha} = \frac{\partial J}{\partial T_n} \cdot \frac{dT_n}{d\alpha}$

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

- 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:

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

$$\hat{J} = J_0 + \sum_i \frac{\partial J}{\partial a_i} a_i$$

"Preconditioning" with SFEM for assessment,

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

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

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

- If the approximation is good, then we need far fewer samples to compute our estimate

Performance of SFEM model

3 parameters: Cp-coolant	Range	Variance	Error variance	# points
■ Random sampling	953.8092 957.5269	1.2901		
■ Linear model	953.7269 957.5761	1.3813	0.0016	
■ SFEM, full	953.8016 957.5245	1.2933	0.0001	12
■ SFEM, truncated	953.8027 957.5273	1.2937	0.0002	4

Performance of SFEM model

6 parameters: Cp-coolant, K-fuel	Range	Variance	Error variance	# points
■ Random sampling	953.8098 957.5273	1.2900		
■ Linear model	953.7528 957.5619	1.3527	0.0008	
■ SFEM, full	953.8031 957.5272	1.2942	1.6105e-5	26
■ SFEM, truncated	953.8020 957.561	1.2942	1.6113e-5	10

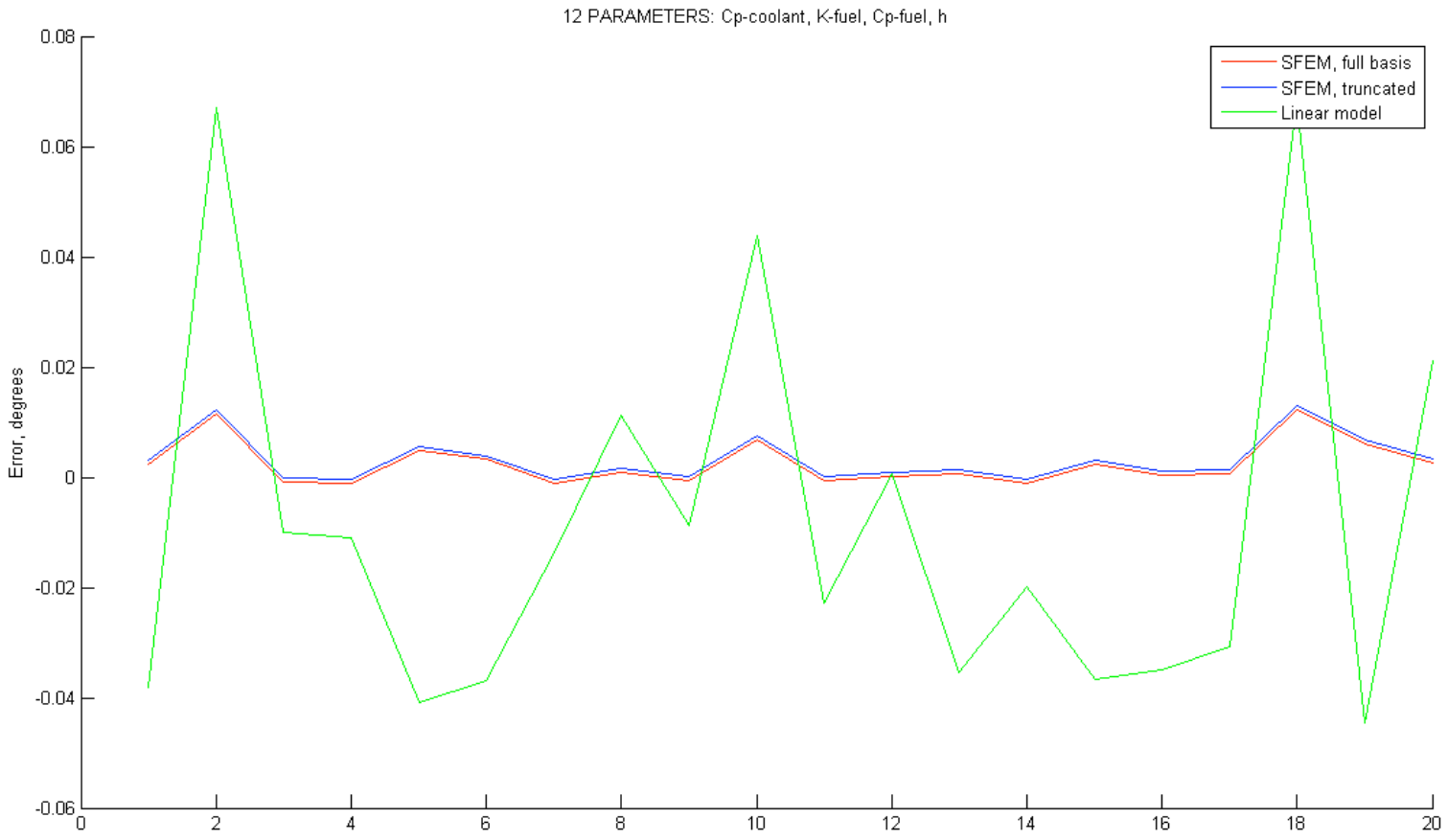
Performance of SFEM model

9 parameters: Cp-coolant, K-fuel, K-coolant	Range	Variance	Error variance	# points
■ Random sampling	953.8162 957.5340	1.2902		
■ Linear model	953.7194 957.6103	1.4115	0.0028	
■ SFEM, full	953.8040 957.5280	1.2941	1.5786e-5	46
■ SFEM, truncated	953.8033 957.5273	1.2941	1.5761e-5	10

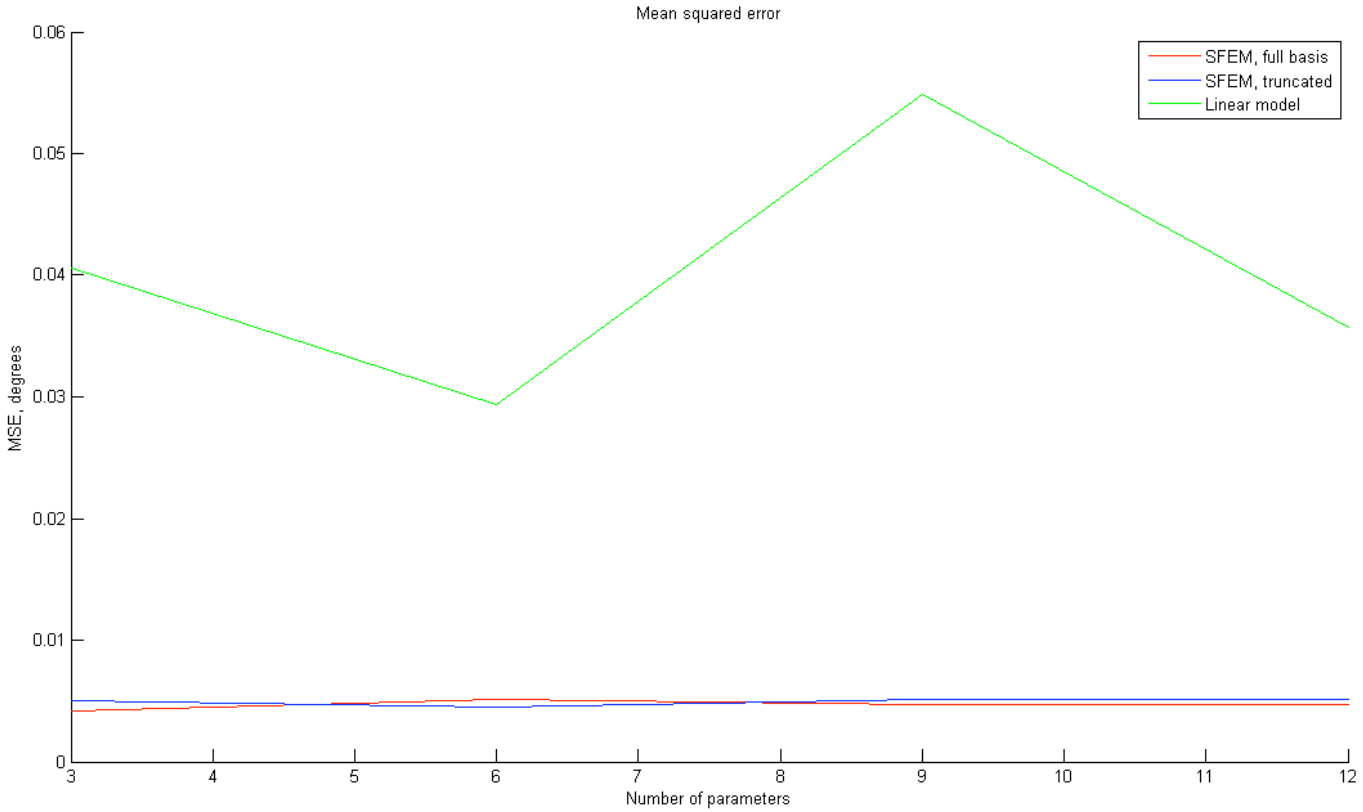
Performance of SFEM model

12 parameters: Cp-coolant, K-fuel, K-coolant, h	Range	Variance	Error variance	# points
■ Random sampling	953.8162 957.5340	1.2902		
■ Linear model	953.7482 957.5786	1.3679	0.0012	
■ SFEM, full	953.8040 957.5280	1.2941	1.5786e-5	72
■ SFEM, truncated	953.8033 957.5273	1.2941	1.5762e-5	11

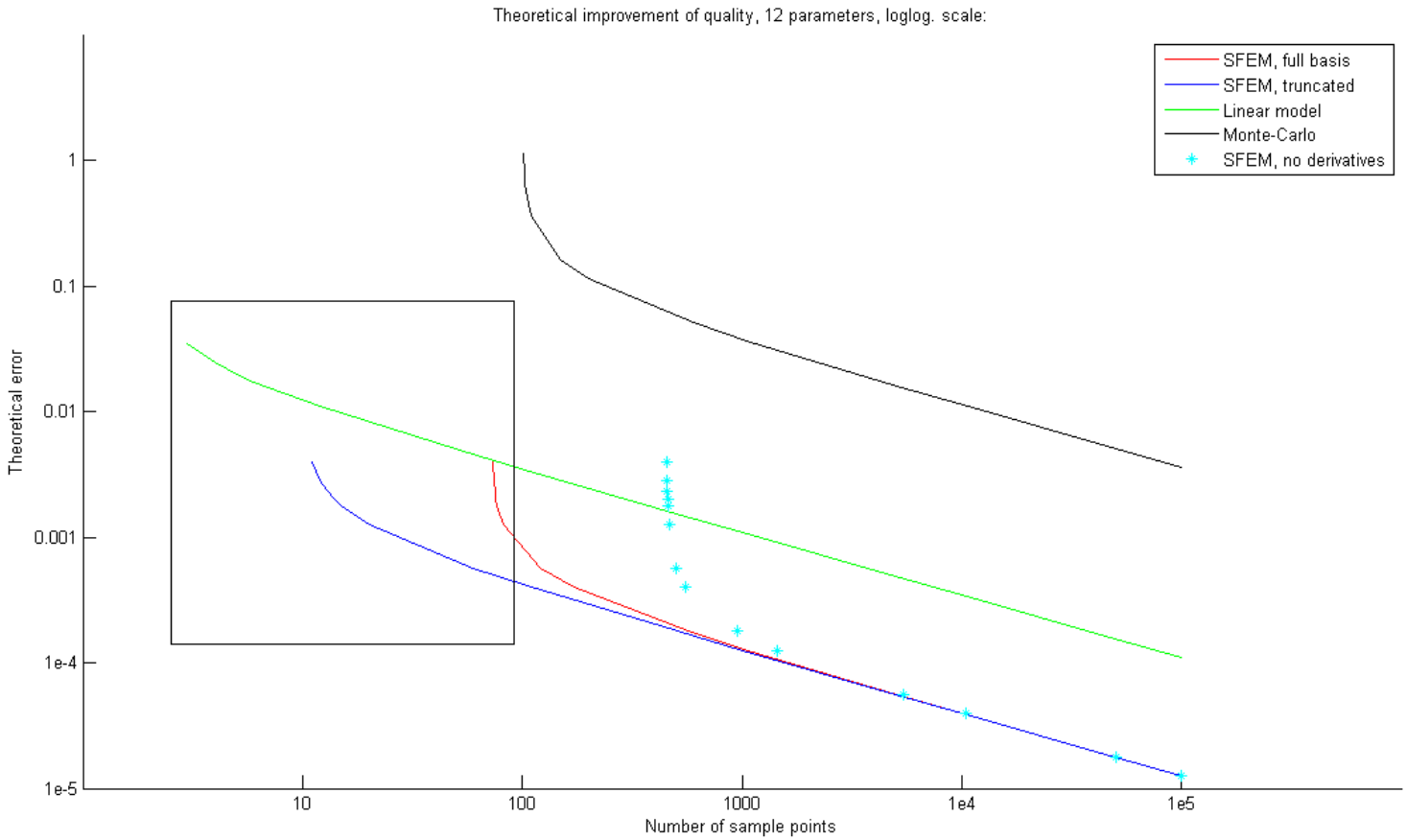
Max temp For 12 parameters:



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.