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Uncertainty quantification using stochastic finite element method.

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Topics of discussion

- Need for uncertainty analysis
- An example of a complex system with uncertain inputs
- Limited applicability of linear model, random sampling
- Applicability of stochastic finite element (SFEM) approach

- Improvement of SFEM performance through the use of goal-oriented polynomial basis, goal-oriented collocation procedure

Uncertainty calculations in high dimensional systems

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

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

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

- *F* could be a coupled system of several differential equations, describing a complex engineering structure, *p* the physical parameters (*p~10,100, 1000...*).
- G could be an observation on performance of the model (*maximal temperature*), or a characteristic function which computes the probability for the observed quantity to be in the prescribed range (*chance of overheating*).

Uncertainty calculations in high dimensional systems

- Computing the correct average is strongly related to approximating the function *G*.

- Available solutions:

- Random sampling (directly evaluate *G* for a sample from parameter space)

  Global, but slow.

- Sensitivity analysis (approximate *G* by a linear function, using derivative information)

Fast, but local, hard to adjust. What if the precision is insufficient?

- Can we create a method that efficiently uses the advantages of both approaches? We think so: using adapted stochastic finite element method fitted with derivative information.

Stochastic Finite Element Method, preview

- A stochastic finite element model model is an explicit approximation $G \approx \hat{J}(\alpha) = \sum x_q \Psi_q$ in basis $\{\Psi(\alpha)\}$, dependent on direct (or derived) uncertain parameters {α}.

- Stochastic Finite Element Method (SFEM):

- Choose a set of multi-variable orthogonal polynomials Ψ. Use some subset $\{\Psi_q\}$ to approximate the output function: $\hat{J} \approx \sum_q x_q \Psi_q$
  $\Psi_q = P_0 + \sum P_i \alpha_i + \sum P_{ij} \alpha_i \alpha_j + \sum P_{ijk} \alpha_i \alpha_j \alpha_k + \ldots$

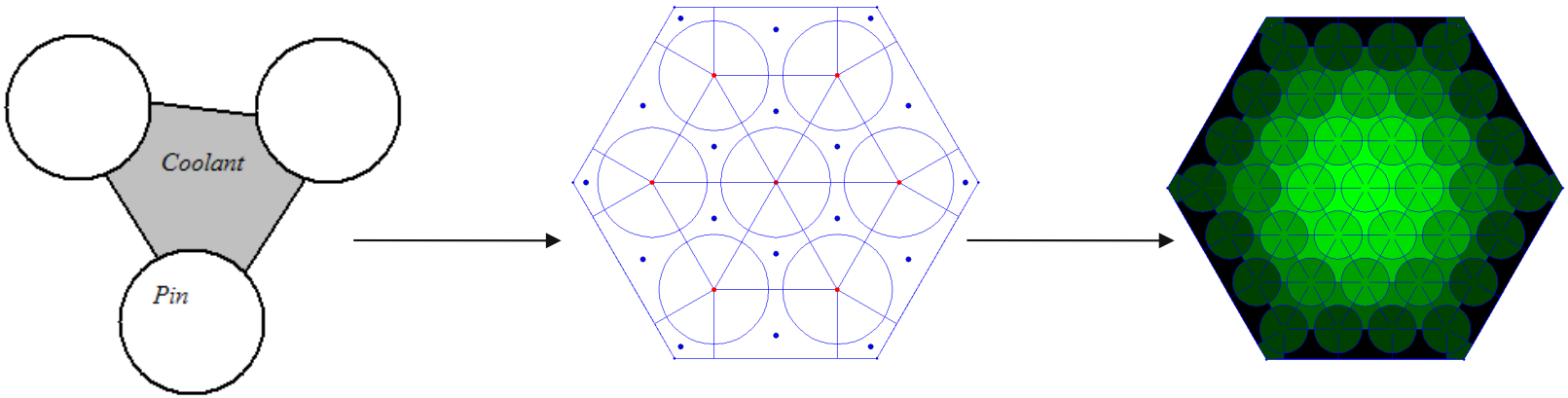
- The coefficients P in the definition of each polynomial are chosen to satisfy the orthogonality condition in some measure π:
  $\int_\Omega \Psi_p \Psi_q d\pi = 0 \quad p \neq q$

- The coefficients x_q are found by solving the collocation equation
  $G(\alpha) = \sum_q x_q \Psi_q(\alpha)$

Distribution and transport of heat in the 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.



Distribution and transport of heat in the reactor 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. Statistical information about the uncertainty may be unavailable.

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

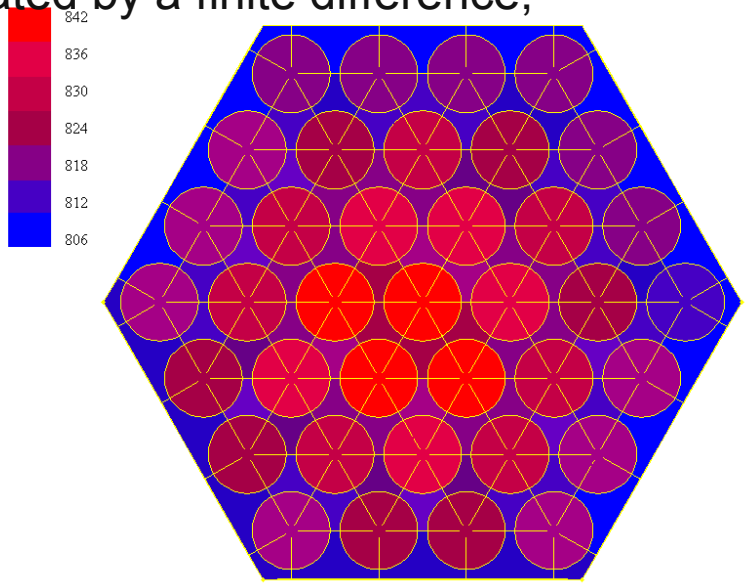
with uncertainty $\frac{\Delta c_p}{c_p}$ estimated at 0.1% at 300 K, 3% at 1000 K, 8% at 2000 K.

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 temperature of the core.

- 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 q''', 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.



Distribution and transport of heat in the reactor core

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

Interface

- When discretized we obtain

Fuel

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

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

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

Fluid

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

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

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

Distribution and transport of heat in the reactor core

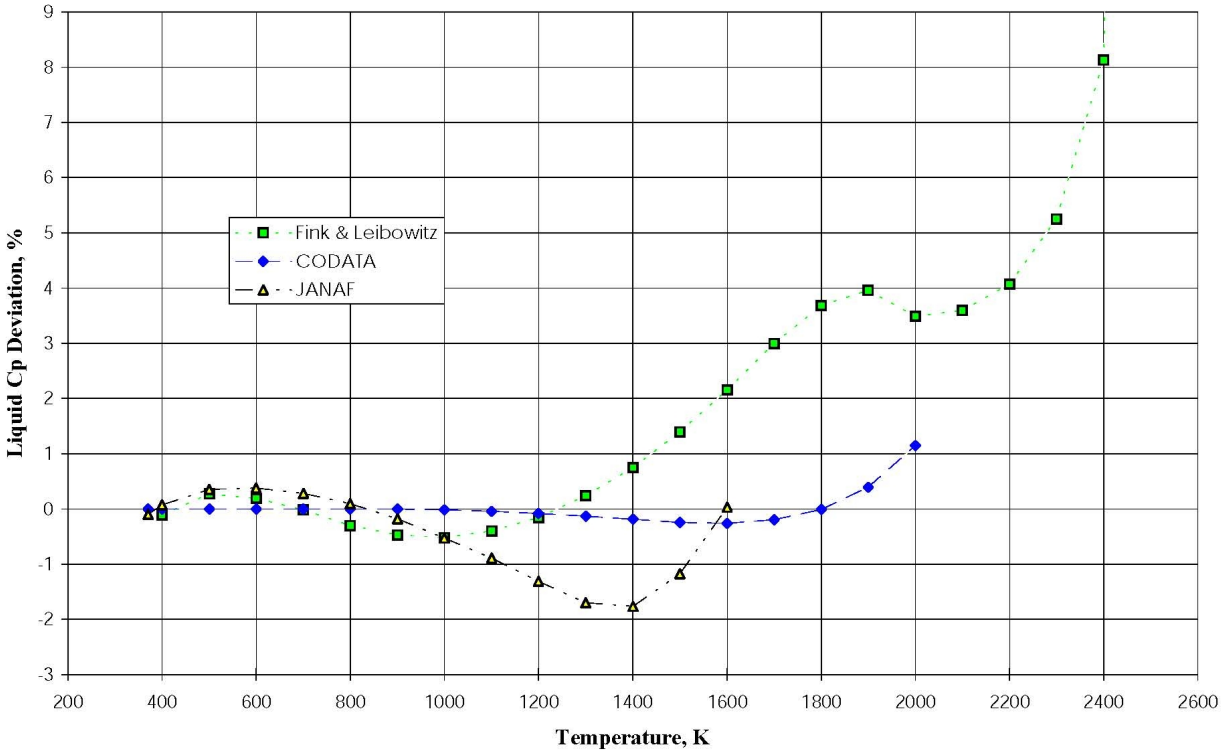


Fig. 1.1-11 Deviations of Values from Other Assessments from the Recomended Values for the Heat Capacity at Constant Pressure of Liquid Sodium

Approximating the output of the model

- Assume a temperature-dependent structure for the uncertainty:

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

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

in the Chebyshev polynomial basis

$$C^{(0)}(T) = 1 \quad C^{(1)}(T) = T + 1 \quad C^{(2)}(T) = 2T^2 - 1$$

$$C^{(3)}(T) = 4T^3 - 3T^2$$

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

- Note: other structures are less suitable for expressing the uncertainty conditions.

$$R = \left(\sum_i r^{(i)} T^i \right) + \left(\alpha_0^{(i)} C^{(0)}(T) + \alpha_1^{(i)} C^{(1)}(T) + \alpha_2^{(i)} C^{(2)}(T) \right)$$

$$R = \sum_i (r^{(i)} + \alpha^{(i)}) T^i$$

Approximating the output of the model

- 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 $\Delta R / R \le \xi\ \%$

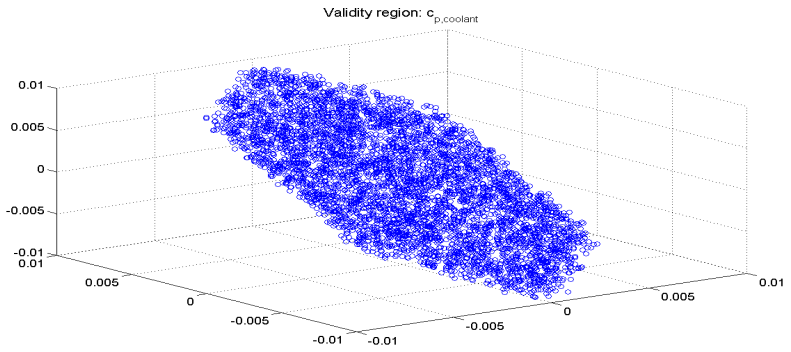
$c_p \approx 1.6582 - 8.470 \cdot 10^{-4} T + 4.4541 \cdot 10^{-7} T^2 - 2992.6 T^{-2}$

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, $\Delta R / R = 1 + \alpha^{(0)} C^{(0)} + \alpha^{(1)} C^{(1)} + \alpha^{(2)} C^{(2)}$

$C = C(T), C = C(Pe(T))$

- Check the uncertainty condition at selected values of T, or of Pe to obtain the uncertainty validity region.



Stochastic Finite Element Method

- Stochastic Finite Element Method (SFEM):
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- The coefficients P in the definition of each polynomial are chosen to satisfy the orthogonality condition in some measure π:
  $\Psi_q = P_0 + \sum P_i \alpha_i + \sum P_{ij} \alpha_i \alpha_j + \sum P_{ijk} \alpha_i \alpha_j \alpha_k + \ldots$
- For Gaussian probability measure, $\int_\Omega \Psi_p \Psi_q d\pi = 0 \quad p \neq q$
  the basis is a set of Hermite polynomials: $\Psi(\alpha_1, \alpha_2, \ldots) = \prod_i H^{(k_i)}(\alpha_i)$

$$H^{(0)}(\alpha) = 1 \quad H^{(1)}(\alpha) = 2\alpha \quad H^{(2)}(\alpha) = 4\alpha^2 - 1$$

$$H^{(3)}(\alpha) = 8\alpha^3 - 12\alpha \quad H^{(4)}(\alpha) = 16\alpha^4 - 48\alpha^{12} + 12$$

- 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.

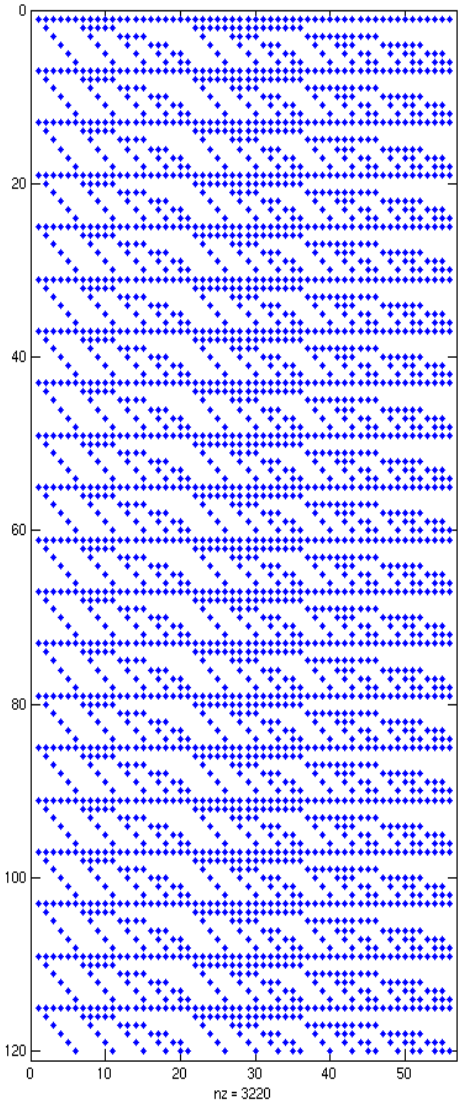
- Suggestions:
  - For each sample point, include derivative information.
  - Use an incomplete basis.

SFEM: Derivative-based Regression

- Collocation with derivative information:

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

- Only right-hand side requires direct evaluations of the model.
- It is possible to evaluate the derivative efficiently, and get blocks of additional information for not even an extra model evaluation cost!



Approximating the output of the model

- 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. 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.

Performance of SFEM model

- Size of the finite volume model: 7 pins, 20 horizontal layers.
- The output function is an estimation of maximal temperature in the centerline of the reactor core (evaluation may require additional calculations).
- The computational budget for the reduced SFEM basis is kept approximately constant. We use 100 exact outputs for validation.
- Linear approximation is defined as a tangent model obtained at a "typical" temperature distribution. $\widehat{J} = J_0 + \sum_i \frac{\partial J}{\partial a_i} a_i$
- We output:
  - Range (lowest and highest observed outputs)
  - Variance (variance of the observed outputs)
  - Error variance (variance of the difference between surrogate and exact outputs)

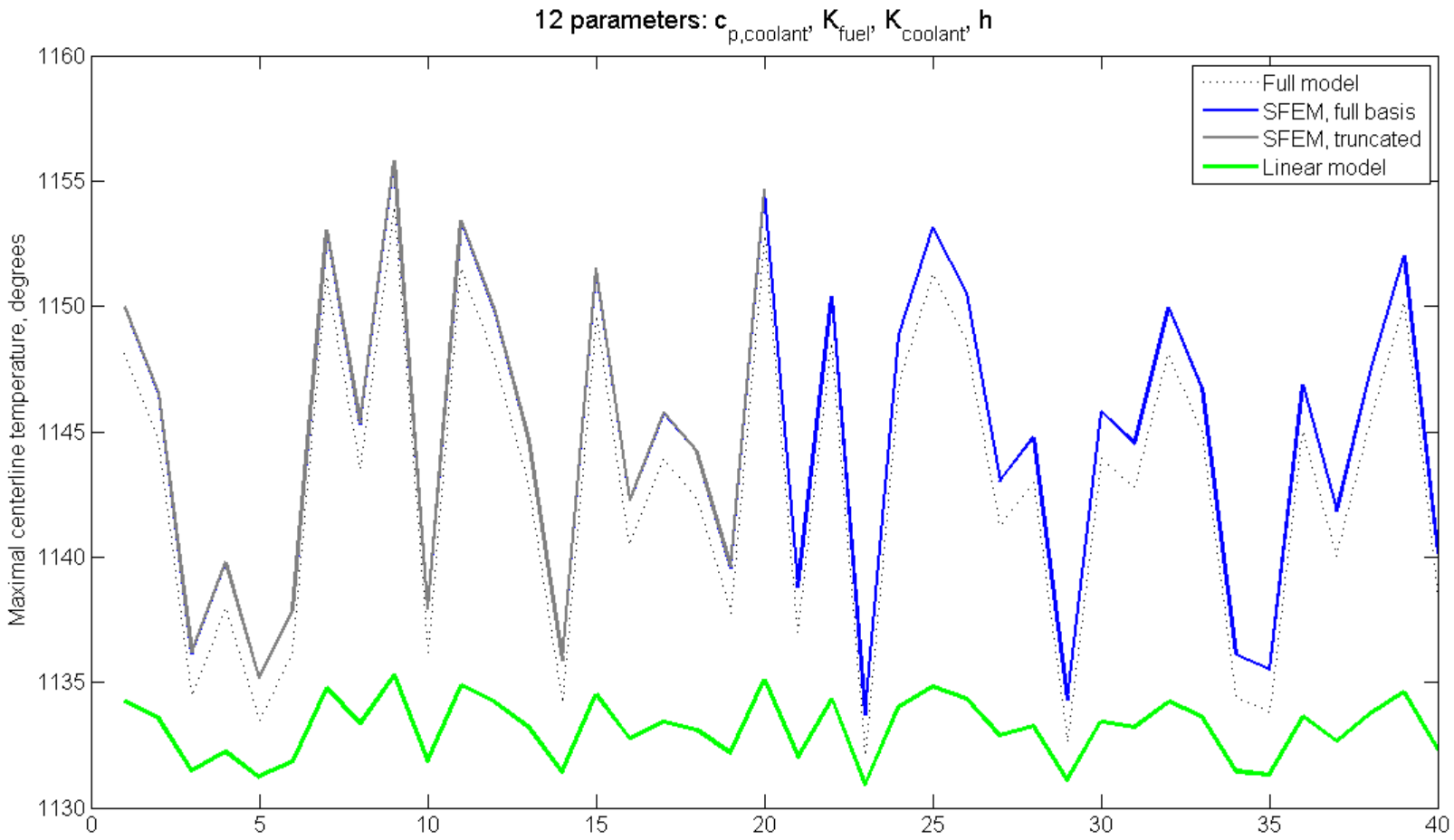
Performance of SFEM model

3 parameters: Cp-coolant	Range	Variance	Error variance	# points
■ Random sampling	1123.11 1144.24	36.86		
■ Linear model	1211.31 1218.62	1.58	23.19	
■ SFEM, full	1124.10 1144.13	36.54	0.0013	12
■ SFEM, truncated	1124.45 1147.66	39.03	0.0015	4

Performance of SFEM model

12 parameters: Cp-coolant, K-fuel, K-coolant, Cp-fuel	Range	Variance	Error variance	# points
■ Random sampling	1132.06 1153.95	39.49		
■ Linear model	1130.92 1135.28	1.57	25.28	
■ SFEM, full	1133.71 1155.75	40.12	0.0032	72
■ SFEM, truncated	1135.81 1155.79	45.21	0.0028	9

Performance of SFEM model



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. This results in an advantage in computational efficiency over a generic SFEM approach.
- For a simplified reactor core model this results in significant improvement in variance over the linear model.
- The method has several challenges: optimal sampling, improvement of the collocation condition number, basis truncation.
- We will extend the developed approach to larger models, incorporating additional physical effects.

Thank you for your attention.

Acknowledgement of information provided to us:

- Nuclear reactor analysis (Duderstadt, Hamilton)
- Thermo-hydraulics of a reactor core (lecture by Paul Fischer)
- Stochastic finite element methods (Ghanem, Spanos)
- Material properties (Fink)

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:

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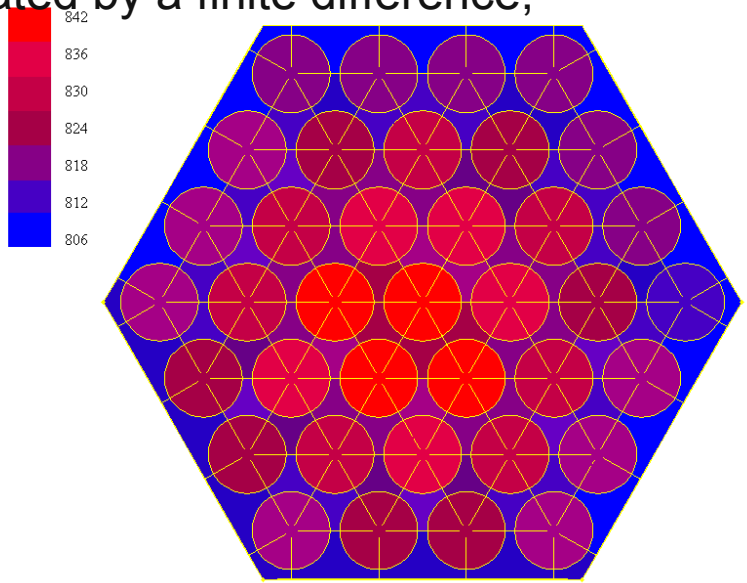

Approximating the output of the model

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- 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 $\Delta R / R \le \xi\ \%$

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$C = C(T), C = C(Pe(T))$

- Check the uncertainty condition at selected values of T, or of Pe.

Approximating the output of the model

- A surrogate model is an explicit approximation $J \approx \hat{J}(\alpha) = \sum x_q \Psi_q$ in some basis $\Psi(\alpha)$.

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  - The coefficients P in the definition of each polynomial are chosen to satisfy the orthogonality condition in some measure π:
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    the basis is a set of Hermite polynomials: $H^{(0)}(\alpha) = 1 \quad H^{(1)}(\alpha) = 2\alpha \quad H^{(2)}(\alpha) = 4\alpha^2 - 1$
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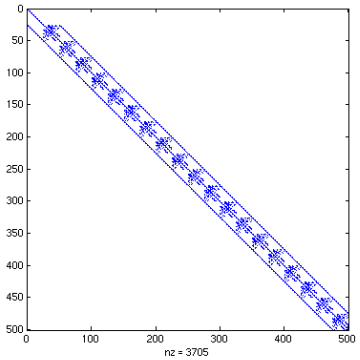
  - The coefficients x_q are found by collocation.

Approximating the output of the model

- The dependencies $J(T), T(\Lambda), \Lambda(R,T), R(T,\alpha)$ 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 $F = \Lambda(\alpha)T - \sum q'''dV$
  - Assemble a system for the adjoint variable λ: $D = \nabla_T F, \quad D^T \lambda = \nabla_T J$
  - Evaluate the expression: $\nabla_\alpha J = -\lambda^T \nabla_\alpha F$

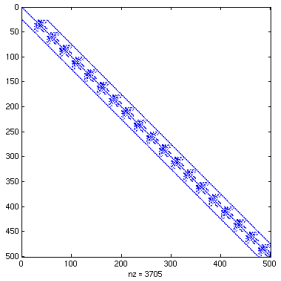


Approximating the output of the model

- 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:

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

Approximating the output of the model

- The required components of the derivatives arrays

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

  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: $\frac{dJ}{d\alpha} = \frac{\partial J}{\partial T_n} \cdot \frac{dT_n}{d\alpha}$

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

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