Uncertainty Quantification in Two-dimensional Simulations of Spent Nuclear Fuel Assemblies

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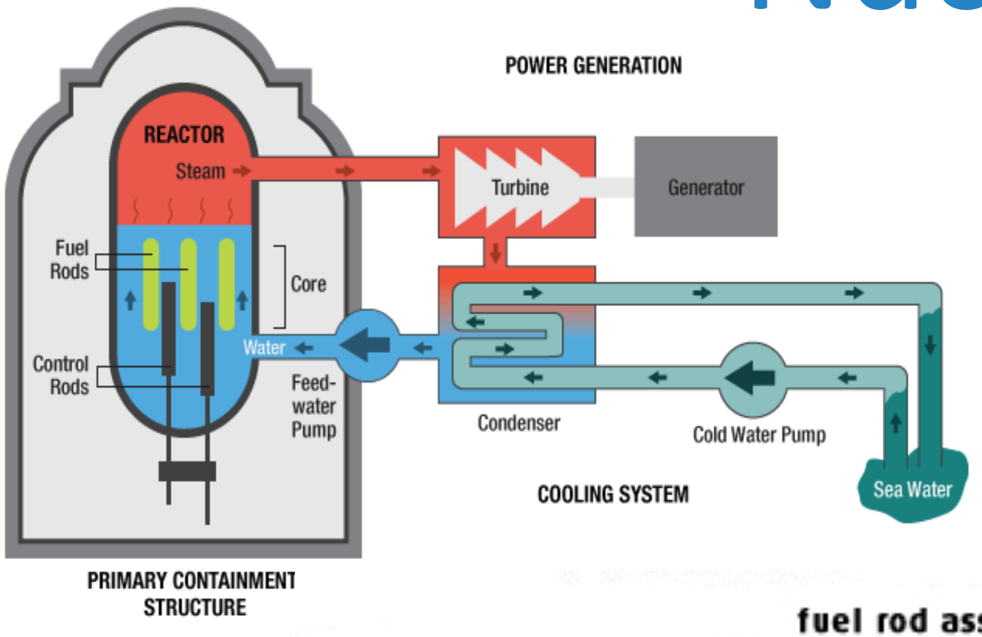
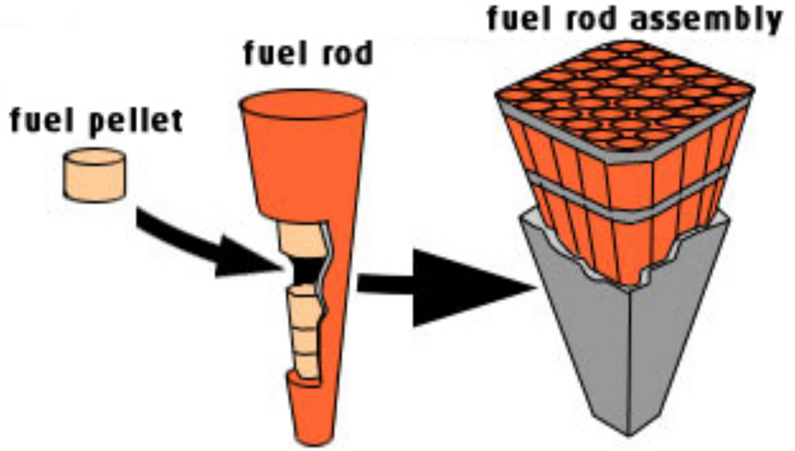
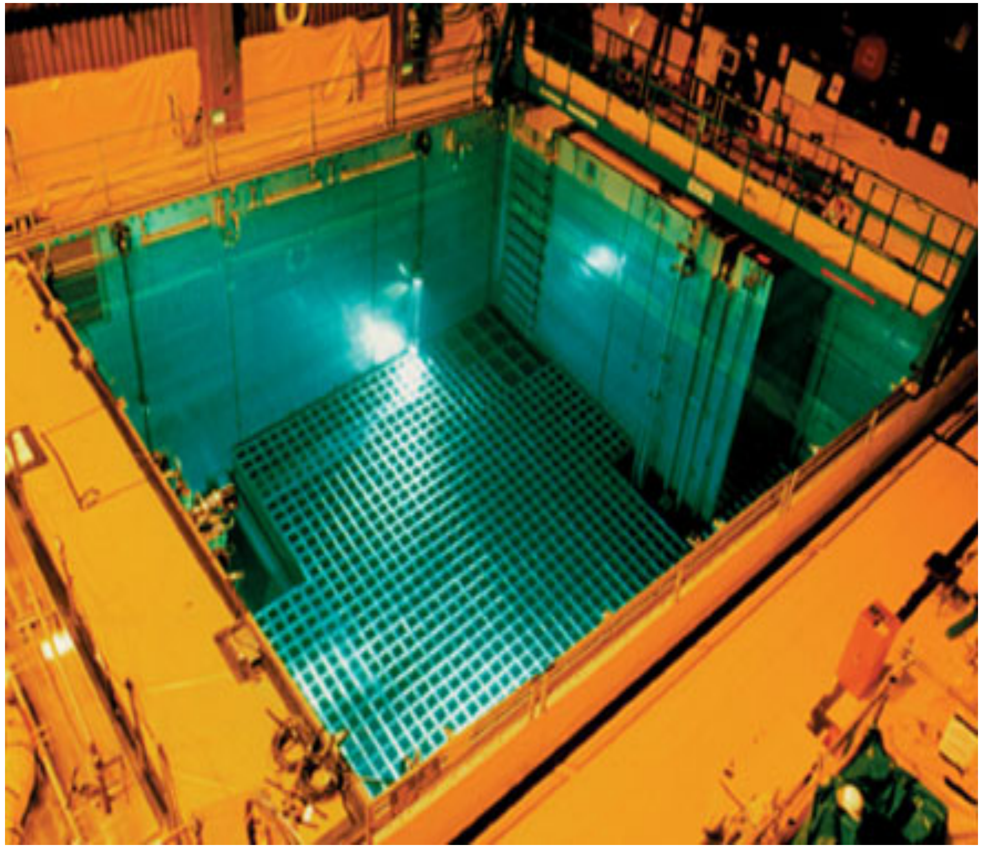
Outline

- Nuclear Energy Background
- 9x9 Fuel Assembly FLUENT Model
- Uncertainty Quantification (UQ) Introduction and Background
- Applying UQ to FLUENT Model
- Results
- Future Work

Nuclear Energy

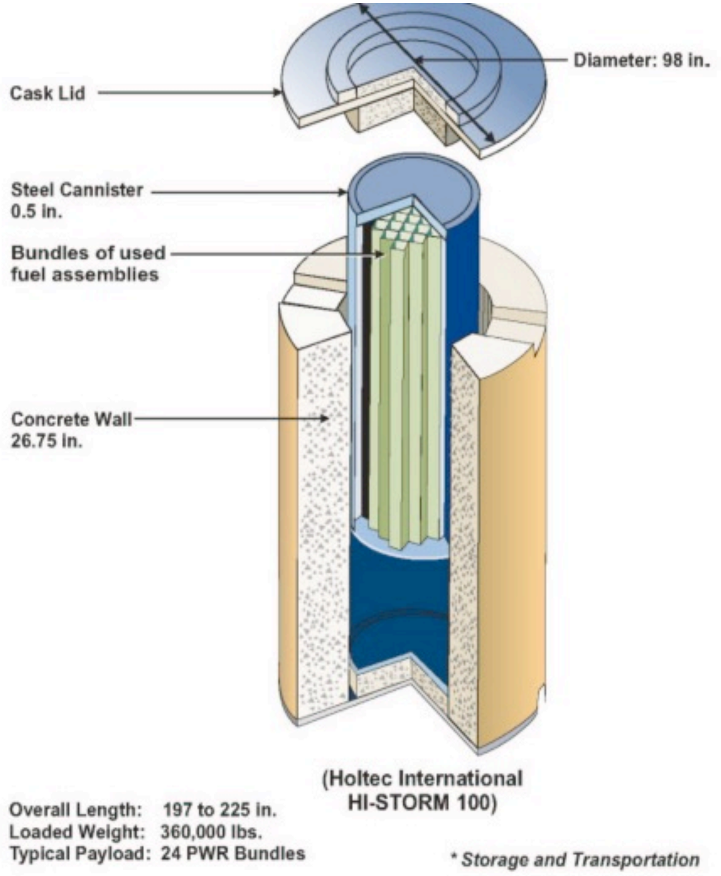




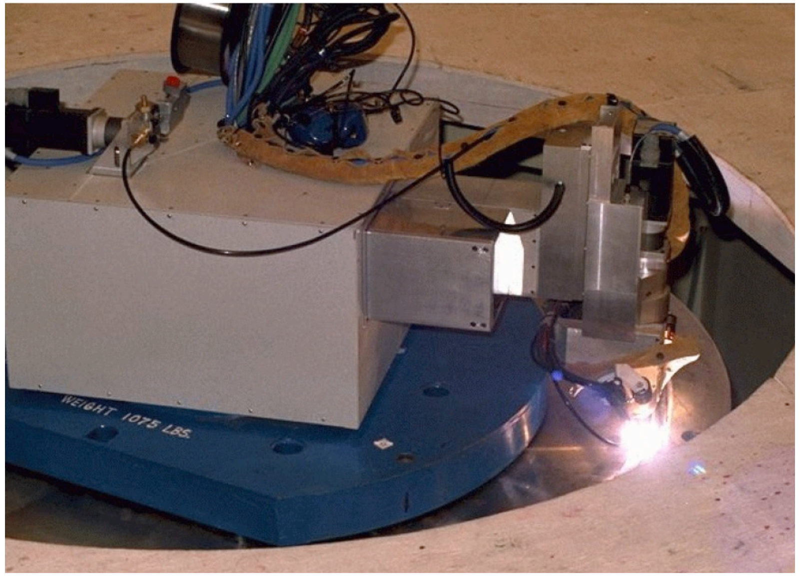


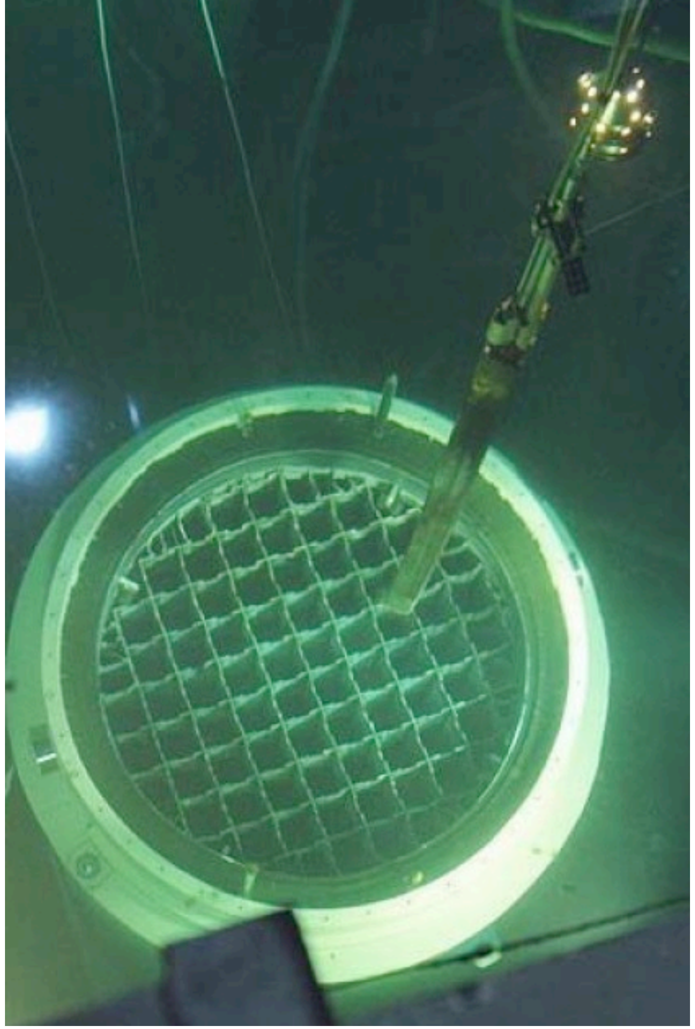
Spent Fuel Pool to Shield Radiation and Cool Fuel Rods

Spent Fuel Storage Casks

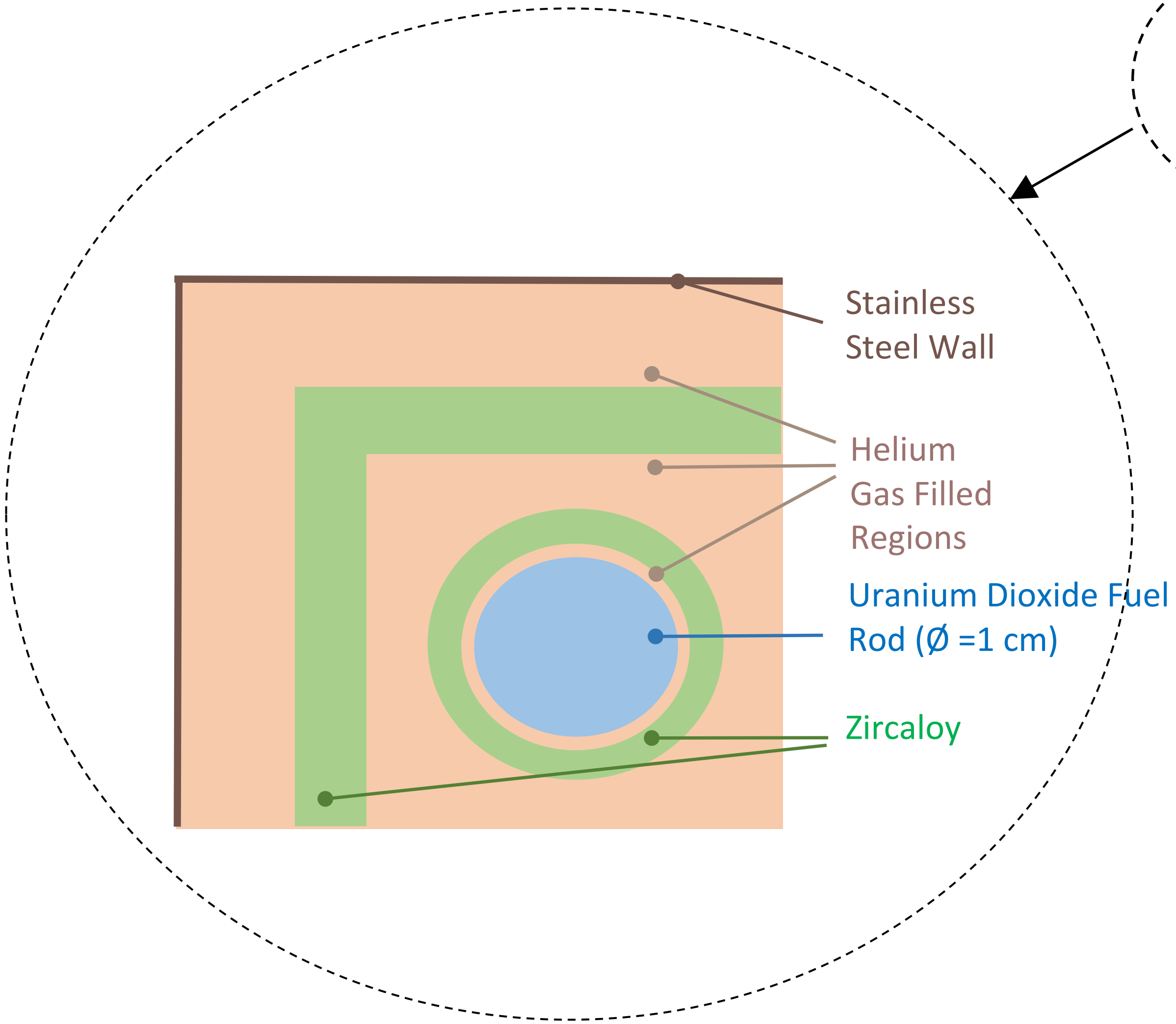


Welding of Canister Lid

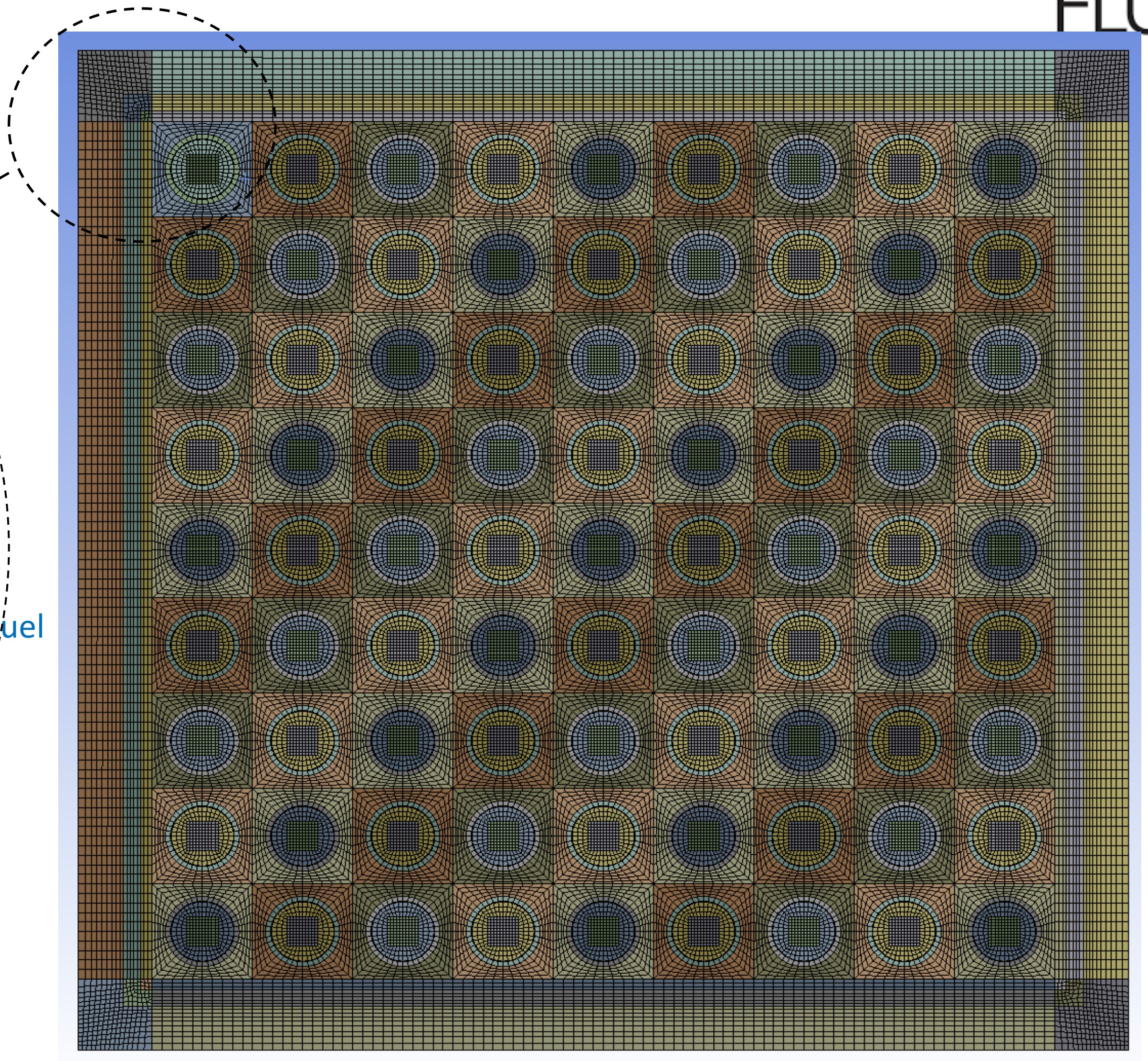




Fluent Geometry



47,944 nodes
47,702 elements



Fluent Model

- Steady State 2D simulations using Pressure-based solver in Fluent
- Gravity in Y direction
- Energy Equation ON to model:
  - Conduction heat transfer in solid region
  - Buoyancy induced gas motion and natural convection heat transfer within the gas filled regions
  - Radiation heat transfer across all gas filled regions

Fluent Model Input and B.C.

Zircaloy
Thermal Conductivity
Specific Heat
Emissivity

Helium
Thermal Conductivity
Specific Heat

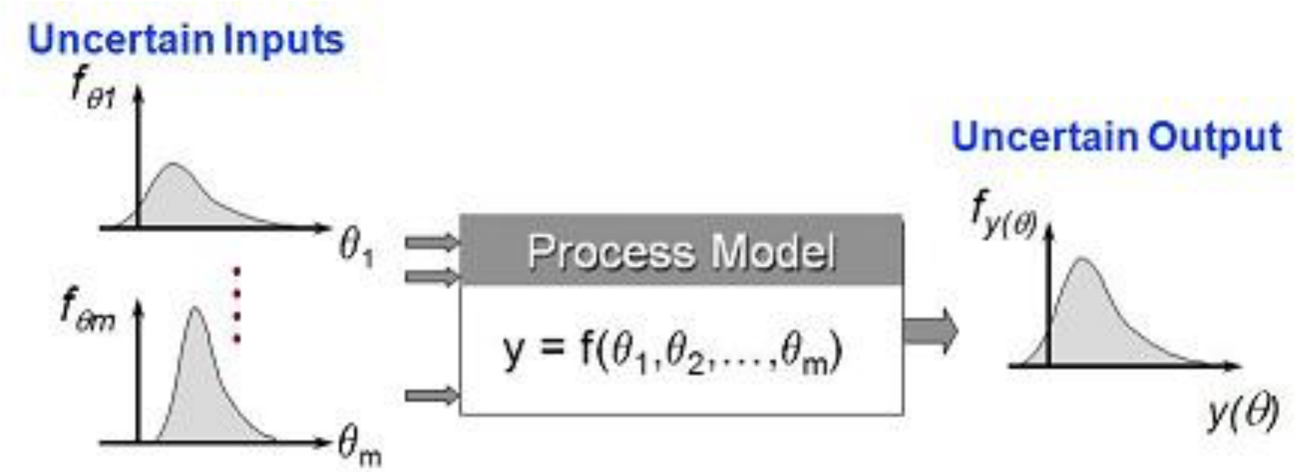
Uranium Dioxide
Thermal Conductivity
Specific Heat
Emissivity
Power

Stainless Steel
Wall Temperature

Uncertainty Quantification

Mathematical models of heat transfer are often challenged by random/uncertain properties

Uncertainty quantification is needed in order to get a predictive fidelity of the simulation



Introduction to PCE

p = N-ord (Highest order Legendre Present).
n = N-dim (Number of uncertain dimensions).

PCE is Polynomial Chaos Expansion

Univariate Case: For one input parameter, we model the propagation of uncertainty through our model

1. Assume our input variable can be expressed as a polynomial expansion. Where ξ represents a uniform random variable, and ψ represents Legendre Polynomials
2. After propagating X through our model we can model the output of the model as a similar expansion
3. We can then perform non-intrusive spectral projection (NISP) to extract the coefficients of this expansion

$$X = \sum_{i=0}^{p} x_i \psi_i(\xi)$$

$$T = \sum_{i=0}^{p} T_i \psi_i(\xi)$$

$$K = \frac{\langle x_i, \psi_i \rangle}{\langle \psi_i, \psi_i \rangle} \qquad T_i = K * T$$

Introduction to PCE

Multivariate Case: For n-input parameters, we model the propagation of uncertainty through our model

p = N-ord (Highest order Legendre Present).
n = N-dim (Number of uncertain dimensions).

1. When modeling the propagation of multiple uncertain parameters we introduce a Multi-index (**M**) showing the ordering of polynomials in the expansion. The number of terms in our expansion is N_pc.
2. Using identical methods from the univariate case we are able to extract an expansion for the output parameter as a function of our multiple input variables

$$N_{pc} = \frac{(n+p)!}{n!p!}$$

$$\begin{aligned} T &= \sum_{i=0}^{N_{pc}} T_i \Psi_i(\Xi) \\ &= \sum_{i=0}^{N_{pc}} T_i \prod_{j=1}^{n} \psi_l^j(\xi^j) \qquad \text{where} \qquad l = M_i^j \end{aligned}$$

Multivariate Case Example

We will now consider the case where Nord = 2, and Ndim = 2.

In this case we will use the nPCETerms equation to see that we expect 6 terms in our output expansion.

$$\text{nPCETerms} = \frac{(2+2)!}{2!2!} = N_{pc} = 6$$

We will then look at our MultiIndex matrix which shows how the terms are paired.

$$M_i^j = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 2 & 0 \\ 1 & 1 \\ 0 & 2 \end{bmatrix}$$

This yields the following general expression for the center temperature expansion:

$$= T_0\psi_0^1\psi_0^2 + T_1\psi_1^1\psi_0^2 + T_2\psi_0^1\psi_1^2 + T_3\psi_2^1\psi_0^2 + T_4\psi_1^1\psi_1^2 + T_5\psi_0^1\psi_2^2$$

Now we refer to the table of Legendre polynomials to see what these basis Functions actually are.

Order (l)	Value
0	1
1	x
2	$\frac{1}{2}(3x^2 - 1)$
3	$\frac{1}{2}(5x^3 - 3x)$

Furthermore, since $\psi_0 = 1$ and $\psi_1 = x$, we can reduce the expansion to:

$$T_c = T_0 + T_1x_1 + T_2x_2 + T_3(\frac{1}{2})(3(x_1)^2 - 1) + T_4x_1x_2 + T_5(\frac{1}{2})(3(x_2)^2 - 1)$$

Matlab-Fluent Interface

- Using user-input, MATLAB can create arbitrarily complex journal files based on a custom dictionary of FLUENT text user-interface commands
- These journal files are sent to the ANSYS - FLUENT environment where they are used to modify model parameters based on their uncertainty
- Solution data is exported after each simulation, these files are then collected by MATLAB and used for UQ data analysis

Sensitivity Analysis

	HeK	HeCp	ZrK	ZrCp	ZrEm	UOK	UOCp	WallT	Power	FuelEm
Minimum	0.1368	4673	13.5	270	0.8	4.5	211.5	323	27000	0.8
Maximum	0.1672	5712	16.5	330	1	5.5	258.5	423	33000	1

- 10 Dimensions & 1st Order Legendre Polynomials
- This allows us to see the relative contribution of each variable to the overall output parameter, be that Temperature, Velocity, Pressure, etc.

Sensitivity Analysis Results

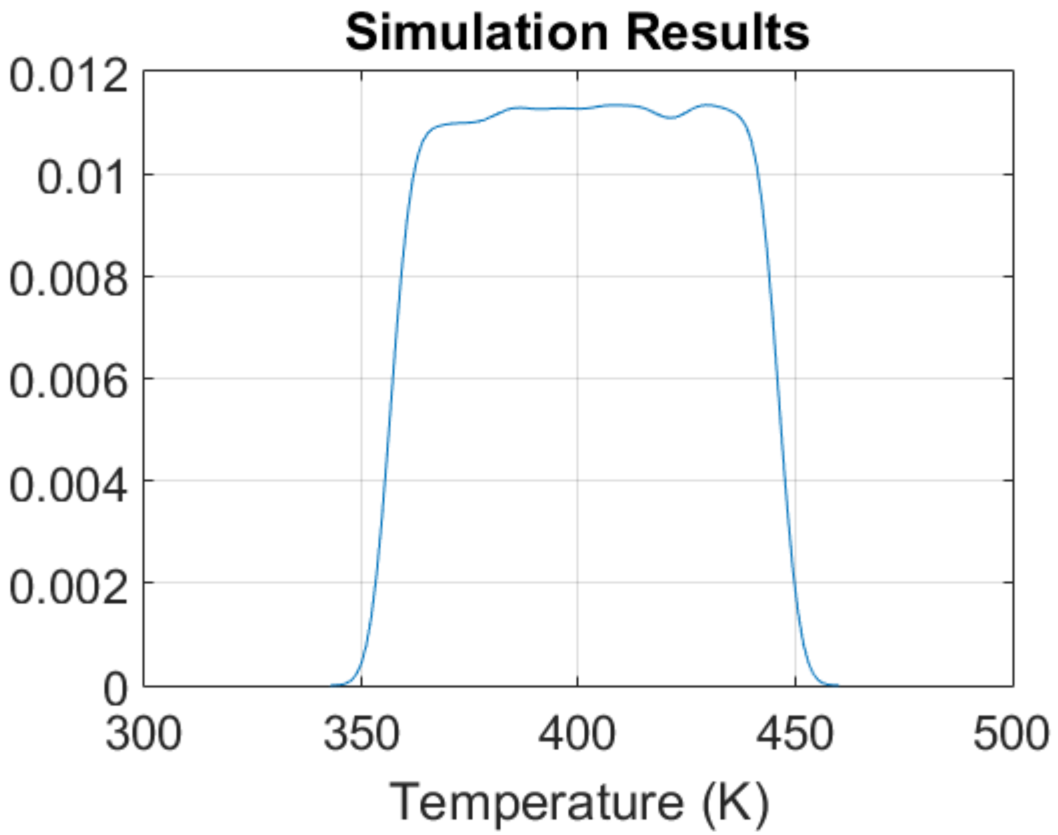
- 1,024 FLUENT Simulations
- Time-to-Run on local machine: Intel Xeon E3 - 4 (8 thread) 3.50GHz cores
  Approximately **16 hours**.
- Coefficients of Significance for Center Temperature

	HeK	HeCp	ZrK	ZrCp	ZrEm	UOK	UOCp	WallT	Power	FuelEm
(Mean)	T1	T2	T3	T4	T5	T6	T7	T8	T9	T10
379.6246	-0.11803	9.08E-03	-0.04534	-1.44E-15	-0.09561	-5.42435	-5.30E-14	48.18958	1.596366	-0.17262

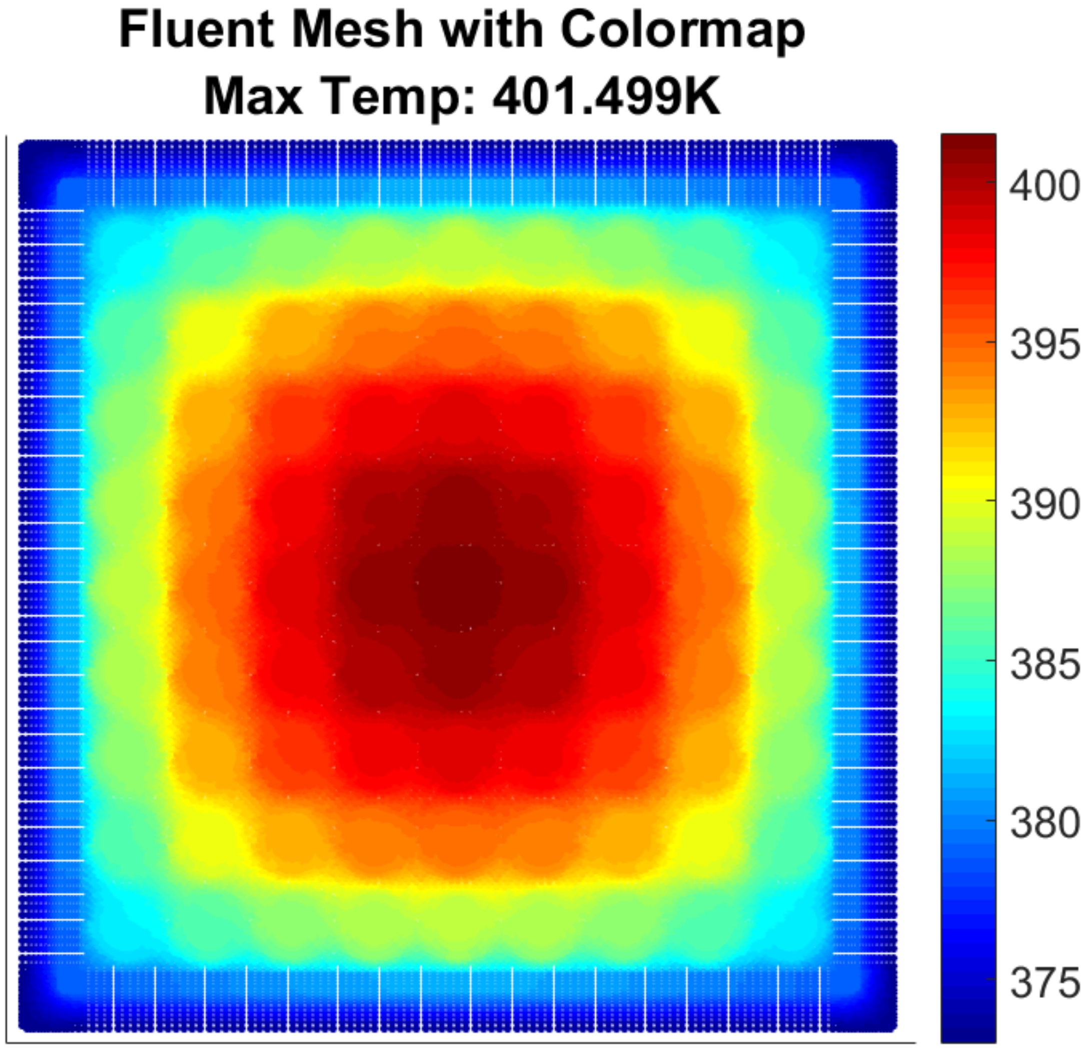
$$T = \sum_{i=0}^{N_{pc}} T_i \Psi_i(\Xi)$$

- ZrCp and UOCp can be dropped (no convection heat transfer in solid)
- HeCp can also be dropped. This could be explained by the dominant conduction/radiation heat transfer modes in gas filled regions (ref. Araya and Greiner)

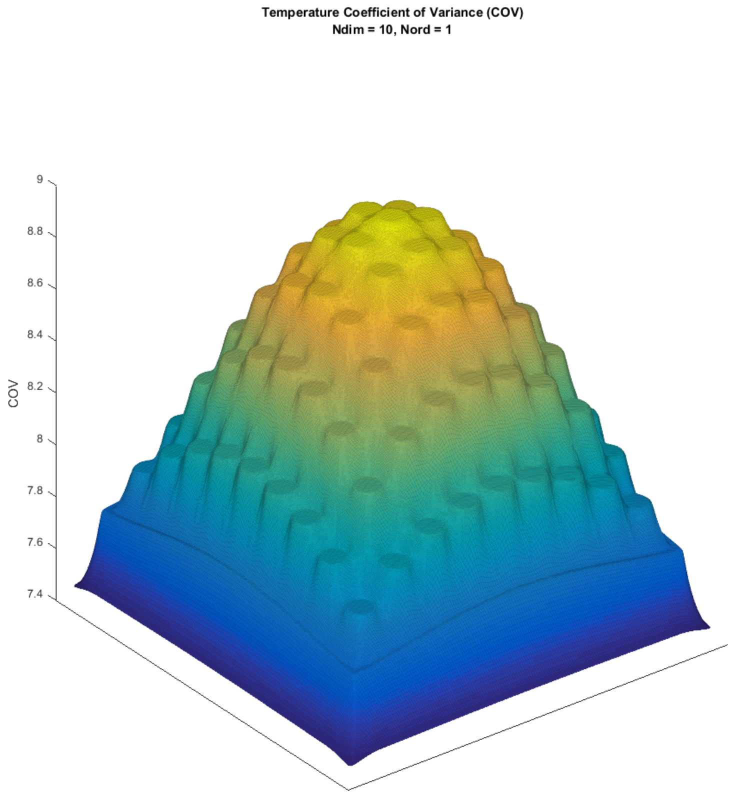
PDF of the Center Temperature Distribution



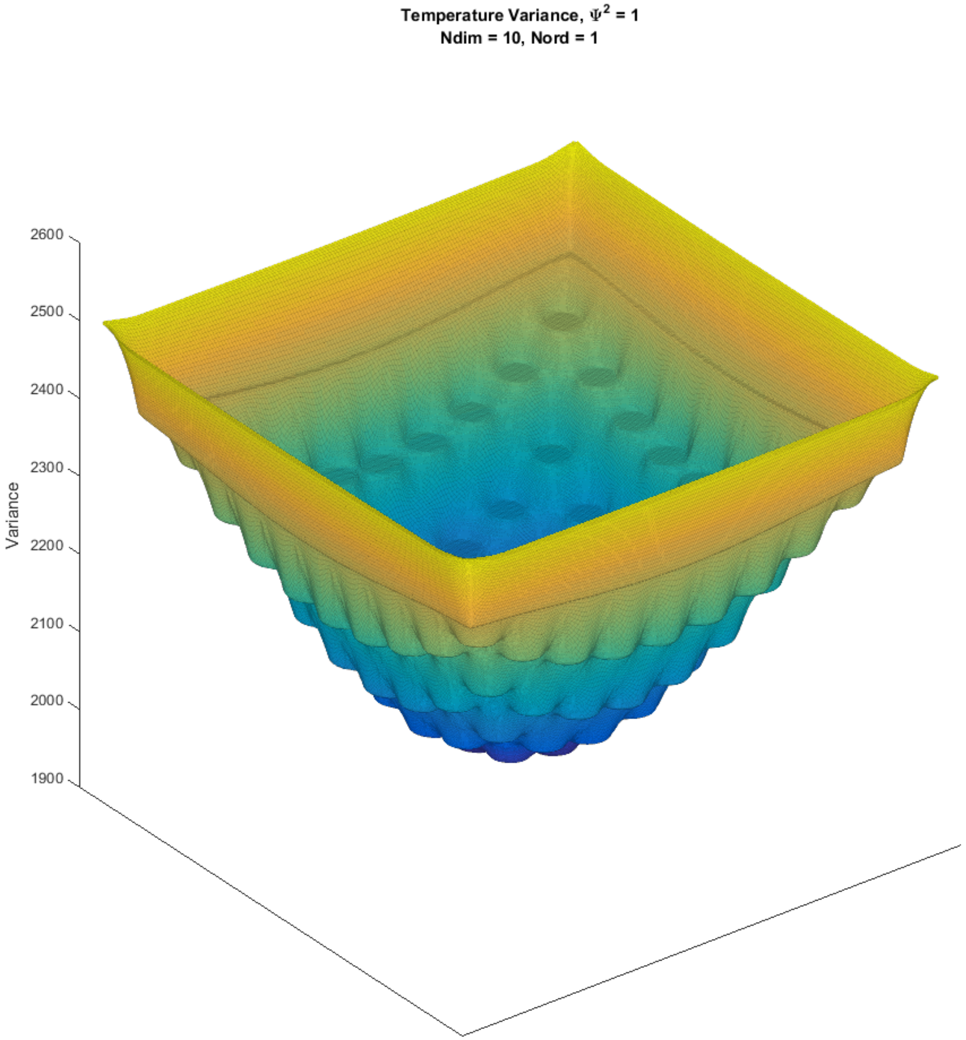
Mean Temperature Distribution



Variance and Coefficient of Variance

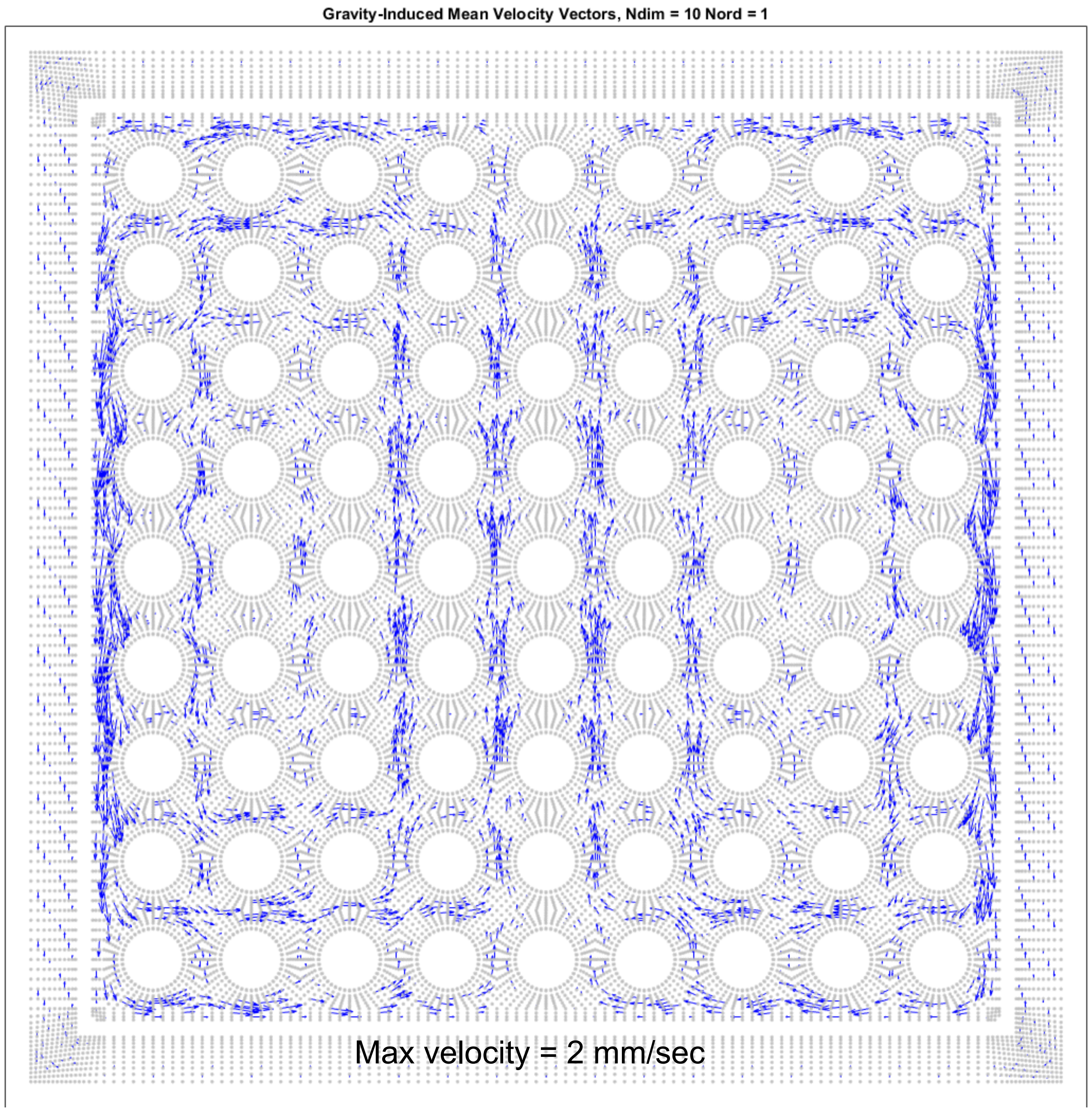


COV = mean /standard deviation



Variance

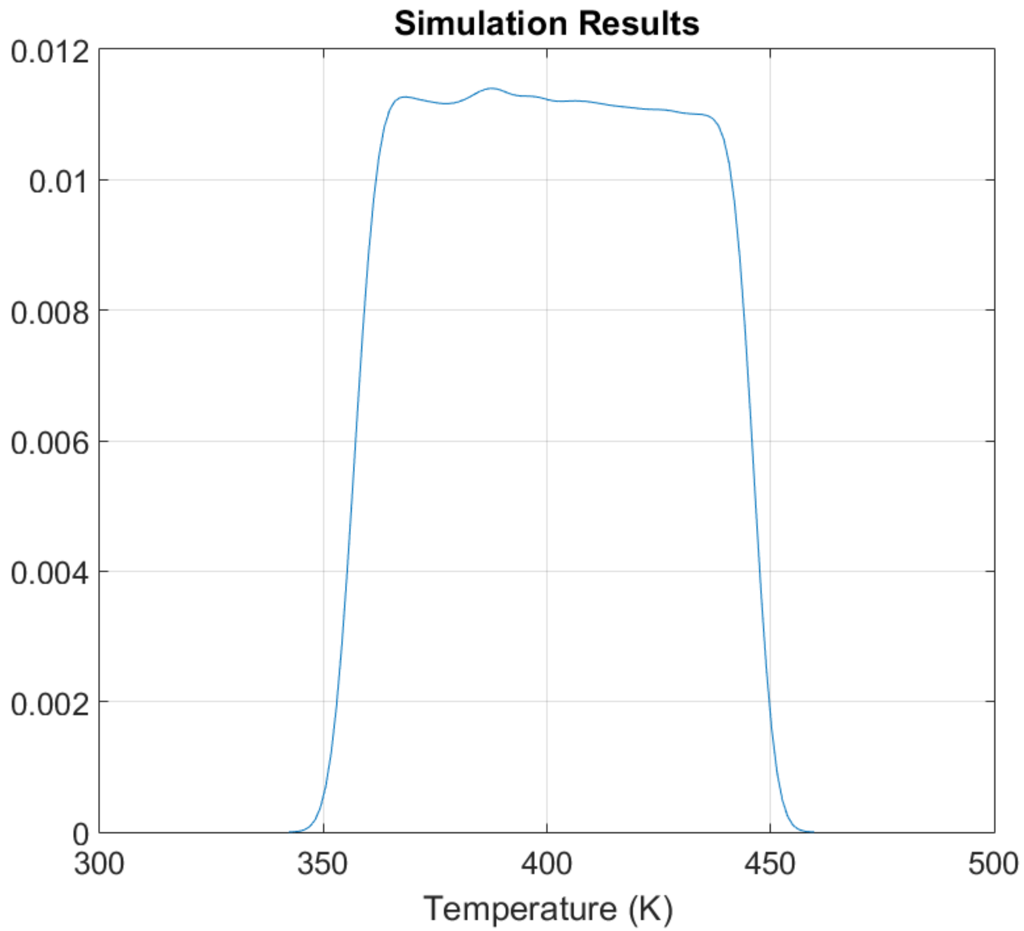
Average Velocity Distribution



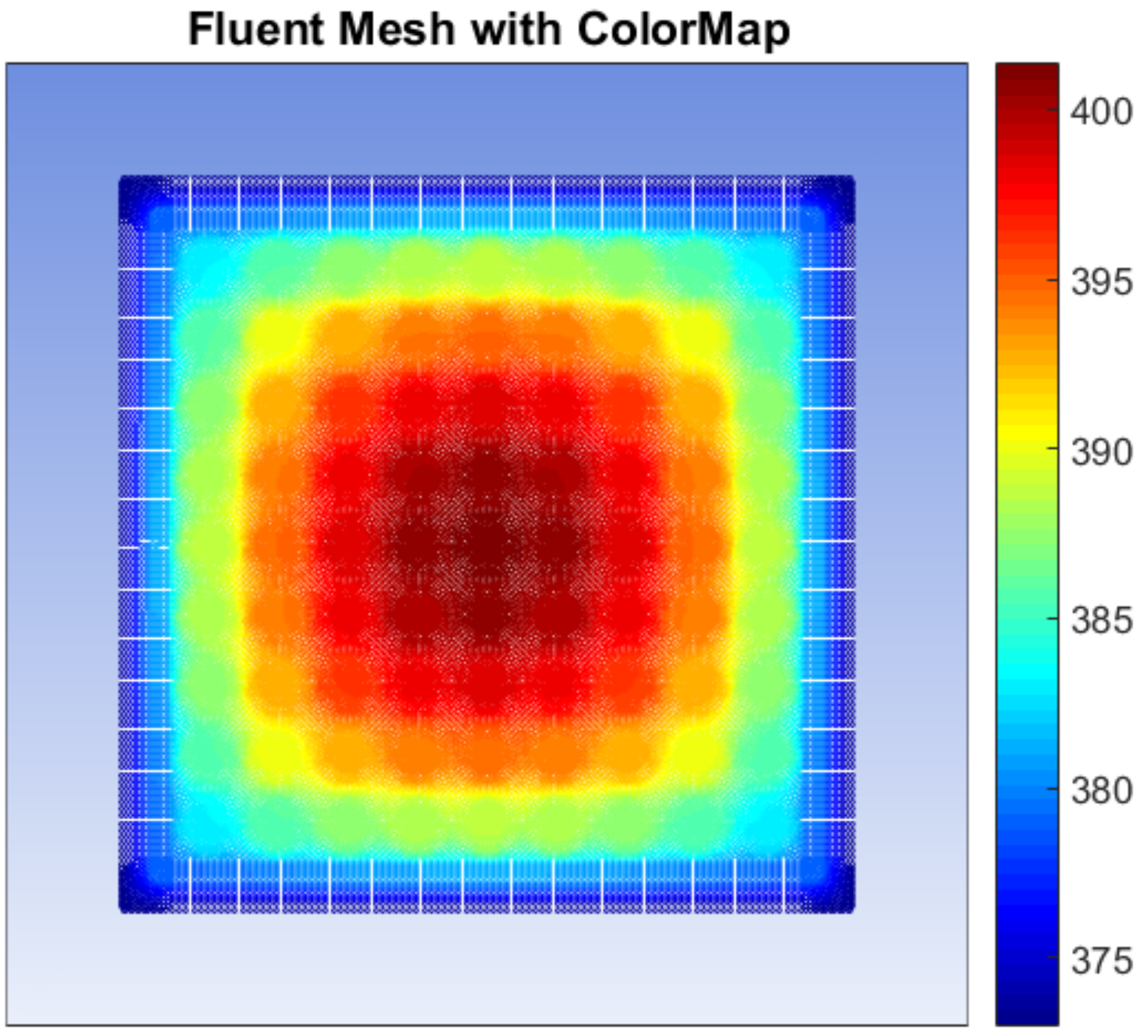
2^{nd} Order PCE Analysis Results

- Reduced Dimensions to 7 after Cp concluded to be insignificant, based on sensitivity analysis.
- 2,187 FLUENT Runs
- Time-to-Run on local machine: less than 2 Days

PDF of the Center Temperature Distribution



Mean Temperature Distribution



Future Work

- Convergence Analysis with 3rd order polynomial
- HPC - run larger, more complex models faster
- Building 3D models of the assemblies