



HTGR PBR Reactor Optimization Methodology

July 2023

Changing the World's Energy Future

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Idaho National Laboratory – Department of Reactor Physics Methods and Analysis

HTGR PBR Reactor Optimization Methodology

Reduced Order models, equilibrium core, DLOFC

DOE ART Gas-Cooled Reactor (GCR) Review Meeting

Virtual Meeting

July 25 – 27, 2023



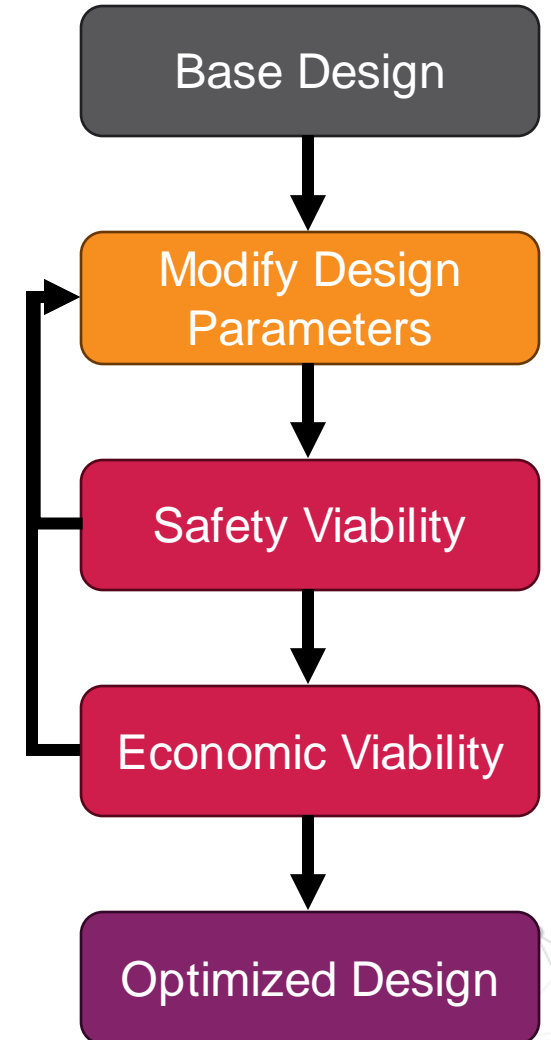


Outline

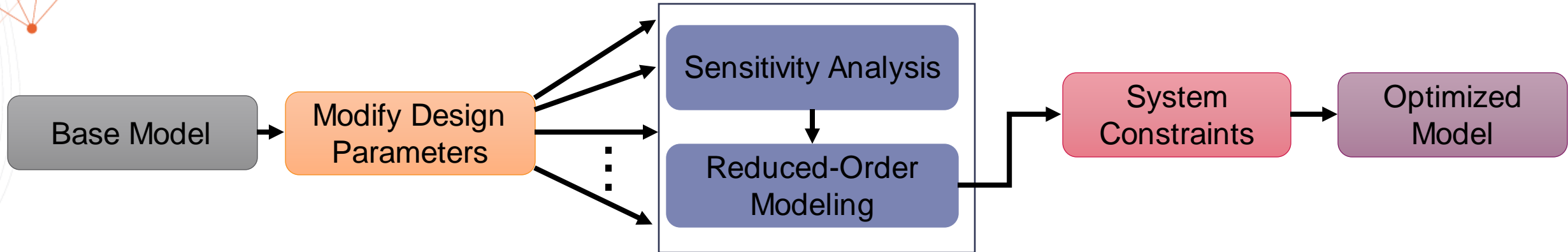
- Purpose
- Model Description
- Sensitivity Analysis
- Reduced Order Modeling
- Conclusions

Purpose

- Reactor designs incur both **safety and economic constraints**
 - Ensuring ALARA principles for certification and preventing damage
 - Keeping development and operational costs low for economic viability
- Safety and economic considerations are **often counteracted**
 - **Higher temperatures** create a more efficient power cycle, but reduce margin for system failure
 - **Higher burnup** reduces fuel costs, but create higher likelihood of fuel failure
 - **Exotic/advanced materials** are more thermally or neutronically efficient, but cost more to integrate
- Modeling and simulation** used to test and analyze different reactor configurations
- Design-basis accident** simulations are common to determine safety features
- Effects of various design considerations are often difficult to determine implicitly, especially when considered together
- Large parameter space** means many different configurations to consider

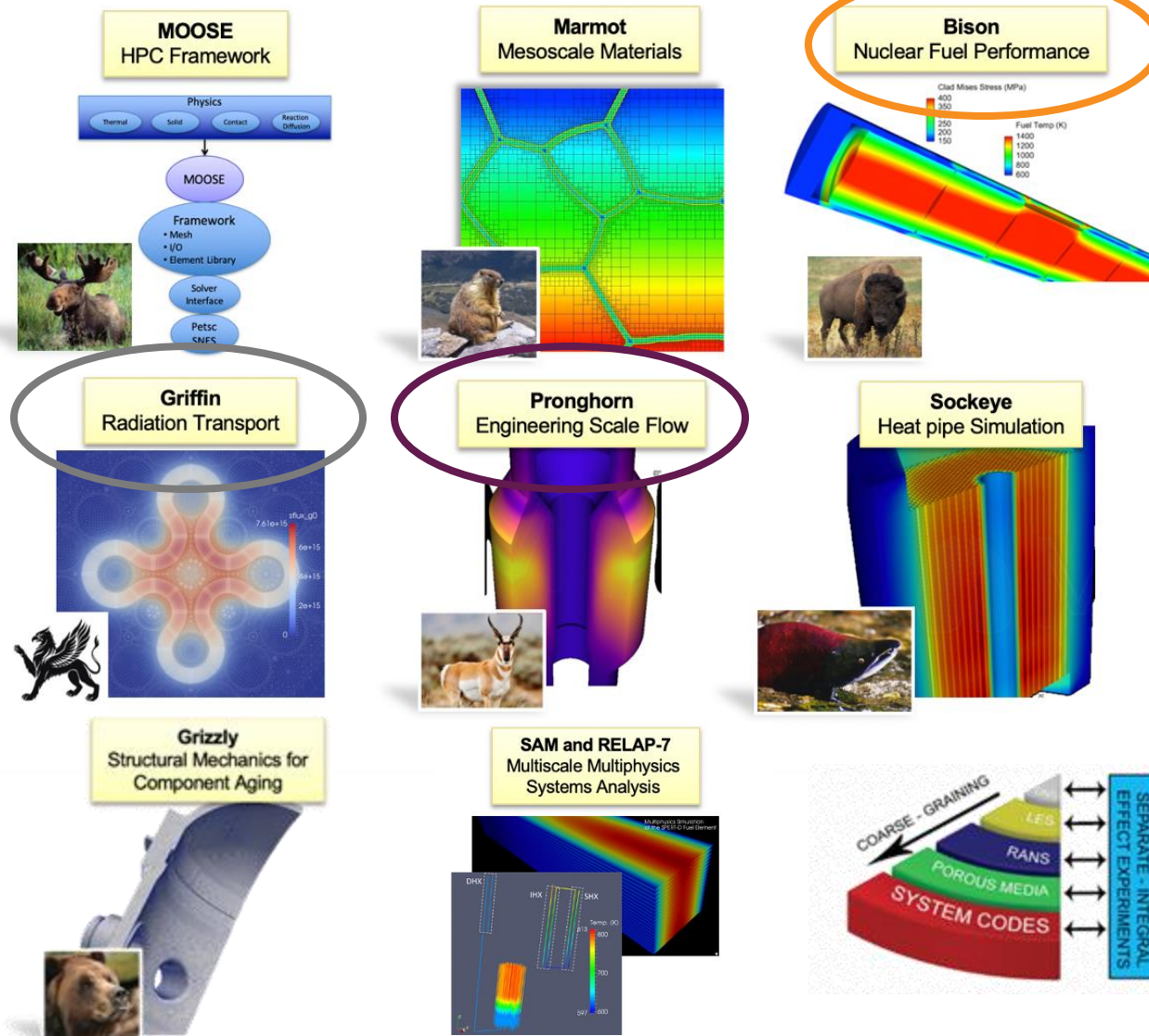


Proposed Methodology

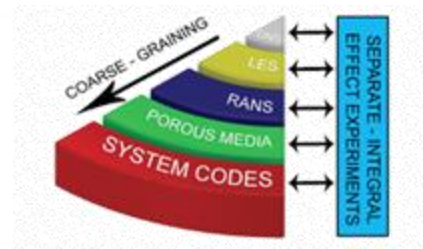


- Base model is coupled neutronics, depletion, thermal-hydraulics, fuel-performance model
 - Includes equilibrium core simulation and protected DLOFC transient
 - Goal is that nominal configuration satisfies system constraints, but not optimized
- Identify appropriate **design parameters and output quantities** related to constraints and optimization
- **Sensitivity analysis** provides insight on how reactor behaves when changing parameters
- **Reduced-order model** provides fast-evaluating surrogate for optimization
- **System constraints** include safety and nonproliferation, reduces space of viable configurations
- **Optimized model** is a minimization problem for factors like fuel utilization/cost

DOE NEAMS MOOSE Based Applications



- **NEAMS:** The Nuclear Energy Advanced Modeling and Simulation Program
- **MOOSE:** Multiphysics Object Oriented Simulation Environment
- **Flexible**
 - 1D, 1DR, 2D, 2DRZ, 3D,
 - Huge variety of physics
 - Adaptive time stepping and sub cycling
 - Multiscale through Multiapp system
 - Easily Extendible to new physics and sales
- **Tunable fidelity**
 - 0D scalar lumped parameters problem
 - 1D systems models
 - Multi D Intermediate “homogenized” geometry
 - High-fidelity “explicit” Geometry
- **Scalable**
 - MOOSE supports hybrid parallelism
 - Scales well on workstation and HPC
 - 2D/RZ models execute in minutes
 - High-fidelity 3D models execute on HPC



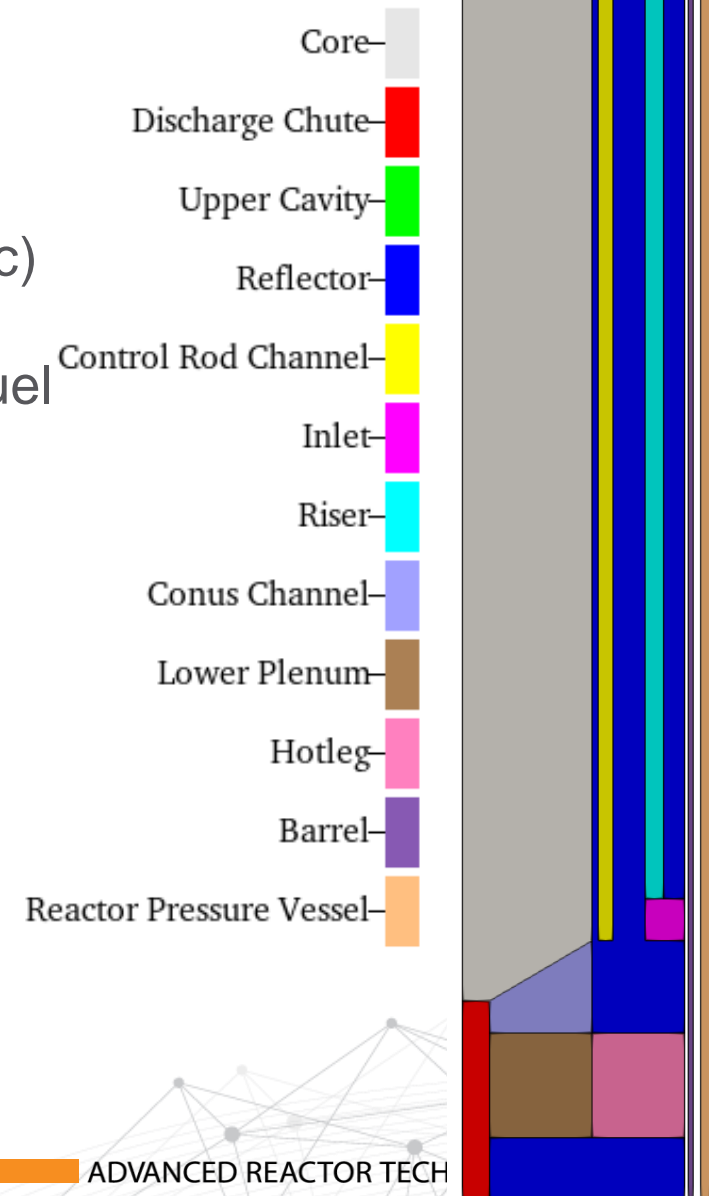
NEAMS Base Reactor Design

- Nominal Characteristics:

- Power: 200 MWth
- Core height/radius: 8.93/1.2 m
- TRISO packing: 9.24% (18,687 per pebble)
- Fuel kernel diameter: 0.435 mm
- Fuel enrichment: 15.5%
- Pebble discharge rate: 1.5 pebbles/min
- Burnup limit: 147.6 MWd/kg_{HM}
- Helium flow rate: 64.3 kg/s
- He inlet temperature: 260 °C
- He outlet pressure: 5.8 Mpa
- RCCS Temperature: 70 °C

- Model Description:

- Mesh: MOOSE reactor module
- Geometry: 2D RZ (axisymmetric)
- Equilibrium core: neutronics, depletion, thermal hydraulics, fuel performance
- Protected DLOFC: depletion, heat conduction, fuel performance
- Codes:
 - **Griffin**: neutronics and depletion
 - **Pronghorn**: thermal hydraulics and heat conduction
 - **Bison**: fuel performance



Multiphysics Coupling

Equilibrium Core (steady-state)

Protected DLOFC (transient)

GRIFFIN – Neutronics + Depletion

- **2D RZ Diffusion:** Pebble bed, upper cavity, reflector, control rod.
- **Cross sections:** 9 Energy groups, 6 tabulation variables (Burnup, Fuel Temperature Moderator temperature, Enrichment, TRISO packing, Fuel kernel radius)
- **Depletion:** 5 streamlines, 295 isotopes + 20 pseudo isotopes, 13 burnup groups

Solid Temperature

Isotopic Composition

PRONGORN + GRIFFIN - DLOFC

- **2D RZ Heat Conduction:** No fluid flow or coolant heat transfer
- **Decay heat:** explicit short-depletion calculation, no neutronics

Pebble Surface Temperature

Fractional Decay Heat

BISON – TRISO HC

- **1D Spherical Heat conduction:** Pebble core-shell model, Average TRISO particle model.
- **3,900 single CPU** subapps, one for each BU group (13) and for each core zone (300)

Fractional Power Density

Fuel Temperature

Moderator Temperature

Pebble Surface Temperature

Reflector Temperature

Total Power Density

BISON – TRISO HC

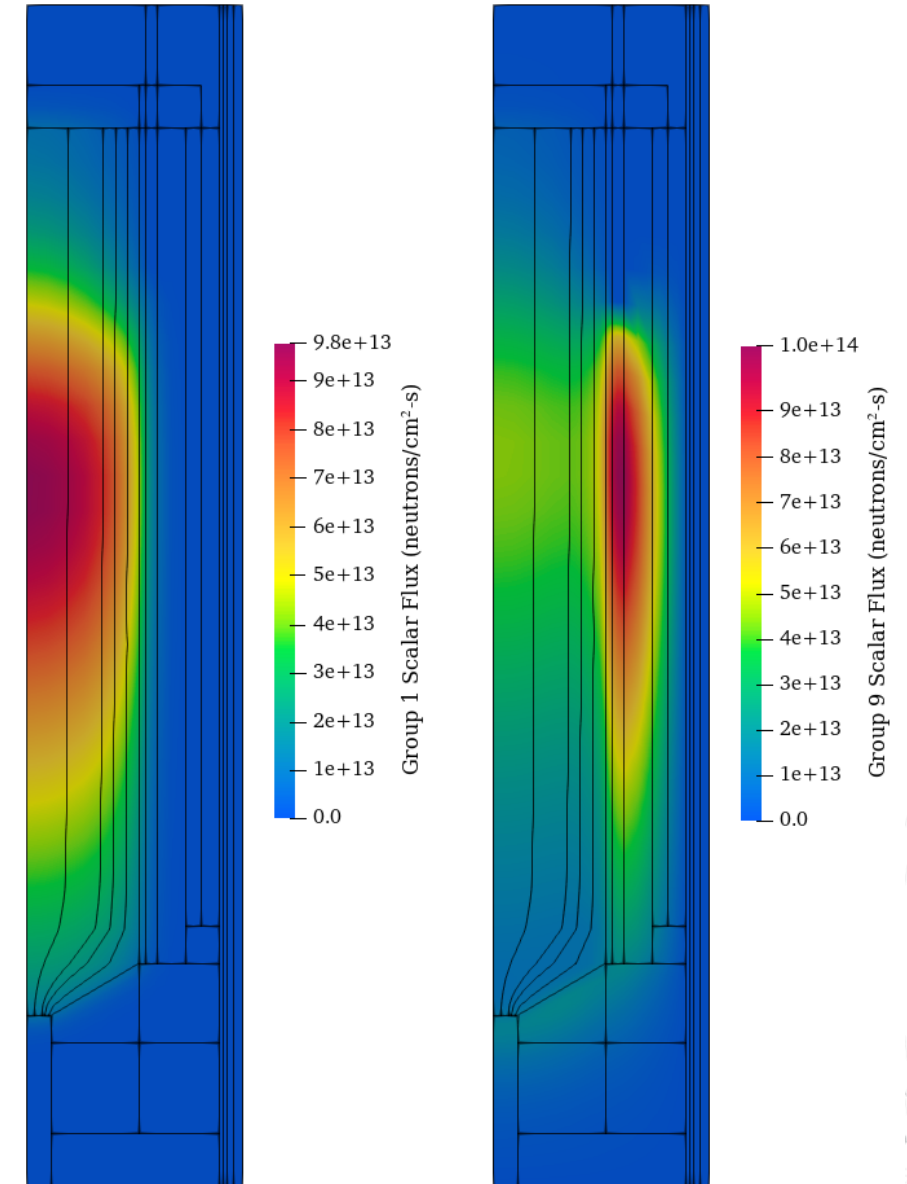
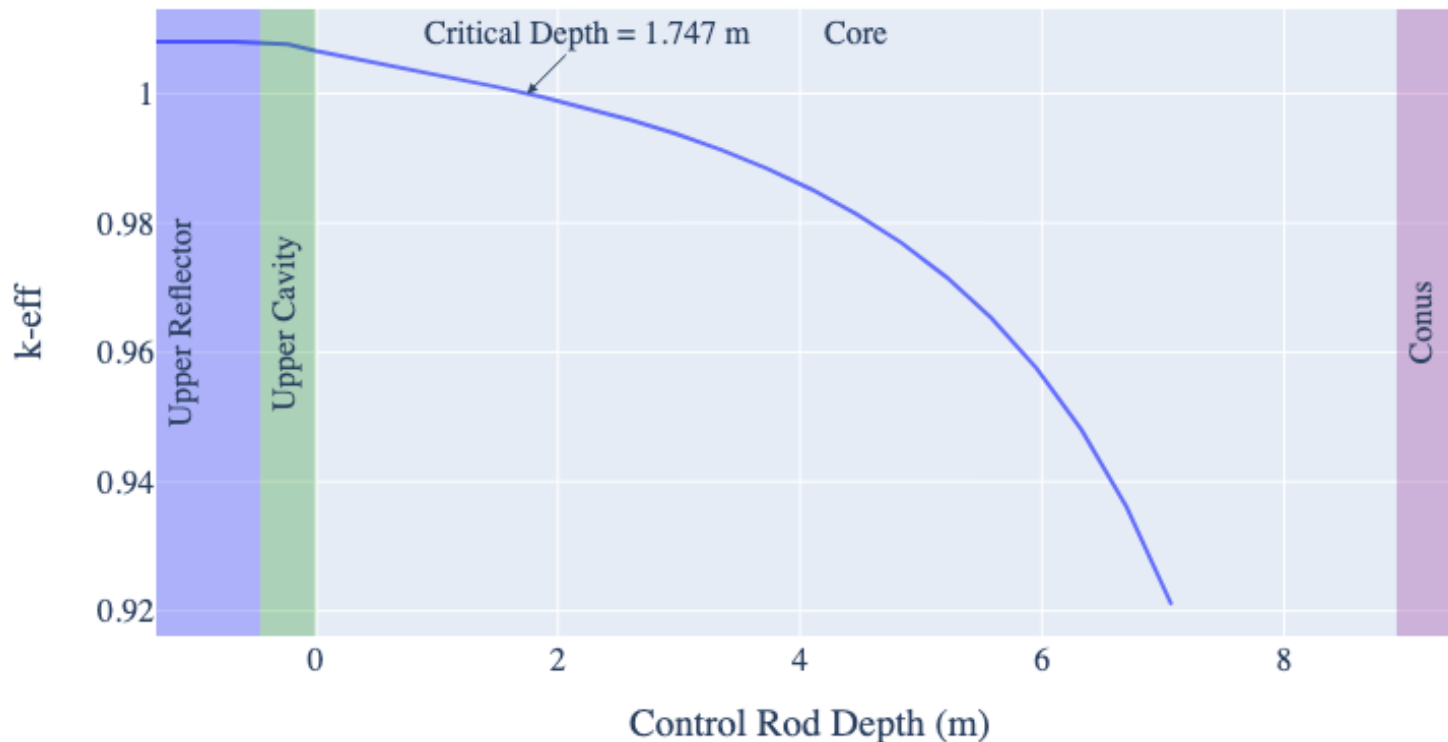
- **1D Spherical Heat conduction:** Pebble core-shell model, Average TRISO particle model.
- **3,900 single CPU** subapps, one for each BU group (13) and for each core zone (300)

PRONGHORN - TH

- **2D RZ porous media:** Pebble bed, cavity, reflector, gaps, barrel, RPV,
- **Gaps treatment:** radiation conduction model for gaps and cavity.

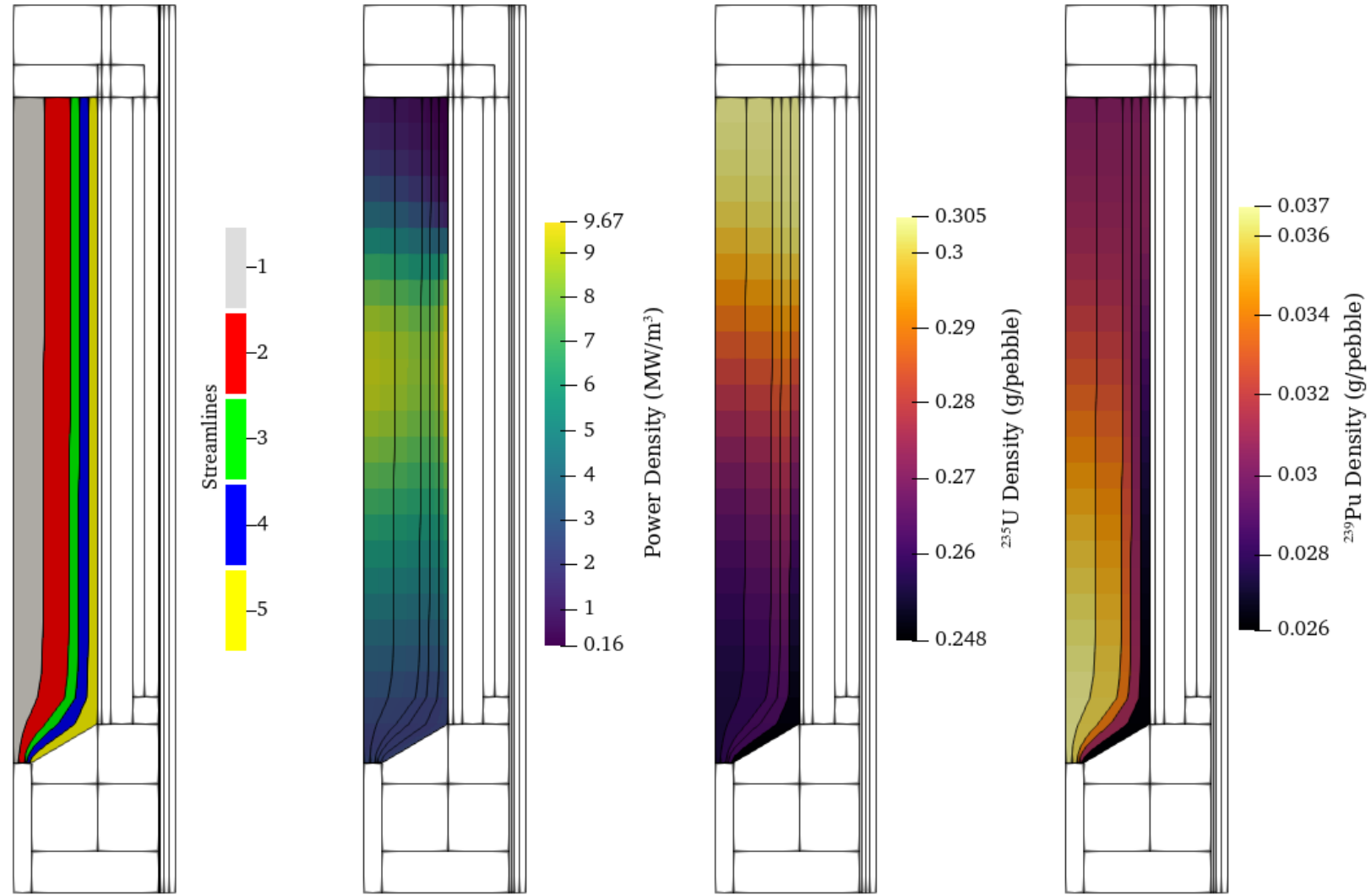
Neutronics Model

- 2D RZ 9-group diffusion model
- Control rod placed at critical configuration
- Simulated k_{eff} : 0.99961
- Excess reactivity: 806 pcm



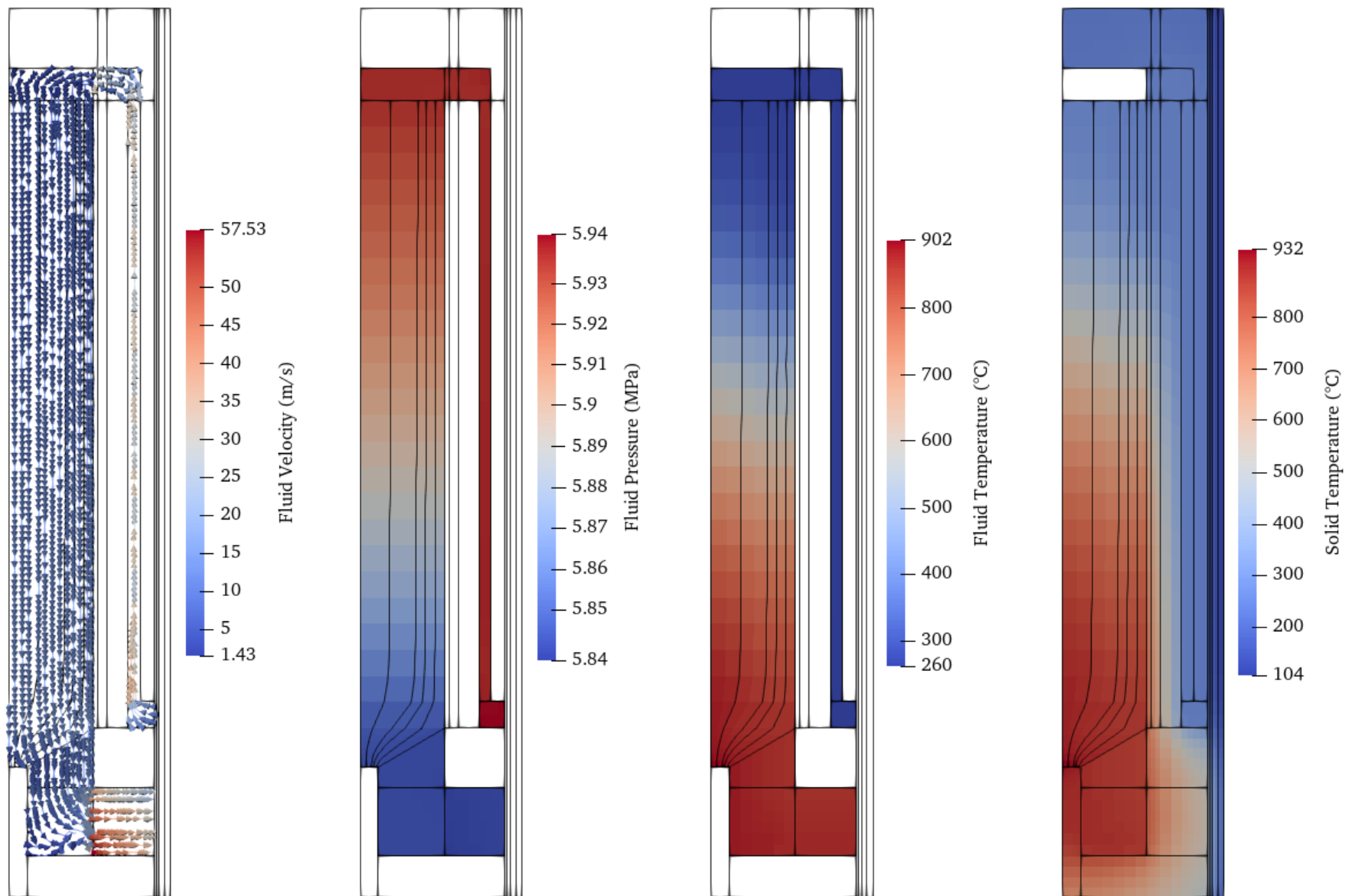
Depletion Model

- Eulerian streamline depletion:
 - 295 isotopes + 20 pseudo isotopes
 - 5 streamlines (processed from DEM calculation)
 - 13 burnup groups (0-196.8 MWd/kg_{HM})
- Max pebble power: 2.67 kW
- Peaking factor: 2.01
- Average fissile Plutonium fraction: 63.2%



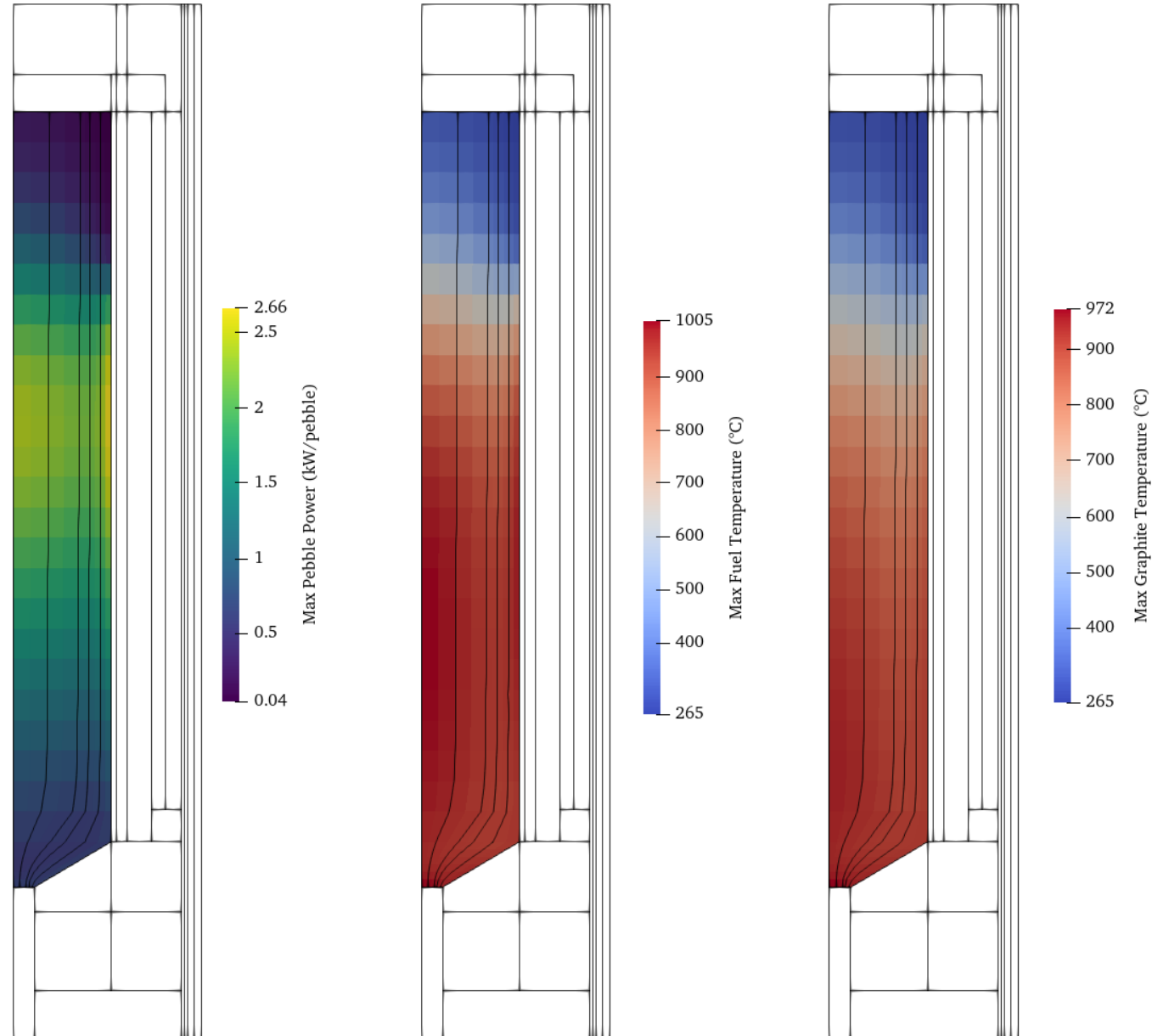
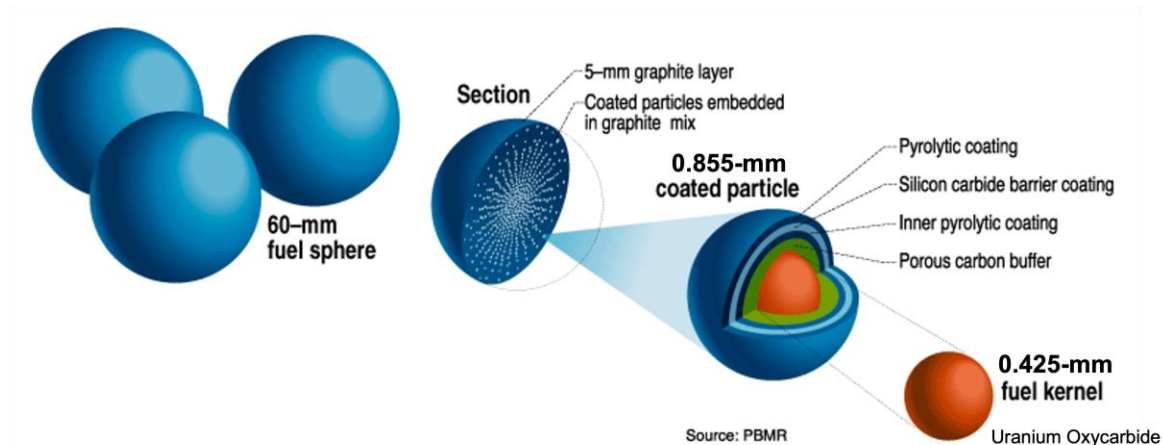
Thermal Hydraulics Model

- 2D RZ coupled porous flow and solid heat conduction



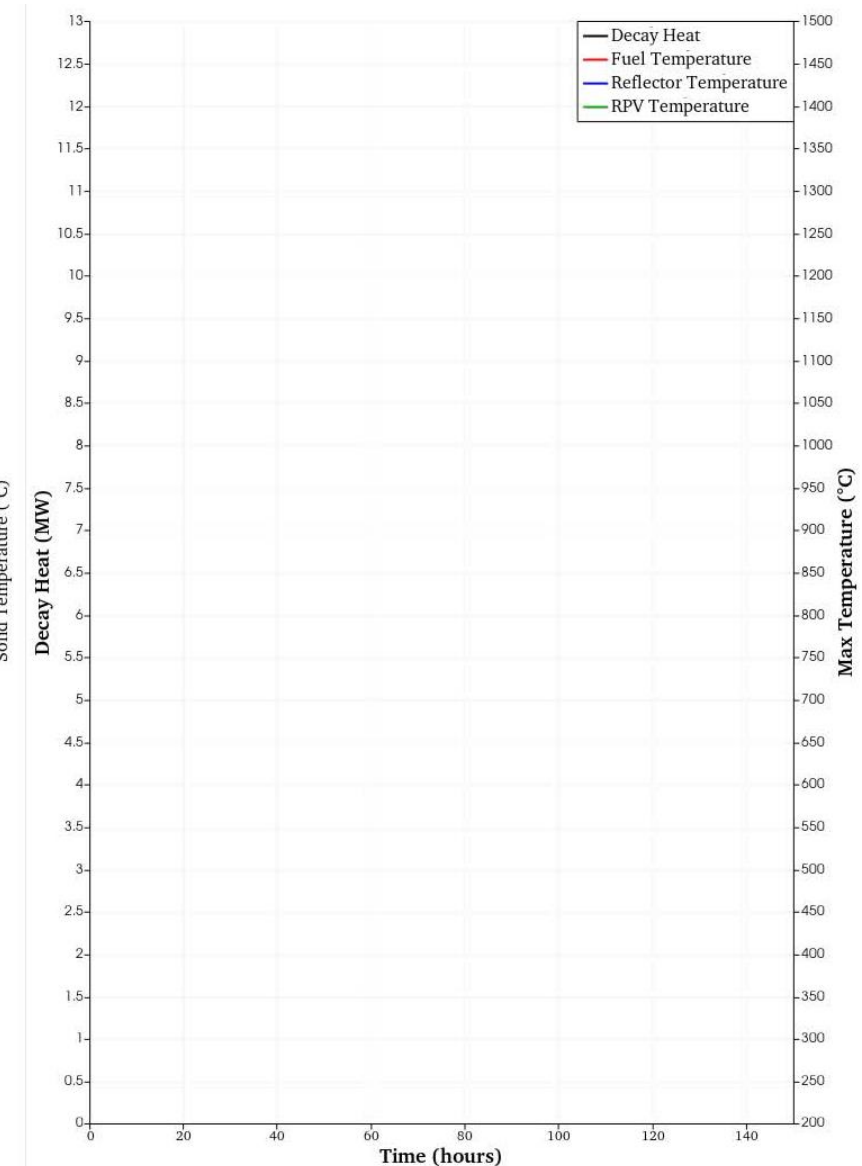
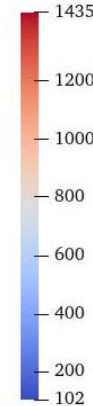
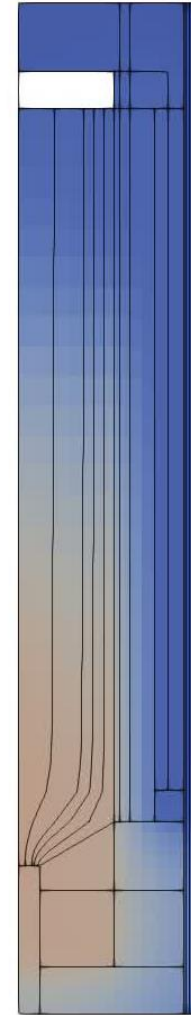
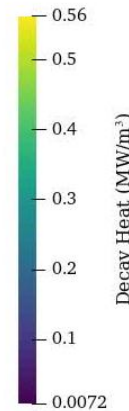
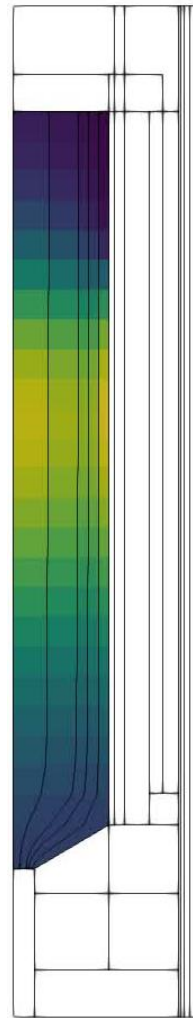
Pebble and TRISO Heat Conduction Model

- 1D R-Spherical heat conduction
- Representative pebble mode for each cell and burnup group (3,900 solves)
- Surface temperature of pebble assigned from TH
- Surface temperature of TRISO assigned from average pebble temperature
- Max fuel temperature: 1009 °C



Protected DLOFC Transient

- Initial solid temperature and isotopic composition taken from equilibrium core calculation
- Decay heat evaluated from explicit depletion solve (assumed instantaneous shutdown)
- Purely solid heat conduction (assumed no coolant)
- Pebble HC computed each timestep (no coupling)
- Initial decay heat: ~6% of full power
- Max fuel temperature: 1438 °C
- Max RPV temperature: 322 °C



Design Parameters and Quantities of Interest

Parameter	Nominal Value	Lower Bound	Upper Bound	Units
Kernel Radius	0.2125	0.15	0.3	mm
Filling Factor	9.34	5	15	%
Enrichment	15.5	5	20	wt%
Feed Rate	1.5	1	3	pebbles/min
Burnup Limit	147.6	131.2	164.0	MWd/kg _{HM}
Total Power	200	180	220	MWth
Core Radius	1.2	1.1	1.3	m
Core Height	8.93	8	10	m

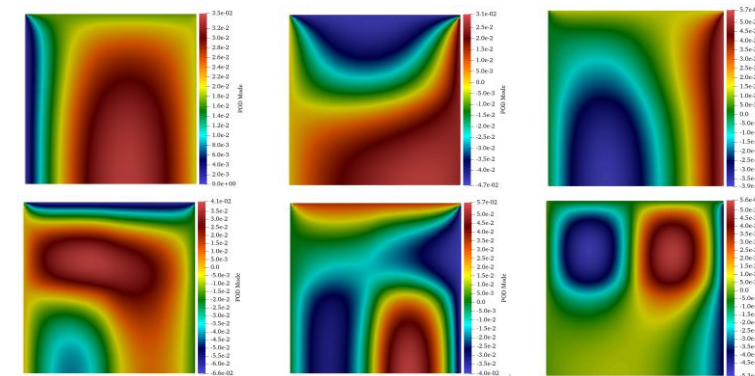
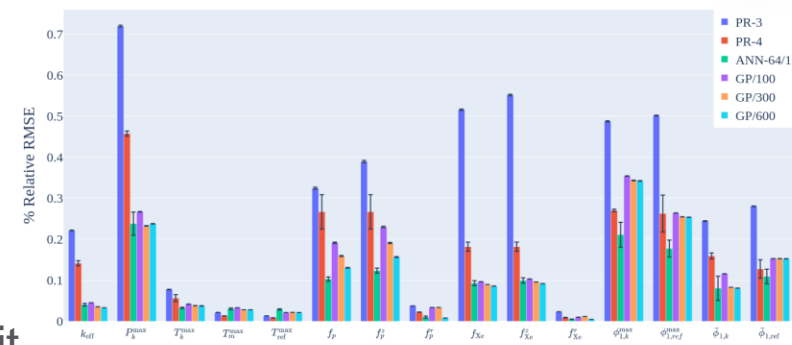
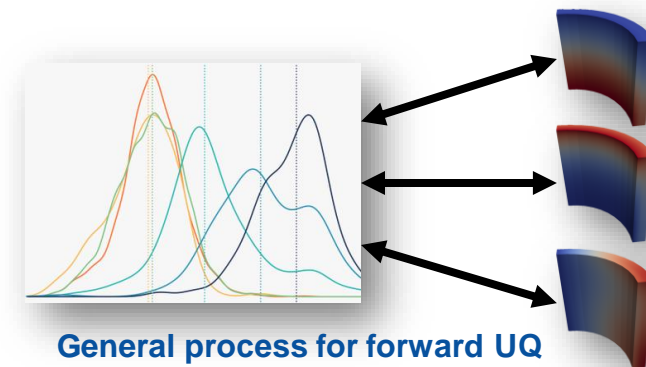
Qol	Nominal Value	Units
k-eff	0.99961	—
Max Pebble Power	2.67	kW
Peaking Factor	2.01	—
Fissile Plutonium Fraction	63.2	%
Max Operating Fuel Temp	1006	°C
Max DLOFC Fuel Temp	1438	°C
Max DLOFC RPV Temp	322	°C

Sensitivity Analysis Methodology

- Goal 1: **Determine the effect of each parameter** on quantities of interest **qualitatively**
 - Sample each parameter **individually**
 - Useful to understand behavior if a parameter was changed one way or another
 - Puts robustness of the model's solver to the test
- Goal 2: **Produce data**
 - **Random sampling** over entire parameter space
 - Data will be used to evaluate global sensitivities and generate reduced-order models
 - Useful to see **how probable edge cases are** to occur
- Goal 3: Evaluate **global sensitivities for each parameter-Qol** pair
 - Utilize **polynomial chaos meta-modeling** to evaluate Sobol indices
 - Quantitatively determines **impact of a parameter on a Qol**
 - Useful for determining important parameters

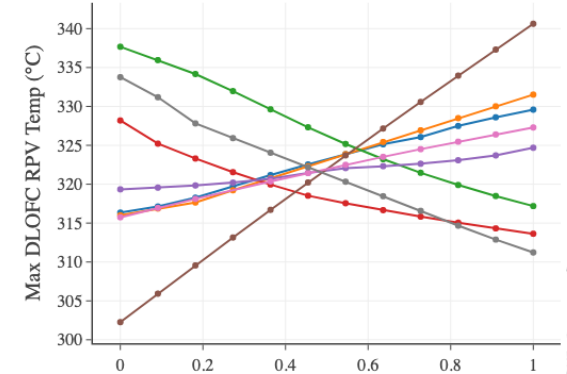
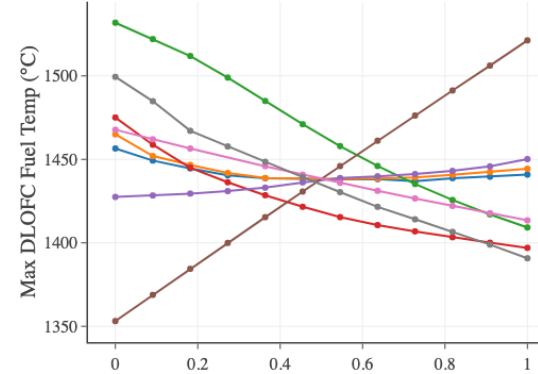
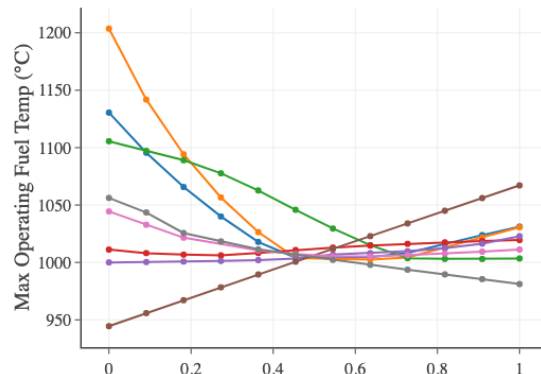
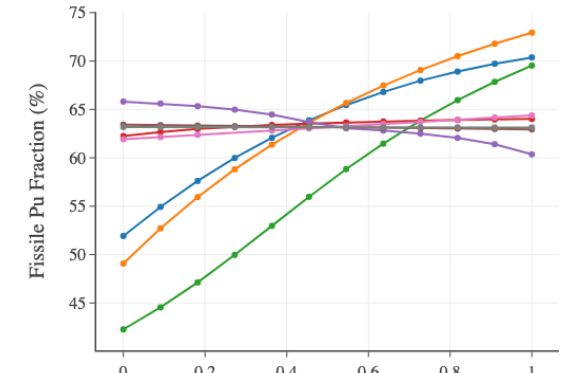
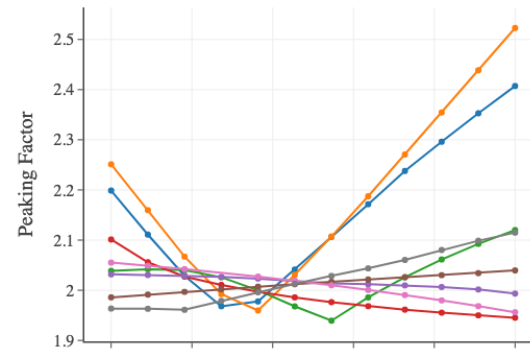
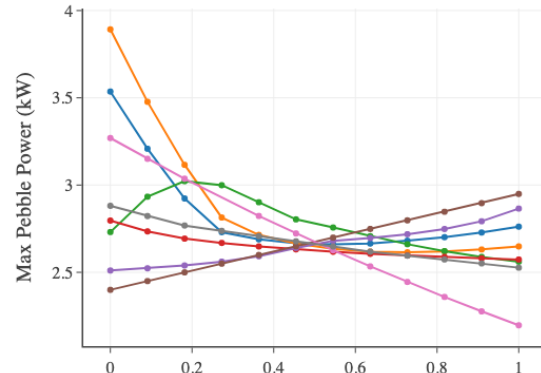
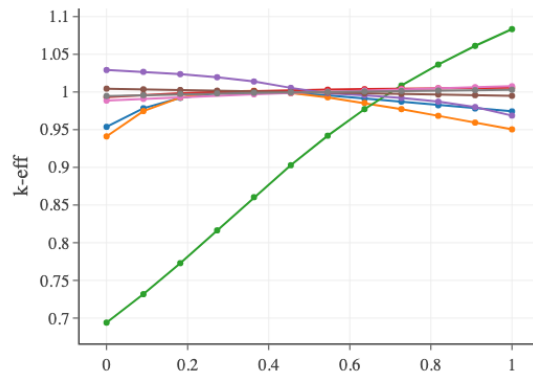
The MOOSE Stochastic Tools Module

- Provide a **MOOSE interface** for performing stochastic analysis on MOOSE-based models.
- Sample parameters, run applications, and gather data that is both **efficient** (memory and runtime) and **scalable**.
- Perform UQ and sensitivity analysis with **distributed data** with **advanced variance reduction** methods
- **Parallel Scalable Inverse Bayesian UQ** for parameter and model error estimation
- Train meta-models to develop fast-evaluating **surrogates** of the high-fidelity multiphysics model
 - Harness advanced machine learning capabilities through the C++ front end of Pytorch
 - Use active learning models for building surrogates
- Provide a **pluggable** interface for these surrogates.
- Use **POD (Proper Orthogonal Decomposition)-based dimensionality reduction** methods to build mappings between solution variables and latent (low-dimensional) spaces



Sensitivity Analysis: Qualitative Analysis

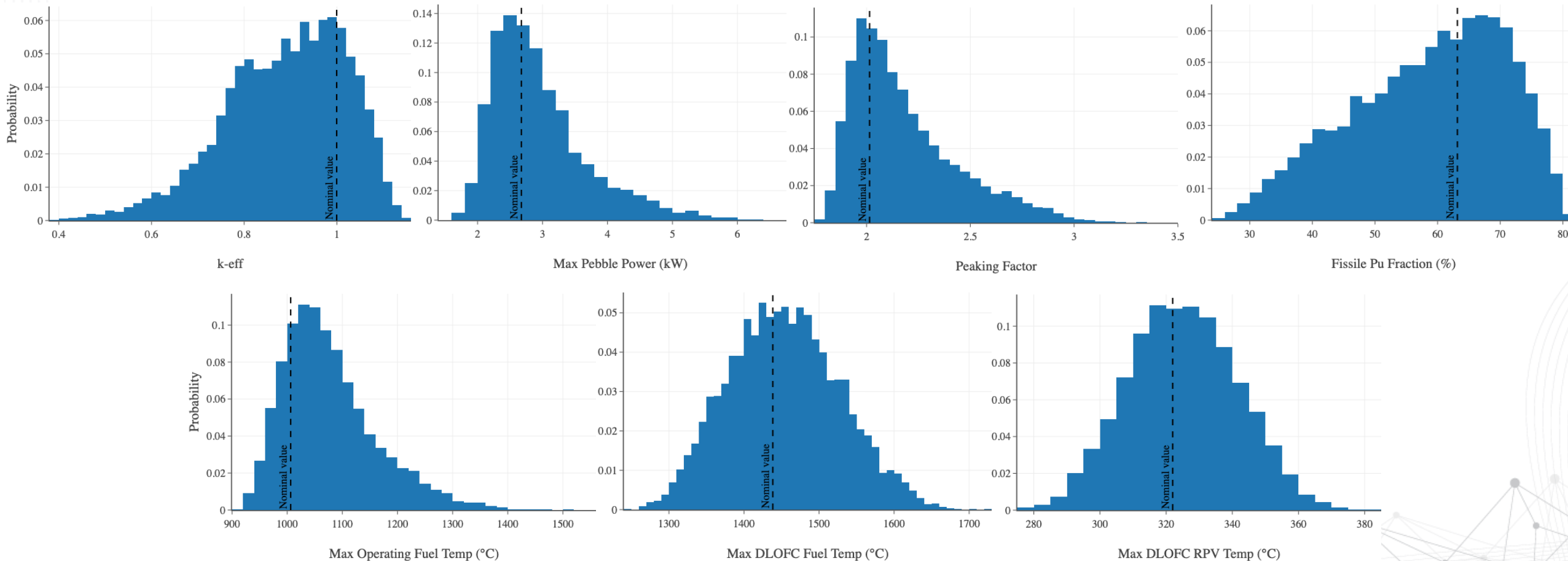
- Each design parameter was changed individually
 - Example: enrichment was changed uniformly between 5-20 wt%, while all other parameters were held at their nominal values
 - 12 points for each parameter: 96 total samples



Normalized Parameter (0=min, 1=max)

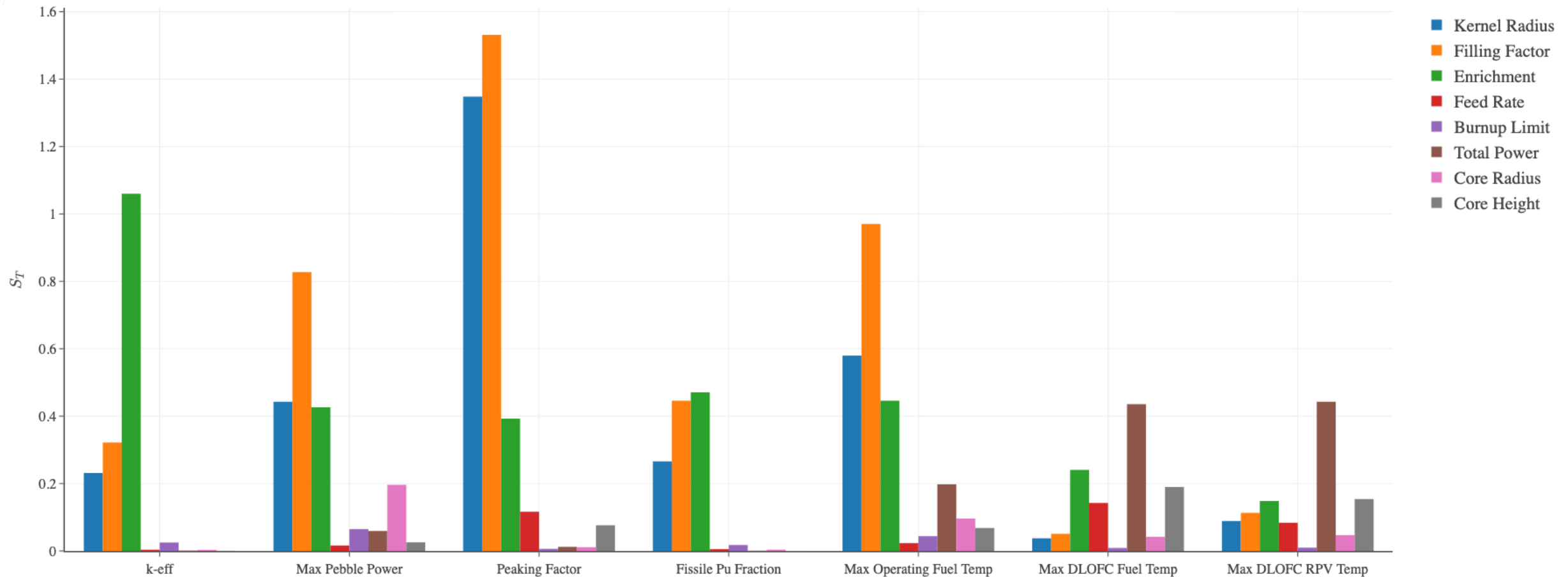
Sensitivity Analysis: Producing Data

- Random sampling of parameter space
 - Latin hypercube (LHS) sampling with 10,000 samples



Sensitivity Analysis: Global Sensitivity

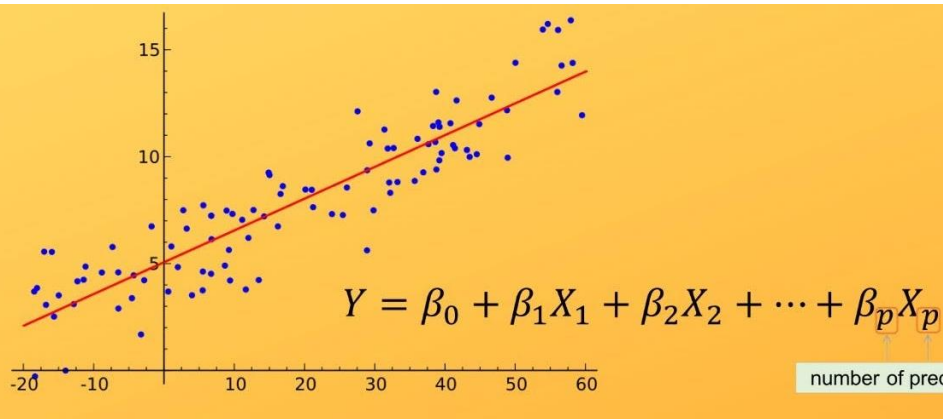
- Total Sobol indices using polynomial chaos expansion
 - Fourth-order monomial expansion
 - Second-order indices also available indicating cross-term sensitivity



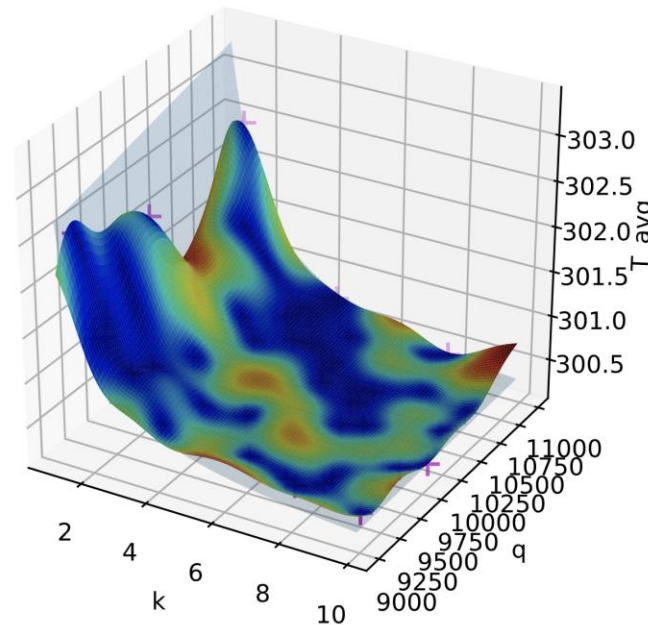
Reduced-Order Model Methodology

- Investigating three different regression techniques

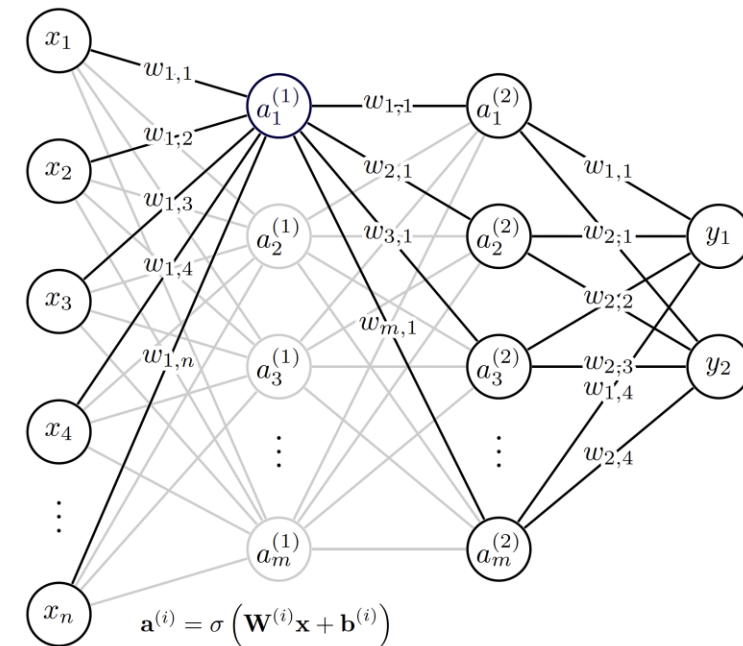
Polynomial Regression



Gaussian Processing

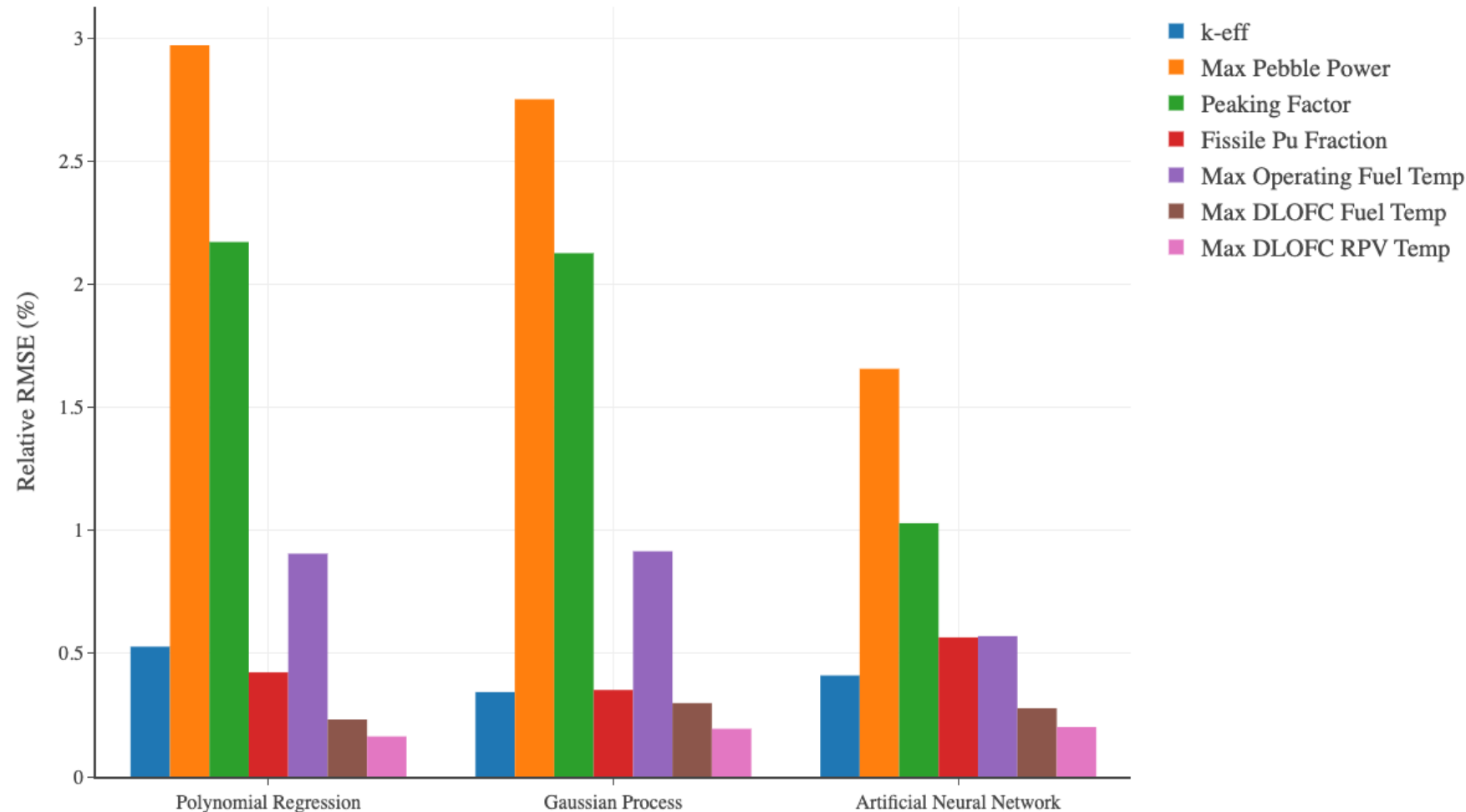


Artificial Neural Network



Reduced-Order Model Comparison

- Split data into training and validation set (3,000 training points)
- Fourth-order monomial for polynomial regression
- Optimized Gaussian Process model
- Three-layer artificial neural network



System Constraints

- Viable configurations defined by constraints on the output of the simulation
- Includes both operational success and risk of failure
- Full Model uses 10,000 sample case and ROMs were run with 100k samples

QoI	Constraint	Fraction of Viable Configurations (%)			
		Full Model	PR	GP	ANN
k-eff	> 0.99200	24.92	25.00	25.03	25.24
Max Pebble Power	< 4.5 kW	95.16	95.61	95.24	95.23
Peaking Factor	< 2.2	62.67	63.55	60.89	61.78
Fissile Pu Fraction	< 70 %	80.30	79.18	79.45	79.21
Max Operating Fuel Temp	< 1100 °C	67.65	68.37	68.43	68.01
Max DLOFC Fuel Temp	< 1600 °C	97.16	97.27	97.25	97.40
Max DLOFC RPV Temp	< 350 °C	93.03	93.14	93.11	93.13
Total	□	13.62	13.91	13.35	13.37



Conclusions

- Summary
 - Defined **workflow** for developing models for **design optimization**
 - Utilized MOOSE tools to build **multiphysics equilibrium core and DLOFC model**
 - Defined core **design parameters and quantities of interest** related to viability
 - Generated a **large dataset** of simulations
 - Performed **sensitivity analysis** to gain insight on parameter behavior
 - Built and compared various **reduced order models**
- Upcoming Work
 - Define core metrics to optimize
 - Utilize reduced order models for optimization
- Future Work
 - Look at optimization for approach to equilibrium core (running-in)
 - More advanced cross section generation