July 27, 2023

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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

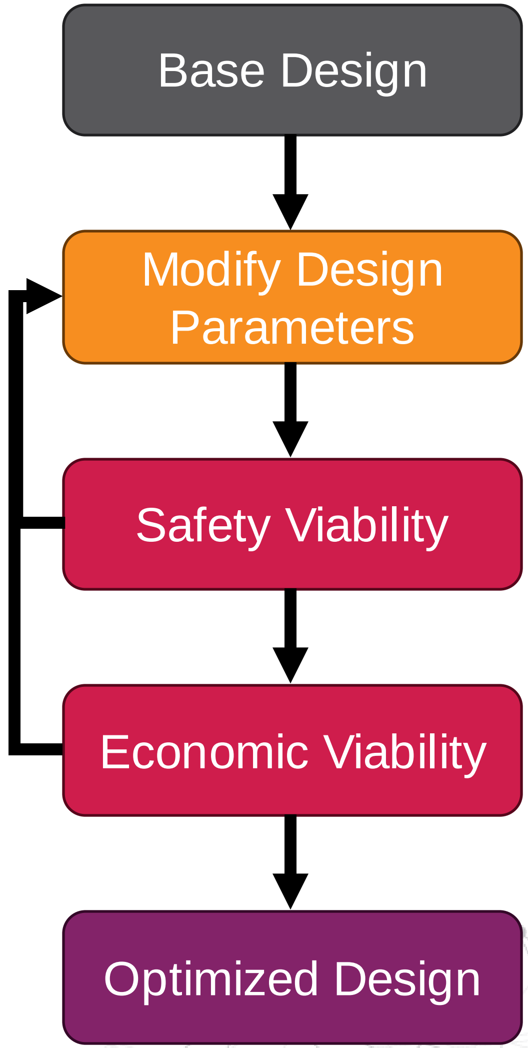
ART
Advanced Reactor Technologies

Outline

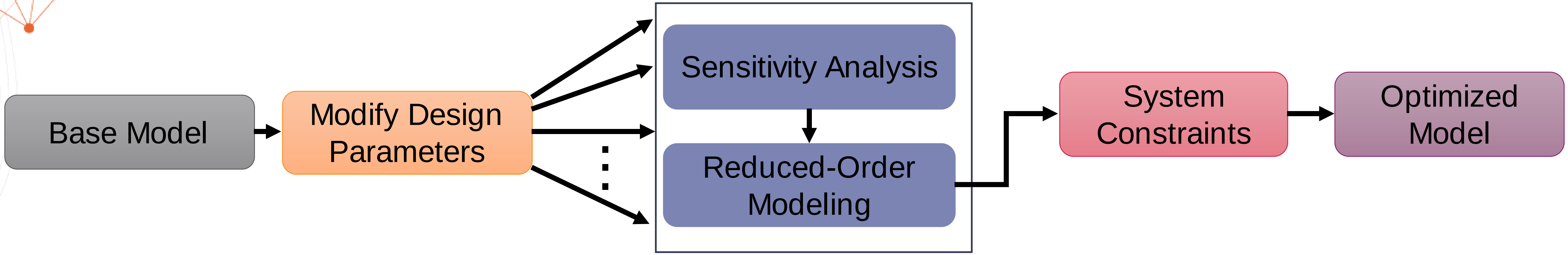
- Purpose
- Model Description
- Sensitivity Analysis
- Reduced Order Modeling
- Conclusions

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

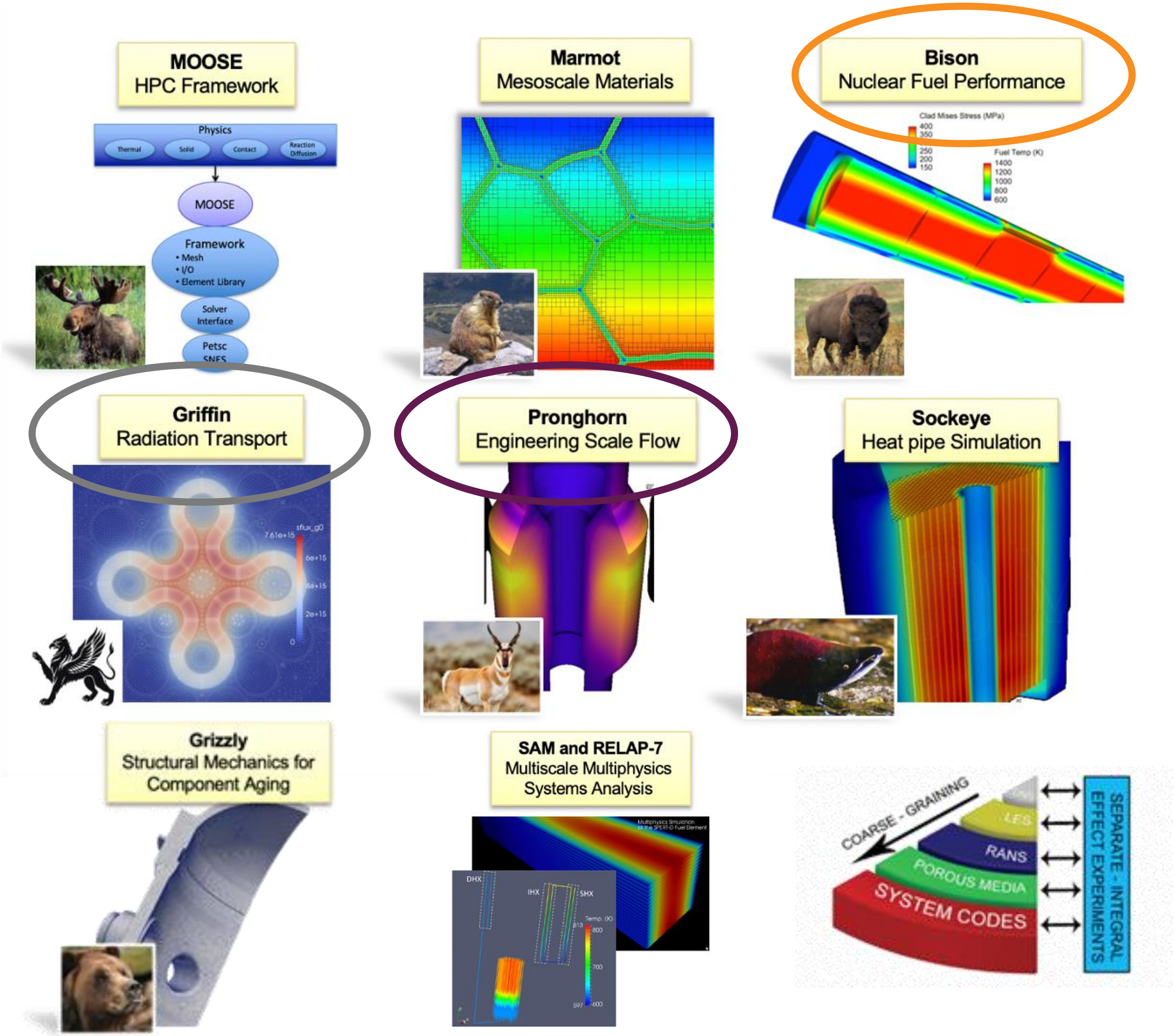


Proposed Methodology



- 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

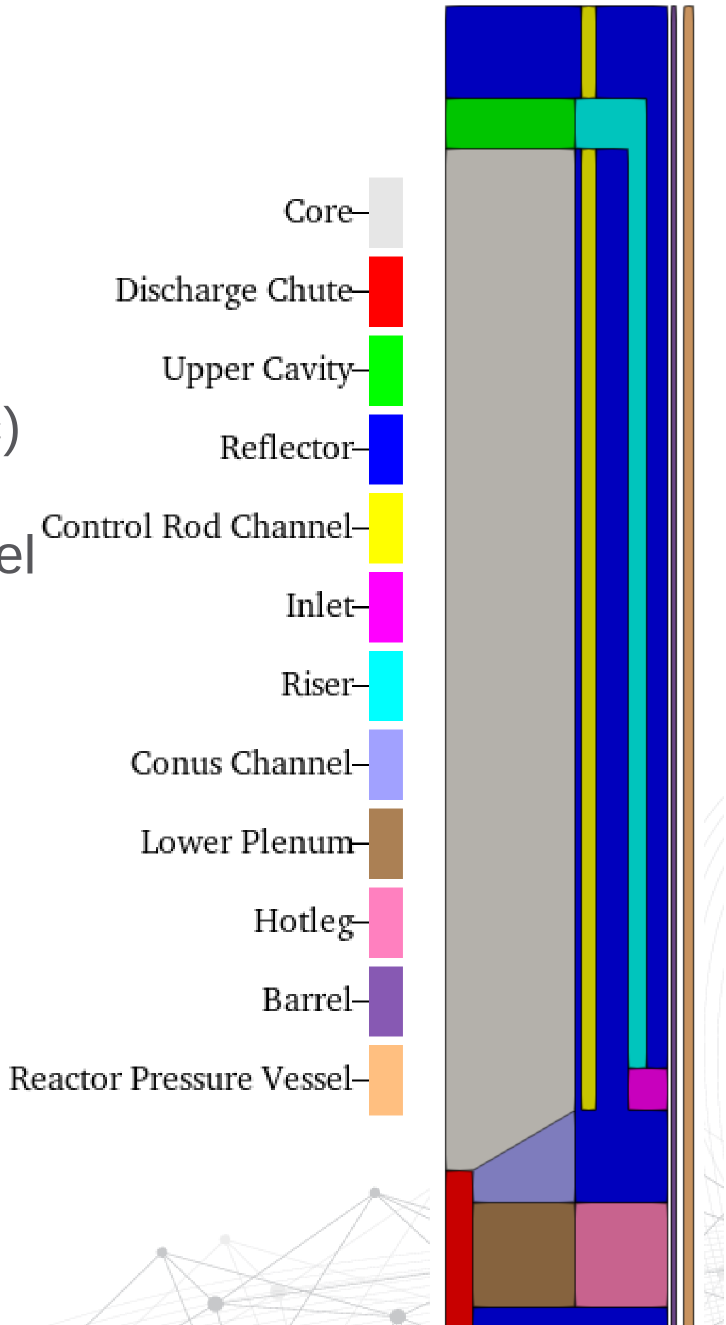
DOE NEAMS MOOSE Based Applications



- **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 ºC
  - He outlet pressure: 5.8 Mpa
  - RCCS Temperature: 70 ºC
- 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)

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

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.

Solid Temperature

Isotopic Composition

Protected DLOFC (transient)

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

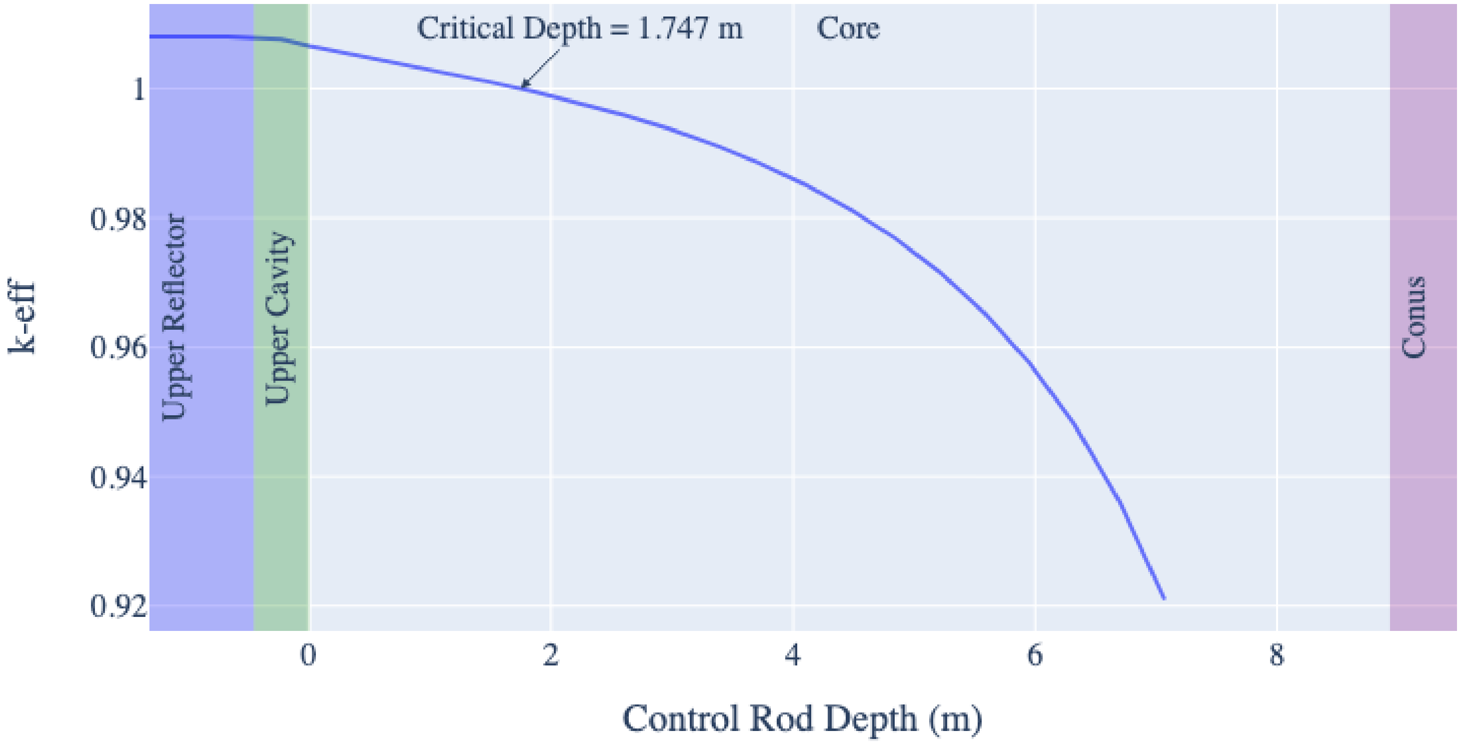
Fractional Decay Heat

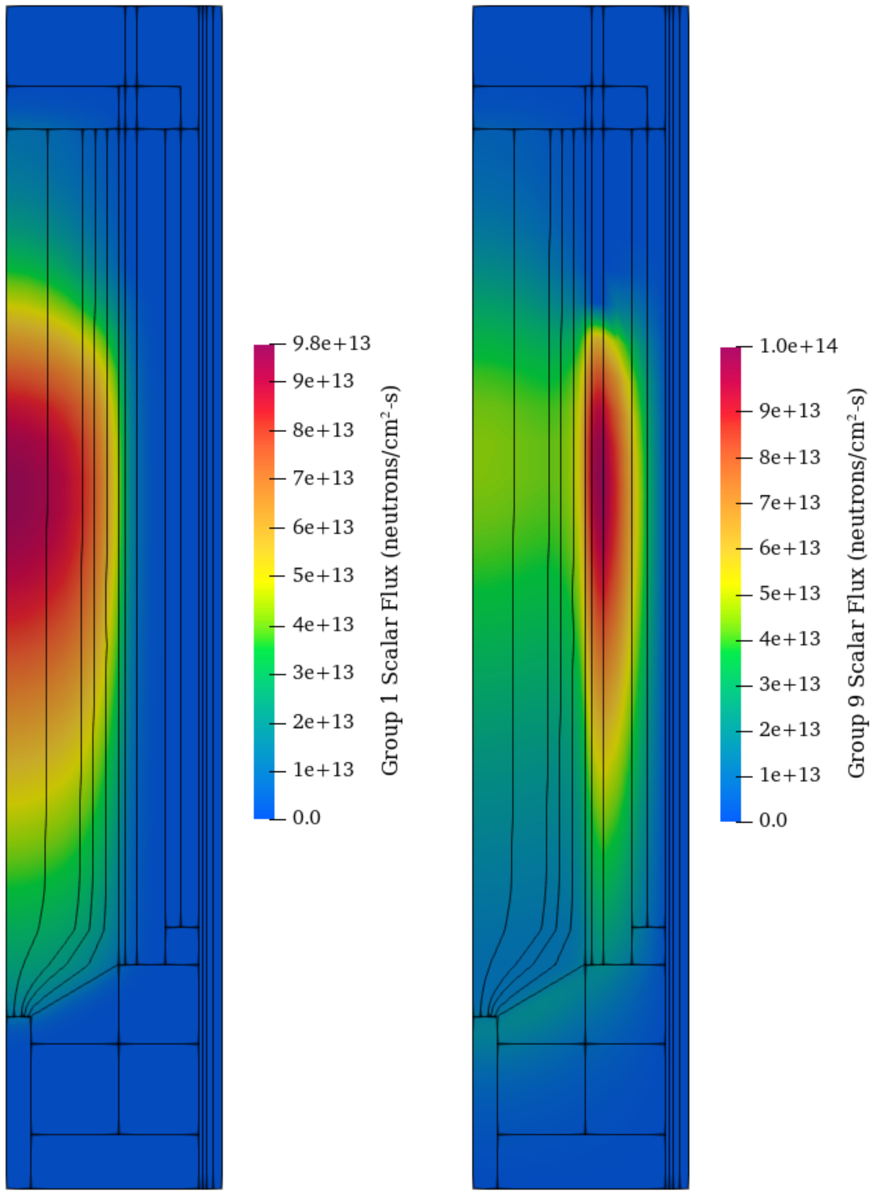
BISON – TRISO HC

- **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)

Neutronics Model

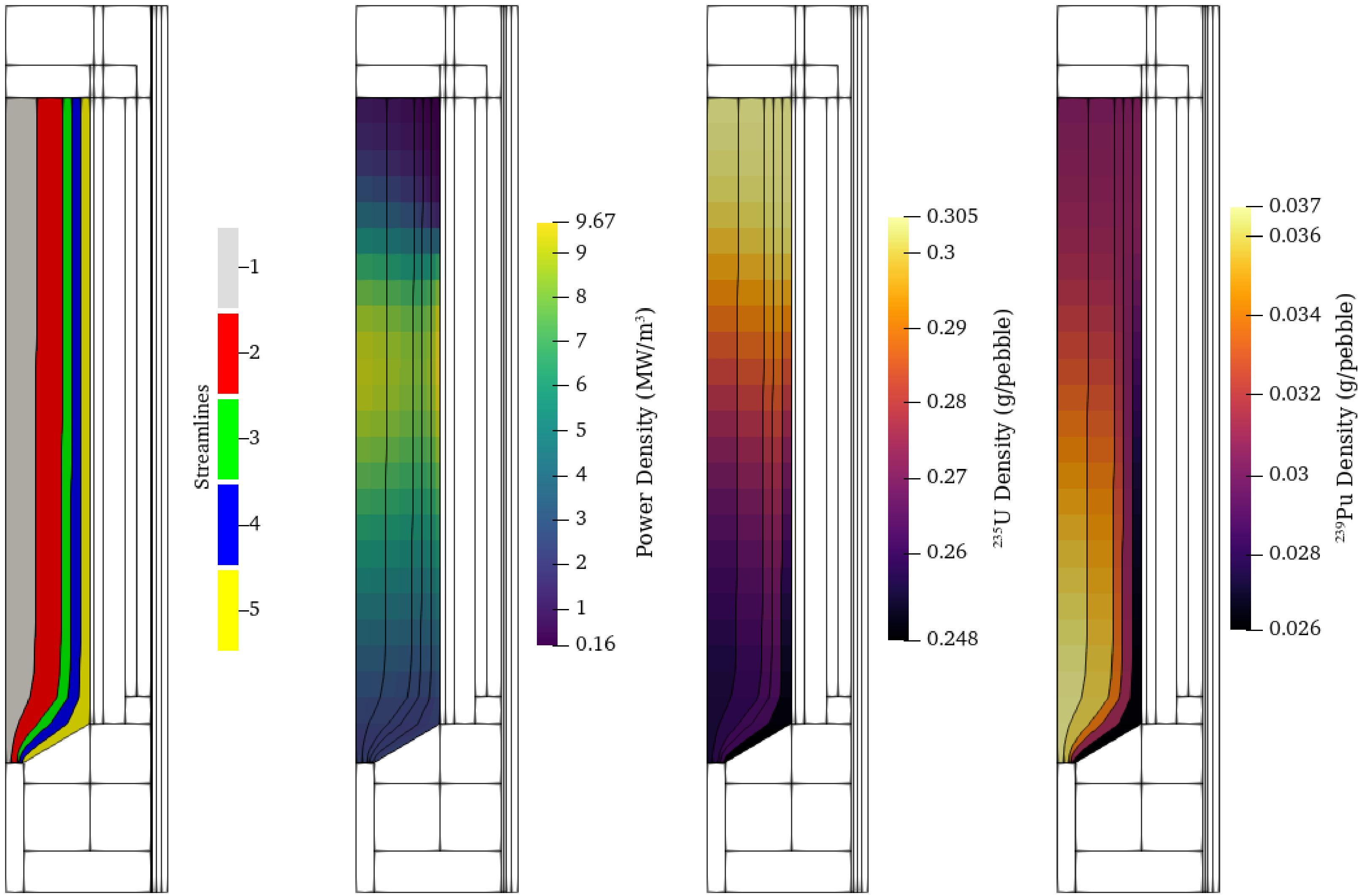
- 2D RZ 9-group diffusion model
- Control rod placed at critical configuration
- Simulated k-eff: 0.99961
- Excess reactivity: 806 pcm





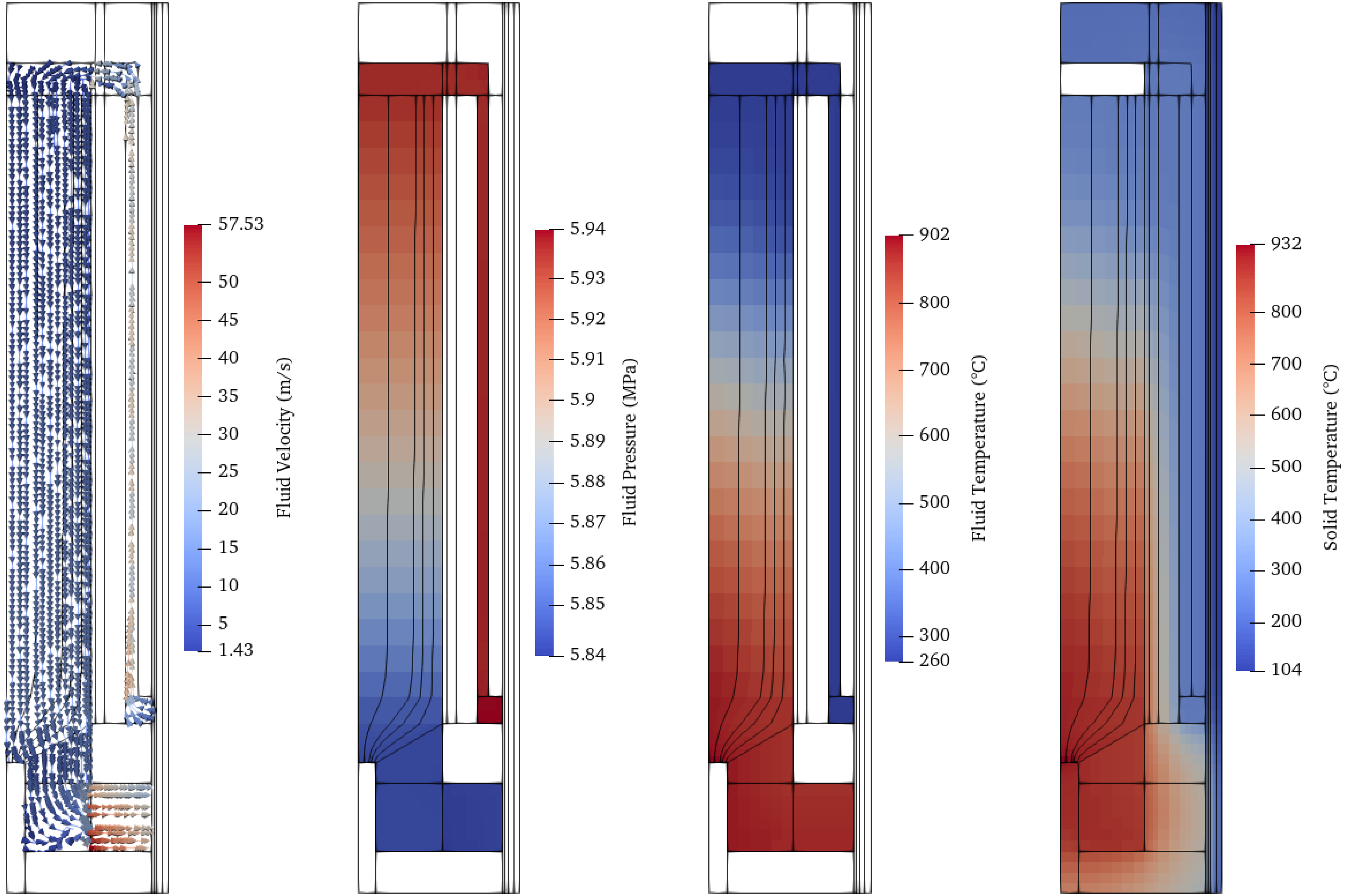
Depletion Model

- 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%



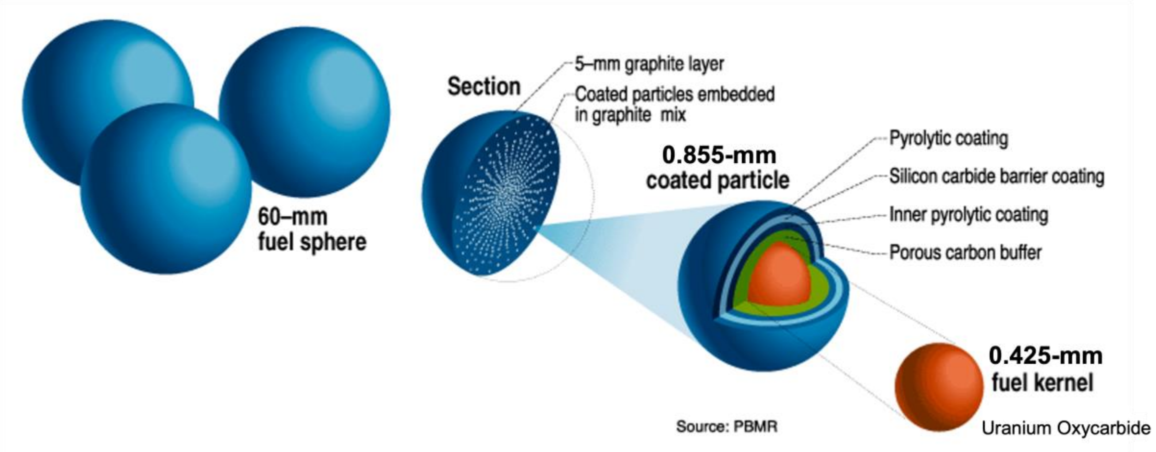
Thermal Hydraulics Model

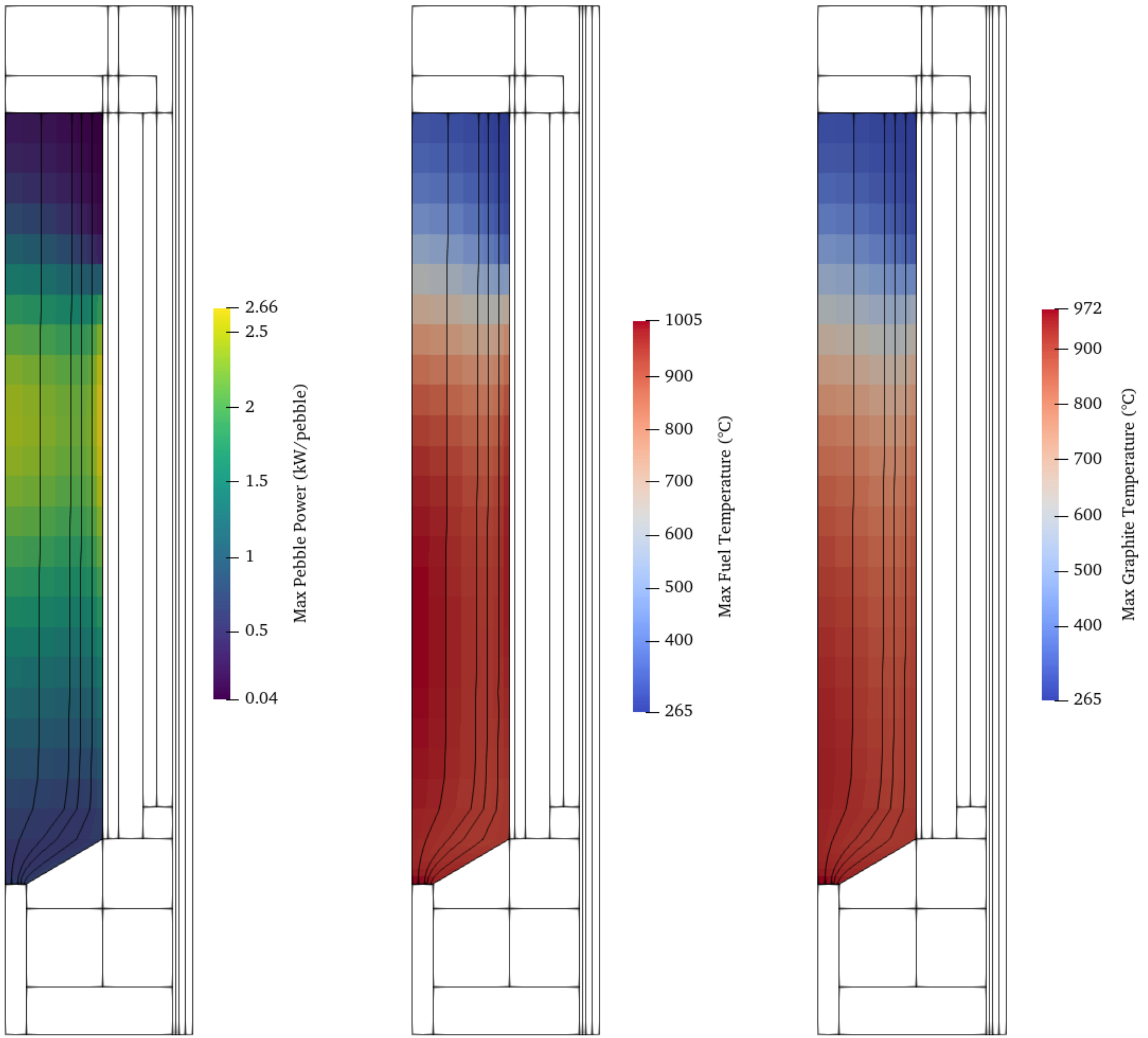
- 2D RZ coupled porous flow and solid heat conduction



Pebble and TRISO Heat Conduction Model

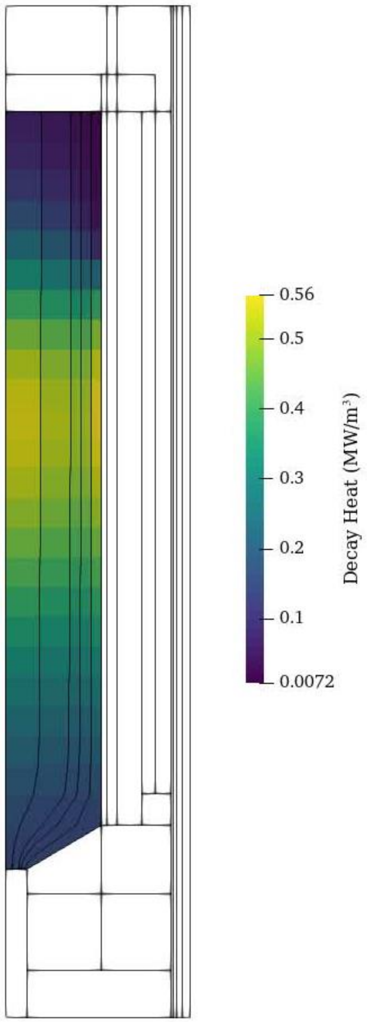
- 1D R-Spherical heat conduction
- Representative pebble mode for each cell and burnup group (3,900 solves)
- Surface temperature of pebble assigned from TH
- Surface temperature of TRISO assigned from average pebble temperature
- Max fuel temperature: 1009 ºC

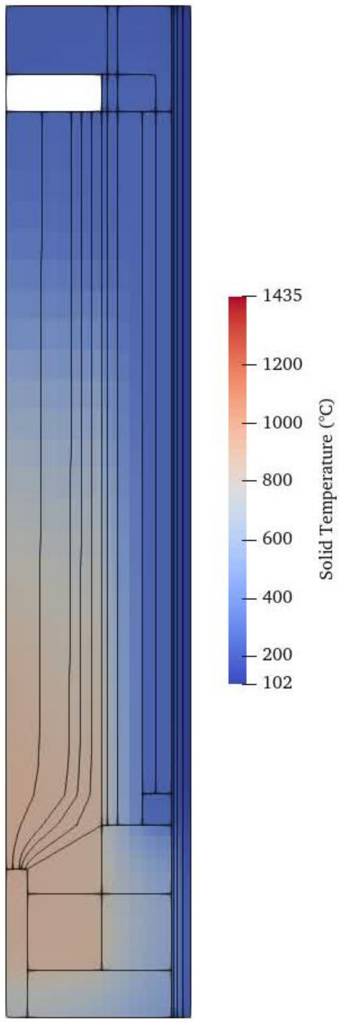


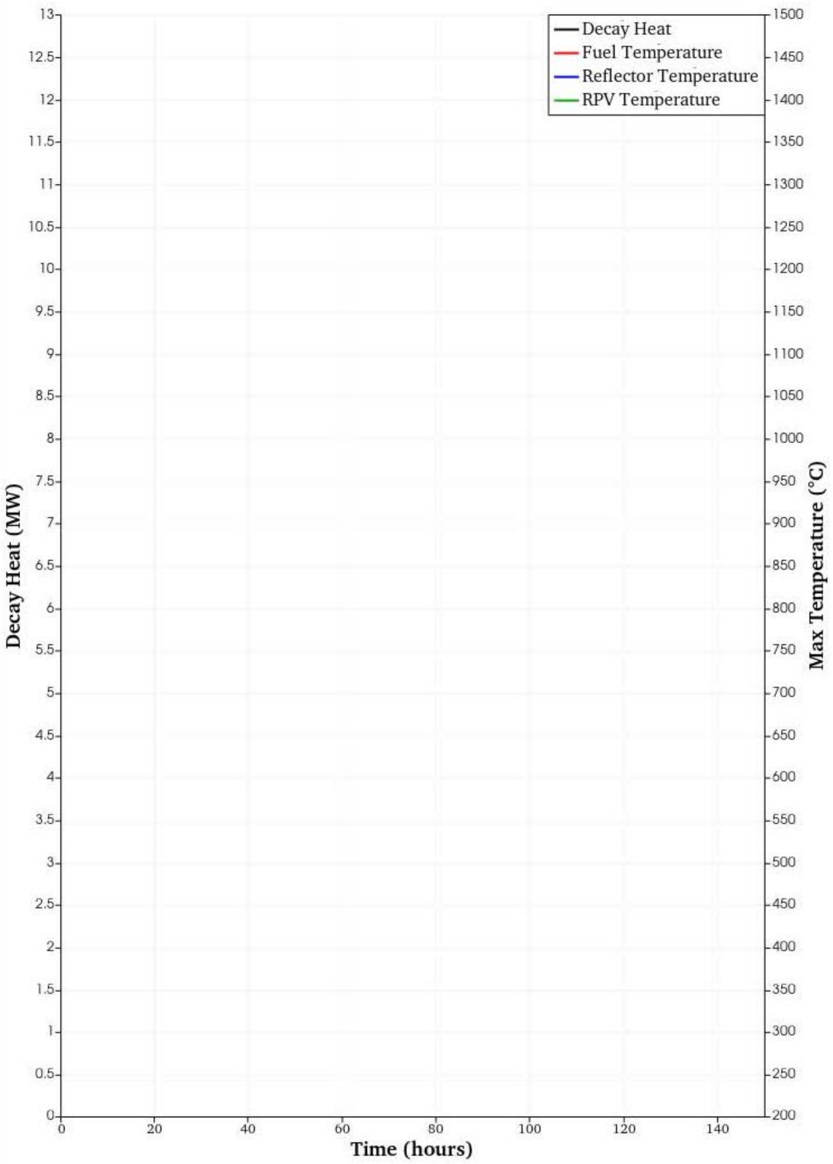


Protected DLOFC Transient

- 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 ºC
- Max RPV temperature: 322 ºC







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

QoI	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	^oC
Max DLOFC Fuel Temp	1438	^oC
Max DLOFC RPV Temp	322	^oC

Sensitivity Analysis Methodology

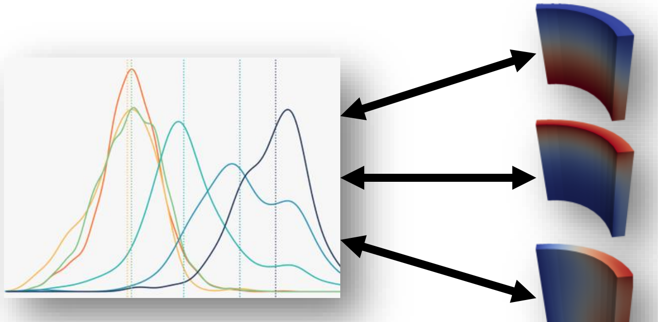
- Goal 1: **Determine the effect of each parameter** on quantities of interest **qualitatively**
  - Sample each parameter **individually**
  - Useful to understand behavior if a parameter was changed one way or another
  - Puts robustness of the model's solver to the test

- 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

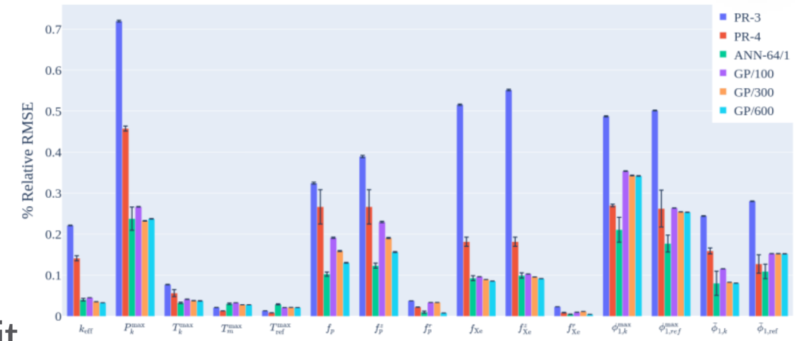
- Goal 3: Evaluate **global sensitivities for each parameter-QoI** pair
  - Utilize **polynomial chaos meta-modeling** to evaluate Sobol indices
  - Quantitively determines **impact of a parameter on a QoI**
  - Useful for determining important parameters

The MOOSE Stochastic Tools Module

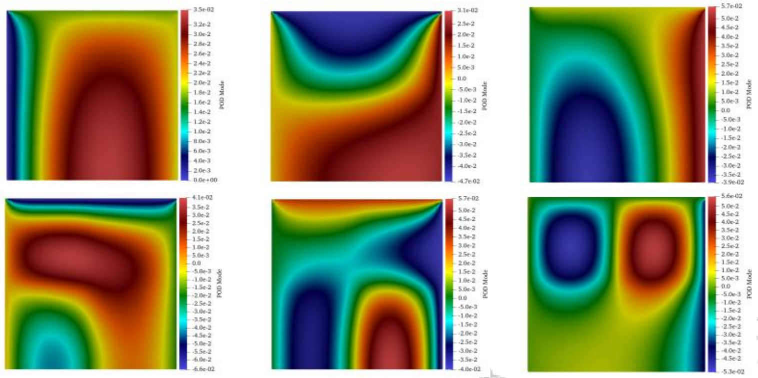
- Provide a **MOOSE interface** for performing stochastic analysis on MOOSE-based models.
- Sample parameters, run applications, and gather data that is both **efficient** (memory and runtime) and **scalable**.
- Perform UQ and sensitivity analysis with **distributed data** with **advanced variance reduction** 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



General process for forward UQ



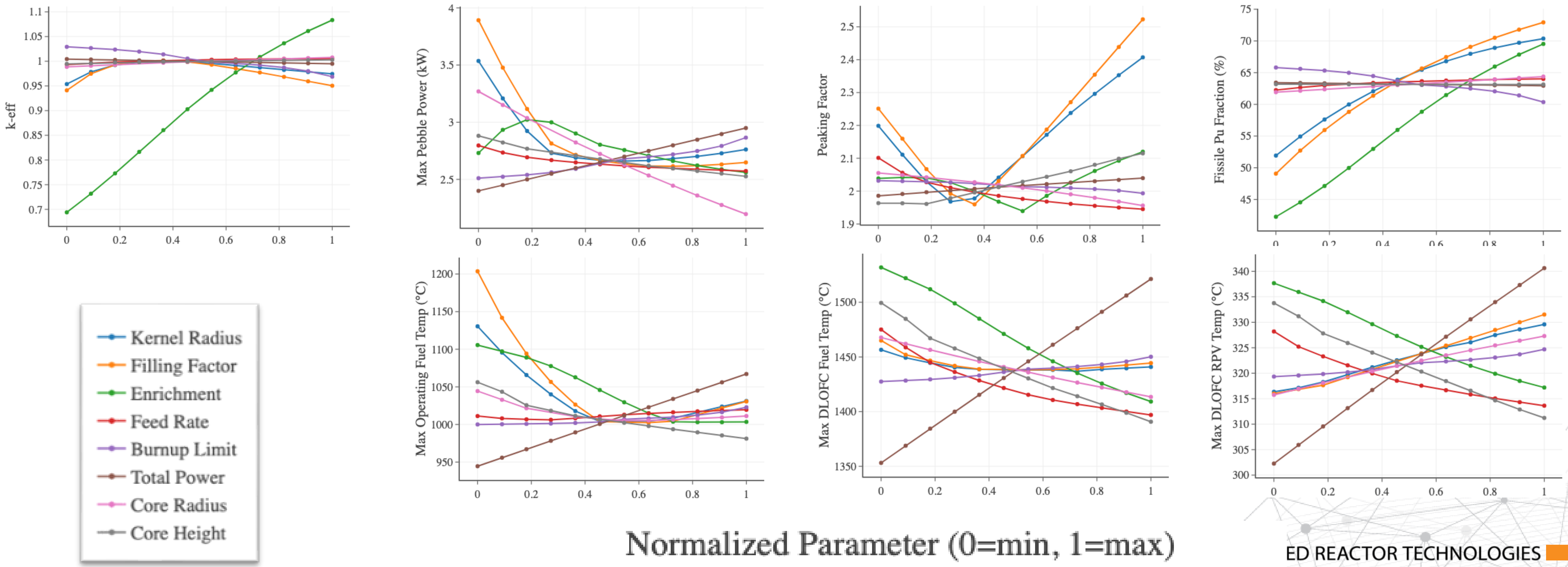
Surrogate Comparison for Reactor Optimization



POD modes of a 2D heat conduction problem

Sensitivity Analysis: Qualitative Analysis

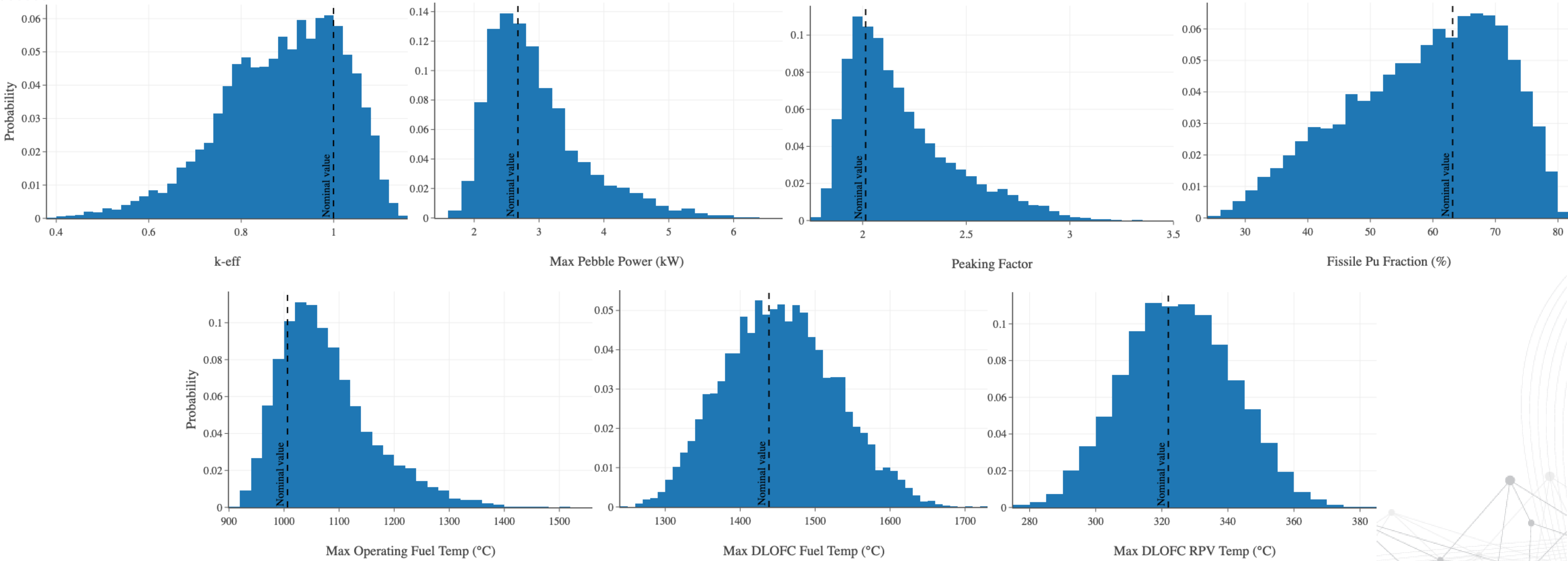
- Each design parameter was changed individually
  - Example: enrichment was changed uniformly between 5-20 wt%, while all other parameters were held at their nominal values
  - 12 points for each parameter: 96 total samples



ED REACTOR TECHNOLOGIES

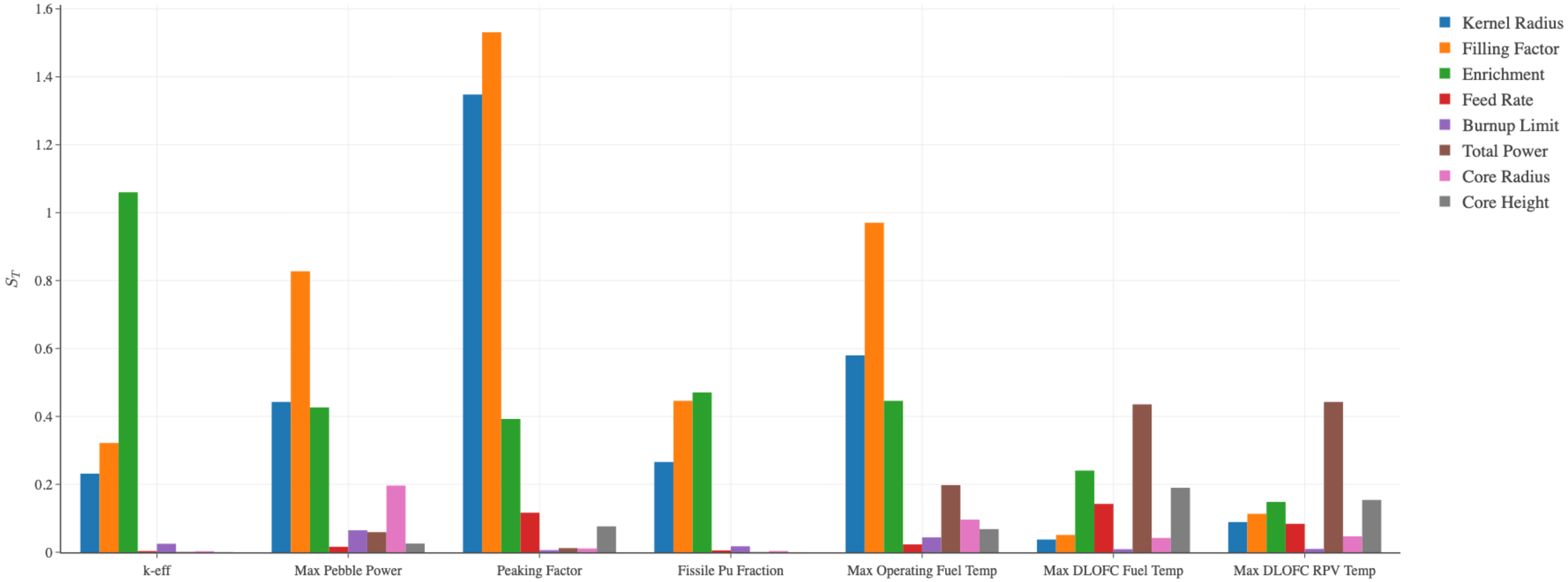
Sensitivity Analysis: Producing Data

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



Sensitivity Analysis: Global Sensitivity

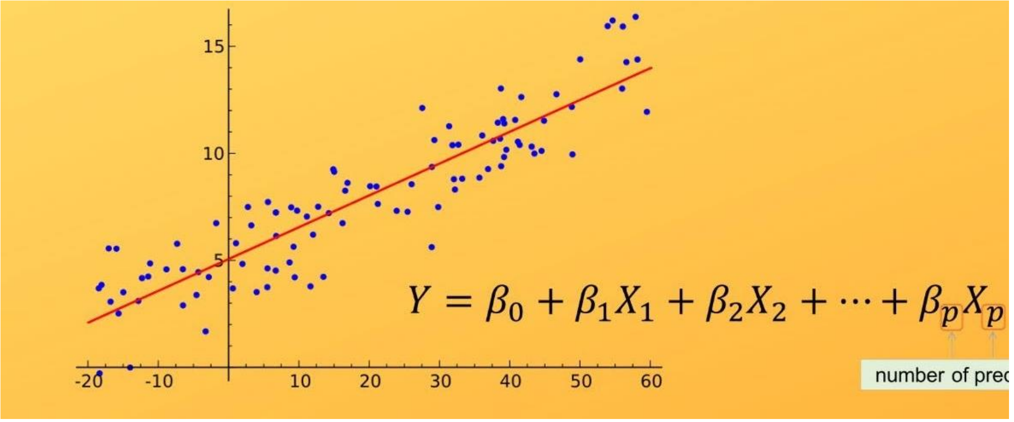
- Total Sobol indices using polynomial chaos expansion
  - Fourth-order monomial expansion
  - Second-order indices also available indicating cross-term sensitivity



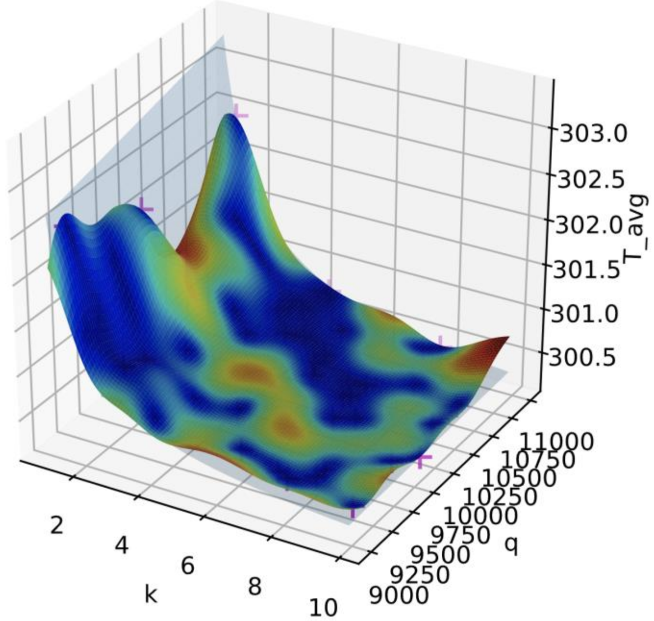
Reduced-Order Model Methodology

- Investigating three different regression techniques

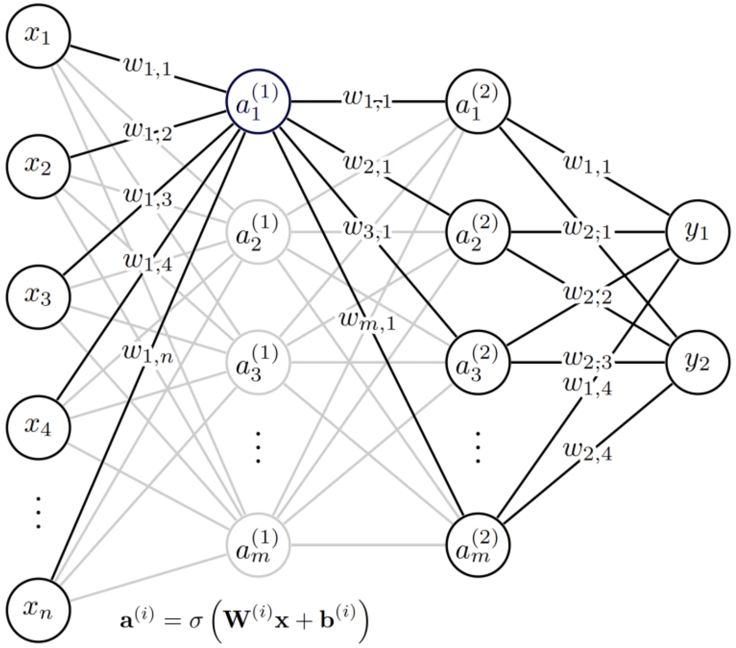
Polynomial Regression



Gaussian Processing

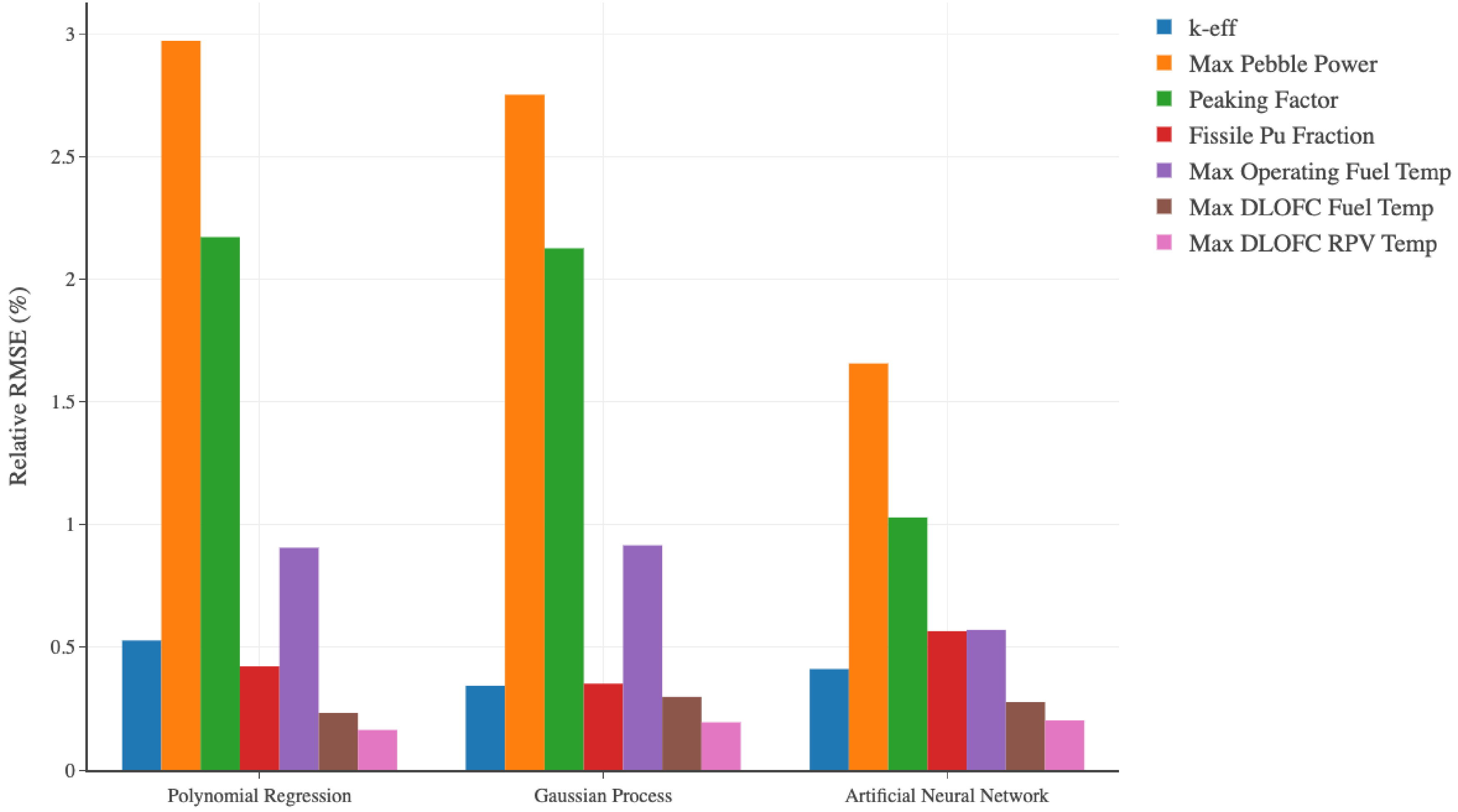


Artificial Neural Network



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 ºC	67.65	68.37	68.43	68.01
Max DLOFC Fuel Temp	< 1600 ºC	97.16	97.27	97.25	97.40
Max DLOFC RPV Temp	< 350 ºC	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