

# A Surrogate Approach Towards Validation and Uncertainty Quantification of Multiphysics Reactor Simulation Codes

## Thesis Prospectus

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# Outline

## 1 Motivation

- Proposed Application

## 2 Building Surrogate Models

## 3 Application of Surrogate Models

# Background

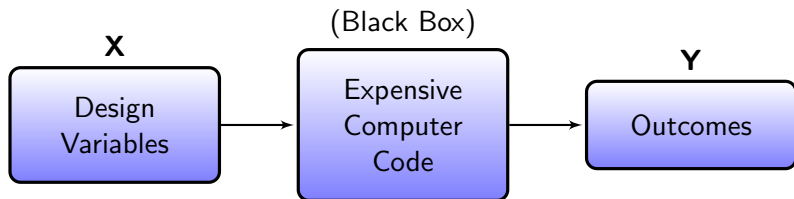
- Physical phenomena is studied by conducting experiments.
- Any data collected represents instances of underlying stochastic processes.
- We build predictive computer models in an attempt to reproduce such observed physical phenomena.
- To accurately capture stochastic element of experiments, computer models should be probabilistic.
- In other words, inputs to computer models have uncertainties associated with them that are propagated to any outputs of interest.
- Running computer simulations should be like conducting physical experiments. Computer experiments.

# Why Surrogates?

- We run computer simulations to meet design objectives under certain constraints.
- Involves numerical optimization, calibration, and performing what-if analyses.
- Also, we're interested in determining which of our design variables have the greatest effects on simulation outcomes.
- Thousands of simulations required to make this possible but...
- Computer simulations that model real phenomenon like nuclear reactors often take  $\mathcal{O}(\text{hours})$  or  $\mathcal{O}(\text{days})$  to complete.
- Building a surrogate model for your expensive computer simulations can make everything listed above possible.

# What is a Surrogate Model?

- A model for the outcomes of (likely) expensive computer simulations that can be rapidly evaluated while simultaneously preserving the predictive capabilities of the original simulations.
- Want to intelligently choose subspace  $\{x_1, x_2, \dots, x_N\} \subset \mathbf{X}$  to sample expensive computer code to get  $\{y_1, y_2, \dots, y_N\} \subset \mathbf{Y}$ .
- Learn fast mapping that approximates  $\mathbf{X} \rightarrow \mathbf{Y}$ .



# Proposed Application to Fuel Performance Modeling

- Fission Gas Release (FGR) refers to the phenomenon where Xenon and Krypton gases formed in  $\text{UO}_2$  fuel rods are released into the rod filling gas.
- Causes pressure build-up and thermal conductivity degradation in the rod filling gas, potentially jeopardizing the safety of the reactor.
- Fission gas atoms generated in the fuel grains diffuse towards the grain boundaries.
- Majority of the gas diffuses into grain-face gas bubbles, giving rise to grain-face swelling.
- Bubble growth brings about bubble coalescence and interconnection, eventually leading to the formation of a tunnel network through which the fission gas is released.

# SIFGRS FGR Model

- Simple Integrated Fission Gas Release and Swelling (SIFGRS)
- Incorporates gas diffusion and precipitation in grains, growth and coalescence of gas bubbles at grain faces, thermal, athermal, steady-state, and transient gas release.
- Through a direct description of the grain face gas bubble development, the fission gas swelling and release are calculated as coupled processes.
- Parameterized by, among others, linear heat rate, gas diffusion coefficient, surface tension of grain face bubbles, hydrostatic pressure, fuel grain radius, fuel porosity, and grain boundary sweeping.

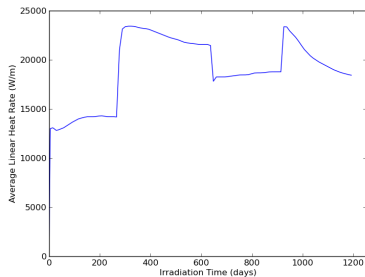
# Risø AN3 Experiment

- Validation case for fuel performance modeling in the Fumex-II database.
- Experiment consists of a base irradiation of four reactor cycles in the Biblis A pressurized water reactor.
- After the base irradiation period, a fuel rod is extracted and refabricated to a shorter length before undergoing a power ramp.
- Refabricated fuel rod is outfitted with various instrumentation such that fuel centerline temperature, FGR and rod internal pressure measurements can be obtained.

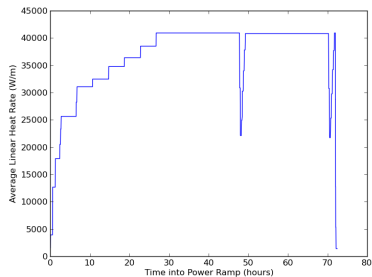


# Risø AN3 Experiment Irradiation Profiles

## Base Irradiation History



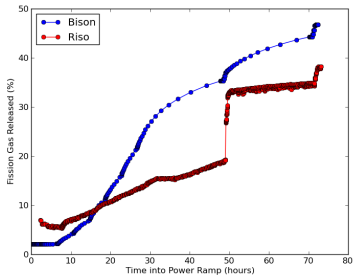
## Power Ramp Experiment



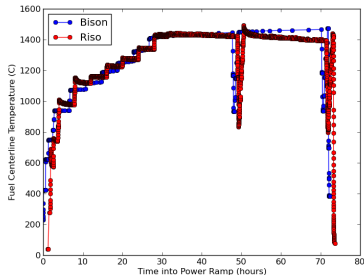
# Modeling Risø AN3 Experiment with BISON

- BISON is a finite-element fuel performance modeling code that utilizes the SIFGRS model.
- SIFGRS parameters are quite generic and uncertain.

Fission Gas Release



Fuel Centerline Temperature



# Modeling Risø AN3 Experiment with BISON/MPACT

- No sense in comparing the output of a computer simulation to experimental data unless the computer simulation is of high fidelity and capable of reproducing the pertinent physics.
- MPACT is a neutronics code that provides detailed intrapin and azimuthally dependent neutronics data in the fuel elements.
- The two-way coupling scheme provided by BISON and MPACT provides the most accurate fuel performance modeling available for a nuclear reactor.
- Expensive!

# Modeling Risø AN3 Experiment with BISON/MPACT

- BISON predictions of FGR and temperature fields stand to be improved by calibrating FGR parameters to experimental data.
- Calibration studies require  $\mathcal{O}(10^3)$  function evaluations, which in this case are the coupled BISON/MPACT computer codes.
- Each simulation of the Risø AN3 experiment will take a few hours.
- It's necessary to construct a surrogate for the calibration study!

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