Multiphysics Reduced Order Modelling

> Parikshi Bajpai

Motivation and Objectives

Background -Reactor Physics 00.01

Parameterised Multiphysics Model

Finite Element Discretisation

Reduced Bas Formulation

Expected
Outcomes and

Multiphysics Reduced Order Modelling Reduced Basis Method for Lead-Cooled Fast Reactor

Parikshit Bajpai

MCSC 6020G - Numerical Analysis October 28, 2019

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Motivation

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The full order simulation of nuclear reactors is extremely costly!

Can we reduce the computational time and cost associated with these simulations without compromising with the accuracy?

Objective of

Multiphysics Reduced Order Modelling

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Develop a Reduced Basis method, with basis functions sampled by a Proper Orthogonal Decomposition technique, to develop a reduced order model of a parametrised Lead-cooled Fast Reactor single-channel.

Lead-cooled Fast Reactor (LFR)

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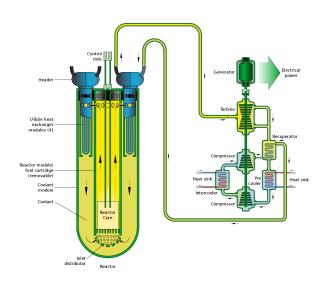
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Expected Outcomes and Results

Neutron balance

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot D\nabla \phi + \nu \Sigma_f \phi - (\Sigma_a + \Sigma_s) \phi$$

 ϕ - Neutron Flux

D - Diffusion Coefficient

 Σ_a - Macroscopic Absorption Cross Section

 Σ_s - Macroscopic Scattering Cross Section

 ν - Fissile Yield (No. of neutrons produced per fission)

 Σ_f - Macroscopic Fission Cross Section

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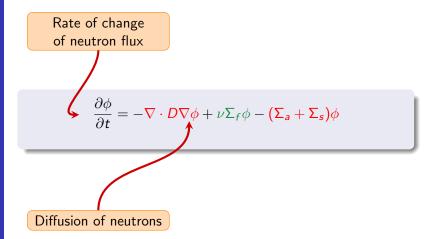
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Expected Outcomes and Rate of change of neutron flux $\frac{\partial \phi}{\partial t} = -\nabla \cdot D\nabla \phi + \nu \Sigma_f \phi - (\Sigma_a + \Sigma_s) \phi$

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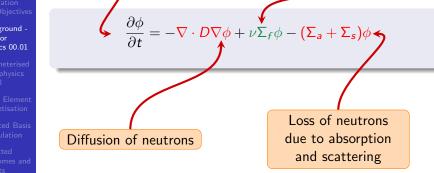
Neutron production Rate of change through fission of neutron flux $\frac{\partial \phi}{\partial x} = 0$ $-\nabla \cdot D\nabla \phi + \nu \overset{\mathbf{v}}{\Sigma}_{f} \phi - (\Sigma_{a} + \Sigma_{s}) \phi$ Diffusion of neutrons

Rate of change

of neutron flux

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Neutron production

through fission

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Energy Balance

$$\frac{\partial T}{\partial t} = \nabla \cdot [(K + K_T)\nabla T] - \rho C_{\rho} \mathbf{v} \cdot \nabla T + Q$$

T - Temperature

K - Thermal Conductivity

 K_T - Turbulent Thermal Conductivity

 C_p - Heat Capacity

v - Velocity of fluid

Q - Source Term

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Rate of change of temperature $\frac{\partial T}{\partial t} = \nabla \cdot [(K + K_T)\nabla T] - \rho C_p \mathbf{v} \cdot \nabla T + Q$

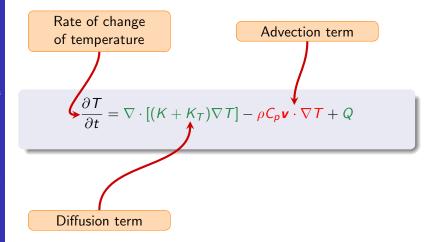
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Rate of change of temperature $\frac{\partial T}{\partial t} = \nabla \cdot [(K + K_T)\nabla T] - \rho C_p \mathbf{v} \cdot \nabla T + Q$ Diffusion term

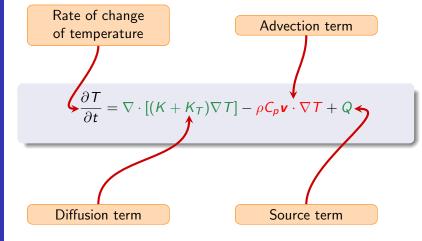
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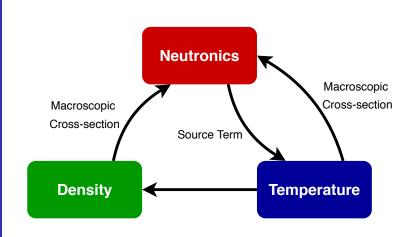
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Multiphysics Model

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Parameterised Multiphysics Model



Parametrised Multiphysics Model

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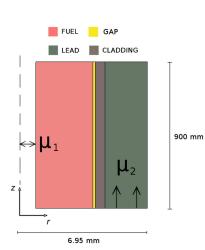
Expected Outcomes and Results

- Parametrised LFR single channel model.
- Rotational symmetry along fuel channel (r-z model).
- Time-independent settings.
- Parameters:
 - Inner radius of fuel pellet

$$\mu_1 \in [0.1, 0.43] \text{ (cm)}$$

Nominal coolant flow rate

$$\mu_2 \in [0.8, 1.6] \text{ (m/s)}$$



Neutronics

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Expected Outcomes and Results The multi-group neutron diffusion equation in stationary formulation is a generalised eigenvalue problem.

$$\left(-\nabla\cdot\overline{\overline{D}}\nabla+\overline{\overline{\Sigma_a}}+\overline{\overline{\Sigma_s}}\right)\overline{\Phi}=\lambda_{\mathit{eff}}\overline{\chi}\overline{\mathit{F}}'\overline{\Phi}$$

$$\overline{\Phi} = \begin{bmatrix} \Phi_1(\mathbf{r}) \\ \vdots \\ \Phi_6(\mathbf{r}) \end{bmatrix} \quad \overline{\overline{D}} = \begin{bmatrix} D_1(\mathbf{r}) & \dots & 0 \\ & \ddots & \\ & \dots & D_6(\mathbf{r}) \end{bmatrix} \quad \overline{\overline{\Sigma_a}} = \begin{bmatrix} \Sigma_a^1(\mathbf{r}) & \dots & 0 \\ & \ddots & \\ & \dots & \Sigma_a^6(\mathbf{r}) \end{bmatrix}$$

$$\overline{\overline{\Sigma_s}} = \begin{bmatrix} \sum_{g' \neq 1} \Sigma_s^{1 \to g'}(\mathbf{r}) & \dots & -\Sigma_s^{6 \to 1} \\ & \ddots & \\ -\Sigma_s^{1 \to 6} & \dots & \sum_{g' \neq 6} \Sigma_s^{6 \to g'} \end{bmatrix} \quad \overline{\chi} = \begin{bmatrix} \chi_1 \\ \vdots \\ \chi_6 \end{bmatrix} \quad \overline{F} = \begin{bmatrix} \nu \Sigma_f^1(\mathbf{r}) \\ \vdots \\ \nu \Sigma_f^6(\mathbf{r}) \end{bmatrix}$$

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$$\left(-\nabla\cdot\overline{\overline{D}}\nabla+\overline{\overline{\Sigma_a}}+\overline{\overline{\Sigma_s}}\right)\overline{\Phi}=\lambda_{\textit{eff}}\overline{\chi}\overline{\textit{F}}'\overline{\Phi}$$

Fuel domain

$$\Sigma(T, \rho) = \frac{\rho}{\rho_0} \left[\Sigma_0 + \alpha \log \left(\frac{T}{T_0} \right) \right]$$

Lead domain

$$\Sigma(T,\rho) = \frac{\rho}{\rho_0} \Sigma_0$$

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The multi-group neutron diffusion equation in stationary formulation is a generalised eigenvalue problem.

$$\left(-\nabla\cdot\overline{\overline{D}}\nabla+\overline{\overline{\Sigma_a}}+\overline{\overline{\Sigma_s}}\right)\overline{\Phi}=\lambda_{\text{eff}}\overline{\chi}\overline{F}'\overline{\Phi}$$

Boundary conditions

Albedo boundary conditions provide a good compromise between accuracy and computational requirements.

$$\overline{n} \cdot (D_{g} \nabla \Phi_{g}) = -\gamma_{z} \phi_{g}$$

$$\overline{n} \cdot (D_{\mathbf{g}} \nabla \Phi_{\mathbf{g}}) = -\gamma_{\mathbf{r}} \phi_{\mathbf{g}}$$

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Expected Outcomes and Results Within the cladding and gap domains the heat transfer is purely conductive.

$$-\nabla \cdot (K\nabla T) = 0$$

Within the fuel domain the heat transfer is purely conductive but has a source term.

$$-\nabla \cdot (\nabla T) = \sum_{g=1}^{6} \Sigma_g^f E_f \Phi_g$$

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Within the lead domain, the heat transfer is has an advective and a conductive term.

$$-\nabla \cdot [(K + K_T)\nabla T] = \rho C_p \mathbf{v} \cdot \nabla T$$

Boundary conditions

- Symmetry conditions at inner radius of the fluid domain and and outerradius of fluid domain.
- Homogeneous Neumann conditions on top and bottom of the domain.

Back to Objective

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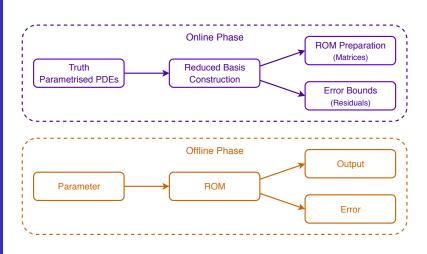
The full-fidelity model can have $\mathcal{O}(10^6-10^9)$ degrees of freedom.

We want to capture the behaviour of the system without using a high-fidelity, computationally expensive discretisation scheme.

Offline/Online Strategy

Multiphysics Reduced Order Modelling

Parameterised Multiphysics Model



Finite Element Discretisation

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Expected
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For a given $\mu\in\mathcal{D}$, find $\overline{\Phi}(\mu)\in V^\mathcal{N}$ and $T(\mu)\in W^\mathcal{N}$ such that

$$\begin{split} \mathrm{a}\left(\overline{\Phi},\overline{\nu};\mu,\Sigma(T)\right) &= \lambda_{\mathit{eff}} \mathrm{m}\left(\overline{\Phi},\overline{\nu};\mu,\Sigma(T)\right) \qquad \forall \overline{\nu} \in V^{\mathcal{N}} \\ \mathrm{d}\left(T,w;\mu\right) &= \mathrm{f}\left(w;\mu,S(\overline{\phi})\right) \qquad \forall w \in W^{\mathcal{N}} \end{split}$$

$$\mathbf{a}\left(\overline{\Phi}, \overline{\nu}; \mu, \Sigma(T)\right) = \int_{\Omega} \overline{\overline{D}} (\nabla \overline{\Phi} \cdot \nabla \overline{\nu}) + (\overline{\overline{\Sigma}_{a}} + \overline{\overline{\Sigma}_{s}}) \overline{\Phi} \overline{\nu} + \int_{\Gamma_{side}} \gamma_{r} \overline{\Phi} \overline{\nu} + \int_{\Gamma_{tot} + \Gamma_{bot}} \gamma_{z} \overline{\Phi} \overline{\nu}$$

$$\mathrm{m}\left(\overline{\Phi}, \overline{\nu}; \mu, \Sigma(T)\right) = \int_{\Omega} \overline{\chi} \overline{F}' \overline{\Phi} \overline{\nu}$$

Finite Element Discretisation

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Finite Element Discretisation

Reduced Basis Formulation

Expected Outcomes and Results For a given $\mu \in \mathcal{D}$, find $\overline{\Phi}(\mu) \in V^{\mathcal{N}}$ and $T(\mu) \in W^{\mathcal{N}}$ such that $\mathrm{a}\left(\overline{\Phi}, \overline{\nu}; \mu, \Sigma(T)\right) = \lambda_{\mathit{eff}} \mathrm{m}\left(\overline{\Phi}, \overline{\nu}; \mu, \Sigma(T)\right) \qquad \forall \overline{\nu} \in V^{\mathcal{N}}$

$$d(T, w; \mu) = \lambda_{\text{eff}} \operatorname{in} (\Psi, \nu; \mu, \Sigma(T)) \qquad \forall \nu \in V$$

$$d(T, w; \mu) = f(w; \mu, S(\overline{\phi})) \qquad \forall w \in W^{\mathcal{N}}$$

$$d(T, w; \mu) = \int_{\Omega} K \nabla T \nabla w + \int_{\Omega_{lead}} K_T \nabla T \nabla w$$

$$\mathrm{f}\left(w;\mu,S(\overline{\phi})\right) = \int_{\Omega_{fool}} Qw + \int_{\Omega_{fool}}
ho C_{
ho}(oldsymbol{v}\cdot
abla T)w$$

Affine Parametric Dependence

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Outcomes and Results

$$\mathrm{a}\left(\overline{\Phi}, \overline{\nu}; \mu, \Sigma(\mathcal{T})\right) = \sum_{q=1}^{Q_{\mathsf{a}}} \Theta_{\mathsf{a}}^{q}(\mu) \mathrm{a}^{q}\left(\overline{\Phi}, \overline{\nu}; \Sigma(\mathcal{T})\right)$$

$$\mathrm{m}\left(\overline{\Phi},\overline{\nu};\mu,\Sigma(T)\right) = \sum_{q=1}^{Q_m} \Theta_m^q(\mu) \mathrm{m}^q\left(\overline{\Phi},\overline{\nu};\Sigma(T)\right)$$

$$d(T, w; \mu) = \sum_{q=1}^{Q_d} \Theta_d^q(\mu) d^q(T, w)$$

$$f\left(w;\mu,S(\overline{\phi})\right) = \sum_{r=1}^{Q_f} \Theta_f^q(\mu) f^q\left(w;S(\overline{\phi})\right)$$

Reduced Basis Model

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The RB method is aimed at constructing reduced order solutions $\overline{\Phi}^{N_f}$ and T^{N_T} such that

$$\mathbf{a}\left(\overline{\Phi}^{N_f}, \overline{\nu}; \mu, \Sigma(T^{N_T})\right) = \lambda_{\text{eff}} \mathbf{m}\left(\overline{\Phi}^{N_f}, \overline{\nu}; \mu, \Sigma(T^{N_T})\right)$$
$$\forall \overline{\nu} \in V^{N_f} \subset V^{\mathcal{N}}$$

$$d\left(T^{N_{T}}, w; \mu\right) = f\left(w; \mu, S(\overline{\phi}^{N_{f}})\right)$$
$$\forall w \in W^{N_{T}} \subset W^{N}$$

Reduced Basis Model

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$$\mathbf{a}\left(\overline{\Phi}^{N_f}, \overline{\nu}; \mu, \Sigma(T^{N_T})\right) = \lambda_{\text{eff}} \mathbf{m}\left(\overline{\Phi}^{N_f}, \overline{\nu}; \mu, \Sigma(T^{N_T})\right)$$
$$\forall \overline{\nu} \in V^{N_f} \subset V^{\mathcal{N}}$$

$$d\left(T^{N_{T}}, w; \mu\right) = f\left(w; \mu, S(\overline{\phi}^{N_{f}})\right)$$
$$\forall w \in W^{N_{T}} \subset W^{\mathcal{N}}$$

The reduced spaces V^{N_f} and W^{N_T} have dimensions N_f and N_T respectively and are defined as:

$$V^{N_f} = \operatorname{span}\left\{\xi_1^f, \dots, \xi_{N_f}^f\right\} \quad W^{N_T} = \operatorname{span}\left\{\xi_1^T, \dots, \xi_{N_T}^T\right\}$$

Reduced Basis Model

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$$\Phi^{N_f} = \sum_{i=1}^{N_f} \phi_{N,i} \xi_i^f \qquad T^{N_T} = \sum_{j=1}^{N_T} T_{N,j} \xi_j^T$$

$$\begin{split} \mathrm{a}(\mathcal{Z}_f \overline{\phi_N}, \overline{\nu}; \mu, \Sigma(\mathcal{Z}_T \overline{T}_N)) &= \lambda_{eff}^N \mathrm{m}(\mathcal{Z}_f \overline{\phi_N}, \overline{\nu}; \mu, \Sigma(\mathcal{Z}_T \overline{T}_N)) \\ \mathrm{d}(\mathcal{Z}_f \overline{T_N}, w; \mu) &= \mathrm{f}(w; \mu, S(\mathcal{Z}_f \overline{\phi_N})) \end{split}$$

$$\mathcal{Z}_f = [\xi_1^f | \dots | \xi_{N_f}^f]$$
 $\mathcal{Z}_T = [\xi_1^T | \dots | \xi_{N_T}^T]$

Offline Phase

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Expected Outcomes and Results

Offline

- Run high fidelity computations to get snapshots.
- Construct matrices \mathcal{Z}_f and \mathcal{Z}_T required to build the matrices of ROM
- Matrices corresponding to the bilinear form of affine decompositions.

Online

- Multiply reduced matrices by proper coefficients and sum together.
- Solve the ROM.

Expected Outcomes and Results

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Reduced Basis

Expected Outcomes and Results Evaluate the errors between the reactivity provided by ROM and FE solution and error vs. number of basis functions.

$$\epsilon_{\lambda}(\mu) = |\lambda_{N}(\mu) - \lambda_{\mathcal{N}}(\mu)|$$

Evaluate the error between the neutron flux provided by the two models.

$$\epsilon_f = \int_{\Omega} (\Phi^{N_f} - \overline{\Phi})^2$$

Evaluate the error between the temperature field provided by the two models.

$$\epsilon_T = \int_{\Omega} (T^{N_f} - T)^2$$

Expected Outcomes and Results

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Expected Outcomes and Results Comparison of computational cost of ROM and FE model.

$$\mathsf{Speed\text{-}up} = \frac{\mathsf{Wall\ time\ of\ ROM\ calculation}}{\mathsf{Wall\ time\ of\ FE\ simulation}}$$

Computational break-even.

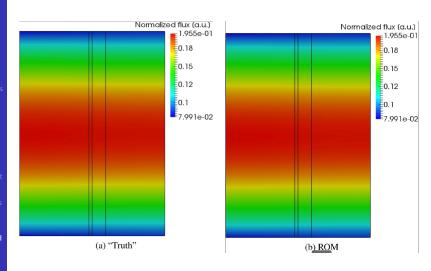
$$\mathsf{Break\text{-}even} = \frac{\mathsf{Total\ Offline\ time}}{\mathsf{Time\ for\ 1\ FE\ simulation}}$$

Sample Results

Multiphysics Reduced Order Modelling

Expected Outcomes and





Sample Results

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