A restarted proper orthogonal decomposition method to integrate the neutron diffusion equation

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1 Introduction

The Proper Orthogonal Decomposition (POD) is a technique to construct reduced order methods (ROMs) widely used in engineering to reduce the dimensionality of complex systems. It involves decomposing high-dimensional data into a lower-dimensional representation while preserving the essential features of the original system. In engineering applications, POD is commonly employed to analyse and model large-scale systems, such as fluid dynamics [1], structural mechanics [2], heat transfer [3], etc.

A significant analysis in the field of nuclear engineering is the quantification of sensitivity and uncertainty in nuclear systems. This implies the efficient simulation of numerous configurations of a reactor core. The computational expense associated with these simulations has led to the adoption of POD reduced order models [4, 5, 6, 7]. This methodology is based on expressing the neutron flux in terms of a basis of a low-dimensional subspace. First, in an offline stage, it extracts the 'mode shapes' or the basis (the POD modes) from a SVD decomposition of experimental data or detailed simulations of high-dimensional systems termed 'snapshots'. Subsequently, in an online stage, the basis are used in Galerkin projections that yield low-dimensional dynamical models. The main issue of this methodology is obtaining a useful spatial representation of the quantity of interest from the set of snapshots in order to extract a basis of low rank that produces a small reduced order model.

Different techniques have been studied to compute the optimal dimension of the expansion required to establish an accurate approximation. Alternatively, this work explores a restarted Proper Orthogonal Decomposition methodology, where the basis of the subspace is updated along the time in accordance with the transient studied. The methodology is developed for the neutron diffusion equation, which has been successfully used to model the neutronic behaviour inside a reactor core. The accuracy and computational efficiency of the proposed POD method are evaluated for a benchmark problem against the full order model (FOM).

This contribution is structured as follows. First, the neutron diffusion equation is briefly described. Second, a proper orthogonal decomposition is developed. Moreover, in this Section, the

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criterion for the selection of snapshots used in this work is explained. Next, a numerical benchmark is presented to test the methodology. Finally, the main conclusions of this work are synthesized.

2 The neutron diffusion equation

Our starting point is the time-dependent neutron diffusion equation for two energy groups [10]

$$\begin{aligned} \mathcal{V}^{-1}\frac{\partial \Phi}{\partial t} + \mathcal{L}\Phi &= (1-\beta)\mathcal{F}\Phi + \sum_{k=1}^{K}\lambda_k^d \mathscr{C}_k \chi, \\ \frac{\mathrm{d}\mathscr{C}_k}{\mathrm{d}t} &= \beta_k \mathcal{F}_1 \Phi - \lambda_k^d \mathscr{C}_k, \qquad k = 1, \ldots, K, \end{aligned} \tag{1}$$

where,

$$\mathcal{L} = \begin{pmatrix} -\vec{\nabla}\cdot(D_1\vec{\nabla}) + \Sigma_{a_1} + \Sigma_{12} & 0 \\ 0 & -\vec{\nabla}\cdot(D_2\vec{\nabla}) + \Sigma_{a_2} \end{pmatrix},$$

$$\mathcal{S} = \begin{pmatrix} 0 & 0 \\ -\Sigma_{12} & 0 \end{pmatrix}, \qquad \mathcal{F} = \begin{pmatrix} \nu\Sigma_{f_1} & \nu\Sigma_{f_2} \\ 0 & 0 \end{pmatrix}, \qquad \mathcal{F}_1 = \begin{pmatrix} \nu\Sigma_{f_1} & \nu\Sigma_{f_2} \end{pmatrix},$$

$$\mathcal{V}^{-1} = \begin{pmatrix} v_1^{-1} & 0 \\ 0 & v_2^{-1} \end{pmatrix}, \qquad \chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \Phi = \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}.$$

In the previous equations, $\Phi = \Phi(\vec{r}, t)$ represents the scalar neutron flux. The remaining coefficients are time and spatial dependent magnitudes that will be determined by the configuration of the reactor.

The finite element method is applied to this equation to discretize the continuous spatial dependence. In particular, a continuous Galerkin method with Lagrange polynomials is used to get a semi-discrete system of the form

$$\begin{aligned} V^{-1}\frac{\mathrm{d}\tilde{\Phi}}{\mathrm{d}t} + L\tilde{\Phi} &= (1-\beta)F\tilde{\Phi} + \sum_{k=1}^{K}\lambda_k^d X C_k, \\ \frac{\mathrm{d}XC_k}{\mathrm{d}t} &= \beta_k F\tilde{\Phi} - \lambda_k^d X C_k, \qquad k = 1, \ldots, K, \end{aligned} \tag{2}$$

where L and F are the matrices obtained from the discretization of operators $\mathcal{L}$ and $\mathcal{F}$, respectively. Vectors $\tilde{\Phi}$ and C_k are the corresponding coefficients of Φ and $\mathcal{C}_k$ in terms of the Lagrange polynomials. The matrices X and V^{-1} are, then, defined as

$$X = \begin{pmatrix} P \\ 0 \end{pmatrix}, \qquad V^{-1} = P\begin{pmatrix} v_1^{-1} & 0 \\ 0 & v_2^{-1} \end{pmatrix},$$

where P is the mass matrix. The system (2) is known as Full Order Model (FOM).

3 The restarted proper orthogonal decomposition

The time-dependent neutron diffusion equation (2) can be approximated by using a proper orthogonal decomposition. It is supposed that $\Phi(\vec{r}, t)$ admits the following expansion

$$\Phi(\vec{r}, t) = \sum_{m=1}^{M} n_m(t)\psi_m(\vec{r}), \tag{3}$$

where $\psi_m(\vec{r})$ is an orthonormal basis, known as POD (spatial) modes, and $n_m(t)$ are their time coefficients.

The expression (3) is substituted into equations (2) and then, the resulting system is multiplied by ψ_l^{T} with $l = 1, \ldots, M$, to obtain the reduced order problem of $M(K+1)$ equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{N} = \mathbf{T}\mathbf{N}, \tag{4}$$

where

$$\mathbf{N} = \begin{pmatrix} n_1 \cdots n_M & c_{11} \cdots c_{M1} & \cdots & c_{1K} \cdots c_{MK} \end{pmatrix}^{\mathsf{T}}, \tag{5}$$

$$\mathbf{T} = \left(\begin{array}{c|ccc} \bar{V}^{-1}(\bar{F} - \bar{L}) & \bar{V}^{-1}\lambda_1^d & \cdots & \bar{V}^{-1}\lambda_K^d \\ \hline \beta_1\bar{F} & -\lambda_1^d I_M & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \beta_K\bar{F} & 0 & \cdots & -\lambda_K^d I_M \end{array}\right), \tag{6}$$

and the elements of the small matrices $\bar{V}$, $\bar{F}$, $\bar{L}$ and the unknowns c_{lk} are given by

$$\begin{aligned} \bar{V}_{lm} &= \langle \psi_l^{\mathsf{T}}, V^{-1}\psi_m \rangle, & \bar{L}_{lm} &= \langle \psi_l^{\mathsf{T}}, L\psi_m \rangle, \\ \bar{F}_{lm} &= \langle \psi_l^{\mathsf{T}}, F\psi_m \rangle, & c_{lk} &= \langle \psi_l^{\mathsf{T}}, XC_k \rangle. \end{aligned} \tag{7}$$

The initial conditions of the reduced problem are set by imposing the initial condition $\Phi(\vec{r}, 0) = \Phi_0$, which implies

$$\begin{aligned} n_m^{\delta}(0) &= \langle \psi_m^{\mathsf{T}}, \Phi_0 \rangle, & m &= 1, \ldots, M \\ c_{mk}^{\delta}(0) &= \frac{\beta_k}{\lambda_k^d} \langle \psi_m^{\mathsf{T}}, F\Phi_0 \rangle, & m &= 1, \ldots, M, \quad k = 1, \ldots, K, \end{aligned}$$

where Φ_0 is the solution of the problem at steady-state.

The neutron flux in a reactor core can suffer strong spatial variations along the transient, which implies the necessity of using a high number of vectors in the decomposition (3) to represent accurately this behaviour, and consequently to solve a large reduced order problem. To avoid an expensive computational cost in the calculation, this work proposes to change the basis during the transient, and for this purpose, the reduced problem must be updated accordingly.

In this restarted POD (RPOD), the time domain is divided into several intervals $[t_i, t_i + \Delta t_i] = [t_i, t_{i+1}]$. In each interval $[t_i, t_{i+1}]$, the neutron diffusion equation can be integrated by using the expansion of the neutron flux Φ in terms on the orthonormal basis ψ^i as

$$\Phi(\vec{r}, t) = \sum_{m=1}^{M_i} n_m^i(t)\psi_m^i(\vec{r}), \tag{8}$$

and, then by solving the reduced order problem

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{N}^i = \mathbf{T}^i\mathbf{N}^i, \tag{9}$$

where

$$\mathbf{N}^i = \begin{pmatrix} n_1^i \cdots n_{M_i}^i & c_{11}^i \cdots c_{M_i 1}^i & \cdots & c_{1K}^i \cdots c_{M_i K}^i \end{pmatrix}^{\mathsf{T}}, \tag{10}$$

$$\mathbf{T}^i = \left(\begin{array}{c|ccc} \bar{V}^{-1}(\bar{F} - \bar{L}) & \bar{V}^{-1}\lambda_1^d & \cdots & \bar{V}^{-1}\lambda_K^d \\ \hline \beta_1\bar{F} & -\lambda_1^d I_{M_i} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \beta_K\bar{F} & 0 & \cdots & -\lambda_K^d I_{M_i} \end{array}\right), \tag{11}$$

and

$$\begin{aligned} \bar{V}^i_{lm} &= \langle \psi^{i,\mathsf{T}}_l, V^{-1}\psi^i_m \rangle, & \bar{L}^i_{lm} &= \langle \psi^{i,\mathsf{T}}_l, L\psi^i_m \rangle, \\ \bar{F}^i_{lm} &= \langle \psi^{i,\mathsf{T}}_l, F\psi^i_m \rangle, & c^i_{lk} &= \langle \psi^{i,\mathsf{T}}_l, XC_k \rangle. \end{aligned} \tag{12}$$

Observe that this system has the same structure as the POD without updating. Nevertheless, the initial conditions (at time t_i) must be reformulated to ensure the continuity of the solution. These initial conditions will depend on the solution in the previous interval $[t_{i-1}, t_i]$ and the basis used in the previous time-step (ψ^{i-1}_m). From the solution obtained in the interval $[t_i, t_{i+1}]$, the solution in the interval $[t_{i+1}, t_{i+2}]$ is calculated, etc.

The initial conditions for n^i_m at time t_i must be defined to solve the problem (11) in the interval $[t_i, t_{i+1}]$. For that purpose, we reconstruct the vector

$$\Phi(t_i) = \sum_{m=1}^{M_{i-1}} n^{i-1}_m(t_i)\psi^{i-1}_m, \tag{13}$$

from the variables $n^{i-1}_m(t_i)$, ψ^{i-1}_m obtaining from the integrating in the interval $[t_{i-1}, t_i]$. As the function $\Phi(t)$ must be continuous on all its domain, one could use the expansion

$$\Phi(t_i) = \sum_{m=1}^{M_i} n^i_m(t_i)\psi^i_m,$$

and obtain the value of $n^i_m(t_i)$, $m = 1, \ldots, M_i$ as

$$n^i_m(t_i) = \langle \psi^{i,\mathsf{T}}_m, \Phi(t_i) \rangle,$$

where $\Phi(t_i)$ is computed from Equation (13).

In order to compute the initial conditions related to the concentration of the precursor k at time t_i, $c^i_{lk}(t_i) = \langle \psi^{i,\mathsf{T}}_l, XC_k \rangle(t_i)$, we use the known $c^{i-1}_{mk}(t_i)$ computed in the previous integration on $[t_{i-1}, t_i]$. We assume that

$$\psi^{i,\mathsf{T}}_l = \sum_{m=1}^{M_{i-1}} a_{lm}\psi^{\mathsf{T},i-1}_m.$$

One could collapse the previous Equation by the left along the direction of ψ^{i-1}_m to obtain that

$$a_{lm} = \langle \psi^{i,\mathsf{T}}_l, \psi^{i-1}_m \rangle. \tag{14}$$

Thus, the concentration of precursors at time t_i, c^i_{lk}, $m = 1, \ldots, M_i$ can be computed as

$$c^i_{lk}(t_i) = \langle \psi^{i,\mathsf{T}}_l, XC_k \rangle(t_i) = \sum_{m=1}^{M_{i-1}} a_{lm}\langle \psi^{\mathsf{T},i-1}_m, XC_k \rangle(t_i) = \sum_{m=1}^{M_{i-1}} a_{lm}c^{i-1}_{mk}(t_i). \tag{15}$$

3.1 Selection of the POD modes

Let $\mathcal{P} = \{\mu_1, \ldots, \mu_{n_s}\}$ be a set of parameter samples where we run full order model simulations. Let $\mathcal{T} = \{t_0, \ldots, t_{N_t}\}$ a set of different time values. Let $U_p = [u^{(0)}(\mu_p), \ldots, u^{(N_t)}(\mu_p)]$, $p = 1, \ldots, n_s$, be a full order model state solution matrix for a sample parameter value μ_p. Then a snapshot matrix, U is defined by concatenating all state solution matrices, i.e.,

$$U \equiv [U_1 \cdots U_{ns}].$$

The POD modes can be obtained by setting $\psi_m = W_m$, where W_m is the mth left singular vector that is obtained by solving the Singular Value Decomposition (SVD)

$$U = W\Sigma V^{\mathsf{T}}.$$

In nuclear engineering, it is usual to study the behaviour of transients defined by the movement of control rods, whose displacement produces an increasing or decreasing of the neutronic power. In this work, each type of bank of rods will be a parameter sample in this problem.

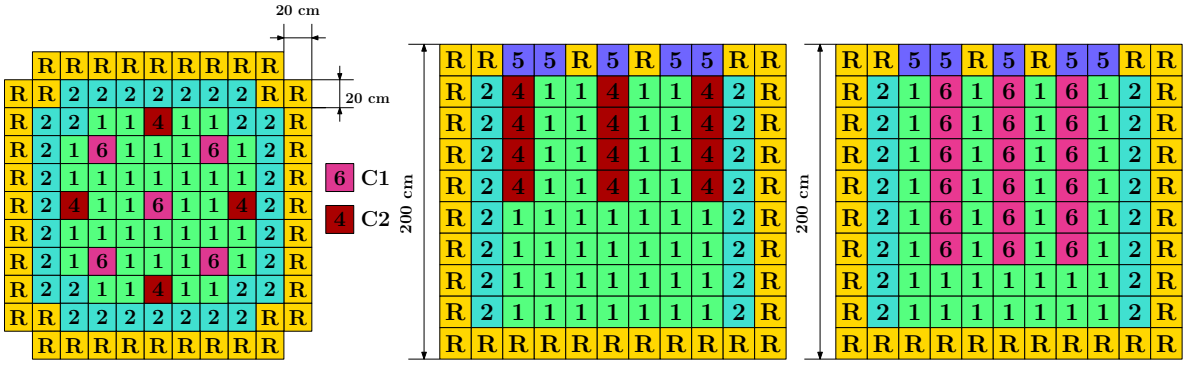
Given a configuration of the reactor, a time-independent eigenvalue problem can be defined by dividing the fission operator $\mathcal{F}$ by a positive number λ transforming the Equation (1) into the λ-modes problem

$$\mathcal{L}\varphi = \frac{1}{\lambda}\mathcal{F}\varphi. \tag{16}$$

The eigenvectors associated with the dominant eigenvalue of this steady-state problem for the different configurations, corresponding to different positions of the control rods of reactor, will define the snapshot matrix.

4 Numerical results

The tridimensional Langenbuch reactor [8] is selected to test the methodology proposed. Figure 1 shows the geometry of the reactor model. The full description of the reactor can be found in [8]. The calculations for the reactor have been performed with a whole core model, using 1170 cells and using finite elements of degree 3. The problem corresponds to an operational transient of the Langenbuch reactor. Materials 4 and 6 represent control rods. It has been initiated by the withdrawal of a bank of four partially inserted control rods (C1 in Figure 1.1(a)) at a rate of 3 cm/s over $0 < t < 26.7$ s. A second bank of control rods (C2 in Figure 1.1(a)) is inserted at the same rate over $7.5 < t < 47.5$ s. The transient is followed during 60 s. As reference, we have computed the solution of the FOM by using a semi-implicit backward method [9].



(a) Radial view (b) Axial profile at $t = 0.0$ (c) Axial profile at $t = 60.0$

Figure 1: Geometry of the Langenbuch reactor.

First, we test the POD without restarting. As the transient is defined by two types of control rods movement, two set of snapshots are obtained by considering equally spaced axial positions of each type of rod bank, from the bottom to the top. The number of positions considered is equal to the number of snapshots. The snapshots are the solutions of steady-state problems associated to each configuration, i.e. position of the bar. Figure 2 shows the neutron power evolution of the reference solution (FOM) with the solution obtained with the POD for a different set of snapshots. This Figure shows the convergence of the POD as the number of snapshots is increased. Moreover,

this graphic shows that the neutron power results of the POD with 5 snapshots (POD-5) are very close to the FOM solution.

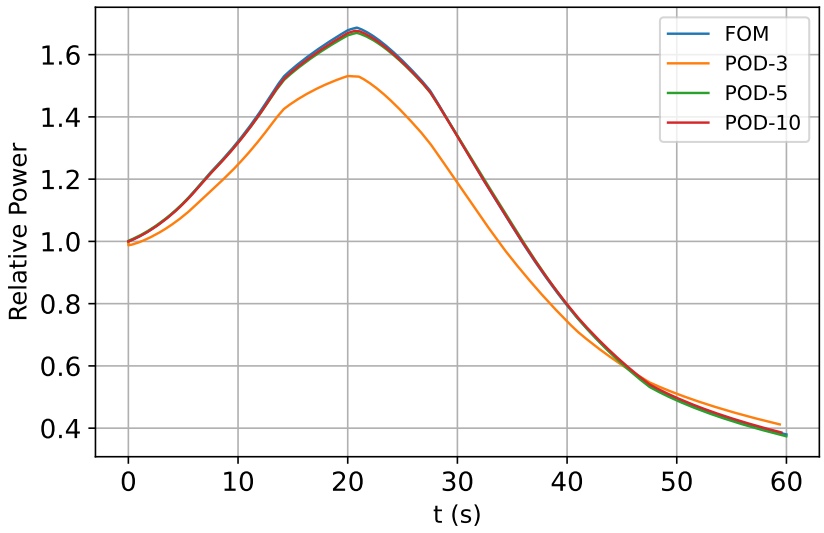


Figure 2: Power evolution of the Langenbuch reactor with the FOM and POD with 3, 5, and 10 snapshots.

Next, we test the restart POD by using three sets of snapshots. In the first 7.5 s, the POD modes are obtained from the snapshots U_1. Then, from 7.5 s to 26.7 s, we use the set of snapshots $U = [U_1, U_2]$, and finally, from 26.7 s to the end of the transient, we use U_2 to extract the POD modes. Figure 3 shows the power evolution of the reference solution of FOM, the solution of POD without restarting and 5 snapshots, and the solution with the restarted POD with 5 snapshots (RPOD-5). This graphic does not show significant differences between the approximations.

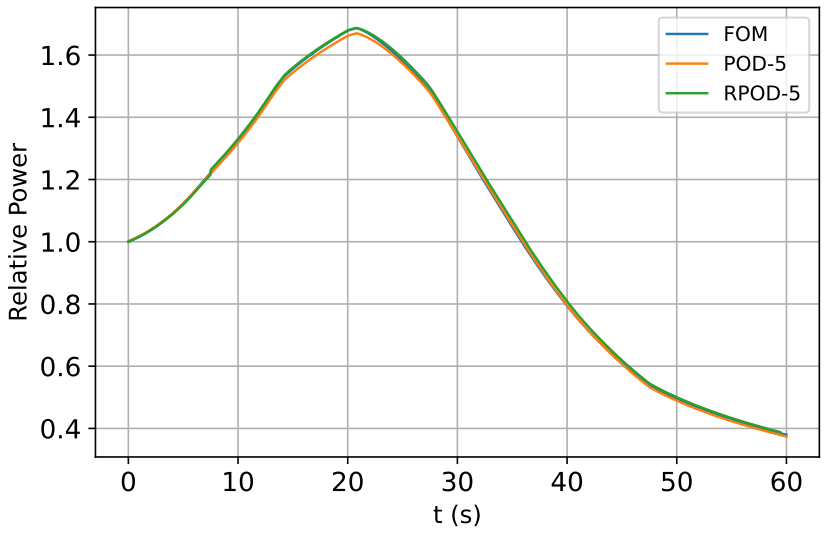


Figure 3: Power evolution of the Langenbuch reactor with the FOM and POD with 5 snapshots, and RPOD with 5 snapshots and restarting.

Finally, Table 1 displays the power errors and CPU time for the different methodologies used in this work. The neutron power error ($\bar{\varepsilon}$) is obtained by computing the mean value between the difference of the power obtained with FOM and the rest of the methods over time.

$$\bar{\varepsilon} = \frac{1}{N_i} \sum_i |P_i - P_{FOM}| \tag{17}$$

The CPU Time of POD also includes the process to obtain the snapshots. As previous graphics show POD with 5 snapshots (POD-5) gives precise results, reducing the CPU time of FOM almost three times. Moreover, this Table shows similar approximations between the POD with and without restart, but in the case where the basis are updated the results are computed faster.

Table 1: Errors and CPU Time (s) obtained for the ROM-3, ROM-5, ROM-10 and RROM-10 against the FOM.

Method	Error ($\bar{\varepsilon}$)	CPU Time
POD-3	0.0648	277 s
POD-5	0.0061	774 s
POD-10	0.0040	2938 s
RPOD-5	0.0097	514 s
FOM		1839 s

5 Conclusions

This work proposes a new approach to integrate the neutron diffusion equation. The methodology is based on the classical POD method and consists of updating the basis of snapshots along the transient to avoid a reduced basis too big. This ensures that the reduced model accurately represents the evolution of the neutron flux within a reactor core. A transient defined by the movement of control rods in a three-dimensional reactor is used to test this approach.

The numerical results show that the ROM-POD method is three times more efficient than applying a time scheme directly to the full model with an error smaller than 1 % of the nominal power. Additionally, restarting the POD method allows the solution to be approximated in a faster way than without restarting.

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