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ANS M&C 2021 - The International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering · Raleigh, North Carolina · October 3–7, 2021

A NON-INTRUSIVE REDUCED ORDER MODEL FOR NEUTRONIC TRANSIENT ANALYSES OF THE ALFRED REACTOR

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ABSTRACT

The safety analysis of Gen-IV lead-cooled fast reactors requires accurate evaluations for different operational and accidental conditions. The FRENETIC code, constituted by a full-core, multi-group nodal diffusion module coupled with a thermal-hydraulics one, allows to perform accurate transient calculations, but it is not suitable for the detailed parametric evaluations required by a thorough safety assessment. To fill this gap in the code performances, a non-intrusive reduced-order model reproducing an accurate approximation of the FRENETIC output with a reduced computational effort is proposed. The results obtained for a stand-alone neutronic transient involving the accidental insertion of a control rod show how the approach adopted is promising for computationally-efficient safety assessments.

KEYWORDS: full-core simulation, lead cooled fast reactors, accidental transient analysis, improved quasi-static, FRENETIC, non-intrusive reduced-order modeling, RBF, POD

1. INTRODUCTION

The development of the Gen-IV reactor designs has introduced the need for more sophisticated reactor physics computational techniques for design and licensing purposes. As a matter of fact, the complexity of such systems requires careful evaluations of the operating and accidental conditions, with particular emphasis on the coupling between neutronics (NE) and thermal-hydraulics (TH) and on the presence of several time, energy and spatial scales. The computational issues related to the presence od such different scales have been traditionally tackled using approximated, reduced-order models. In neutronics, for example, the traditional approach for dealing with the spatial and energy scales consists in solving the steady-state neutron transport equation over a fine-group energy grid at the pin lattice level, in order to estimate the multi-group, spatially homogenized constants, which are then employed as input data for multi-group nodal diffusion models applied to the full-core [1].

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As regards the time scale, one of the standard methods is the quasi-static approach [2], which assumes that the neutron flux can be factorised into two functions: the flux amplitude, dependent on time and related to the neutron population size, and the flux shape, mosty accounting for the phase space evolution on a longer time scale. This method takes advantage of the fact that the shape, which is governed by a computationally expensive model (i.e., a partial differential equation in the phase space), evolves on a time scale slower than the amplitude, which instead is described by a set of coupled ordinary differential equations in time, much cheaper to solve.

In principle, similar computational strategies can be devised also for the thermal-hydraulics equations, but the time scales of such phenomena are much slower than the neutron lifetime scale. This aspect is fundamental in a multi-physics simulation framework, like the one implemented in the FRENETIC (Fast REactor NEutronics/Thermal-hydraulICs) code, developed at Politecnico di Torino in the last decade [3–5]. In this code, designed for the operational and accidental full-core transient analysis of lead-cooled fast reactors, there is a continuous information exchange in time between the two physical modules. In a transient, the slowest time scale is the dominant one, thus coupled simulations are usually much heavier than stand-alone neutronics transients, which are anyway quite computationally demanding.

In spite of its state-of-the-art algorithms and of potential NE/TH coupling improvements, the use of FRENETIC for thorough parametric transient analyses like the ones required, for example, in the licensing phase, would be too computationally demanding. A promising strategy to reduce the computational cost is represented by Parametrised Non-Intrusive Reduced Order Models (P-NIROM) [6]. This approach allows to build a meta-model that reproduces the full-order model (i.e. the FRENETIC output, in this case) interpolating a set of training solutions,also called *snapshots*, previously computed. The off-line calculations are usually computationally demanding, as they require to compute the solution snapshots for an exhaustive set of parameters, but they are performed only once, to train the model. When the model approximation error becomes acceptable, the P-NIROM can be used for estimating the code outcome even over untrained points, with a reduced computational cost and without any modification of already validated codes. In this work, the P-NIROM is applied to a purely neutronic transient in FRENETIC, to test the feasibility of this approach for the time-dependent analysis of lead fast reactors.

2. ALFRED REACTOR TEST CASE

In order to assess the Reduced-Order Model (ROM) performances in reducing the computational burden associated to the simulations of accidental transients with FRENETIC, a 3D full-core model of the ALFRED (A Lead Fast Reactor European Demonstrator) core design [7] is considered as a case of study. The multi-group constants employed in FRENETIC are spatially homogenised to represent the regions sketched in Figure 1 and are collapsed over the six-group energy grid presented in Table 1 using the Serpent 2 Monte Carlo code [8].

The transient considered in this paper is the accidental insertion of a control rod (CR), starting from a close-to-critical reactor initial configuration, obtained with an insertion of the control rods to 45 cm with respect to the active zone bottom plane. The initial k_{eff} computed by FRENETIC, 1.00045, is in very good agreement with the one computed by Serpent 2, 1.00008(24). The CR (indicated in Figure 1 with the X symbol) accidental insertion is assumed to reach the height of 57 cm and 67 cm in two different time instants, called t_1 and t_2, which are assumed to be the free

Table 1: Six-group energy grid adopted to perform the macroscopic cross sections energy collapsing [5].

Energy [MeV]	$2.000 \cdot 10^{1}$	$1.353 \cdot 10^{0}$	$1.832 \cdot 10^{-1}$	$6.738 \cdot 10^{-2}$	$9.119 \cdot 10^{-3}$	$2.000 \cdot 10^{-5}$	$1.000 \cdot 10^{-11}$

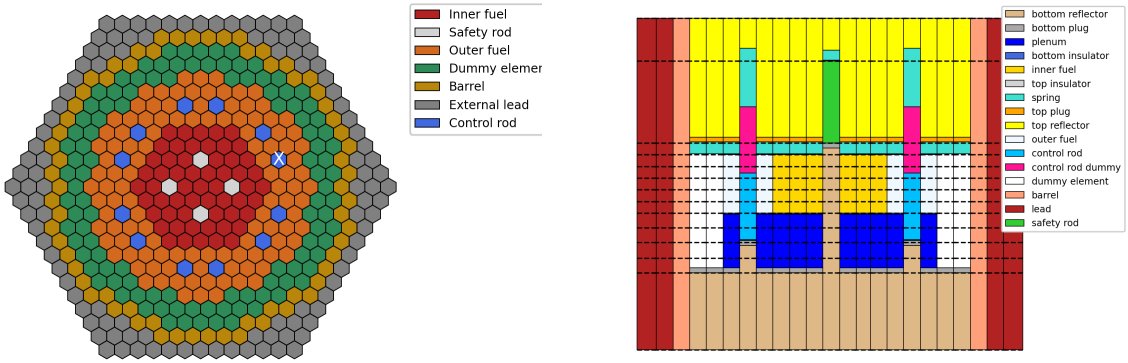

Figure 1: Radial section (left) and axial regions (right) of ALFRED 3D model employed in the study. The X symbol identifies the control rod inserted during the transient.

parameters of the transient for the identification of the training set. The control rod insertion speed is constant in each time step.

3. NON-INTRUSIVE PARAMETRIC REDUCED ORDER MODELING

In this section, the main steps required for the construction of the meta-model are described. Due to its non-intrusive nature, the P-NIROM only requires to gather a set of high-fidelity simulations, suitably chosen to cover the input parameter space, and then to construct a set of hyper-surfaces to reproduce the full-order model solutions [6].

3.1. Parameter space sampling

In order to efficiently draw the points needed for the training simulations from a p-dimensional parameter space $\mathbb{R}^p$ (here $p = 2$, i.e. the two time intervals for the CR insertion), it is a common practice to employ sparse grids. Here, a grid based on the Chebyshev polynomials extrema is built using Smolyak's algorithm [9]. This technique, originally conceived for interpolating high-dimensional functions with a few points on hypercubes, allows to select the most important points from the tensor products of unidimensional grids. Since the Chebyshev polynomials extrema are nested sets, one can choose an arbitrarily low grid approximation level $\vec{p}$ for the parameter space and then increase *a posteriori* the number of training points, automatically including the already existing simulations. Figure 2 shows the two-dimensional sparse grid constructed for the training phase up to the $4-$th approximation level. It is assumed that both the time intervals, defined as $\Delta t_1 = t_1 - 0$ and $\Delta t_2 = t_2 - t_1$, range from 0.5 to 10 s.

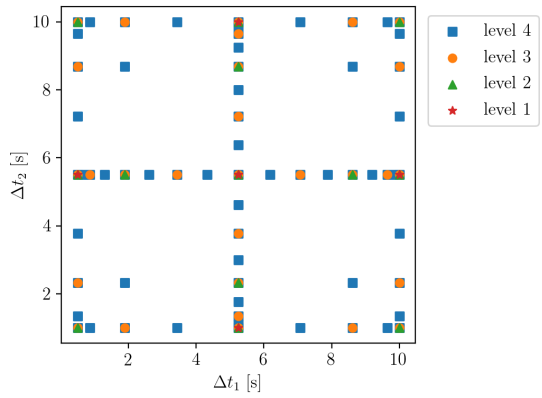

Figure 2: Smolyak sparse grid built to train the ROM. As can be seen, the points of level $n+1$ include the points of level n.

3.2. High fidelity simulations

After the selection of the training points, the high-fidelity simulations are carried out with FRENETIC. Since the aim of the paper is testing the ROM performances, only standalone neutronic calculations are performed. The neutronic module currently available in FRENETIC implements a coarse mesh nodal diffusion model, which is solved at the assembly level for each axial discretisation node. The black dashed lines visible in Figure 1 (right) define the core regions where the multi-group constants are axially homogenised. Each training transient simulation, solved up to 35 s using the Improved Quasi-Static (IQS) method, requires about three hours on a commercial laptop.

3.3. Model reduction and training

Once the computationally intensive phase is concluded, a set of time snapshots is obtained per each parameter training point. For the sake of conciseness, in this work only the thermal power density produced by fission $\dot{Q}(x, y, z, t)$ is considered among the different output quantities evaluated by FRENETIC. The purpose of such choice is two-fold. Firstly, it is of paramount importance for safety evaluations. Secondly, it allows to easily evaluate the total power $\dot{Q}_T(t)$, which can be used to assess the impact of the ROM approximation errors on a macroscopic integral parameter.

The first step needed for the P-NIROM construction is reducing the data dimensionality via the Proper Orthogonal Decomposition (POD) [10]. Given a set of discrete time snapshots $\dot{Q}(x, y, z, t_i)$ $(i = 1, \ldots, N_t)$ for each training point $\vec{p}_j$ $(j = 1, \ldots, P)$, POD can provide, via the Singular Value Decomposition (SVD), a set of K basis functions ψ that best approximate, in a L_2-norm sense, the original solution:

$$\dot{Q}(x, y, z, \vec{p}_j, t) \approx \sum_{k=1}^{K} a_k(\vec{p}_j, t)\psi_k(x, y, z, \vec{p}_j)_i \quad j = 0, ..., P, \tag{1}$$

where $a_k(\vec{p}_j, t)$ is the set of time-dependent coefficients associated to the j-th training parameter

point. These coefficients represent the solution dynamics in a reduced-order space. The advantage of this approach is that, usually, a limited number of POD modes is needed to get a sufficiently accurate representation of the original snapshots [10].

The second step required for constructing the P-NIROM is the definition of a set of interpolant, which are needed to approximate the solutions over new, untrained parameters. This task is accomplished using the full-order model snapshots to train a set of Radial Basis Functions (RBF), i.e. functions whose value depends on the L_2 distance between their centers and the new parameter point $\vec{p}_n$. Since both the POD coefficients $a_k(\vec{p}_j, t)$ and basis $\psi_k(x, y, z, \vec{p}_j)$ depend on the parameters, a two-level RBF interpolation is needed to retrieve the set $\{a_k, \psi_k\}$, $k = 1, \ldots, K$ for the new parameter $\vec{p}_n$:

$$a_k(\vec{p}_n, t) = \sum_{j=1}^{P} f_a(||\vec{p}_j - \vec{p}_n||, \sigma_a)\vec{w}_{a,j,k}, \tag{2}$$

$$\psi_k(x, y, z, \vec{p}_n) = \sum_{j=1}^{P} f_\psi(||\vec{p}_i - \vec{p}_n||, \sigma_\psi)\vec{w}_{\psi,j,k}. \tag{3}$$

The RBF weighting coefficients $\vec{w}_{a,j,k}$ and $\vec{w}_{\psi,j,k}$ can be determined forcing the RBF interpolants to be centred on the training parameters, i.e. to be able to reproduce the coefficients and basis functions at the training points. In this paper, the RBF are taken as Hardy inverse multiquadric functions, i.e. $\sqrt{(\sigma^2 + ||\vec{p}_i - \vec{p}_n||)}^{-1}$, where σ is the RBF shape factor, a tuning parameter that can be found optimising the RBF interpolation capability.

Once the training phase is completed, the ROM approximation to the full-order solution on $\vec{p}_n$ can be expressed as:

$$\dot{Q}(x, y, z, \vec{p}_n, t) \approx \sum_{k=1}^{K} \left(\sum_{j=1}^{P} f_a(||\vec{p}_i - \vec{p}_n||, \sigma_a)\vec{w}_{aj,k} \right) \left(\sum_{j=1}^{P} f_\psi(||\vec{p}_i - \vec{p}_n||, \sigma_\psi)\vec{w}_{\psi\,j,k} \right). \tag{4}$$

As it can be noticed from eq. 4, this model only needs the FRENETIC varying input parameters and its output solutions.

4. RESULTS

The POD/RBF parametrised non-intrusive ROM is trained using the first four levels of the Smolyak sparse grid in Figure 2, for a total of 65 points. In order to tune and validate the ROM, an additional set of independent 100 simulations is carried out. Among these, 80 are taken from the points of the $5-$th level of the Smolyak grid, excluding the ones already used for the training, while 20 are sampled randomly, extracting 5 points per each quadrant. Each simulation is composed of 71 time snapshots, which span uniformly the interval $t \in [0, 35]$ s. The snapshots are scored over the 171 fuel assemblies on 10 axial nodes uniformly distributed along the active height. A number of 30 out of 71 POD pairs $\{a_k, \psi_k\}$ is considered for the dimensionality reduction, allowing to spare computational time for the evaluation of the P-NIROM in eq. (4). With these settings, the ROM requires a few seconds to provide the approximation to the FRENETIC solution on new parameter points.

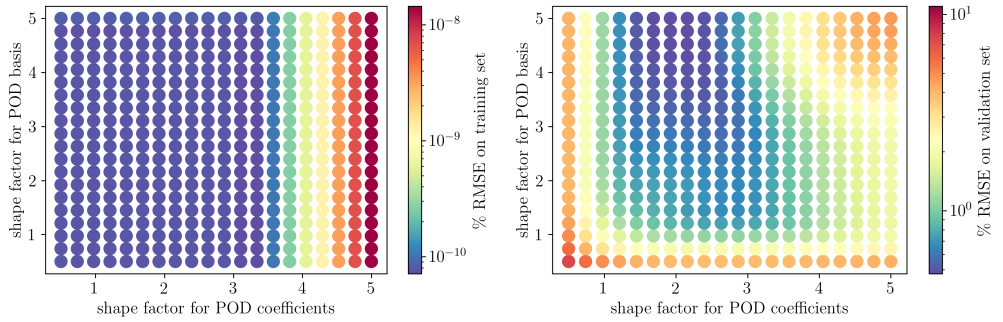

Figure 3: Root Mean Square Error for the training (left) and validation (right) simulations as a function of different shape factors σ.

The validation set allows to tune the shape parameters of the two RBF nets in order to maximise their interpolation capability. Due to the so-called "RBF uncertainty principle" [11], the choice of this parameter has to be a trade-off between the net interpolation capability and the RBF system numerical stability. Increasing σ usually enhances the interpolation capability of the net, but also worsen the condition number of the RBFs, leading to larger approximation errors for the training points, as visible in Figure 3 (left). In this paper, the optimal values of the shape factors for the POD coefficients and basis is chosen to minimise the Root Mean Square Error (RMSE) between ROM and FRENETIC for the validation points, represented on the right of Figure 3. By inspection, it is possible to see that the optimal set of shape factors lays around the point (σ_a, σ_ψ)=(1.9, 5). Figure

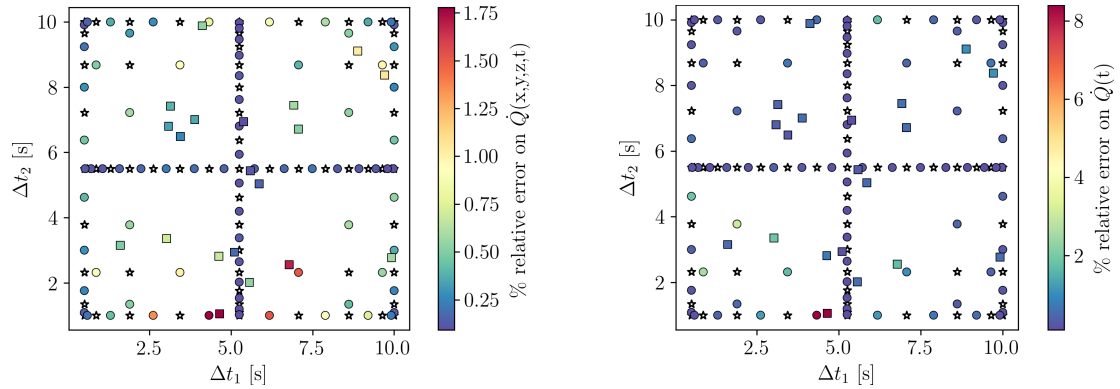

Figure 4: % relative error between FRENETIC and P-NIROM for all the points belonging to the validation set. Black stars: training points; dots: validation subset drawn from the Smolyak algorithm; squares: points sampled randomly in each quadrant.

4 displays the L_2-norm error between the power density and the total power between FRENETIC and the ROM for the whole transient time interval.

In spite of the limited number of training samples (65), the agreement between the ROM and FRENETIC is very good, almost always below 1% for the power density field. This accuracy is

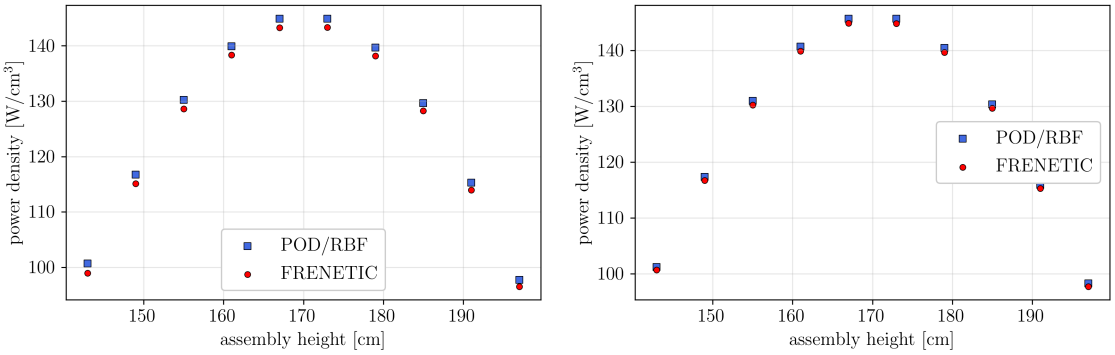

Figure 5: Power density axial profile in the central SA at time instant with the largest error (t=3 s) for the cases with (Δt_1, Δt_2)=(3.13 s, 7.42 s) (left) and (Δt_1, Δt_2)=(3.02 s, 3.35 s) (right).

acceptable for fast, parametric transient analyses needed for the safety evaluations, and it could be further reduced if more simulations were added to the training set. The agreement is remarkable also when the total power is considered, with the exception of the two points featured by the largest error on the power density (around Δt_1 = 4.8 s and Δt_2=0.5 s). In these cases, the errors on the total power is around 9%. Most of the points have an error lower than 4%, hence the P-NIROM seems able to reproduce also a global parameter like the total power with an acceptable accuracy, in spite of the errors on the local power density distribution.

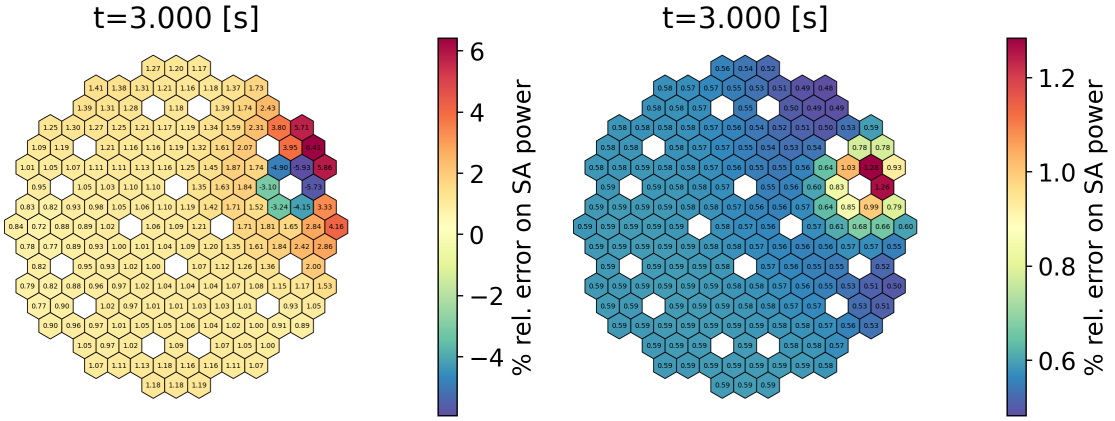

Figure 6: Relative $\%$ error on the SAs power at time instant with the largest error (t=3 s) for the cases with (Δt_1, Δt_2)=(3.13 s, 7.42 s) (left) and (Δt_1, Δt_2)=(3.02 s, 3.35 s) (right).

Figures 5 to 7 show, with a decreasing spatial detail, the agreement between the P-NIROM approach and FRENETIC for two cases belonging to the random validation points, i.e. (Δt_1, Δt_2) =(3.13 s, 7.42 s) and (Δt_1, Δt_2)=(3.02 s, 3.35 s). Figure 5 displays the power density axial profile in the hottest SA, i.e. the central one, which plays a fundamental role in the safety evaluations.

In spite of the low training point density around these two untrained points, the ROM is able to mimic the full-order model with a good accuracy. Figure 6 represents the radial distribution of the relative error on the total power per SA at the time featured by the largest discrepancy. It is interesting to notice that the error has an almost uniform behaviour, with the exception of the assemblies surrounding the CR that is inserted during the accidental transient. Finally, Figure 7 shows the comparison between the total power evolution during the whole transient computed by the ROM and FRENETIC, respectively.

The overall results presented and discussed in this section show that the P-NIROM based on the POD and RBF techniques is suitable for the typical parametric simulations required for the design safety assessment, providing an accurate yet very fast tool.

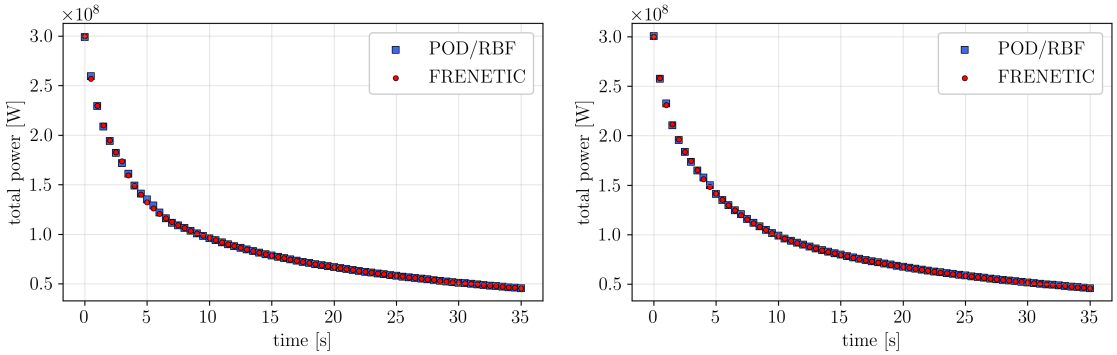

Figure 7: Total power evolution for the cases with (Δt_1, Δt_2)=(3.13 s, 7.42 s) (left) and (Δt_1, Δt_2)=(3.02 s, 3.35 s) (right).

5. CONCLUSIONS AND FUTURE PERSPECTIVES

In this paper, a Parametrised Non-Intrusive Reduced Order Model based on POD and on a two RBF interpolation levels has been applied in order to reduce the computational burden associated to the full-core nodal diffusion code FRENETIC. In order to test the P-NIROM performances, the accidental insertion of a control rod in a close-to-critical initial configuration of the ALFRED core design has been considered as a test problem. Due to the full-core nature of the transient, the Improved Quasi-Static method is used to generate the high-fidelity solution snapshots, needed to train the ROM. The two time steps needed for the full control rod insertion are considered to be the free parameters in the system, while the power density, for safety analysis purposes, is taken as the output quantity of interest.

In spite of the relatively low number of samples, the ROM shows a good accuracy (below 2 %) with respect to the full-order model for the validation points considered, on both the local and global spatial scales and for the whole transient duration. From the computational burden point of view, excluding the off-line training phase, which is though very limited, due to the fairly low number of training points, the ROM outperforms FRENETIC, providing the full-core power density time snapshots in less than a dozen of seconds, with respect to the 3 hours required by the code.

As a future development, efforts will be devoted to improve the training parameters sampling, trying to reduce the number of samples needed to match the target accuracy. Since the Smolyak grid based on the Chebyshev polynomials used in the paper is more dense at the corners, the sampling performances could be improved a lot considering alternative point distributions, like the evenly-space Clenshaw-Curtis points. Moreover, in order to completely characterise the ROM performances, a transient featured by a larger parameter spaces will be considered, e.g. more than one control rod moving and variable insertion heights. Finally, the ROM will be improved to fully exploit the time adaptivity feature of the IQS algorithm, thus considering only the snapshots that are more significant for the reactor dynamics, in contrast to the uniform time binning employed in this work.

ACKNOWLEDGEMENTS

Computational resources were provided by HPC@POLITO, a project of Academic Computing within the Department of Control and Computer Engineering at the Politecnico di Torino. The Authors wish to thank the colleague G.F. Nallo for his guidance into the FRENETIC code.

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