

6th European Conference on Computational Mechanics (ECCM 6)
7th European Conference on Computational Fluid Dynamics (ECFD 7)
1115 June 2018, Glasgow, UK

REDUCED ORDER MODELLING USING A POD-BASED IDENTIFICATION METHOD FOR PARAMETRIZED PDES

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Key words: CFD, least-squares method, proper orthogonal decomposition, identification, reduced-order models

Abstract. To reduce the computational cost of high-fidelity simulations, model reduction techniques have been developed to approximate parametrized Partial Differential Equations (PDEs) for Computational Fluid Dynamics (CFD) problems. Typically, a Galerkin projection is performed to obtain a reduced order model (ROM). In that case, the governing equations are projected onto the reduced basis space generated by applying a Proper Orthogonal Decomposition (POD) approach on snapshots of the full order simulation. The main issue of this method is its intrusiveness: the construction of the reduced matrices requires access to the full order matrices and thus knowledge of the solvers discretization and solution algorithm. Therefore, a non-intrusive reduced-order method for parametric CFD problems is proposed in this work, which is applicable regardless of the solver. This POD-based identification (PODI) method identifies reduced matrices of the same form as in the POD-Galerkin method using the least-squares technique. This identification uses the set of known time-dependent coefficients obtained by projecting all snapshots on the POD basis in the offline phase. Parameterization of the reduced system requires full order simulations for different parameter values. The resulting reduced system of equations is then solved online for a given set of parameters. The offline-online decomposition of the POD-Galerkin method is thus maintained. To demonstrate the proposed method, numerical results are presented for the convection-diffusion equation, using the finite volume method. The results are compared with the POD-Galerkin method and the benefits and limitations of the presented method are discussed. As the reduced basis is the same for the PODI method and the POD-Galerkin method, also the reduced matrices obtained through respectively identification and projection can be compared.

1 INTRODUCTION

Computational Fluid Dynamics (CFD) simulations are widely used in industry to solve fluid problems. Commercial and open-source codes such as ANSYS Fluent and OpenFOAM, respectively, use the Finite Volume Method (FVM) for the spatial discretization of the governing equations that describe the physical model [1, 2]. These high-fidelity simulations can contain millions of degrees of freedom and are therefore computationally expensive. Model reduction techniques have been developed to approximate the (parametrized) Partial Differential Equations (PDEs) to reduce the CPU time and computer memory usage.

Different types of reduction techniques for fluid problems can be found in literature. A family of techniques are those based on a reduced basis where a low dimensional subspace, containing the essential dynamics of the full order system, is constructed. The Proper Orthogonal Decomposition (POD) is the most often used method in fluid dynamics literature as it can be applied to nonlinear models [3]. The full order model (FOM) is sampled at several points in time to construct the so-called snapshot matrix. Next a reduced basis space is created through a Singular Value Decomposition (SVD). For unsteady problems POD is typically combined with the Galerkin projection to obtain a reduced order model where the full order matrices are projected onto the low-dimensional subspace of POD modes and the difference with the snapshots are minimized [4]. The main issue of this method is its intrusiveness because the construction of the reduced matrices requires access to the full order matrices and thus knowledge of the solvers discretization. For that reason projection-based methods cannot be used for commercial solvers as ANSYS Fluent.

To avoid this intrusiveness, data-driven reduction techniques could be used instead, such as System Identification (SI) where a low-dimensional system is identified to describe the dynamics of a high-dimensional system. This is a black-box approach where the problem is treated as a system that processes a set of inputs and yields a set of outputs. The input/output data is then used to determine a set of low-order ordinary differential equations (ODEs) that approximately describe the input/output relationship of the FOM [5]. A disadvantage of this method is that the obtained system does not have a physical meaning and consistency issues can occur for parameterized problems [6]. Therefore a non-intrusive reduced-order method for parametric CFD problems is proposed in this work, which is applicable regardless of the solver. This POD-based identification (PODI) method identifies reduced matrices of the same form as in the POD-Galerkin method using the least-squares technique. This identification method uses the set of known time-dependent coefficients obtained by projecting all snapshots on the POD basis in the offline phase.

2 The Full Order Model

The linear unsteady convection-diffusion equations are used to demonstrate the proposed PODI method. For heat transfer, the general equations are given in a domain Ω

by

$$\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{u}T) = \nabla \cdot (\alpha \nabla T) + \frac{\dot{q}_v}{\rho c_p} \quad (1)$$

where T is the temperature, α is the thermal diffusivity, ρ is the mass density of the fluid, c_p is the specific heat capacity, \mathbf{u} is the flow velocity vector, \dot{q}_v is the volumetric heat source term and t is the time. For simplicity the diffusion coefficient, α , is constant in time and space and no heat sources or sinks are present. The given velocity field, \mathbf{u} , should satisfy the continuity equation (incompressible flow) $\nabla \cdot \mathbf{u} = 0$. Proper boundary and initial conditions are applied.

Discretizing in space using the FVM, rearranging in matrix form and parameterizing the problem leads to the following system of equations where the diffusivity coefficient, α , and the magnitude of the velocity field, $\|\mathbf{u}\|$, are the two parameters considered

$$\dot{\mathbf{T}} + \|\mathbf{u}\| \mathbf{C} \mathbf{T} = \alpha \mathbf{D} \mathbf{T} \quad (2)$$

where the dot indicates the time derivative and \mathbf{C} and \mathbf{D} are the convective and diffusive matrices, respectively.

3 Proper Orthogonal Decomposition

Both reduction methods, the Galerkin projection and the proposed PODI method, are POD based. Therefore a short description of the POD method is given first in this section.

The POD method is a commonly used basis extraction tool for fluid problems as it is applicable to both linear and non-linear problems [4]. The main assumption of the POD method is that there exists an approximation $T_r(\mathbf{x}, t)$ to the full order solution $T(\mathbf{x}, t)$ that can be expressed as linear combination of orthogonal spatial modes $\phi_i(\mathbf{x})$ multiplied by time-dependent coefficients $a_i(t)$ [7] as given by

$$T(\mathbf{x}, t) \approx T_r(\mathbf{x}, t) = \sum_{i=1}^{N_r} \phi_i(\mathbf{x}) a_i(t) \quad (3)$$

where a_i are the time-dependent coefficients and N_r is the dimension of the reduced basis space. The spatial modes $\phi_i(\mathbf{x})$ are determined using a snapshot technique where a snapshot matrix Y is generated, in this case by numerical simulations, containing a set of snapshot solutions of T at some selected times t^n for $n = 0, \dots, N_t$

$$Y = [T(t^0), T(t^1), \dots, T(t^{N_t})] \in \mathbb{R}^{N_x \times N_t} \quad (4)$$

where N_x is the spatial dimension and the snapshot times t_n do not necessarily have to correspond with the time steps for which the full order solution is calculated. However, the snapshots do need to capture the entire dynamics of the system within a specified range. One way to compute the POD modes is by taking the Singular Value Decomposition (SVD) of the snapshot matrix, $Y = U \Sigma V^T$. The POD modes are given by the columns of matrix $U \in \mathbb{R}^{N_x \times N_x}$, which is a square matrix of N_x left singular vectors. In addition, these modes are orthogonal to each other as $\langle \phi_i(\mathbf{x}), \phi_j(\mathbf{x}) \rangle_{l^2} = \delta_{i,j}$, where $\langle \cdot, \cdot \rangle_{l^2}$ is the l^2 inner

product over the domain Ω . The matrix $V \in \mathbb{R}^{N_t \times N_t}$ is a square matrix of right singular vectors. The diagonal matrix $\Sigma \in \mathbb{R}^{N_x \times N_t}$ has as entries the singular values of the snapshot matrix which is a measure of the relative energy of each mode [8]. These singular values are sorted in descending order, meaning that the first modes contain the most energy. The decay of the normalized singular values can then be used to retain the first N_r (with $N_r < N_t$) left singular vectors of matrix U for the POD modes given a certain tolerance for the truncation error [9]. The time-dependent coefficients are obtained by projecting all snapshots on the POD basis functions and the temperature field can be reconstructed according to equation (3). The l^2 error between the FOM and reconstruction can be computed [9] by

$$\|e\|_{l^2} = \sqrt{\frac{\langle (T - T_r), (T - T_r) \rangle_{l^2}}{\langle T, T \rangle_{l^2}}} \quad (5)$$

The SVD approach could become more computationally expensive when the dimension of the grid, used to discretize the domain, is increased (spatial). It is then recommended to solve an eigenvalue problem using the correlation matrix $\mathbf{C}_{corr} \in \mathbb{R}^{N_t \times N_t}$ of the snapshots to have no longer a dependency on N_x . For a more detailed explanation the reader is referred to [8, 9].

4 Reduced Order Modelling methods

In this section the classical Galerkin projection is described shortly and the proposed PODI method is described in some more detail.

4.1 Galerkin projection

By substituting the approximation equation (3) in the governing equations (2) and applying a Galerkin projection on the POD basis functions gives the following reduced order representation of the parameterized system of equations

$$\dot{\mathbf{a}} = \alpha \mathbf{D}_r \mathbf{a} - \|\mathbf{u}\| \mathbf{C}_r \mathbf{a} \quad (6)$$

where \mathbf{a} is a vector containing all temporal coefficients $a_i(t)$, \mathbf{D}_r is the reduced matrix of the diffusion term and \mathbf{C}_r is the reduced matrix of the convection term with

$$\mathbf{D}_r = \Phi^T \mathbf{D} \Phi \quad (7)$$

$$\mathbf{C}_r = \Phi^T \mathbf{C} \Phi. \quad (8)$$

where Φ is the transformation matrix containing the first N_r dominant POD modes

$$\Phi = [\phi_1, \dots, \phi_{N_r}] \in \mathbb{R}^{N_x \times N_r} \quad (9)$$

where N_x is the spatial dimension of the FOM.

The variables in this dynamical system are the time dependent coefficients \mathbf{a} . The ordinary differential equations (6) are discretized in time and solved using the backward Euler method. For more details the reader is referred to [3, 8, 9].

4.2 POD-based identification

The main issue of the POD-Galerkin method is its intrusiveness as described in the introduction. The POD-based identification method is proposed as a non-intrusive reduced-order method for parametric CFD problems. This PODI method uses the set of known time-dependent coefficients, $a_i(t)$, obtained by projecting all snapshots on the POD basis, $\phi_i(\mathbf{x})$, in the offline phase as follows

$$\mathbf{a}(t) = \Phi^T T(\mathbf{x}, t) \quad (10)$$

where Φ is the transformation matrix containing the first N_r dominant POD modes as given by equation (9).

This method is similar to the Dynamic Mode Decomposition (DMD) technique where the snapshots with linear dynamics are fitted on a reduced order subspace, typically POD modes, to capture the dynamics of the system. For nonlinear problems the DMD technique can be combined with direct subspace techniques to construct an input-output reduced order model or so called state space model (for more details see [10] and [11]).

The PODI method proposed here does not construct a state space model, but identifies the reduced matrices of the same form as in the POD-Galerkin method using a least-squares technique such as normal equations, QR-decomposition or SVD. A set of ordinary differential equations, still describing the physical model, is obtained. The resulting reduced system of equations is then solved online for a given set of parameters.

The offline-online decomposition of the POD-Galerkin method is thus maintained. In case multiple distinguishable matrices with a multiplication parameter are present in the FOM (as in equation (2)), then as many full order simulations as number of distinguishable matrices are required to determine the reduced matrices with the least-squares approach. For the example given in this paper, where the thermal diffusivity and input velocity are taken as the parameters, a minimum of two sets of simulations are required to distinguish the reduced matrices for the convection and diffusion part. This is one of the disadvantages of the proposed PODI method. The Galerkin method requires only one full order simulation. However, this advantage of the Galerkin method will be less for parameterized problems with high dimensionality as in practice multiple full order simulations for different parameter sets are added to the snapshot matrix to improve the reduced solutions away from the snapshots.

5 Simulation set-up

5.1 Offline phase

A Matlab [12] code has been written to solve the 2D full order model for the convection-diffusion equations as given by (1), with no sources or sinks present, using the finite volume method on a Cartesian grid, $\Omega = (0, 1) \times (0, 1)$. The uniform grid consists of 25×25 control volumes. An upwind scheme is included for the convective term and an implicit time discretization scheme is applied to enhance stability. Homogeneous Neumann boundary

conditions are applied on all boundaries Γ and the initial condition is given by the function

$$T(0, x, y) = \sin\left(\frac{1}{2}\pi x\right) \cdot \sin\left(\frac{1}{2}\pi y\right). \quad (11)$$

The first parameter set is given by a thermal diffusivity of $\alpha = 1 \times 10^{-6} \text{ m}^2/\text{s}$ and a uniform time-independent velocity field in space where the velocity in the x-direction equals the velocity in the y-direction with $\|\mathbf{u}\| = 0.01 \text{ m/s}$. The simulation is run until $t = 2 \text{ s}$ with a constant time step of $\Delta t = 2 \times 10^{-2} \text{ s}$. Snapshots are taken at every time step, resulting in a total of 101 snapshots per parameter set.

Next the POD basis is created as described in section 3 using economy-size singular value decomposition in Matlab [12]. Then the Galerkin-projection and identification method with the QR-decomposition as least-squares approach are applied as described in sections 4.1 and 4.2, respectively. The Galerkin method requires only one full order simulation to be able to determine the reduced matrices. However the PODI method requires at least as many full order simulations as the number of reduced matrices to be distinguished for the parametrized problem. As there are two parameters, two full order simulations are needed. Therefore a second full order simulation is done for $\alpha = 1 \times 10^{-5} \text{ m}^2/\text{s}$ and $\|\mathbf{u}\| = 0.02 \text{ m/s}$. The snapshots of the two different simulations are used to create the POD basis.

5.2 Online phase

The two ROMs, POD-Galerkin and PODI, are constructed as described in previous sections. The calculation of the ROM solutions is performed in MATLAB using a backward substitution method. The ROM computational time depends on the number of modes used and no longer on the degrees of freedom of the FOM. Finally the results of the PODI method are compared with the POD-Galerkin method and the benefits and limitations are discussed. As the reduced basis is the same for the PODI method and the POD-Galerkin method, also the reduced matrices obtained through respectively identification and projection are compared. Finally intermediate values are chosen for the parameters to test the ROM. The values chosen are $\alpha = 7 \times 10^{-5} \text{ m}^2/\text{s}$ and $\|\mathbf{u}\| = 0.0125 \text{ m/s}$ and these have thus not been used to create the snapshot matrix.

6 Results and Discussion

In this section the accuracy of the ROMs for the non-parametric case is tested and the eigenvalues of reduced matrices obtained for both methods are compared. The same is done later on for the parametric case and the results are discussed.

Firstly one full order simulation is performed for the first parameter set. The initial temperature field at $t = 0 \text{ s}$ and the final field at $t = 2 \text{ s}$ are shown in figure 1. The modes are determined with the POD approach and the decay of the normalized POD eigenvalues is shown in figure 2 in order to determine the number of basis functions needed to create the reduced subspace. The figure shows that 8 basis functions are needed to have a truncation error less than 10^{-4} and that is sufficient for this specific case. The

parametrization is not considered yet and thus only one reduced matrix, containing all linear terms, has to be determined with the Galerkin projection and the PODI method.

Furthermore simulations are done for the obtained set of ODEs and the full order solution is reconstructed. The accuracy of the ROMs is checked by calculating the l^2 error of the temperature field, as shown in figure 3, for the two reduction methods and comparing them with the error given by the projection of the snapshots onto the POD basis, called here the basis projection. The l^2 errors, which are of the order 10^{-3} , are varying slightly over the investigated time interval and are on top of each other, indicating that the ROMs describe the same system as the FOM. The ROM-Galerkin solution is as accurate as the basis projection, because the discretized equations (given by (2)) are projected rather than the original continuous equations (given by (1)).

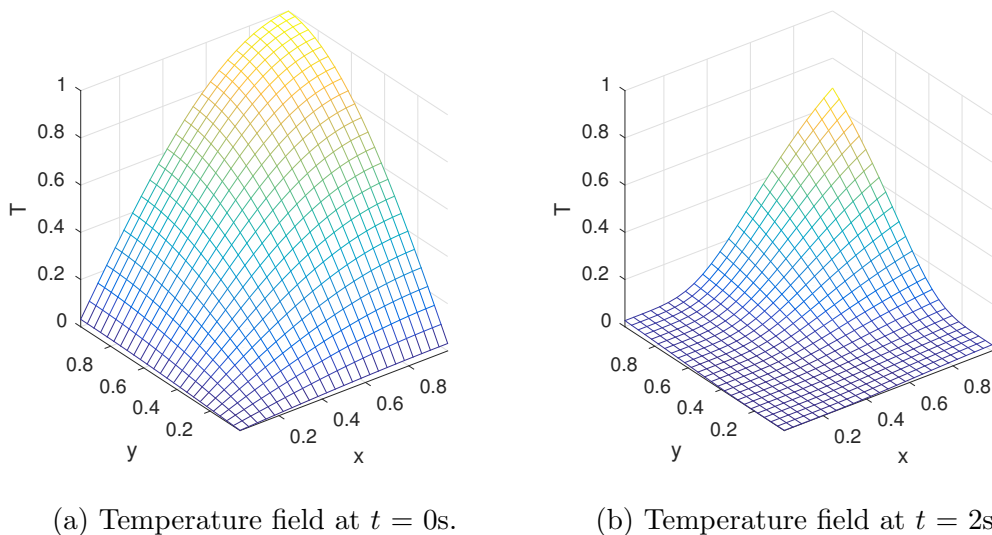


Figure 1: Full order simulation for $\alpha = 10^{-6} \text{ m}^2/\text{s}$ and $\|u\| = 0.01 \text{ m/s}$.

The fact that the PODI method leads to the same reduced system as the Galerkin method is also shown by the comparison of the eigenvalues of the reduced matrices obtained through identification and projection in figure 4 where the eigenvalues are the same for both methods. Also the time to calculate the POD basis functions is the same for both ROMs. However the time to set-up the reduced order system for the PODI method is about 5 times longer than the Galerkin projection for the non-parametrized case.

In case of the parametrized problem, the PODI method requires two parameter sets in order to distinguish two reduced matrices; one for the diffusion term and one for the convective term. Therefore a full order simulation is done for the second parameter set and the results of both sets are used to create a new snapshot matrix set and the POD basis functions. Again 8 modes are used for the creation of the reduced subspace. The ROM set-up takes about 7 times longer for the PODI method compared to the classic Galerkin-projection method, due to the extra set of equations that had to be solved for the PODI method to distinguish the reduced matrices.

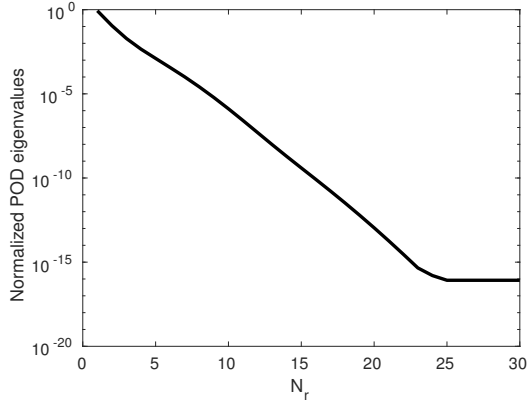


Figure 2: Normalized POD eigenvalues for $\alpha = 1 \times 10^{-6} \text{ m}^2/\text{s}$ and $\|\mathbf{u}\| = 0.01 \text{ m/s}$

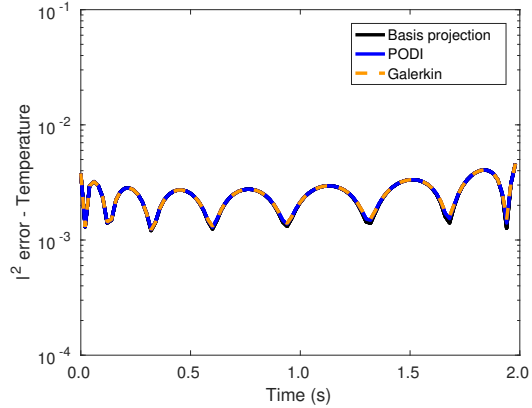


Figure 3: l^2 error of the reconstructed temperature with $N_r = 8$ for the ROMs. Non-parametrized case.

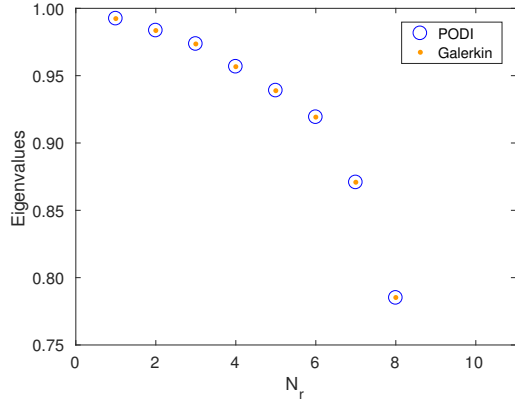


Figure 4: Eigenvalues of the reduced matrices for the non-parametrized case.

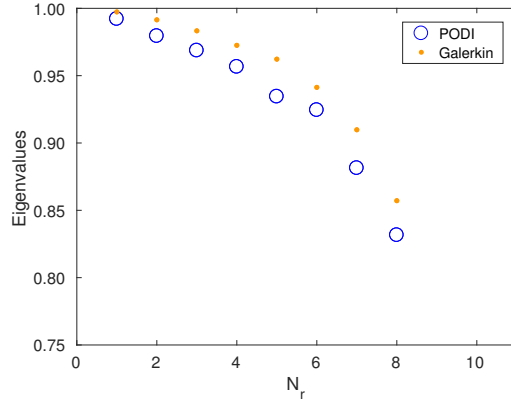


Figure 5: Eigenvalues of the reduced matrices for $\alpha = 7 \times 10^{-5} \text{ m}^2/\text{s}$ and $\|\mathbf{u}\| = 0.0125 \text{ m/s}$

Finally intermediate values are chosen for the parameters to test the accuracy of the parameterized ROMs: $\alpha = 7 \times 10^{-5} \text{ m}^2/\text{s}$ and $\|\mathbf{u}\| = 0.0125 \text{ m/s}$. These values have not been used to create the snapshot matrix. The eigenvalues of the reduced matrices are plotted in figure 5. For the PODI method the eigenvalues are lower than those for the Galerkin-projection method, but that does not result in a large deviation of the l^2 error as shown in figure 6. The PODI method performs even better than the Galerkin projection method. However, for both methods the l^2 error is of the order 10^{-2} and increases slightly over the time interval, meaning that the methods are less stable for a parameter set that has not been used for the snapshot creation.

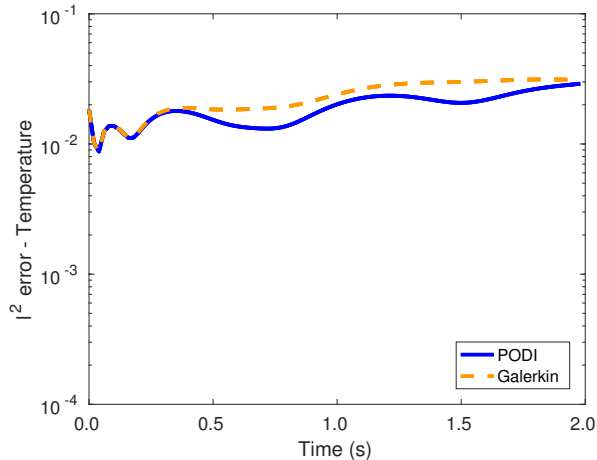


Figure 6: l^2 error of the reconstructed temperature field with $N_r = 8$ for the ROMs. $\alpha = 7 \times 10^{-6} \text{ m}^2/\text{s}$ and $\|\mathbf{u}\| = 0.0125 \text{ m/s}$.

7 CONCLUSIONS

The PODI method presented here in this paper is a non-intrusive reduction method that can be applied to parametric CFD problems using the FVM. This method leads to the same set of ODEs as the classic POD-Galerkin projection, meaning that the reduced model is still describing the physical behavior of the system that has been reduced. The results for the non-parameterized linear unsteady convection-diffusion equations are promising as the relative error of the main variable, namely the temperature, is corresponding to the error given by the projection of the snapshots onto the POD basis. However, the set-up time for the PODI method is larger than for the Galerkin method as an overdetermined system of equations has to be solved rather than applying a projection. The total offline time could be reduced further by, for instance, optimizing the POD method.

The results for the parameterized case are about one order less accurate compared to the non-parameterized case for both methods. However, the PODI method performs slightly better than the Galerkin projection, but the set-up time for the PODI method is larger, compared to the non-parametrized case, due to the extra set of equations that had to be solved in order to distinguish the reduced matrices.

As the PODI method is based on the classic Galerkin method it might encounter the same challenges and difficulties as already exploited in literature for the POD-Galerkin method applied to the FVM. Examples are non-homogeneous Dirichlet boundary conditions, long time integrations and instabilities. For more details the reader is referred to [4, 8, 9, 13].

Further work will include the application of the PODI for non-linear parametric problems. Non-linear problems, as for example the convective term in the Navier-Stokes equations, require at least as many reduced matrices as there are modes to be stored in the offline phase [7, 8, 9]. The reduced problem is then growing with the cube of the number of modes, but the offline-online decomposition would be maintained. Further-

more, the stability of the method has to be studied. Finally the method will be tested on full order results obtained from software as for example OpenFOAM or ANSYS Fluent to demonstrate the non-intrusiveness of the method.

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