EXTENSION AND COMPARISON OF TECHNIQUES TO ENFORCE BOUNDARY CONDITIONS IN FINITE VOLUME POD-GALERKIN REDUCED ORDER MODELS FOR FLUID DYNAMIC PROBLEMS

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Abstract. A Finite-Volume based POD-Galerkin reduced order model is developed for fluid dynamic problems where the (time-dependent) boundary conditions are controlled using two different boundary control strategies: the control function method, whose aim is to obtain homogeneous basis functions for the reduced basis space and the penalty method where the boundary conditions are enforced in the reduced order model using a penalty factor. The penalty method is improved by using an iterative solver for the determination of the penalty factor rather than tuning the factor with a sensitivity analysis or numerical experimentation. The boundary control methods are compared and tested for two cases: the classical lid driven cavity benchmark problem and a Y-junction flow case with two inlet channels and one outlet channel. The results show that the boundaries of the reduced order model can be controlled with the boundary control methods and the same order of accuracy is achieved for the velocity and pressure fields. Finally, the speedup ratio between the reduced order models and the full order model is of the order 10³ for the lid driven cavity case and of the order 10² for the Y-junction test case.

1. Introduction

Solving complex fluid dynamic problems using discretization methods such as Finite Difference, Finite Element, Finite Volume (FV) or spectral element methods almost in real time for use in applications as on-the-spot decision making, (design) optimization or control is, in practice, not so feasible. The high fidelity Computational Fluid Dynamics (CFD) tools, used for numerical simulations of the Navier–Stokes equations, are too computationally expensive for those purposes. This has motivated the development of reduced order modeling techniques. However, low degree-of-freedom models that are solely based on input-output data do not represent the physics of the underlying systems adequately and, moreover, may be sensitive to operating conditions [1]. Therefore, techniques, as Reduced Basis (RB) methods, have been developed that retain the essential physics and dynamics of a high fidelity model that consists of discretized Partial Differential Equations (PDEs) describing the fluid problem [2, 3]. The basic principle

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of these reduced order methods is to project the (parametrized) PDEs onto a low dimensional space, called the reduced basis space, in order to construct a physics-based model that is reduced in size and, therefore, in computational cost [4, 5, 6]. Fluid flows can be controlled in several ways. As an example, the system configuration can be manipulated by modifying the physical properties. However, in this work the focus is on controlling boundary conditions (BC) that are essential for defining flow problems.

An example of a boundary control application from the nuclear field is the coupling of thermal-hydraulic system codes, i.e. transient simulations that are based on one-dimensional models of physical transport phenomena, with three-dimensional CFD codes [7, 8]. These type of system codes are, in general, based upon the solution of six balance equations for liquid and steam that are coupled with conduction heat transfer equations and that are supplemented by a suitable set of constitutive equations[9]. One of the main purposes of this coupling is to speed up the CFD calculations by only including the region of interest in the CFD model and the rest of the domain in the much faster system code. However, the gain in computational time of such a coupled model is still limited by the CFD part. To overcome this burden, the system codes can be coupled with reduced order models (ROM) of the high fidelity CFD codes. For transient problems, time-dependent boundary conditions of the ROM are then to be controlled based on the BCs obtained from the systems codes.

For industrial applications, the Finite Volume discretization method is widely used by commercial software and open-source codes, as the method is robust [10] and satisfies locally the conservation laws [11, 12].

By using a RB technique, the non-homogeneous BCs are, in general, no longer satisfied at the reduced order level. Furthermore, the BCs are not explicitly present in the ROM and therefore they cannot be controlled directly [13]. In literature [13, 14, 15, 16], different approaches to control the ROM BCs can be found of which two common approaches are extended and compared in this work: the control function method and the penalty method. The aim of the control function method [14, 16] is to homogenize the BCs of the basis functions contained in the reduced subspace, while the penalty method [14, 13, 15, 17] weakly enforces the BCs in the ROM with a penalty factor. A disadvantage of the penalty method is that it relies on a penalty factor that has to be tuned with a sensitivity analysis or numerical experimentation [17]. Therefore, an iterative method is presented for tuning the penalty factor, which is, to the best of the authors’ knowledge, introduced here for the first time in the context of Finite-Volume based POD-Galerkin reduced order methods. The novelty of this method is that a error tolerance for the enforced BC has to be set instead of an arbitrary value for the factor. Also the factor is determined automatically by iterating rather than manually via numerical experimentation.

The work is organized as follows: in Section 2 the formulation of the full-order approximation of the PDEs is given and the methodology of the POD-based Galerkin projection is addressed in Section 3. In Section 4 the two boundary control methods, the control function method and the iterative penalty method, are presented. In Section 5 the set-up of two numerical experiments, lid driven cavity and a Y-junction test case, are given and the results are provided and discussed in Section 6 and 7, respectively. Finally, conclusions are drawn in Section 8 and an outlook for further developments is provided.
2. FULL ORDER MODEL OF THE INCOMPRESSIBLE NAVIER-STOKES EQUATIONS

The fluid dynamic problem is physically described by the unsteady incompressible Navier-Stokes equations. In an Eulerian framework on a domain $\Omega \subseteq \mathbb{R}^d$ with $d = 2, 3$ and boundary $\Gamma = (\Gamma_{D,U} \cup \Gamma_{N,U}) \cap (\Gamma_{D,p} \cup \Gamma_{N,p})$, the governing system of equations is given by

$$
\begin{align*}
\begin{cases}
\mathbf{u}_t + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) - \nabla \cdot (\nu \nabla \mathbf{u}) &= -\nabla p + \mathbf{F} & \text{in } \Omega \times [0, T], \\
\nabla \cdot \mathbf{u} &= 0 & \text{in } \Omega \times [0, T], \\
\mathbf{u}(x, 0) &= k(x) & \text{in } \Omega \times \{0\}, \\
\mathbf{u}(x, t) &= \mathbf{f}(x, t) & \text{on } \Gamma_{D,U} \times [0, T], \\
(\nabla \mathbf{u}(x, t)) \cdot \mathbf{n} &= 0 & \text{on } \Gamma_{N,U} \times [0, T], \\
(p(x, t)) \mathbf{n} &= h(x) & \text{on } \Gamma_{D,p} \times [0, T], \\
(\nabla p(x, t)) \mathbf{n} &= 0 & \text{on } \Gamma_{N,p} \times [0, T], \\
\end{cases}
\end{align*}
$$

where $\mathbf{u}$ is the vectorial velocity field, $p$ is the normalized scalar pressure field, which is divided by the fluid density $\rho$, $\nu$ is the kinematic viscosity and $\mathbf{F}$ is a body force term. For velocity, the (time-dependent) non-homogeneous Dirichlet boundary condition on $\Gamma_{D,U}$ is represented by $\mathbf{f}(x, t)$ and $k(x)$ denotes the initial condition for the velocity at time $t = 0$ s. On $\Gamma_{N,U}$ a homogeneous Neumann boundary condition for velocity is applied and $\Gamma_{D,p}$ and $\Gamma_{N,p}$ are the Dirichlet- and homogeneous Neumann boundary conditions for pressure. $T$ is the total simulation time.

The equations are presented here in a general format. The problem-specific (boundary) conditions are specified in Section [5] in which the numerical experiments are presented.

2.1. Pressure Poisson equation. Standard Galerkin projection-based reduced order models are unreliable when applied to the non-linear unsteady Navier-Stokes equations [18]. Furthermore, the ROMs need to be stabilized in order to produce satisfactory results for both the velocity and pressure fields [19, 20, 21, 17, 22]. Two different stabilization techniques are compared in [23]; the supremizer enrichment of the velocity space in order to meet the inf-sup condition (SUP) and the exploitation of a pressure Poisson equation during the projection stage (PPE). The SUP-ROM performed about an order worse with respect to the PPE-ROM for what concerns the velocity field but better for what concerns the pressure field. This difference can be explained by the fact that within a supremizer stabilization technique, the POD velocity space is enriched by non-necessary (for the correct reproduction of the velocity field) supremizer modes. As the focus of this work is on controlling velocity boundary conditions, it is decided to use the PPE approach for stabilizing the ROM.

For fluid problems that are solved numerically using a Finite Volume discretization technique [11, 24], often a Poisson Equation is solved for pressure as there is no dedicated equation for pressure in [21]. The PPE is obtained by taking the divergence of the momentum equations and subsequently exploiting the divergence free constraint $\nabla \cdot \mathbf{u} = 0$. The resulting set of governing full order equations is then given by

$$
\begin{align*}
\begin{cases}
\mathbf{u}_t + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) - \nabla \cdot (\nu \nabla \mathbf{u}) &= -\nabla p + \mathbf{F} & \text{in } \Omega \times [0, T], \\
\Delta p &= -\nabla \cdot (\nabla \cdot (\mathbf{u} \otimes \mathbf{u})) + \nabla \cdot \mathbf{F} & \text{in } \Omega \times [0, T], \\
\mathbf{n} \cdot \nabla p &= -\nu \mathbf{n} (\nabla \times \nabla \times \mathbf{u} + \partial_t \mathbf{f}) + \mathbf{n} \cdot \mathbf{F} & \text{on } \Gamma \times [0, T], \\
\end{cases}
\end{align*}
$$

In order to simplify the problem, no body force term, $\mathbf{F}$, is considered in this work. For more details on the derivation of the PPE the reader is referred to J.-G Liu et al. [25]. These equations are discretized with the Finite Volume method and solved using a
PIMPLE [26] algorithm for the pressure-velocity coupling, which is a combination of SIMPLE [27] and PISO [28].

3. POD-Galerkin reduced order model of the incompressible Navier-Stokes equations

There exist several techniques in literature for creating a reduced basis space onto which the full order system (2.1) is projected such as the Proper Orthogonal Decomposition (POD), the Proper Generalized Decomposition (PGD) and the Reduced Basis (RB) method with a greedy approach. For more details about the different methods the reader is referred to [2, 4, 5, 29]. In this work, the Proper Orthogonal Decomposition method is used to create a reduced set of basis functions, or so-called modes, governing the essential dynamics of the full order model (FOM). For this, full order solutions are collected at certain time instances, the so-called snapshots. These snapshots do not necessarily have to be collected at every time step for which the full order solution is calculated.

Subsequently, it is assumed that the solution of the FOM can be expressed as a linear combination of orthonormal spatial modes, \((\varphi_i, \varphi_j)_{L^2(\Omega)} = \delta_{ij}\), multiplied by time-dependent coefficients. The \(L^2\)-norm is preferred for discrete numerical schemes [23, 30] with \((\cdot, \cdot)_{L^2(\Omega)}\) the \(L^2\) inner product of the fields over the domain \(\Omega\). For the velocity and pressure fields, the approximations are given, respectively, by

\[
(3.1) \quad u(x, t) \approx u_r = \sum_{i=1}^{N_u} \varphi_i(x) a_i(t), \quad p(x, t) \approx p_r = \sum_{i=1}^{N_p} \chi_i(x) b_i(t),
\]

where \(\varphi_i\) and \(\chi_i\) are the modes of the velocity and pressure, and respectively \(a_i\) and \(b_i\) the corresponding time-dependent coefficients. \(N_u\) is the number of velocity modes and \(N_p\) is the number of pressure modes and thus it is assumed that velocity and pressure at reduced order level are approximated with a different number of temporal coefficients. The optimal POD basis space for velocity, \(E^{POD}_{N_u} = \text{span}(\varphi_1, \varphi_2, \ldots, \varphi_{N_u})\) is then constructed by minimizing the difference between the snapshots and their orthogonal projection onto the basis for the \(L^2\)-norm [31]. This gives the following minimization problem:

\[
(3.2) \quad E^{POD}_{N_u} = \text{arg min} \frac{1}{N_u} \sum_{n=1}^{N_u} \left\| u_n(x) - \sum_{i=1}^{N_u} (u_n(x), \varphi_i(x))_{L^2(\Omega)} \varphi_i(x) \right\|_{L^2(\Omega)}^2,
\]

where \(N_u\) is the number of collected velocity snapshots and \(N_u > N_p\). The POD modes are then obtained by solving the following eigenvalue problem on the snapshots [32, 23, 16]:

\[
(3.3) \quad CQ = Q\Lambda,
\]

where \(C_{ij} = (u_i, u_j)_{L^2(\Omega)}\) for \(i,j = 1, \ldots, N_u\) is the correlation matrix, \(Q\) is a square matrix of eigenvectors and \(\Lambda\) is a diagonal matrix containing the eigenvalues. The POD modes, \(\varphi_i\), can then be constructed as follows

\[
(3.4) \quad \varphi_i(x) = \frac{1}{N_u \sqrt{\lambda_i}} \sum_{n=1}^{N_u} u_n(x) Q_{i,n} \quad \text{for} \quad i = 1, \ldots, N_u,
\]

of which the most energetic (dominant) modes are selected. The procedure is the same for obtaining the pressure modes.

To obtain a reduced order model, the POD is combined with the Galerkin projection,
for which the full order system of equations (2.2) is projected onto the reduced POD basis space. For more details about POD and Galerkin Projection methods the reader is referred to [33, 16, 23]. The following reduced system of momentum equations is then obtained

\[(3.5) \quad M_r \dot{a} + C_r(a)a - \nu A_r a + B_r b = 0,\]

where

\[(3.6) \quad M_{rij} = (\varphi_i, \varphi_j)_{L^2(\Omega)}, \quad A_{rij} = (\varphi_i, \Delta \varphi_j)_{L^2(\Omega)}, \quad B_{rij} = (\varphi_i, \nabla \chi_j)_{L^2(\Omega)}.
\]

These reduced matrices can be precomputed during an offline stage except for the non-linear term \(C_r\), which is given by

\[(3.7) \quad C_{rijk} = (\varphi_i, \nabla \cdot (\varphi_j \cdot \varphi_k))_{L^2(\Omega)}.
\]

This non-linear term is stored as a third order tensor [34, 16] and the contribution of the convective term to the residual of Eq. (3.5), \(R\), is evaluated at each iteration during the ROM simulations, or so-called online stage, as

\[(3.8) \quad R_i = a^T C_{r_{im}} a.
\]

The dimension of the tensor (3.7) is growing with the cube of the number of modes used for the velocity space and therefore this approach may lead in some cases, especially when a large number of basis functions are employed, to high storage costs. Other approaches, such as EIM-DEIM [35, 36] or Gappy-POD [37] may be more affordable [23]. As the pressure gradient term is present in the momentum equation the system is also coupled at reduced order level [16]. The projection of the PPE leads to the following reduced system

\[(3.9) \quad D_r b + G_r(a)a - \nu N_r a - T_r b = 0,\]

where

\[(3.10) \quad D_{r_{ij}} = (\nabla \chi_i, \nabla \chi_j)_{L^2(\Omega)}, \quad G_{r_{ijk}} = (\nabla \chi_i, \nabla \cdot (\varphi_j \otimes \varphi_k))_{L^2(\Omega)}, \quad T_{r_{ij}} = \langle \chi_i, n \cdot \varphi_j \rangle_{L^2(\Gamma_D)}, \quad N_{r_{ij}} = \langle n \times \nabla \chi_i, \nabla \cdot \varphi_j \rangle_{L^2(\Gamma_D)}.
\]

Following the same strategy as in Equation (3.8), the non-linear term in Equation (3.9) is evaluated by storing the third order tensor \(G_r\). Equation (3.10) consists only of first order derivatives as integration by parts of the Laplacian term is used together with exploiting the pressure boundary condition after the PPE is projected onto the POD space spanned by the pressure modes. In that way, the numerical differentiation error can be reduced [23].

3.1. Initial conditions. The initial conditions (IC) for the reduced system of Ordinary Differential Equations (3.5) are obtained by performing a Galerkin projection of the full order initial conditions onto the POD basis spaces as follows

\[(3.11) \quad a_i(0) = (\varphi_i(x), u(x, 0))_{L^2(\Omega)}, \quad b_i(0) = (\chi_i(x), p(x, 0))_{L^2(\Omega)},\]

for velocity and pressure, respectively.
3.2. Relative error. Three types of fields are considered: the full order fields, \( X_{\text{FOM}} \), the projected fields, \( X_r \), which are obtained by the \( L^2 \)-projection of the snapshots onto the POD bases and the prediction fields obtained by solving the ROM, \( X_{\text{ROM}} \). For every time instance, \( t \), the basis projection error, \( \| \hat{e} \|_{L^2(\Omega)} \), is given by

\[
\| \hat{e} \|_{L^2(\Omega)}(t) = \frac{\| X_{\text{FOM}}(t) - X_r(t) \|_{L^2(\Omega)}}{\| X_{\text{FOM}}(t) \|_{L^2(\Omega)}},
\]

and the prediction error \( \| e \|_{L^2} \), is determined by

\[
\| e \|_{L^2(\Omega)}(t) = \frac{\| X_{\text{FOM}}(t) - X_{\text{ROM}}(t) \|_{L^2(\Omega)}}{\| X_{\text{FOM}}(t) \|_{L^2(\Omega)}},
\]

where \( X \) is either representing the velocity or pressure fields.

4. Non-homogeneous (time-dependent) Dirichlet boundary conditions of the incompressible Navier-Stokes equations

In a POD-based ROM, the non-homogeneous BCs are, in general, not satisfied by the ROM, as the basis functions, and in the same way their BCs, are a linear combination of the snapshots. Furthermore, the BCs are not explicitly present in the reduced system and therefore they cannot be controlled directly [13]. Two common approaches are presented in this section for handling the BCs: the control function- and the penalty method [14]. The aim of the control method is to have homogeneous POD modes and to enforce the BCs by means of a properly chosen control function in the ROM. On the other side, the penalty method enforces the BCs in the ROM with a penalty factor. In this work only the velocity BCs are controlled with the two methods.

4.1. The control function method. With the control function method, the velocity snapshots are made homogeneous by subtracting suitable control functions from all of them on which then the POD is performed. The result is a set of velocity modes with homogeneous BCs. The functions to be chosen are system-specific and they have to satisfy two constrains: the control functions must be divergence free in order to retain the divergence-free property of the basis functions and the functions need to satisfy the remaining BCs of the FOM. One way to generate a control function, \( \tilde{\zeta}_c(x) \), satisfying both constraints is by solving a problem, as close as possible to the full order problem, where the boundary of interest is set to its value and everywhere else to a homogeneous BC. As one of the characteristics of the POD modes is that they are orthonormal, the control functions are normalized as follows

\[
\zeta_c(x) = \frac{\tilde{\zeta}_c(x)}{\| \tilde{\zeta}_c(x) \|_{L^2(\Omega)}},
\]

before subtracting them from all snapshots and applying POD. The snapshots are then modified accordingly

\[
u'(x, t) = u(x, t) - \sum_{j=1}^{N_{BC}} \zeta_{cj}(x) u_{BCj}(t),
\]

where \( N_{BC} \) is the number of non-homogeneous BCs, \( \zeta_c(x) \) the normalized control functions and \( u_{BC} \) is the normalized value of the corresponding Dirichlet boundary condition. The POD modes, \( \varphi_i \), are obtained by solving the following eigenvalue problem on the homogenized snapshots \( u'(x, t) \) and the control functions are then added as
additional modes to the reduced system. Finally, the velocity fields are approximated by

\[(4.3) \quad u_r(x, t) = \sum_{j=1}^{N_{BC}} \zeta_c_j(x) u_{BC,j}(t) + \sum_{i=1}^{N_u} \varphi_i(x) a_i(t),\]

which satisfy the boundary conditions of the problem. \(u_{BC}\) can be time-dependent and be parametrized. For more details on the control function the reader may take a look at [16, 33].

The overall algorithm for the control function method is given below.

**Algorithm 1: Control function method**

**Solve full order model:**
1. Generate snapshots over a time period \([t_1, t_N]\) by solving the full order problem of Eq. 2.1;

**Obtain the control functions:**
2. Generate the control functions by solving a flow problem:
   
   \[
   \text{for } i = 1 \text{ to } N_{BC} \text{ do}
   \]
   
   \[
   \text{for } j = 1 \text{ to } N_{BC} \text{ do}
   \]
   
   \[
   \text{if } i = j \text{ then } u|\Gamma_{D_j} = 1; \text{ else } u|\Gamma_{D_j} = 0
   \]
   
   \[
   \text{end for}
   \]
   
   \[
   \text{end for;}
   \]
3. Normalize the control functions to obtain \(\zeta_c\) as in Eq. 4.1;
4. Subtract the normalized control functions from the velocity snapshots as in Eq. 4.2;

**Perform POD:**
5. Retrieve the correlation matrix \(C\) from the solution snapshots;
6. Solve the eigenvalue problem of Eq. 3.3 to obtain the POD modes using Eq. 3.4;
7. Add the normalized control functions, \(\zeta_c\), as additional modes to the velocity POD modes \(\varphi\);

**Solve reduced order model:**
8. Project the initial field for the parametrized BC onto the POD basis to get the initial condition for the ROM using Eq. 3.11;
9. Solve the reduced order problem of Eq. 3.5 with the reduced Poisson equation, Eq. 3.9 for pressure for the time period \([t_1, t_N]\);
10. Reconstruct the full order fields from the obtained coefficients using Eq. 4.3;

**4.2. The iterative penalty method.** For the penalty method, no modification of the snapshots is needed as the velocity Dirichlet BCs are directly enforced as constraints in the reduced system in the following way

\[(4.4) \quad M_r \dot{a} - \nu B_r a + a^T C_r a + K_r b + \sum_{l=1}^{N_{BC}} \tau_l (u_{BC,l}(t) P_{1,l} - P_{2,l} a) = 0,\]

where \(\tau\) is the penalty factor [17] and

\[(4.5) \quad P_{1,li} = \langle \varphi_i, 1 \rangle_{L^2(\Gamma_l)} \quad \text{for } l = 1, \ldots, N_{BC} \text{ and } i = 1, \ldots, N_u,
\]

\[
\text{and}\]

\[
P_{2,ij} = \langle \varphi_i, \varphi_j \rangle_{L^2(\Gamma_l)} \quad \text{for } l = 1, \ldots, N_{BC} \text{ and } i, j = 1, \ldots, N_u.
\]
are evaluated for each boundary separately. In order to have an asymptotically stable solution, the penalty factors $\tau$ should be larger than 0. In case $\tau \to \infty$ a strong imposition would be approached and the ROM becomes ill-conditioned. Therefore, it is important to find a penalty factor as small as possible, which is usually done by numerical experimentation. In this work the experimentation is optimized using a first-order iterative optimization scheme to determine the factors. The penalty factors, $\tau$, are updated each iteration $k$, as follows

\begin{equation}
\tau_{k+1} = \tau_k \frac{|r_k(\hat{t})|}{\epsilon} = \tau_k \frac{|\hat{u}_{BC_l}(\hat{t}) - u_{BC_l}(\hat{t})|}{\epsilon}
\end{equation}

for $l = 1, ..., N_{BC}$,

with $r_k(\hat{t})$ the residual between $\hat{u}_{BC_l}^k$, the value of a certain boundary at the $k^{th}$ iteration, and $u_{BC_l}$, the enforced boundary condition, at an evaluated time $\hat{t}$. $\epsilon > 0$ is the given error tolerance for the residual which has to be set. The penalty method is therefore no longer based on an arbitrary value for the penalty factor. As long as $|\hat{u}_{BC_l}^k(\hat{t}) - u_{BC_l}(\hat{t})| > \epsilon$ the penalty factors grow every update and converge to the smallest penalty factors that satisfy the required tolerance. Thus, if the initial guess for the factor is below the minimum value for $\tau$ for which the boundary condition is enforced in the ROM, the factor is approached from below using this method. For time-dependent problem it is not needed to determine a penalty factor for all time steps. Often the factor determined after the first couple of time steps can be used for the whole ROM solution.

The step-by-step demonstration of the iterative function method is given below by Algorithm 2.

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**Algorithm 2: Iterative penalty method**

**Solve full order model:**
1. Generate snapshots over a time period $[t^1, t^{Ns}]$ by solving the full order problem of Eq. 2.4.

**Perform POD:**
2. Retrieve the correlation matrix $C$ from the solutions;
3. Solve the eigenvalue problem of Eq. 3.3 to obtain the POD modes using Eq. 3.4.

**Impose BCs with penalty method:**
4. Project the modes on the reduced basis at the boundary of the domain to determine $P1$ and $P2$ for each non-homogeneous Dirichlet boundary condition as in Eq. 4.5;
5. Solve iteratively for the penalty factor using Eq. 4.6.

**Solve reduced order model:**
6. Project the initial field for the parametrized BC onto the POD basis to get the initial conditions $a^0$ for the ROM using Eq. 3.11;
7. Solve the reduced order problem of Eq. 3.5 with the reduced Poisson equation, Eq. 3.9, for pressure for the time period $[t^1, t^{Ns}]$;
8. Reconstruct the full order fields from the obtained coefficients using Eq. 3.1.

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5. **Numerical simulation tests**

In this section the set-up of two cases are described for which the boundary control methods, the control function method and the iterative penalty method, are tested. The first one test case is the classical lid driven cavity benchmark and the second one is a
Y-junction with two inlets and one outlet channel whose time-dependent inlet boundary conditions are controlled.

5.1. Lid-driven cavity flow problem. The first test case consists of a lid driven cavity problem. The simulation is carried out on a two-dimensional square domain of length \( L = 0.1 \) m on which a \((200 \times 200)\) structured mesh with quadrilateral cells is constructed. The boundary is subdivided into two different parts \( \Gamma = \Gamma_{LID} + \Gamma_w \) and the boundary conditions for velocity and pressure are set according to Figure 1. The pressure reference value is set to 0 Pa at coordinate \((0,0)\). At the top of the cavity a constant uniform and horizontal velocity equal to \( \mathbf{u} = (U_{LID},0) = (1,0) \) m/s is prescribed. The kinematic viscosity is equal to \( \nu = 1 \cdot 10^{-4} \) m\(^2\)/s and the corresponding Reynolds number is 1000, meaning that the flow is considered laminar.

The unsteady full order equations are iteratively solved by the FV method with the \textit{pimpleFoam} solver of the open source C++ library OpenFOAM 6 \[39\]. The PIMPLE algorithm is used for the pressure-velocity coupling \[26\]. For the full order simulations the space discretization is performed with a central differencing scheme and the time discretization is treated using a second order backward differencing scheme (BDF2). A constant time step of \( \Delta t = 5 \cdot 10^{-4} \) s has been applied and the total simulation time is 10 s. Snapshots of the velocity and pressure fields are collected every 0.01 s, resulting in a total of 1000 snapshots. The initial condition field with \( U_{LID} = 1 \) m/s is used as a control function.

For this test case the same boundary conditions are applied in the ROM as in the FOM for which the snapshots are collected. The time discretization of the ROM is performed with a first order backward differencing scheme.

5.2. Y-junction flow problem. Junctions are often used for the combination or separation of fluid flows and can be found in all types of engineering applications from gas transport in pipes till micro flow reactors. As a second test case a Y-junction with one outlet channel and two inlet channels is modeled. The angle between each inlet and
the horizontal axis is 60 degrees, as shown in Figure 2 on the left [41]. The length of the channels is 2 m. The 2D geometry is split in 6 zones as depicted in Figure 2 on the left. On the three rectangular zones a mesh with quadratical cells is constructed. The remaining three zones are meshed with hexagonal cells. The different meshes are depicted in Figure 2 on the right. The total number of cells is 13046. The boundary is subdivided into four different parts $\Gamma = \Gamma_{i1} \cup \Gamma_{i2} \cup \Gamma_o \cup \Gamma_w$. The two inlets, $\Gamma_{i1}$ and $\Gamma_{i2}$, have a width of 0.5 m, while the outlet, $\Gamma_o$, has a width of 1 m. The kinematic viscosity is equal to $\nu = 1 \cdot 10^{-2}$ m$^2$/s meaning that the Reynolds number at the inlet is 50 and the flow is considered laminar. The uniform inlet velocities are time dependent and the velocity magnitude of the flow at the inlets is set according to figure 3.

![Figure 2.](image)

A homogeneous Neumann boundary condition is applied for pressure at the inlet and wall boundaries. At the outlet, $\Gamma_o$, $p = 0$ Pa together with a homogeneous Neumann BC for velocity. A no slip BC is applied at the walls, $\Gamma_w$.

As initial conditions the steady state solution for a velocity magnitude of 1 m/s at both inlets is chosen. As done previously for the lid driven cavity case, the unsteady governing equations are iteratively solved by the FV method with the *pimpleFoam* solver of OpenFOAM 6 [39]. For the full order simulations, the discretization in space is performed with a central differencing scheme for the diffusive term and a combination of a second order central-differencing and upwinding schemes for the convective term. The time discretization is treated using a second order backward differencing scheme (BDF2). A constant time step of $\Delta t = 5 \cdot 10^{-4}$ s has been applied and the total full order simulation time is 12 s for which snapshots of the velocity and pressure fields are collected every 0.03 s, resulting in a total of 401 snapshots. The inlet velocity BCs are time-dependent and the velocity magnitude of, alternately, inlet 1 or 2 is increased or decreased linearly between 1 m/s to 0.5 m/s as shown in Figure 3 on the left.
In that way the ROM is trained for all possible combinations of inlet velocities within the specified range. The inlet boundary conditions of the ROM are then controlled according to figure 3 on the right, where the inlet velocity magnitude is increased or decreased linearly over time between the maximum of 1 m/s and minimum of 0.5 m/s. The magnitude of the inlet velocities of the ROM decreases and increases faster or slower over time compared to the training run. Also the ROM is tested for a longer time period, 18 s, compared to the full order simulation of 12 s. In that way the ROM performance can be tested on the long term.

The time discretization of the ROM is performed with a first order backward differencing scheme.

Both the iterative penalty method and control function method are tested. The control functions are determined by solving for a potential flow field problem given by

\[
\begin{align*}
\nabla \cdot u &= 0 & \text{in } \Omega, \\
\nabla^2 p &= 0 & \text{in } \Omega, \\
(p(x) I) n &= 0 & \text{on } \Gamma_o, \\
(\nabla p(x,t)) n &= 0 & \text{on } \Gamma \not\subset \Gamma_o, \\
(\nabla u(x)) n &= 0 & \text{on } \Gamma_o, \\
(\nabla u(x)) n &= 0 & \text{on } \Gamma_w, \\
u(x) &= g_1(x) & \text{on } \Gamma_{i1}, \\
u(x) &= g_2(x) & \text{on } \Gamma_{i2},
\end{align*}
\]

(5.1)

with the magnitude of the inlet velocity at inlet 1, \( \Gamma_{i1} \), set to 1 m/s while inlet 2, \( \Gamma_{i2} \), is kept at 0 m/s as shown in figure 4 for the first control function. To obtain the second control function \( \|u\| = 0 \) at \( \Gamma_{i1} \) and 1 m/s at \( \Gamma_{i2} \). Both control functions are shown in Figure 4.

The test case of a Y-junction is more complicated than the lid driven cavity case as not only one, but two boundaries need to be controlled, which are also time dependent. Furthermore, as the channel inlets are placed under an angle, one needs to take into account that the inlet velocity can be decomposed in an x- and a y-direction. Therefore, the vectorial control functions are split into their components before normalization. Also in case of the penalty method, four penalty factors are determined; one for each inlet and each direction. This will be further discussed in section 7.
6. RESULTS AND ANALYSIS

6.1. Lid driven cavity flow problem. First the full order simulation for the lid driven cavity test case is performed and 1001 velocity and pressure snapshots are collected, including the initial conditions, which are then used to create the POD basis functions. Stabile and Rozza [23] concluded in their research that 10 velocity and pressure modes are enough to retain 99.99% of the energy contained in the snapshots. Therefore the same number of modes for the reduced basis creation are used in this work.

Reduced order models are constructed with both the control function- and penalty method and compared with a ROM without boundary enforcement. With the use of the iterative procedure a penalty factor of 0.058 is determined within 2 iterations by evaluating only the first five time steps with a maximum error tolerance, $\epsilon$, of $10^{-5}$ for the value of the boundary condition of the ROM and starting from an initial guess of $10^{-6}$. For a similar study of the lid driven cavity benchmark, Lorenzi et. al. [13] had found a factor between $10^{-2}$ and $10^{5}$ using numerical experimentation. The value found here using the iterative method is thus within the same range and near their minimum value. A higher value for the penalty factor can be used, but it is then more likely that the ROM becomes ill-conditioned.

The obtained ROMs are tested for the same initial and boundary conditions as the high fidelity simulation. The evolution in time of the relative $L^2$-error between the reconstructed fields and the full order solutions is plotted in Figure 5 together with the basis projection.

In case no boundary enforcement method is used the flow field remains zero throughout the simulation and therefore the relative error is 1. When either the control function- or penalty method is used the relative $L^2$-error for both the velocity and pressure fields are about the order of $10^{-1}$ due to the relatively low number of snapshots acquired during the initial part of the transient. The snapshots are equally distributed in time, while this time span exhibits the most non-linear behavior. Therefore one should concentrate the snapshots in this time span to enhance the performance of the ROM [23]. After about 2 seconds of simulation time, for both boundary control methods, the relative error drops till about the order of $10^{-3}$. At the final time of the simulation the penalty method is performing slightly better than the control function method, but the order
is the same. Contrary to velocity, the relative error for pressure stays about $4 \cdot 10^{-1}$ after 2 s of simulation time, while the projection error drops till about $10^{-3}$. This has been previously acclaimed by Stabile et. al. in [10]. The PPE stabilization method is less accurate concerning pressure compared to the supremizer enrichment method. Furthermore, the absolute error between the FOM and the ROMs is shown in Figure 5 and 7 for velocity magnitude and pressure, respectively. It is observed that both methods lead, for velocity, to an absolute error between the FOM and the ROM of the order $10^{-2}$ at the beginning of the simulation and about $10^{-3}$ once the flow has reached its steady state solution. Furthermore, the velocity error slightly increases between 5 and 10 s of simulation time. This can also be observed in the $L^2$-error analysis over time in Figure 5. For pressure, the error is largest near the top corners of the cavity and are of the order $10^{-3}$. Note that the scale does not show the whole range of absolute errors. This is done to better visualize the error. The maximum error for pressure is about $5 \cdot 10^{-2}$ Pa at the top right corner. As the pressure relative to its reference point at $(0,0)$ plotted in Figure 7 is always less than 1 Pa, the relative error plotted in Figure 5 is greater than the absolute error plotted in Figure 7. Furthermore, the error distribution, for both the velocity and pressure fields, is similar all over the domain, meaning the methods are performing the same, as previously confirmed by the $L^2$-error analysis over time in Figure 5.

The relative error for the total kinetic energy is determined and plotted in Figure 8. The order is more or less the same for both boundary control methods. From time to time the penalty method is performing slightly better and the other way around and the relative velocity error is less than $10^{-2}$ for the vast part of the simulation. Finally, the computational times for performing the full order simulation (Eq. 2.1), calculating the POD modes (Eq. 3.1 - 3.4), the reduced matrices (Eq. 3.6, 3.7, Eq. 3.10) and performing the simulation at reduced level (Eq. 3.5 (control function method) or Eq. 4.4 (penalty method) & Eq. 3.9) are all listed in Table 1. Calculating the POD modes, reduced matrices and the ROM solutions takes more time in case of the control function method as the reduced basis space consists of an additional mode, namely the normalized control function for the boundary with the lid, compared to the penalty method. Determining the penalty factor with the iterative method takes only 0.11 s. The speedup ratio between the ROM and the FOM is about 270 times for the control method and 308 times for the penalty method.
Table 1. Computational time (clock time) for the FOM simulation, POD, calculating reduced matrices offline (Matrices), determining penalty factor with iterative method (Penalty) and ROM simulation.

| Method   | FOM     | POD | Matrices | Penalty factor | ROM |
|----------|---------|-----|----------|----------------|-----|
| Control  | 37 min. | 50 s| 8.2 s    | -              | 8.2 s|
| Penalty  | 37 min. | 45 s| 6.8 s    | 0.11 s         | 7.2 s|

Figure 6. Comparison of the full order velocity magnitude fields (1st column), the ROM fields obtained with the control function method (2nd column) and penalty method (4th column) and the difference between the FOM and ROM fields obtained with the control function method (3rd column) and penalty method (5th column) at $t = 0.2, 1, 5$ and $10$ s (from top to bottom) for the lid driven cavity problem.
Figure 7. Comparison of the full order pressure fields (1st column), the ROM fields obtained with the control function method (2nd column) and penalty method (4th column) and the difference between the FOM and ROM fields obtained with the control function method (3rd column) and penalty method (5th column) at $t = 0.2, 1, 5$ and $10$ s (from top to bottom) for the lid driven cavity problem.

Figure 8. Kinetic energy relative $L^2$-error for the ROM with control function and with penalty method.
6.2. **Y-junction flow problem.** A full-order simulation is performed for the Y-junction test case with varying inlet velocities (magnitude) according to figure 3 on the left. In total 400 velocity and pressure snapshots are collected, which are then used to create the POD basis functions. To determine the number of basis functions necessary for the creation of the reduced subspace, the cumulative eigenvalues (based on the first 20 most energetic POD modes) are listed in Table 2. 5 velocity and pressure modes are sufficient to retain 99.99% of the energy contained in the snapshots. These first five (homogenized) velocity and pressure modes are plotted in Figure 9. The first velocity magnitude mode has a symmetric pattern and is close to the time-averaged solution when it has non-homogeneous BCs and looks more like a fluctuation around the mean when it has homogeneous BCs. From the third mode and higher, the modes are more or less alike, whether the modes have homogeneous BCs or not.

**Table 2.** The cumulative eigenvalues for the Y-junction test case. The second and third columns report the cumulative eigenvalues (total of the first 20 modes) for the velocity and pressure fields, respectively.

| N modes | u          | p          |
|---------|------------|------------|
| 1       | 0.976478   | 0.967073   |
| 2       | 0.998492   | 0.989840   |
| 3       | 0.999724   | 0.998781   |
| 4       | 0.999859   | 0.999741   |
| 5       | 0.999924   | 0.999933   |
| 6       | 0.999967   | 0.999975   |
| 7       | 0.999989   | 0.999995   |
| 10      | 0.999999   | 0.999999   |

In Figure 10 for each number of modes the time-averaged relative $L^2$-error between the FOM and the basis projection is plotted, on the left for velocity and on the right for pressure. For velocity this is repeated with a set of homogenized snapshots. As there are two inlet boundary conditions, the first two modes are the normalized control functions and all sequential modes are then the homogeneous basis functions obtained with the POD method. Therefore the average $L^2$-error is still above the order $10^{-1}$ as these modes do not contain any information about the full order solution. The figure shows that 11 velocity basis functions and 10 pressure basis functions are required to have a truncation error less than $10^{-3}$. Taking also into account previous observation, these number of modes are used for calculating the ROM matrices.

After applying the Galerkin projection with the obtained modes, the penalty factors are determined using the iterative procedure. Starting from an initial guess of $10^{-6}$ the penalty factors found are $5.9 \cdot 10^{-8}$ and $88.3$ for inlet 1 and $1.1 \cdot 10^{-7}$ and 125 for inlet 2 in the x- and y-direction, respectively. The factors are determined within 41 iterations for an error tolerance of $10^{-5}$ and only the first five time steps are evaluated. However, it took only 15 iterations to have an error of $1.00009 \cdot 10^{-5}$ with penalty factors $0.0327$, $88.3$, $0.048$, $124.5$. So one could relax the criteria for the error a bit for a faster convergence. Thereafter, three ROMs are obtained; one without boundary enforcement method, one with the control function method and one with the penalty method. These are then consecutively tested for the time-dependent boundary conditions of Figure 4. The evolution in time of the $L^2$ relative error between the reconstructed fields is plotted in Figure 11.
In case no boundary enforcement method is used, the relative error for both velocity and pressure is of the order 1 and larger for the vast part of the simulation. The relative error is more or less the same for both boundary control methods, as also was observed previously for the lid driven cavity test case, except around 9 s of simulation time. Then the difference in relative error for pressure between the two methods is the largest; the penalty method is about $2 \cdot 10^{-1}$ larger than the error obtained with the control function method. However, on the long term the penalty method performs slightly better as also can also be concluded by having a look at the kinetic energy relative error in Figure 12. Other than that, the relative velocity error is of the order $10^{-2}$ and for pressure $10^{-1}$. Furthermore, there is about one order of difference between the minimum and maximum relative error for both variables.

Furthermore, the absolute error between the FOM and the ROMs is shown in Figure 13 and 14 for velocity magnitude and pressure, respectively. For velocity the absolute error between the FOM and the ROM is of the order $10^{-2}$ for all plotted simulation times and the absolute error for pressure is of the order $10^{-1}$. For pressure, the error is indeed larger in case of the penalty method compared to the control function method at 9 s of simulation time, as previously observed in Figure 11 but in general, the error distribution, for both the velocity and pressure fields, is similarly distributed over the domain, and thus the methods are performing the same.
Finally, the computational times for performing the full order simulation (Eq. 2.1), calculating the POD modes (Eq. 3.1 - 3.4), the reduced matrices (Eq. 3.6, 3.7, Eq. 3.10) and performing the simulation at reduced level (Eq. 3.5 (Control function method) or Eq. 4.4 (penalty method) & Eq. 3.9) are listed in Table 3. Calculating the reduced matrices and the ROM solutions takes more time in case of the control function method as the reduced basis space consists of four additional modes, namely the normalized control functions, compared to the penalty method. Determining the penalty factor with the iterative method takes 1.4 s. The speedup ratio between the ROM and the FOM is about 13 times for the control method and 24 times for the penalty method.
Figure 12. Kinetic energy relative $L^2$-error for the ROM with control function and with penalty method for the Y-junction flow problem.

Figure 13. Comparison of the full order velocity magnitude fields (1st column), the ROM fields obtained with the control function method (2nd column) and penalty method (4th column) and the difference between the FOM and ROM fields obtained with the control function method (3rd column) and penalty method (5th column) at $t = 3, 9$ and $18$ s (from top to bottom) for the Y-junction flow problem.
Figure 14. Comparison of the full order pressure fields (1st column), the ROM fields obtained with the control function method (2nd column) and penalty method (4th column) and the difference between the FOM and ROM fields obtained with the control function method (3rd column) and penalty method (5th column) at $t = 3, 9$ and $18$ s (from top to bottom) for the Y-junction flow problem.

Table 3. Computational time (clock time) for the FOM simulation, POD modes, calculating reduced matrices offline (Matrices), determining penalty factor with iterative method (Penalty) and ROM simulation.

| Method  | FOM   | POD   | Matrices | Penalty | ROM  |
|---------|-------|-------|----------|---------|------|
| Control | 13 min| 7.6 s | 9.2 s    | -       | 59 s |
| Penalty | 13 min| 7.9 s | 4.7 s    | 1.4 s   | 33 s |
7. DISCUSSION

The results have shown that the control function method and penalty method perform equally and lead to similar results. However, they have their own advantages and drawbacks. A disadvantage of the penalty methods is that the penalty factor cannot be determined a priori [14]. The implementation of an iterative solver to determine the penalty factor does however save time compared to performing numerical experimentation manually. On the other hand, even though a control function(s) can be determined beforehand, it may be hard to find a function that will lead to an accurate ROM and therefore extensive testing of ROMs for different functions can be needed. In this work, the control functions are obtained by solving a potential flow problem and are thus physics-based unlike the penalty factor, which is an arbitrary value. Moreover, this value needs to be chosen above a certain threshold to enforce the BCs in the ROM, but can lead to an inaccurate ROM solution if it is too high [17]. In that case, the penalty method fails for that specific problem.

Finally, an advantage of the penalty method stated in literature [13] is that long-time integration and initial condition issue are less of a problem compared to a control function method. Here the ROMs have not been tested for long-term integration, so further research is needed in order to confirm this statement. However, as tested for the Y-junction test case, the ROM is accurate and does not exhibit instabilities even outside the time domain in which snapshots were collected.

For both cases tested in this study, only one full order simulation has been performed for collecting the snapshots. However, in case the BCs of the Y-junction are not time-dependent, snapshots from at least two different offline solves are required for the penalty method. The reason for this is that the boundary conditions are a linear combination of snapshots and the boundary conditions can therefore only be scaled and not be set to any arbitrary value in case only snapshots from one full order simulation are used for the POD. When several sets of snapshots for different boundary values are required, one can optimize the POD procedure by using a nested POD approach [33].

In theory the penalty method can be used to adjust the direction of the inlet flow in the ROM. This is, however, not possible with the control function method as then four control functions are required, one for each direction. Using the current approach, these control functions are then unphysical, what would lead to unstable ROMs. So, the control function method is only suitable, in this case, to control the inlet flow magnitude and not the direction of the flow.

Moreover, both methods can, in theory, also be used for controlling pressure boundary conditions, but this is not studied in this work.

In this study, the exploitation of a pressure Poisson equation has been incorporated in the ROM as a stabilization method. Even though the ROMs are indeed stable, the relative error for pressure is about an order higher than for velocity. A supremizer enrichment of the velocity space technique is another technique to stabilize the ROM and could lead to more accurate pressure fields. [23]

Finally, for the Y-junction test case, the full order snapshots and the ROM solutions all have inlet velocities between an identical maximum and minimum value. The ROM could become less stable and accurate in case it is tested for values outside this range. Therefore it is recommended to collect snapshots for the same range as for which the ROM boundary needs to be controlled.
8. CONCLUSIONS AND PERSPECTIVES

Two boundary control methods are tested: the control function method and the iterative penalty method for controlling the velocity boundary conditions of FV-based POD-Galerkin ROMs. The penalty method has been improved by using an iterative solver for the determination of the penalty factors, rather than using numerical experimentation. The factors are determined by the iterative solver in about a second for both test cases. The results of the reconstructed velocity and pressure fields show that both methods are performing equally. Moreover, the reduced order model of which the boundary conditions are controlled with the iterative penalty method is about two times faster compared to the control function method for the Y-junction flow case.

A pressure Poisson equation approach is applied for the reconstruction of the pressure field and to stabilize the ROM. For time-dependent boundary problems, an additional term is added to the ROM formulation. The accuracy of the reconstructed pressure fields can be improved by using a suprenizer enrichment approach rather than solving the Pressure Poisson Equation.

Finally, a speed-up factor of about 40 and 300 has been obtained for the ROM compared with the FOM simulation times on a single processor for the Y-junction and the lid driven cavity test case, respectively.

For further development, the model will be extended for turbulent flows, which will be essential to simulate industrial flow problems. Furthermore, the control of the pressure boundary conditions needs to be investigated, which may be required when coupling 3D CFD problems with 1D system codes.

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