# Optimisation–Based Coupling of Finite Element Model and Reduced Order Model for Computational Fluid Dynamics

Ivan Prusak[0009−0008−2882−0576], and
Davide Torlo[0000−0001−5106−1629], and
Monica Nonino[0000−0002−5503−705X] and
Gianluigi Rozza[0000−0002−0810−8812]

**Abstract** With the increased interest in complex problems, such as multiphysics and multiscale models, as well as real–time computations, there is a strong need for domain–decomposition (DD) segregated solvers and reduced–order models (ROMs). Segregated models decouple the subcomponents of the problems at hand and use already existing state–of–the–art numerical codes in each component. In this manuscript, starting with a DD algorithm on non–overlapping domains, we aim at the comparison of couplings of different discretisation models, such as Finite Element (FEM) and ROM for separate subcomponents. In particular, we consider an optimisation–based DD model on two non–overlapping subdomains where the coupling on the common interface is performed by introducing a control variable representing a normal flux. Gradient-based optimisation algorithms are used to construct an iterative procedure to fully decouple the subdomain state solutions as well as to locally generate ROMs on each subdomain. Then, we consider FEM or ROM discretisation models for each of the DD problem components, namely, the triplet state1–state2–control. We perform numerical tests on the backward–facing step Navier-Stokes problem to investigate the efficacy of the presented couplings in terms of optimisation iterations and relative errors.

Ivan Prusak
Sissa, Mathematics Area, mathLab, International School for Advanced Studies, via Bonomea 265, 34136 Trieste, Italy, e-mail: iprusak@sissa.it

Davide Torlo
Sissa, Mathematics Area, mathLab, International School for Advanced Studies, via Bonomea 265, 34136 Trieste, Italy, e-mail: dtorlo@sissa.it

Monica Nonino
University of Vienna, Department of Mathematics,Oskar-Morgenstern-Platz 1, 1090 Vienna, Austria, e-mail: monica.nonino@univie.ac.at

Gianluigi Rozza
Sissa, Mathematics Area, mathLab, International School for Advanced Studies, via Bonomea 265, 34136 Trieste, Italy, e-mail: grozza@sissa.it

# 1 Introduction

In recent years, different techniques have been developed to reduce the computational costs in numerical simulations. Domain decomposition (DD) achieves this goal by using different solvers on different subcomponents of the domain, for example, using discretisations of much smaller dimensions or already existing codes. Reduced Order Models (ROMs) can be applied for multi–query or real–time tasks. They split the computational effort into two stages: the offline stage, which contains the most expensive part of the computations, and the online stage, which performs fast computational queries using structures that were pre–computed in the offline stage.

The DD–ROM combination is very promising when dealing with different discretisation techniques on different subdomains. This small contribution inspired by [1] aims at expanding the optimisation–based DD–ROM methods investigated in [2, 3] to the hybrid numerical models, where separate subcomponents of the DD problem can be approximated by either a full order model based on Finite Element method (FEM) or a reduced order model.

The rest of the paper is constructed as follows. In Section 2, starting with a formulation monolithic discretised Navier–Stokes equation we describe an optimisation–based discrete DD model at each time step and we derive the optimality system of the resulting optimal control problem. In section 3, we discuss the ROM based on Proper Orthogonal Decomposition (POD) and the different FEM and/or ROM coupling techniques. Finally, in Section 4 we provide numerical tests on the backward–facing step Navier-Stokes problem and draw some conclusions.

# 2 Problem formulation

In this section, starting with a monolithic formulation of the time–dependent incompressible Navier–Stokes equations, we introduce a discretised optimisation–based domain decomposition (DD) problem employing the implicit Euler time–stepping scheme and Finite Element method (FEM). The resulting optimal control problem is set up at each time step, aiming at minimising the distance between the subdomain velocity fields by finding an optimal normal flux at the interface.

## 2.1 Monolithic formulation

Let $\Omega$ be a physical domain of interest: we assume $\Omega$ to be an open subset of $\mathbb{R}^2$ and $\Gamma$ to be the boundary of $\Omega$. We also consider a finite time interval $[0, T]$ with $T > 0$. Let $f : \Omega \times [0, T] \to \mathbb{R}^2$ be the forcing term, $\nu$ the kinematic viscosity, $u_D$ a given Dirichlet datum to be imposed on $\Gamma_D \subset \Gamma$ and $u_0$ a given initial condition.

Following [2, 3], we can define usual Lagrangian FE spaces on a triangulation $\Omega_h$ of $\Omega$ as follows:

- $V_h \subset \left[H^1(\Omega)\right]^2, \quad ||\cdot||_{V_h} = ||\cdot||_{\left[H^1(\Omega)\right]^2}$,
- $V_{0,h} \subset \left\{v \in \left[H^1(\Omega)\right]^2 : v|_{\Gamma_D=0}\right\}, \quad ||\cdot||_{V_{0,h}} = ||\cdot||_{\left[H^1(\Omega)\right]^2}$,
- $Q_h \subset L^2(\Omega), \quad ||\cdot||_{Q_h} = ||\cdot||_{L^2(\Omega)}$

and a time discretisation, through the time step $\Delta t > 0$, and we assume the following time interval partition: $0 = t_0 < t_1 < .... < t_M = T$, where $t_n = n\Delta t$ for $n = 0, ..., M$.

The discretised problem with FEM and implicit Euler reads as follows at each time step: find the velocity field $u_h^n : \Omega\times[0,T] \to \mathbb{R}^2$ and the pressure $p_h^n : \Omega\times[0,T] \to \mathbb{R}$ s.t.

$$\frac{m(u_h^n - u_h^{n-1}, v_h)}{\Delta t} + a(u_h^n, v_h) + c(u_h^n, u_h^n, v) + b(v_h, p_h^n) = (f^n, v_h)_\Omega \quad \forall v_i \in V_{0,h}, \tag{1a}$$

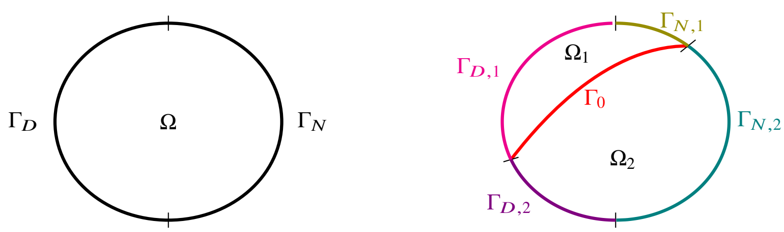
$$b(u_h^n, q_h) = 0 \qquad \forall q_h \in Q_h, \tag{1b}$$

$$u^n = u_{D,h}^n \qquad \text{on } \Gamma_D, \tag{1c}$$

where

- $m : V_h \times V_{0,h} \to \mathbb{R}, \quad m(u_h, v_h) := (u_h, v_h)_\Omega$,
- $a : V_h \times V_{0,h} \to \mathbb{R}, \quad a(u_h, v_h) := \nu(\nabla u_h, \nabla v_h)_\Omega$,
- $b : V_h \times Q_h \to \mathbb{R}, \quad b(v_h, q_h) := -(\mathrm{div} v_h, q_h)_\Omega$,
- $c : V_h \times V_h \times V_{0,h} \to \mathbb{R}, \quad c(u_h, w_h, v_h) := ((u_h \cdot \nabla)w_h, v_h)_\Omega$.

Moreover, since Navier–Stokes equations have a saddle–point structure, we require the pairs of spaces $V_h - Q_h$ and $V_{0,h} - Q_h$ to be inf–sup stable and this is achieved by using, for example, the Taylor–hood $\mathbb{P}_2 - \mathbb{P}_1$ FE spaces.




(a) Physical domain (b) Domain Decomposition

Fig. 1: Domain and boundaries

## 2.2 Discrete Domain Decomposition formulation

As mentioned in the introduction, we resort to the optimisation–based approach for DD as described in [2, 3]. Let $\Omega_i,\ i = 1, 2$, be open subsets of $\Omega$, such that

$\overline{\Omega} = \overline{\Omega_1 \cup \Omega_2}$, $\Omega_1 \cap \Omega_2 = \emptyset$. Denote $\Gamma_i := \partial\Omega_i \cap \Gamma$, $i = 1, 2$, and $\Gamma_0 := \overline{\Omega_1} \cap \overline{\Omega_2}$. In the same way, we define the corresponding boundary subsets $\Gamma_{i,D}$ and $\Gamma_{i,N}$, $i = 1, 2$, see Fig. 1b.

Next, following [2, 3], we assume to have at hand two well–defined triangulations $\mathcal{T}_1$ and $\mathcal{T}_2$ over the polygonal domains $\Omega_1$ and $\Omega_2$ respectively, and a one–dimensional discretisation $\mathcal{T}_0$ of the interface $\Gamma_0$. We assume meshes $\mathcal{T}_1, \mathcal{T}_2$ and $\mathcal{T}_0$ to be conforming on the interface $\Gamma_0$ in the sense that they all share the same degrees of freedom (Dofs) on the interface.

We can then define the restriction of the FE spaces $V_h$, $V_{h,0}$, $Q_h$ onto the subdomain $\Omega_{i,h}$ as $V_{i,h}$, $V_{0,i,h}$, $Q_{i,h}$ and we define a FE space for the interface as

$$X_h \subset \left[L^2(\Gamma_0)\right]^2, \quad ||\cdot||_{X,h} = ||\cdot||_{\left[L^2(\Gamma_0)\right]^2}.$$

Similarly, we define the restriction of the bilinear and trilinear forms onto the restricted FE spaces as $m_i$, $a_i$, $b_i$, $c_i$.

Also in the subcomponents, we choose the Taylor–hood $\mathbb{P}_2 - \mathbb{P}_1$ FE spaces to be inf-sup stable. Concerning the space $X_h$, our choice is to use $\mathbb{P}_2$ FE space implying that the space $X_h$ share the DoFs with the spaces $V_{i,h}, i = 1, 2$ on the curve $\Gamma_0$.

The discretised optimisation–based DD formulation of the problem (1) then reads as follows: for $n \geq 1$ *minimise over* $g_h \in X_h$ *the functional*

$$\mathcal{J}(u^n_{1,h}, u^n_{2,h}; g_h) = \frac{1}{2}\int_{\Gamma_0} \left| u^n_{1,h} - u^n_{2,h} \right|^2 d\Gamma \tag{2}$$

*subject to the variational problem:*
*for* $i = 1, 2$ *find* $u_{i,h} \in V_{i,h}$ *and* $p_{i,h} \in Q_{i,h}$ *satisfying*

$$\begin{aligned} \frac{m_i(u^n_{i,h} - u^{n-1}_{i,h}, v_{i,h})}{\Delta t} + a_i(u^n_{i,h}, v_{i,h}) + c_i(u^n_{i,h}, u^n_{i,h}, v_i) \\ + b_i(v_{i,h}, p^n_{i,h}) = (f^n_i, v_{i,h})_{\Omega_i} + \Big((-1)^{i+1} g_h, v_{i,h}\Big)_{\Gamma_0} \end{aligned} \qquad \forall v_i \in V_{i,0,h}, \tag{3a}$$

$$b_i(u^n_{i,h}, q_{i,h}) = 0, \qquad \forall q_{i,h} \in Q_{i,h} \tag{3b}$$

$$u^n_i = u^n_{i,D,h} \qquad \text{on } \Gamma_{i,D}, \tag{3c}$$

where $u^n_{i,D,h}$ is the Galerkin projection of $u_D$ onto the trace–space $V_{i,h}|_{\Gamma_{i,D}}$.

## 2.3 Optimality system and the gradient of the objective functional

This section aims at providing the necessary elements to set up a gradient–based iterative optimisation algorithm of the DD minimisation problem (2)– (3). For this purpose, in order to deal with variational constraint optimal control problem, we use the Lagrangian functional and sensitivity derivatives approaches; we refer to [2, 3, 4, 5] for more details.

The optimality system arising for the optimal control is defined as follows:

- state problem (3),
- adjoint problem: for $i = 1, 2$, find $\xi_{i,h} \in V_{i,0,h}$ and $p_{i,h} \in Q_{i,h}$ satisfying

$$\frac{m_i(\eta_{i,h}, \xi_{i,h})}{\Delta t} + a_i(\eta_{i,h}, \xi_{i,h}) + c_i(\eta_{i,h}, u^n_{i,h}, \xi_i) + c_i(u^n_{i,h}, \eta_{i,h}, \xi_{i,h}) \tag{4a}$$
$$+b_i(\eta_{i,h}, \lambda_{i,h}) = ((-1)^{i+1}\eta_{i,h}, u^n_{1,h} - u^n_{2,h})_{\Gamma_0} \quad \forall \eta_{i,h} \in V_{i,0,h},$$
$$b_i(\xi_{i,h}, \mu_{i,h}) = 0 \qquad \forall \mu_{i,h} \in Q_{i,h}. \tag{4b}$$

- optimality condition:

$$(r_h, \xi_1 - \xi_2)_{\Gamma_0} = 0 \qquad \forall r_h \in X_h. \tag{5}$$

Resorting to the sensitivity derivatives approach [2, 3] allows us to obtain the gradient representation of the objective functional (2): for a given $g_h \in X_h$ the gradient is defined as

$$\frac{d\mathcal{J}}{dg}(u^n_{1,h}, u^n_{2,h}; g_h) = \xi_{1,h}\big|_{\Gamma_0} - \xi_{2,h}\big|_{\Gamma_0}, \tag{6}$$

where $u^n_{i,h}, i = 1, 2$ are the solutions to the state equations (3) and $\xi_{i,h}, i = 1, 2$ are the solutions to the adjoint equations (4). Please note that the optimality condition (5) ensures that the solutions to the coupled optimality system (3)– (5) are the stationary points of the functional (2).

## 3 Reduced Order Model setting and FEM–ROM couplings

As highlighted in Section 1, reduced–order methods are efficient tools for significant reduction of the computational time for parameter–dependent PDEs. This section deals with the reduced–order model for the problem obtained in the previous section, where the state equations, namely Navier–Stokes equations, are assumed to be dependent on a set of physical parameters. We study then different coupling options choosing for each subcomponent of the DD problem either the FEM or the ROM.

### 3.1 Reduced Order Model setting

In this section, we will list all the necessary components to set–up a reduced order model. All the details can be found in [2, 3].

Our goal is to generate linear low–dimensional subspaces of the FE spaces presented in Section 2.2. We rely on the Proper Orthogonal Decomposition (POD) compression technique; see, for instance, [2, 3, 6]. The POD procedure is based on the sampling of the parameter space $\mathcal{P}$ with a discrete set $\mathcal{P}_M$ and storing the snapshots associated with each parameter $\mu \in \mathcal{P}_M$ and each time instance. Since we aim at constructing linear spaces, we need to introduce parameter–dependent lifting functions $l^n_{i,h}(\mu) \in V_{i,h}$, for $\mu \in \mathcal{P}_M$, such that $l^n_{i,h}(\mu) = u_{i,D,h}$ on $\Gamma_{i,D}$ and define homogenised snapshots $u^n_{i,0,h}(\mu) := u^n_{i,h}(\mu) - l^n_{i,h}(\mu)$ which implies that $u^n_{i,0,h}(\mu)$ belongs to $V_{i,0,h}$. The reduced spaces $V_N^{u_1}, V_N^{p_1}, V_N^{u_2}, V_N^{p_2}$ and $V_N^g$ are then built as it is described in [2, 3] together with the velocity supremiser technique [7] in order to guarantee the inf–sup stability of the velocity–pressure reduced spaces.

Having at our disposal the reduced spaces, we perform the Galerkin projection of the state problem (3): for a given parameter $\mu \in \mathcal{P}$ and $g_N \in V_N^g$, find $u^n_{i,N} = u^n_{i,0,N} + l^n_{i,N}$ with $u^n_{i,0,N} \in V_N^{u_i}$ and $p_{i,N} \in V_N^{p_i}$ satisfying

$$\begin{aligned} &\frac{m_i(u^n_{i,N} - u^{n-1}_{i,N}, v_{i,N})}{\Delta t} + a_i(u^n_{i,N}, v_{i,N}) + c_i(u^n_{i,N}, u^n_{i,N}, v_{i,N}) \\ &\qquad + b_i(v_{i,N}, p^n_{i,N}) = (f^n_i, v_{i,N})_{\Omega_i} + \left((-1)^{i+1} g_N, v_{i,N}\right)_{\Gamma_0} \qquad \forall v_{i,N} \in V_N^{u_1}, \quad (7a) \\ &\qquad b_i(u^n_{i,N}, q_{i,N}) = 0 \qquad \forall q_{i,N} \in V_N^{p_i}, \quad (7b) \end{aligned}$$

where $l^n_{i,N}$ is the Galerkin projection of the lifting function $l^n_{i,h}$ to the finite dimensional space $V_N^{u_i}$ and $i = 1, 2$.

In a similar way we can write the reduced counterpart of the adjoint equations (4): for a given parameter $\mu \in \mathcal{P}$ and $u^N_{i,N} \in V_N^{u_i} + \{l^n_{i,N}\}$, find $\xi_{i,N} \in V_N^{u_i}$ and $\lambda_{i,N} \in V_N^{p_i}$ satisfying

$$\begin{aligned} &\frac{1}{\Delta t} m_i(\eta_{i,N}, \xi_{i,N}) + a_i(\eta_{i,N}, \xi_{i,N}) + c_i\left(\eta_{i,N}, u^n_{i,N}, \xi_i\right) + c_i\left(u^n_{i,N}, \eta_{i,N}, \xi_{i,N}\right) \quad (8a) \\ &\qquad + b_i(\eta_{i,N}, \lambda_{i,h}) = ((-1)^{i+1}\eta_{i,N}, u^n_{1,N} - u^n_{2,N})_{\Gamma_0}, \quad \forall \eta_{i,N} \in V^{u_i}_{i,N}, \\ &\qquad b_i(\xi_{i,N}, \mu_{i,N}) = 0, \qquad \forall \mu_{i,N} \in V^{p_i}_{i,N}. \quad (8b) \end{aligned}$$

where $i = 1, 2$.

### 3.2 FEM–ROM couplings: exploring different options

In this section, we will provide a setting where different types of models, i.e. FEM or ROM, can be chosen for each of the components of the DD problem, namely the triplet state1–state2–control. In particular, we investigate four different scenarios — FEM–FEM–FEM, FEM–ROM–FEM, FEM–ROM–ROM and ROM–ROM–ROM. Each of these choices is characterised by a different optimisation problem.

To proceed we need to define the following parameter–dependent projection and lifting operators from the reduced spaces onto the FE spaces:

- $\Pi_i^n(\mu) : V_{i,h} \to V_N^{u_i} + \{l_{i,N}^n(\mu)\}, \quad (\Pi_i^n(\mu))^T : V_N^{u_i} + \{l_{i,N}^n(\mu)\} \to V_{i,h}$,
- $\Pi_{i,0} : V_{i,0,h} \to V_N^{u_i}, \quad \Pi_{i,0}^T : V_N^{u_i} \to V_{i,0,h}$.

Now, we will list the minimising problem and the corresponding expression of the objective functional gradient for each of the scenarios mentioned above:

- FEM–FEM–FEM (FFF) coupling: minimise over $g_h \in X_h$ the functional (2) under the constraints (3). The gradient in this case is given by the formula (6).
- FEM–ROM–FEM (FRF) coupling: minimise over $g_h \in X_h$ the functional

$$\mathcal{J}(u_{1,h}^n, u_{2,N}^n; g_h) = \frac{1}{2}\int_{\Gamma_0} \left| u_{1,h}^n - (\Pi_2^n(\mu))^T u_{2,N}^n \right|^2 d\Gamma, \tag{9}$$

  where $u_{1,h}$ is the FEM solution to (3) with $i = 1$ and $u_{2,N}$ is the ROM solution to (7) with $i = 2$. The gradient in this case is defined as

$$\frac{d\mathcal{J}}{dg}(u_{1,h}^n, u_{2,N}^n; g_h) = \xi_{1,h}\big|_{\Gamma_0} - \left[\Pi_{2,0}^T \xi_{2,N}\right]\Big|_{\Gamma_0}, \tag{10}$$

  where $\xi_{1,h}$ is the solution to (4) with $i = 1$ and $\xi_{2,N}$ is the solution to (8) with $i = 2$.
- FEM–ROM–ROM (FRR) coupling: minimise over $g_N \in V_N^g$ the functional

$$\mathcal{J}(u_{1,h}^n, u_{2,N}^n; g_N) = \frac{1}{2}\int_{\Gamma_0} \left| \Pi_1^n(\mu) u_{1,h}^n - u_{2,N}^n \right|^2 d\Gamma, \tag{11}$$

  where $u_{1,h}$ is the FEM solution to (3) with $i = 1$ and $u_{2,N}$ is the ROM solution to (7) with $i = 2$. The gradient in this case is defined as

$$\frac{d\mathcal{J}}{dg}(u_{1,h}^n, u_{2,N}^n; g_N) = \left[\Pi_{1,0}\xi_{1,h}\right]\Big|_{\Gamma_0} - \left[\xi_{2,N}\right]\Big|_{\Gamma_0}, \tag{12}$$

  where $\xi_{1,h}$ is the solution to (4) with $i = 1$ and $\xi_{2,N}$ is the solution to (8) with $i = 2$.
- ROM–ROM–ROM (RRR) coupling: minimise over $g_N \in V_N^g$ the functional

$$\mathcal{J}(u_{1,N}^n, u_{2,N}^n; g_N) = \frac{1}{2}\int_{\Gamma_0} \left| u_{1,N}^n - u_{2,N}^n \right|^2 d\Gamma, \tag{13}$$

  where $u_{i,N}$ is the ROM solution to (7) with $i = 1, 2$. The gradient in this case is defined as

$$\frac{d\mathcal{J}}{dg}(u_{1,N}^n, u_{2,N}^n; g_N) = \xi_{1,N}\big|_{\Gamma_0} - \xi_{2,N}\big|_{\Gamma_0}, \tag{14}$$

  where $\xi_{i,N}$ is the solution to (8) with $i = 1, 2$.

# 4 Numerical results

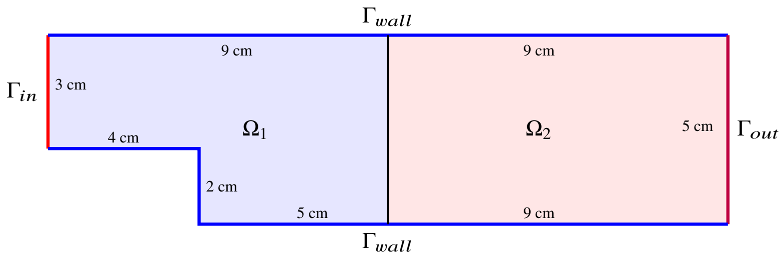
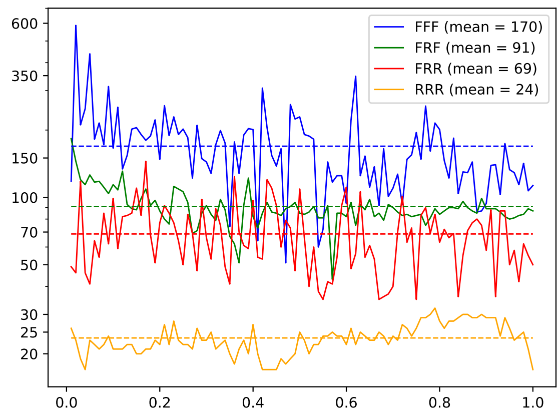



Fig. 2: Physical domain and domain decomposition for the backward–facing step problem

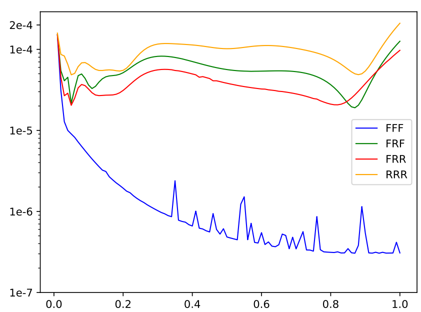
We consider the backward–facing step flow test case presented in [3]. Fig. 2 represents the physical domain of interest and the two–domain decomposition performed by dissecting the domain by a vertical segment. In the offline phase, we consider two physical parameters:the viscosity $\nu \in [0.4, 2]$ and the maximal magnitude $\bar{U} \in [0.5, 4.5]$ of the inlet profile $u_{in}(x, y) = \left(\bar{U} \cdot \frac{4}{9}(y-2)(5-y), 0\right)^T$ on $\Gamma_{in} = \{(x, y) : x = 0, y \in [2, 5]\}$.

In our test case, the FOM FEM solutions are obtained on discrete state problems with a total of 27,890 DoFs carrying out the minimisation in the interface space $X_h$ with 130 DoFs by the limited–memory Broyden–Fletcher–Goldfarb-–Shanno (L–BFGS–B) optimisation algorithm [8] using the `scipy` library [9]. Snapshots are sampled from a training set of 64 parameters randomly sampled from the 2–dimensional parameter space for 100 time steps with $\Delta t = 0.01$ and $T = 1$.

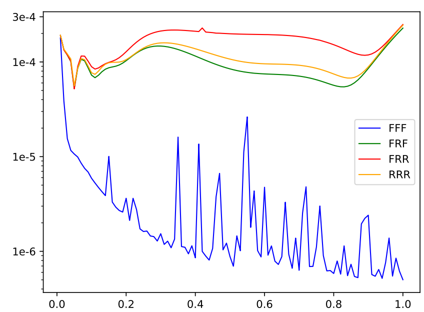
We perform a numerical analysis of the four couplings described in Section 3.2 for a test parameter value $\left(\bar{U}, \nu\right) = (4.5, 0.4)$. For the couplings using the ROM model, we choose the following number of reduced basis modes: 30 for $u_1$, 12 for $u_2$, and 5 for each of $p_1$ and $p_2$ and the corresponding supremisers. Fig. 3 shows the number of optimisation iterations over time for couplings FFF, FRF, FRR and RRR, and the relative error of each state subcomponent with respect to the monolithic solution of the Navier–Stokes problem (1). It can be easily seen that the FFF coupling has the overall highest number of iterations while the RRR coupling has the lowest, and the FRF and FRR are in between the other two. This is because the optimisation in the case of ROM model for the control variable is carried out over a much smaller set of admissible solutions, which is constructed on preliminary physical information, i.e., FEM snapshots. On the other hand, as expected, this is balanced by the relative errors as it is shown in Fig. 3, where the relative error in the FFF coupling scenario is much smaller (at least for the velocity fields $u_1$ and $u_2$) than for other types of coupling. The irregular nature of the relative errors for the pressure fields $p_1$ and $p_2$, which are nevertheless sufficiently low, is most probably due to the fact that we



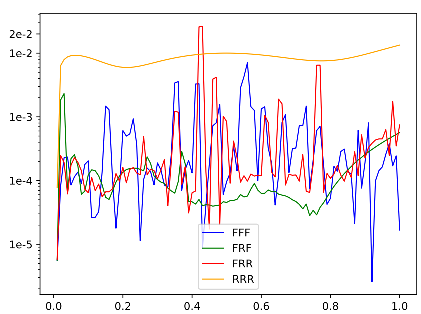

(a) Iterations of the optimization at each time step



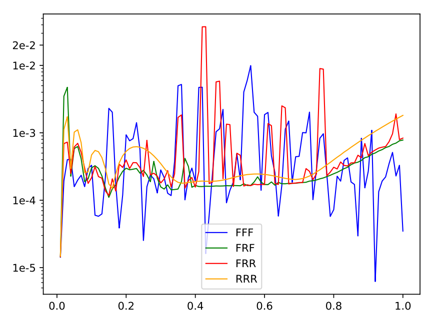

(b) Relative error for $u_1$




(c) Relative error for $u_2$




(d) Relative error for $p_1$




(e) Relative error for $p_2$

Fig. 3: Iterations and relative errors of FFF, FRF, FRR, and RRR solutions w.r.t. the monolithic solution

use a “black–box” optimisation algorithm. Indeed, we do not have access to how the search direction for the control variable representing the approximation of the normal flux on the interface is chosen. We believe this can be ameliorated by the use of different minimisation algorithms where we can have more control over the iterative procedure and impose some additional constraints also on the pressures, e.g., relative error reduction of the pressure with respect to the previous optimisation iteration.

Overall, we can conclude that already choosing one state variable to be in the reduced space can alleviate the costs of the optimization by a factor of 2. Nevertheless, a fully ROM approach gives a much–improved optimization process using only a seventh of the original number of iterations, while in terms of errors all reduced approaches are comparable and lead to an overall good approximation.

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