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A data-driven partitioned approach for the resolution of time-dependent optimal control problems with dynamic mode decomposition

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Abstract

This work recasts time-dependent optimal control problems governed by partial differential equations in a Dynamic Mode Decomposition with control framework. Indeed, since the numerical solution of such problems requires a lot of computational effort, we rely on this specific data-driven technique, using both solution and desired state measurements to extract the underlying system dynamics. Thus, after the Dynamic Mode Decomposition operators construction, we reconstruct and perform future predictions for all the variables of interest at a lower computational cost with respect to the standard space-time discretized models. We test the methodology in terms of relative reconstruction and prediction errors on a boundary control for a Graetz flow and on a distributed control with Stokes constraints.

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1 Introduction

Scientific and industrial contexts need to represent natural phenomena through mathematical models. Historically, this role has been played by partial differential equations (PDEs) and by their numerical simulations. Yet, the model equations, in some frameworks, are not enough to well describe the complexity of the natural phenomenon one is dealing with. To increase the reliability of a proposed PDEs-based model, a very classical and elegant mathematical tool has been exploited: optimal control. This technique responds to the need for reducing the gap between PDEs and collected data. Indeed, the data information, given by some previous knowledge on the

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system, is exploited in order to achieve a *desired configuration*: a convenient profile similar to the behaviour observed or expected in nature. Namely, through a PDE-constrained minimization strategy, optimal control problems (OCPs) are able to steer the solution of the problem at hand towards a target profile. OCPs governed by PDEs are widespread in many scientific applications: some examples in shape optimization may be found in [10, 17, 26] or, in fluid dynamics, in [8, 9, 28] where a parametrized setting is discussed. In the same framework, we can cite biomedical applications [3, 14, 13, 23, 40, 47], or environmental ones [4, 30, 31, 36, 39]. From these references, it is clear that OCPs are of indisputable usefulness in many applications. Yet, they still are very complex to analyse and to simulate, most of all if time-dependency is taken into consideration, since it requires larger computational costs. Despite these difficulties, time-dependent OCPs have been treated in many works: here a far from exhaustive list [18, 21, 24, 34, 35, 37, 38, 39]. In contrast with the aforementioned works, we tackle the study of the evolution of OCPs through the employment of dynamic mode decomposition with control (DMDC) [29], which is a data-driven technique for system identification in the context of feedback and control. The idea is to use the desired state from the OCPs framework as forcing term within the DMDC. Then, with a partitioned approach, we use the solution snapshots to construct different DMDC operators. With such operators, given new actuation snapshots, we perform future predictions for all the variables of interest, in a data-driven fashion. This results in great advantages in terms of computational time, keeping the accuracy within a certain threshold, as usual in the reduced order modeling framework [32]. The main novelty of this work, thus, is the recasting of an OCP in a DMDC framework: to the best of our knowledge, indeed, this is the first time that it is highlighted and investigated. We propose two test cases: a boundary control governed by a Graetz flow and a distributed control with Stokes constraints.

2 Time-dependent optimal control problems

We provide the continuous formulation for general time dependent OCP. Let us consider the spatial domain $\Omega \subset \mathbb{R}^d$, with $d = 2, 3$: here, the analysed physical phenomenon, described by a linear time-dependent PDE, is taking place in the time interval $[0, T]$. Furthermore, we denote with Γ_D and Γ_N two non-overlapping boundary portions where homogeneous Dirichlet and Neumann boundary conditions apply. In the context of constrained optimization, we consider an Hilbert space Y such that $Y \hookrightarrow H \hookrightarrow Y^*$ for some suitable H . Moreover, we define

$$\mathcal{Y}_t = \{y \in L^2(0, T; Y) \text{ such that } y_t \in L^2(0, T; Y^*) \text{ with } y(t) = 0\} \subset \mathcal{Q},$$

with $\mathcal{Q} = L^2(0, T; Y)$. The problem *state variable* y is sought in \mathcal{Y}_0 . In addition, we need to define $\mathcal{U} = L^2(0, T; U)$ as the space for the *control variable* u , with U another suitable Hilbert space.

The control acts on $\Omega_u \subseteq \Omega$ of a portion of its boundary, say $\Gamma_C \subset \partial\Omega$ with $\Gamma_C \cap \Gamma_N \cap \Gamma_D = \emptyset$ while $\Gamma_D \cup \Gamma_N \cup \Gamma_C = \partial\Omega$. In the first case, we say that the control problem is *distributed*, while in the second case, we say that the problem is a *boundary control*. With no distinctions, from now on, we will call Ω_u or Γ_C the *control domain*.

In order to change the classical solution behaviour, we need to define a *controlled system* of the following form, for all q in \mathcal{Q} , considering once again y_0 as initial condition

$$\int_0^T \langle y_t, q \rangle_{Y^*, Y} dt + \int_0^T a(y, q) dt = \int_0^T c(u, q) dt + \int_0^T \langle G, q \rangle_{Y^*, Y} dt, \quad (1)$$

with initial condition y_0 where, $a : Y \times Y \rightarrow \mathbb{R}$ is a coercive and continuous bilinear form and $G \in Y^*$ represents the forcing and the boundary terms of the problem at hand, and $c : U \times Y \rightarrow \mathbb{R}$ is the L^2 product on the control domain. For the sake of notation, we define the controlled equation as $\mathcal{E} : (\mathcal{Y} \times \mathcal{U}) \times \mathcal{Q} \rightarrow \mathbb{R}$. Namely, (1) is verified when $\mathcal{E}((y, u), q) = 0$ for all q in \mathcal{Q} .

The goal of an OCP is to steer the solution towards a desired profile $y_d \in \mathcal{Z} \supseteq \mathcal{Y}$ by minimizing a convex *cost functional* $J : \mathcal{Y}_0 \times \mathcal{U} \rightarrow \mathbb{R}$ over $\mathcal{Y}_0 \times \mathcal{U}$ such that (1) is verified. The functional $J(y, u)$ must be defined case by case. For the well-posedness of the problem, the interested reader may refer to [20]. The minimization problem can be recast in an unconstrained fashion exploiting a Lagrangian approach [20, 43]. Thus, let us consider an arbitrary *adjoint variable* $z \in \mathcal{Y}_T \subset \mathcal{Q}$ and define the following Lagrangian functional

$$\mathcal{L}(y, u, z) = J(y, u) + \mathcal{E}((y, u), z)$$

. It is well known in literature [20], that the aforementioned minimization of problem is equivalent to the following system: find $(y, u, z) \in \mathcal{Y}_0 \times \mathcal{U} \times \mathcal{Y}_T$ such that

$$\begin{cases} D_y \mathcal{L}(y, u, z)[\omega] = 0 & \forall \omega \in \mathcal{Q} & \text{(adjoint equation),} \\ D_u \mathcal{L}(y, u, z)[\kappa] = 0 & \forall \kappa \in \mathcal{U} & \text{(optimality equation),} \\ D_z \mathcal{L}(y, u, z)[\zeta] = 0 & \forall \zeta \in \mathcal{Q} & \text{(state equation).} \end{cases} \quad (2)$$

In this context, the terms D_y, D_u and D_z will denote the differentiation with respect to the state, the control and the adjoint variables. We underline that, over the control domain, the optimality equation in strong form reads:

$$\alpha u - z = 0, \quad (3)$$

where the role of α will be clarified in the next sections. We decided to solve (2) using a *space-time discretization*. The space-time techniques have been successfully applied in many contexts, from parabolic equations [15, 44, 45, 46] to time-dependent PDE-constrained optimization [18, 19, 37, 39, 38]. For the sake of brevity, we are not presenting the details of such an approach. The main idea is to treat the three-equations system (2) as a steady one, where all the time instances are sought all-at-once by means of a direct solver. The reader may refer to the previous cited bibliography for an insight to the method.

For our purposes, it is enough to define a time discretization over $[0, T]$ divided in N_t sub-intervals. Namely, we consider $\Delta t > 0$ and the time instance $t_k = k\Delta t$ for $k = 0, \dots, N_t$. Let us focus on the state, adjoint and control variables evaluated at t_k . At each t_k , the variables can be expressed through the corresponding spatial bases, in our case Finite Element (FE) bases. From now on, for the sake of notation, y_k will denote the column vector of FE coefficients of the FE expansion. The same argument applies to control and adjoint variables at t_k , denoted by u_k and p_k . We remark that state and adjoint have been discretized with the same discretized function space [37] to guarantee the well-posedness of the problem (2). To simulate the solution of the OCP we solve a system of dimension $N_t(2\mathcal{N}_y + \mathcal{N}_u) \times N_t(2\mathcal{N}_y + \mathcal{N}_u)$ through a direct solver. This may lead to time consuming simulations to understand the field dynamic. To lighten these computational costs, one may use multigrid approaches combined with proper preconditioners, see e.g. [5, 33, 35] and the references therein. However, these iterative methods might only partially solve this issue. DMD-based techniques respond to the need of a fast prediction tool to avoid a complete simulation over the time interval $[0, T]$.

3 Dynamic mode decomposition with control

Dynamic mode decomposition (DMD) is a powerful method to identify and approximate dynamical systems using only few spatiotemporal coherent structures [6, 22]. It is ideally suited for time-dependent problems, and its data-driven nature makes it very versatile, also in industrial contexts [11, 41, 42].

When dealing with actuated systems, unfortunately, DMD fails to properly reconstruct the underlying dynamics since it is incapable of incorporating the contribution of the forcing term. To this end, dynamic mode decomposition with control (DMDc) [29] has been developed to overcome this issue. By including the actuation snapshots in the analysis it is able to provide reduced order representations for input-output systems. The DMDc method quantifies the effect of control inputs on the state of the system and computes the underlying dynamics without being confounded by the effect of external control. Recently, an extension for quantum control problems, called bilinear DMD, has been proposed in [16]. A local version of DMDc for predictive control of hydraulic fracturing can be found in [27], while for compressive system identification see [2].

Let us denote the snapshot representing the state of a system at the i -th time instant with $x_i \in \mathbb{R}^{\mathcal{N}}$, where \mathcal{N} represents the number of degrees of freedom of our system. We collect a set of N_t equispaced snapshots $\{x_i\}_{i=1}^{N_t}$ and we arrange them by column in two matrices, X and X' , where X' is the time-shifted version of X . We also collect the input control snapshots $\{\eta_i\}_{i=1}^{N_t-1}$, with $\eta_i \in \mathbb{R}^{\mathcal{L}}$, in the matrix Υ , obtaining the following matrices:

$$X = \begin{bmatrix} | & | & \dots & | \\ x_1 & x_2 & \dots & x_{N_t-1} \\ | & | & \dots & | \end{bmatrix}, \quad X' = \begin{bmatrix} | & | & \dots & | \\ x_2 & x_3 & \dots & x_{N_t} \\ | & | & \dots & | \end{bmatrix}, \quad \Upsilon = \begin{bmatrix} | & | & \dots & | \\ \eta_1 & \eta_2 & \dots & \eta_{N_t-1} \\ | & | & \dots & | \end{bmatrix}.$$

We remark that the snapshots can represent data coming from experiments, from simulations, or even sensors and acquired in real-time.

DMDc is a regression-based approach to system identification that is able to disambiguate the intrinsic dynamics, described by the matrix A , and the effects of control, described by the matrix B , as in the following

$$X' \approx AX + B\Upsilon = \begin{bmatrix} A & B \end{bmatrix} \begin{bmatrix} X \\ \Upsilon \end{bmatrix} := G\Xi. \quad (4)$$

We seek an approximation of the linear mappings A and B using only the three data matrices. We start by computing the SVD of the matrix Ξ in 4, which contains both the state and control snapshot information, as $\Xi \approx U\Sigma V^*$. With the symbol $*$ we denote the conjugate transpose, and we truncate the SVD keeping only the first r_Ξ modes. We can thus express the best-fit matrix $G \in \mathbb{R}^{\mathcal{N} \times (\mathcal{N} + \mathcal{L})}$ as

$$G \approx X'\Xi^{-1} = X'V\Sigma^{-1}U^*. \quad (5)$$

By rewriting $U^* = \begin{bmatrix} U_1^* & U_2^* \end{bmatrix}$, and by computing the SVD of the output matrix $X' \approx U_{X'}\Sigma_{X'}V_{X'}^*$, we can compute the reduced order approximation of A and B as

$$\tilde{A} = U_{X'}^* X' V \Sigma^{-1} U_1^* U_{X'}, \quad (6)$$

$$\tilde{B} = U_{X'}^* X' V \Sigma^{-1} U_2^*. \quad (7)$$

We remark that the truncation rank $r_{X'}$ of the SVD of the output matrix has to be less or equal to r_Ξ . With this reduced order operators we can write $\tilde{x}_{k+1} = \tilde{A}\tilde{x}_k + \tilde{B}\eta_k$, where $\tilde{x}_k = U_{X'}x_k$. The dynamic modes of A can be computed from the eigenvectors w of \tilde{A} as

$$\phi = X'V\Sigma^{-1}U_1^*U_{X'}w. \quad (8)$$

4 A partitioned approach for time-dependent OCPs

In this section we are going to explain how to handle OCPs with DMDc. Our goal is to characterize the relationship between the current measurements of the time-dependent OCP x_k , the future one x_{k+1} , and the current input η_k , given by the desired state y_d at each time instant t_k for a finite number of steps $k = 1, \dots, N_t$:

$$x_{k+1} = Ax_k + B\eta_k, \quad \forall k = 1, \dots, N_t - 1$$

. We remark that the current input for our OCP system is the desired state y_d . In fact, it represents the target state that we want to achieve and hence all the OCP variables (state, control, and adjoint) depend on it. Due to such a dependency, a modification in the desired state will cause a change in the other variables. We present a *partitioned approach* in order to identify two separate dynamical systems: one for the state, and one for the adjoint variables. The control can then be reconstructed through α and the adjoint variable by using the linear relation in (3). For the state variable, we use as measurement matrices $X_y \in \mathbb{R}^{\mathcal{N}_y \times (N_t - 1)}$ and $X'_y \in \mathbb{R}^{\mathcal{N}_y \times (N_t - 1)}$ given by:

$$X_y = \begin{bmatrix} | & | & & | \\ y_1 & y_2 & \dots & y_{N_t-1} \\ | & | & & | \end{bmatrix}, \quad X'_y = \begin{bmatrix} | & | & & | \\ y_2 & y_3 & \dots & y_{N_t} \\ | & | & & | \end{bmatrix}, \quad (9)$$

where each row represents the time series of the state measurement for a particular spatial point given by the space-time discretization. On the other hand, each column contains the coefficients of the FE expansion of the state space-time variable. The final model we obtain is:

$$X'_y = A_y X_y + B_y \Upsilon_d. \quad (10)$$

For the adjoint variable we have that $X_z \in \mathbb{R}^{\mathcal{N}_z \times (N_t - 1)}$, $X'_z \in \mathbb{R}^{\mathcal{N}_z \times (N_t - 1)}$ where each row represents the time series of the adjoint measurement and each column collects the coefficients of the FE expansion of the adjoint space-time variable. We obtain the DMDc model as:

$$X'_z = A_z X_z + B_z \Upsilon_d. \quad (11)$$

We emphasize that the input matrix Υ_d is the same for all the models.

5 Numerical results

In this section, we present the numerical results to validate the DMDC approach applied to OCPs. The first example takes into consideration an unsteady Graetz Flow boundary OCP. A second test case deals with a time-dependent OCP governed by Stokes equations. The experiments validate the performances of DMDC strategy in term of reconstruction and prediction. Indeed, we define the time-pointwise relative error E_k as:

$$E_k = \frac{\|x_k - \tilde{x}_k\|_2}{\|x_k\|_2}, \quad (12)$$

where x_k represents the generic true snapshot at time t_k , and \tilde{x}_k the approximated variable. This error is shown for the reconstruction analysis. For the prediction, we average (12) over all the time instances in the test data set. We vary the size of the training data set and we keep fixed 20 as dimension for the test data set, to understand sensitivity of the method with respect to the data needed for an accurate prediction. For the computations we used the following libraries: multiphenics [1], which is an implementation in FEniCS [25] for block-based systems, and PyDMD [12].

5.1 Boundary OCP governed by a Graetz Flow

Let us consider a boundary control governed by a Graetz Flow in the time interval $[0, T] = [0, 1]$ and in the rectangular space domain $\Omega = [0, 3] \times [0, 1] \in \mathbb{R}^2$ as depicted in Figure 1. The control

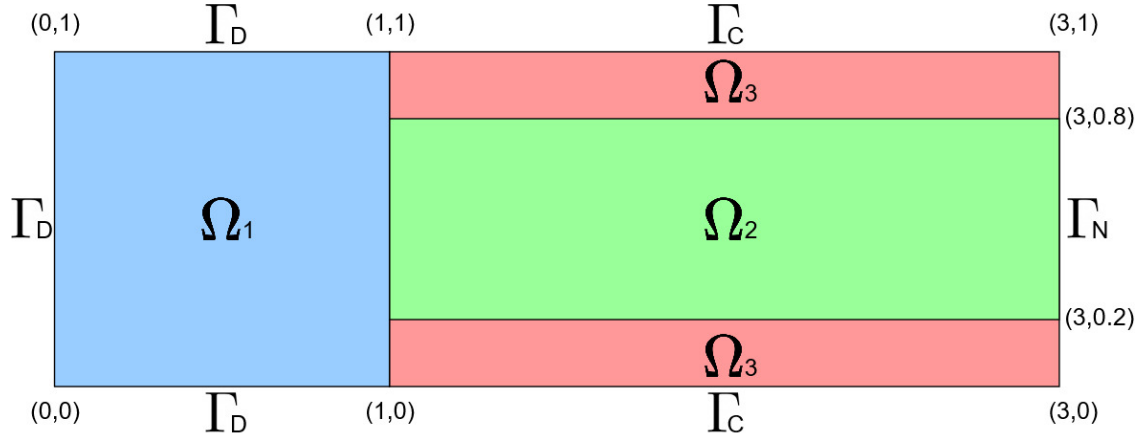


Figure 1: *Graetz Flow*: space domain.

domain is

$$\Gamma_C = ([1, 3] \times \{0\}) \cup ([1, 3] \times \{1\}),$$

while the observation domain is

$$\Omega_3 = ([1, 3] \times [0, 0.2]) \cup ([1, 3] \times [0.8, 1]).$$

The Neumann and the Dirichlet conditions are applied, respectively, to

$$\Gamma_N = \{3\} \times [0, 1] \text{ and } \Gamma_D = \partial\Omega \setminus (\Gamma_C \cup \Gamma_N).$$

We recall that $Y = H_{\Gamma_D}^1(\Omega)$, i.e. the set of functions that are H^1 in the domain but null on Γ_D , and the control space $U = L^2(\Gamma_C)$. We recall that we can recover an homogeneous problem of the form presented in section 2 after a lifting procedure [30]. Thus, the Lagrangian formulation of this OCP reads: find $(y, u) \in \mathcal{Y}_0 \times \mathcal{U}$ which solves:

$$\min_{(y,u) \in \mathcal{Y}_0 \times \mathcal{U}} J(y, u) = \frac{1}{2} \int_0^T \int_{\Omega_3} (y - y_d)^2 dxdt + \frac{\alpha}{2} \int_0^T \int_{\Gamma_C} u^2 dsdt \quad (13)$$

constrained to

$$\begin{cases} y_t - \epsilon \Delta y + \beta \cdot \nabla y = 0 & \text{in } \Omega \times (0, T), \\ y = 1 & \text{on } \Gamma_D \times (0, T), \\ \epsilon \frac{\partial y}{\partial n} = u & \text{on } \Gamma_C \times (0, T), \\ \epsilon \frac{\partial y}{\partial n} = 0 & \text{on } \Gamma_N \times (0, T), \\ y = y_0 & \text{in } \Omega \times \{0\}, \end{cases} \quad (14)$$

where $\epsilon = \frac{1}{12}$, the vector field β is defined as $[x_2(1 - x_2), 0]$, and x_2 as vertical spatial coordinate. The desired state profile is $y_d = 1 + t$, $\alpha = 10^{-2}$ is a penalization parameter on the control, and y_0 is a null function verifying the boundary conditions. For the discretization, we employed \mathbb{P}^1 elements for all the variables with $\mathcal{N}_y = \mathcal{N}_u = 2304$. Moreover, in terms of time discretization, we consider $\Delta t = 0.02$, leading to $N_t = 50$ time instances for the time interval $[0, 1]$. Thus, the global space-time dimension is 345600. In the left panel of Figure 2 we plotted the relative reconstruction error E_k for all the variables of interest and for every $k = 1, \dots, 50$. We used 4 DMD modes for the state and 3 for the adjoint. The mean relative error for the state is 1.3%, while for the adjoint variable is 3.2%.

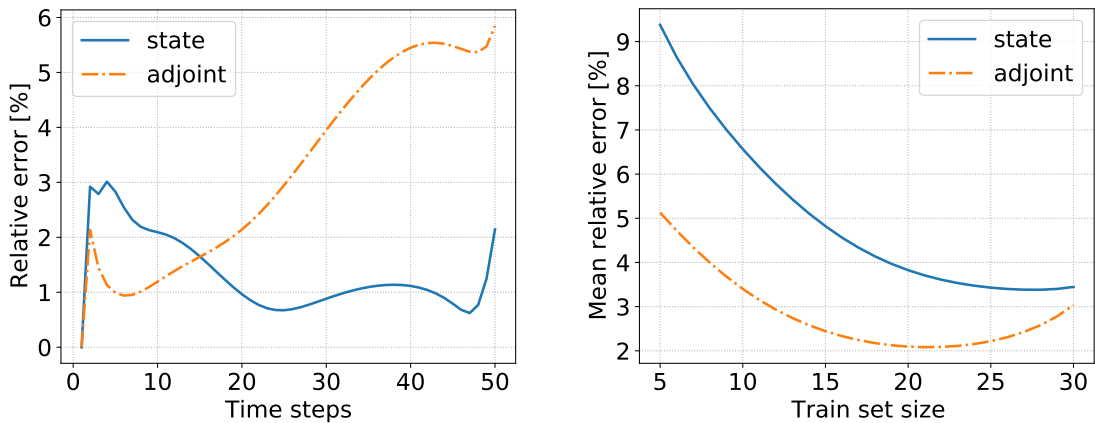


Figure 2: On the left the L^2 relative reconstruction error for the Graetz case for state and adjoint variables. On the right the L^2 mean relative prediction error. The average is done over 20 snapshots in the future.

In Figure 2 (right panel) we plotted the L^2 mean relative prediction error over 20 future states for the state, and adjoint variable, varying the dimension of the train dataset. We see that for the state variable we need at least 20 snapshots in order to have a satisfactory prediction accuracy below 4%, while for the adjoint variable 10 snapshots are sufficient.

5.2 OCP governed by time-dependent Stokes Equations

We now deal with a distributed control problem governed by time-dependent Stokes equation. Let us consider the spatial domain Ω as the unit square in \mathbb{R}^2 and the time interval $[0, 1]$. For this specific case $\Gamma_D = \partial\Omega$, and we consider

$$\mathcal{V}_0 \doteq \{v \in L^2(0, T; V) \text{ such that } v_t \in L^2(0, T; V^*) \text{ such that } v(0) = 0\}$$

with

$$V \doteq [H_{\Gamma_D}^1(\Omega)]^2 \text{ and } \mathcal{P} = L^2(0, T; L_0^2(\Omega)),$$

where $L_0^2(\Omega)$ is the space of functions that have null mean over Ω with L^2 regularity¹. We seek the state-control variable in $\mathcal{Y}_0 \times \mathcal{U}$ where $\mathcal{Y}_0 = \mathcal{V}_0 \times \mathcal{P}$ and $\mathcal{U} = [L^2(\Omega)]^2$. The specific problem

¹Numerically, to enforce the condition of null mean for the state pressure variable, we employed Lagrange multipliers. Namely, the condition is weakly imposed in integral form

$$\int_{\Omega} p \lambda \, dx = 0, \quad \forall \lambda \in \mathbb{R}. \quad (15)$$

we are dealing with is to find the minimum of

$$\min_{((v,p),u) \in \mathcal{Y}_0 \times \mathcal{U}} J((v,p),u) := \frac{1}{2} \int_0^T \int_{\Omega} (v - v_d)^2 dx dt + \frac{\alpha}{2} \int_0^T \int_{\Omega} u^2 dx dt, \quad (16)$$

constrained to the equations:

$$\begin{cases} v_t - \Delta v + \nabla p = u & \text{in } \Omega \times (0, T), \\ -\nabla \cdot v = 0 & \text{in } \Omega \times (0, T), \\ v = 0 & \text{on } \partial\Omega \times (0, T), \\ v(0) = 0 & \text{in } \Omega \times \{0\}, \end{cases} \quad (17)$$

where

$$v_d = \left[10(1+t) \left(1 + \frac{1}{2} \cos(4\pi t - \pi) \right), 0 \right] \in L^2(0, T; [L^2(\Omega)]^2) \quad (18)$$

is considered on the whole space-time domain, and $\alpha = 10^{-5}$. For the space discretization we employed $\mathbb{P}^2 - \mathbb{P}^1$ polynomials for the velocity and pressure fields both for the state and the adjoint variables, while for the control we used \mathbb{P}^2 polynomials. Thus, the FE dimension is 674 for state/adjoint velocity and control variables, while it is 337 for the state and adjoint pressure. In terms of time discretization, in the interval $[0, 1]$ we considered $N_t = 50$ time instances, with $\Delta t = 0.02$. The final dimension of the system is 134800.

In the left panel of Figure 3 we plotted the relative reconstruction error E_k for all the variables of interest and for every $k = 1, \dots, 50$. The error at the first time step is exactly 0, while the spike at the last time instant is due to the nature of DMD which divides the snapshots data into two shifted matrices and we have the accumulation of all the residuals. The maximum error is registered for the adjoint velocity and it is below 1.5%, while on average all the variables present an error below 0.6%. We remark that the adjoint pressure snapshots have been normalized removing the mean of all the states before applying the DMDc. Even if such preprocessing can be done only for reconstruction, we emphasize that the adjoint pressure in this case is not a variable of interest for prediction purposes since only the adjoint velocity affects the control in the optimality equation. Nonetheless we present its relative reconstruction error in order to show that the partitioned approach is able to deal also with such variable.

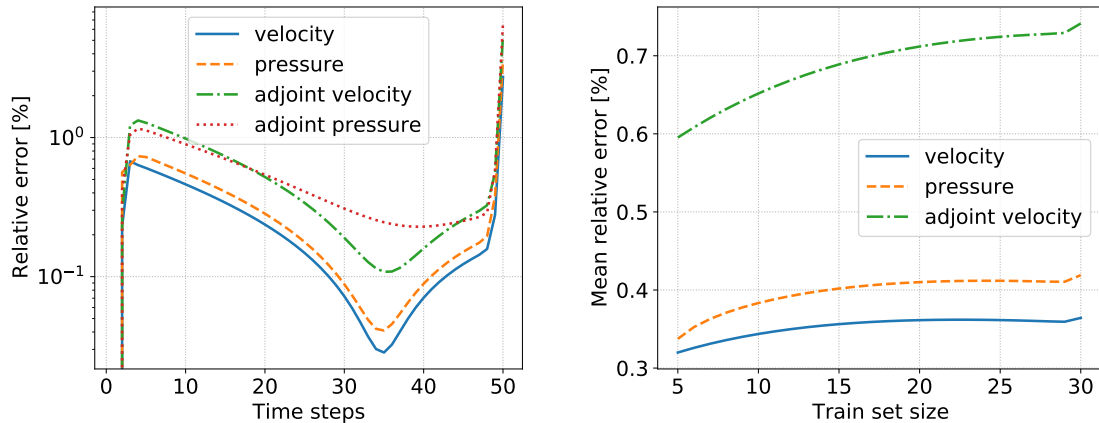


Figure 3: On the left the L^2 relative reconstruction error for the Stokes case for velocity, pressure, and the adjoint variables. On the right the L^2 mean relative prediction error. The average is done over 20 snapshots in the future.

In Figure 3 (right panel) we plotted the L^2 mean relative prediction error over 20 future states for velocity, pressure, and adjoint velocity, varying the dimension of the train dataset. We notice an almost stationary behaviour of the mean error for all the variables of interest, with all the values below 0.8%. This suggests that the future state prediction is robust with respect to the amount of available data.

This constraint reflects in the derivation of the adjoint equation and an extra term appears in the divergence free constraint in weak form.

5.3 Speedup considerations

The computational gain provided by the data-driven approach is considerable for both the test problems. The one-shot approach takes between 13 and 18 minutes, depending on the problem at hand, in order to compute all the variables. The partitioned approach exploiting DMDC, instead, requires less than 1 second for the construction of the reduced operators, and approximately 2 seconds to predict all the quantities on interest for the entire time spans considered. This results in a speedup $\sim \mathcal{O}(10^2)$.

6 Conclusions and perspectives

In this work we showed the potential of data-driven methods for the resolution of time-dependent optimal control problems with PDE constraints. A further improvement of the work might concern a deeper analysis of the sensitivity of the problems with respect to the penalization parameter α which drastically changes the magnitude of the adjoint variable. Another possible approach could be to use the data-driven sparse identification of nonlinear dynamics with control method [7], instead of DMDC. Lastly, we stress that even if the test cases are quite academic, we believe in the potential of such an approach in more complex setting based on data collection. Indeed, this represents a first attempt for a deeper study of this formulation, which might be of interest in many interdisciplinary research fields.

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