MODEL ORDER REDUCTION OF PARAMETER-DEPENDENT
PARTICLE LADEN FLOWS

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Abstract
In this contribution, we extend our previously-developed framework for model order reduction of transport-dominated systems towards parameterized cases. The method combines the shifted proper orthogonal decomposition with interpolation via artificial neural networks. The resulting framework is an a-posteriori one, i.e., for parameterized systems, time-dependent solutions for several parameter values are required for the construction of the reduced-order model (ROM). The ROM can then be cheaply evaluated to predict the solution for previously unseen parameter values. The method is suitable for industry-relevant transport-dominated systems, such as particle-laden flows, where traditional mode-based methods, such as proper orthogonal decomposition (POD), often fail.

Keywords: Model order reduction, shifted POD, artificial neural networks, CFD-DEM, OpenFOAM.

1 Introduction
Systems comprising a fluid and a dispersed solid phase, that is, particle-laden flows, are prevalent in both nature and industry, with examples ranging from pneumatic conveying to transport of sediments in river beds [1, 2]. However, these systems are usually transport-dominated and exhibit non-linear behavior [3], which is transferred into their governing equations. Both these characteristics may incur severe limitations when attempting efficient and accurate model order reduction (MOR). First, the transport dominance leads to a slowly decaying Kolmogorov $n$-width of the system [4], which results in a requirement of a high-dimensional reduced basis of the system when conventional reduced order modeling (ROM) techniques, e.g. proper orthogonal decomposition (POD) [5] are employed. Second, the nonlinearity of the system further reduces the applicability of conventional ROM approaches as these are based on the assumption of modal linear superposition [6].

In the present contribution, we aim to enable the solution of a parameterized time-dependent simulation of a laminar particle-laden flow with a low number of individual particles that will be computationally feasible for real-time or multi-query scenarios. As the full order model, we consider an Eulerian-Lagrangian framework combining computational fluid dynamics (CFD) and discrete element method (DEM) described in [3]. However, the presented findings are transferable to any standard fully resolved CFD-DEM simulation such as the ones described in [7] or [8].

Although an efficient MOR for DEM is still an open issue, we are particularly interested in the MOR of fluid flow with the specifics caused by the combination of CFD and an immersed boundary method [9] to include a moving solid phase. The flow is described by the Navier-Stokes equations and their parameterized numerical solution is used to generate a matrix of snapshots $Y = [y(x, (t_j, \mu_p))], Y \in \mathbb{R}^{m \times NP}$, where $m$ is the dimension stemming from the spatial discretization of the system, $N$ number of temporal snapshots and $P$ number of values of the parameter $\mu \in \mathbb{R}$ used.

However, because the particle-laden flows tend to be transport-dominated, the decay of their Kolmogorov $n$-width is slow and the singular value decay of the matrix $Y$ is slow as well. To allow for the construction of a low-dimensional, yet sufficiently accurate reduced basis, we employ the idea of transport reversal (e.g. [10]). We utilize the shifted proper orthogonal decomposition (sPOD) by Reiss et al. [11], an optimization algorithm capable of treating systems with multiple transports that reconstructs $Y$ as a superposition of data in multiple frames of reference. The
fundamental assumption of the sPOD application is that in these frames of reference, the decay of the Kolmogorov $n$-width is significantly faster.

To extend the prepared reduced-basis applicability to non-linear parameterized systems, we construct the reduced-order model by using artificial neural networks as a data-driven replacement for standard projection techniques. First, the usage of artificial intelligence in the field of MOR is growing, with more complex architectures allowing more complex tasks, see, e.g., [6, 12, 13]. Second, we have already introduced an analogous framework for non-parameterized systems in our previous contributions [14, 15]. A similar method for parameterized systems has since been applied in Burela et al. [16], where they treated models of the spread of forest fires.

This paper is structured as follows: in the first part, we briefly explain the general model order reduction goals and the construction of the reduced basis. We discuss the specifics of the basis construction for transport-dominated systems and sPOD that we use for the task. Afterwards, we examine the construction of the reduced order model itself via artificial neural networks. In the results section we present parameterized von Kármán vortex street, where POD can be used successfully, and a second model of two discs traveling through the fluid, on which the shifted POD variant will be demonstrated.

2 Methods

The general goal of model order reduction is to decrease the computational complexity of a system by reducing its degrees of freedom (DoFs). Let us consider a parametric system stemming from a spatial discretization of a general PDE, which can be written in the form of

\[ \dot{y}(t, \mu) = Ay + b(t, \mu, y(t, \mu)), \quad t \in [0, T], \quad y(0, \mu) = y_0(\mu), \]

where $y : [0, T] \times \mathbb{R}^p \rightarrow \mathbb{R}^m$ is the semi-discrete variable of interest, whose dimension $m$ depends on the used spatial discretization. By $A \in \mathbb{R}^{m \times m}$ and $b : [0, T] \times \mathbb{R}^p \times \mathbb{R}^m \rightarrow \mathbb{R}^m$ we mark, in order, the linear and non-linear parts of mapping on the right-hand side of (1). Finally, $t \in [0, T]$ and $\mu \in \mathbb{R}^p$ are the system independent variable (time) and parameters, respectively. We seek to replace this system with a low-dimensional alternative. For simplicity, let us consider a case with only one parameter $\mu \equiv \mu \in \mathbb{R}$.

The selected MOR approach is an a posteriori one, that is, we use the known time-dependent solution for several values of the parameter $\mu_p, p = 1, \ldots, P$, to construct the reduced-order model. The solution is saved into a matrix of snapshots,

\[ Y = [y(t_1, \mu_1), \ldots, y(t_N, \mu_1), \ldots, y(t_1, \mu_P), \ldots, y(t_N, \mu_P)] \in \mathbb{R}^{m \times N \times P}, \]

where $N$ is the number of temporal snapshots and $P$ the number of pre-evaluated parameter values. The efficiency and accuracy of the prepared reduced order model are determined by two factors, (i) the selection of a reduced basis (RB) required to obtain a low-rank approximation of $Y$, and (ii) the approach to use the selected RB for ROM construction.

Reduced basis construction The fundamental assumption is that although the solution of a parameterized system (1) belongs to a high-dimensional space, it lies in a low-dimensional solution manifold embedded in this space. This assumption is leveraged to seek and identify a suitable basis of the solution manifold that can be truncated to obtain a reduced basis spanning an approximate trial manifold. A standard choice for the RB construction is the proper orthogonal decomposition (POD) by Pearson [5], which can be written as

\[ Y \approx Y^\ell = \Psi^\ell \Sigma^\ell (V^T)^\ell = \Psi^\ell \Sigma^\ell, \quad \Psi^\ell \in \mathbb{R}^{m \times \ell}, \quad \Sigma^\ell \in \mathbb{R}^{\ell \times \ell}, \quad (V^T)^\ell \in \mathbb{R}^{\ell \times N \times P}, \]

where $\ell \ll \min(m, N \times P)$ is the chosen rank of truncation, $\Sigma^\ell = \text{diag}(\sigma_1, \ldots, \sigma_\ell)$ the matrix of singular values sorted from largest to smallest and $\Psi^\ell$ and $(V^T)^\ell$ are matrices comprising orthonormal vectors. The relative error in Frobenius norm of the approximation $Y \approx Y^\ell$ is

\[ \mathcal{E}_F(Y, Y^\ell) = 1 - \sum_{r=1}^{\ell} \frac{\sigma_r^2}{\sum_{r=1}^{\min(m, N \times P)} \sigma_r^2}. \]
Consequently, the faster the decay of singular values, the lesser rank \( \ell \) is sufficient for a given approximation error. In other words, the faster the decay on the Kolmogorov \( n \)-width of the system is, the better choice is POD for the RB construction.

The matrix \( \Psi^f \) serves as the reduced basis of \( Y \). It consists of orthonormal vectors \( \psi_r, r = 1, \ldots, \ell \). The decomposition (3) can be interpreted as each vector \( \psi_r \), representing a spatial structure, topos. Then, the matrix \( H^f \),

\[
H^f = \Sigma^f (V^T)^\ell, \quad H^f = \begin{bmatrix} \eta_1(t_1, \mu_1) & \cdots & \eta_1(t_N, \mu_1) & \cdots & \eta_1(t_{NP}, \mu_1) \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \eta_P(t_1, \mu_1) & \cdots & \eta_P(t_N, \mu_1) & \cdots & \eta_P(t_{NP}, \mu_1) \end{bmatrix} = \begin{bmatrix} \eta_1^T \\ \vdots \\ \eta_P^T \end{bmatrix},
\]

where \( \eta_r \in \mathbb{R}^{NP}, r = 1, \ldots, \ell \) is a time and parameter-dependent amplitude. Note that \( \eta_r^T = [(\eta_r^{\mu_1})^T, \ldots, (\eta_r^{\mu_P})^T] \) with \( \eta_r^{\mu_p} \in \mathbb{R}^N, p = 1, \ldots, P \), is a purely time-dependent chronos for the parameter \( \mu_p \). We denote a mode a pair of \( \psi_r \) and \( \eta_r \).

**Transport-dominated systems** For transport-dominated systems with no special treatment, the fundamental assumption used for RB construction is not valid, the decay of Kolmogorov \( n \)-width of \( Y \) is extremely slow [10]. Here, we treat the transport within the framework proposed by Reiss et al. [11], further extended in [17], and applied in [16]. In particular, the data saved in matrix \( Y \), which we assume contains \( N_t \) types of transport (in our case, \( N_t \) particles), is sorted into \( \{Y_k\}_{k=1}^{N_t}, Y_k \in \mathbb{R}^{m \times NP} \), where each \( Y_k \) is treated in its own co-moving frame of reference. The matrix \( Y \) is then approximated by shifted superposition of these frames as

\[
Y = \sum_{k=1}^{N_t} T^{-\Delta_k} (Y_k) \approx \sum_{k=1}^{N_t} T^{-\Delta_k} (Y_k^f) = \sum_{k=1}^{N_t} T^{-\Delta_k} (\psi_k^f H_k^f),
\]

where \( T \) is the transport operator. In the algorithm, the data is first shifted into the co-moving frames of reference \( T^{-\Delta_k}(t, \mu)(y(t, \mu, x)) = y(t, \mu, x - \Delta_k(t, \mu)) \). In those frames of reference, transport is compensated for, and the decay of Kolmogorov \( n \)-width of each \( Y_k \) is significantly faster. For the \( Y \) reconstruction, a reverse transport operator \( T^{\Delta_k} \) is applied.

The shifts \( \{\Delta_k\}_{k=1}^{N_t} \) are time and parameter dependent and analogously to \( \eta_r \), they are in the form

\[
\Delta_k^f(t, \mu) = [(\Delta_k^{\mu_1})^T, \ldots, (\Delta_k^{\mu_P})^T], \quad \Delta_k \in \mathbb{R}^{NP \times d},
\]

where \( d \in \{1, 2, 3\} \) is the spatial dimension of the system and \( (\Delta_k^{\mu_p})^T \in \mathbb{R}^{NP \times d}, p = 1 \ldots P \), is the purely time-dependent part of the shift for parameter value \( \mu_p \). While POD is purely data-driven, sPOD needs at least discrete versions of the shift operators \( T^{\Delta_k}, k = 1 \ldots N_t \) for the sorting.

**Reduced-order modeling** As the next step, a continuous reduced-order dynamic system is modeled. Traditionally, when POD is used to construct the reduced basis, the dynamic system is modeled by the Galerkin projection, which uses matrix \( \Psi^f \) to project the system (1) onto the low-dimensional solution manifold [18],

\[
\dot{y}^f = A^f y^f + b^f(t, \mu, \Psi^f y^f), \quad y^f(t) \in \mathbb{R}^\ell, \quad t \in (0, T], \quad y^f(0, \mu) = y_0^f(\mu)
\]

\[
A^f = (\Psi^f)^T A \Psi^f, \quad b^f(t, \mu, \Psi^f y^f) = (\Psi^f)^T b(t, \mu, y^f),
\]

where \( y^f : [0, T] \to \mathbb{R}^\ell \) is the new variable of interest in the reduced-order subspace, \( A^f \in \mathbb{R}^{\ell \times \ell} \) is the linear part of the new mapping and \( b^f : [0, T] \times \mathbb{R} \to \mathbb{R}^\ell \) the non-linear part. Alternatively, POD-Galerkin can be combined with discrete empirical interpolation method or similar method for further reduction of the system non-linearities [19, 20].

However, sPOD does not produce a single \( \Psi^f \) suitable for the Galerkin projection, but rather \( \{\Psi_k^f\}_{k=1}^{N_t} \). This limitation compels us to use a purely data-driven approach for reduced dynamics modeling instead. In particular, to approximate the mapping \( (t, \mu) \to \eta_{r,k}(t, \mu) \), respectively \( (t, \mu) \to \Delta_k(t, \mu) \), we combine sPOD with artificial neural networks. The training
data for the network consists of the vectors $\eta_{r,k} \in \mathbb{R}^{NP}$, $r = 1 \ldots \ell$, $k = 1 \ldots N_t$, respectively $\Delta_k \in \mathbb{R}^{NP \times d}$, $k = 1 \ldots N_t$, used as labels, and the features in the form of

$$X = [(t_1, \mu_1), \ldots, (t_N, \mu_1), \ldots, (t_1, \mu_P), \ldots, (t_N, \mu_P)]^T \in \mathbb{R}^{NP \times 2}. \quad (9)$$

As a surrogate, we have used a deep feedforward network implemented in the Python library TensorFlow [21], with architecture inspired by [16]. It comprised 3 hidden layers with 50, 70 and 80 neurons, respectively. The differences between our network and the architecture used in [16] were that hyperbolic tangent was employed as the activation function, instead of the Exponential Linear Unit (ELU) and Leaky Rectified Linear Unit (LeakyReLU). For the training, we have chosen the mean squared error as the loss function and utilized the Levenberg-Marquardt algorithm, taken from [22], for its minimization.

After the training, in the online phase, the networks can be used to predict the estimate

$$\tilde{Y}^{\mu_{\text{new}}} = \sum_{k=1}^{N_t} T^{-\Delta_k} \left( \tilde{Y}_{k}^{\ell, \mu_{\text{new}}} \right) = \sum_{k=1}^{N_t} T^{-\Delta_k} \left( \Psi_k \tilde{H}_k^{\ell, \mu_{\text{new}}} \right), \quad \tilde{Y}^{\mu_{\text{new}}} \in \mathbb{R}^{m \times N}, \quad (10)$$

where $\left( \tilde{H}_k^{\ell, \mu_{\text{new}}} \right)^T = [\tilde{\eta}_{1, \mu_{\text{new}}}, \ldots, \tilde{\eta}_{N, \mu_{\text{new}}}] \in \mathbb{R}^{\ell \times N}$. The tildes above some of the variables signify that the ANN was used for their construction.

**Overall framework** Our resulting method is called the shifted proper orthogonal decomposition with interpolation via artificial neural networks (sPODIANN). It relies heavily on the offline-online split, where the relatively time-consuming shifted POD, as well as the training of the neural network, are performed offline. The online evaluation stage of the method comprises prediction via the trained network, $N_t$ matrix multiplications to reconstruct the frames $\tilde{Y}_{k}^{\ell, \mu_{\text{new}}}$, and shifting the frames using $T^{-\Delta_k}$. A more comprehensive description for non-parameterized systems can be found in our previous contribution [14].

### 3 Examples

In the following paragraphs, we present model order reduction of two parameterized full order models stemming from CFD computations based on the finite volume method (FVM). The first case presented is the laminar von Kármán vortex street with $\mu \equiv \text{Re}$, which is not transport-dominated and (non-shifted) POD was sufficient. The case is used to evaluate the PODIANN capability to treat parameterized systems. The second case is focused on the particle-laden flow and utilizes the full sPODIANN framework. The system comprises two discs traveling through a fluid with different prescribed velocities. Here, the parameter $\mu$ describes the velocities of the discs.

**Full order models description** Both the above-listed numerical examples were simulated using our in-house CFD-DEM solver for particle-laden flows implemented in the C++ library OpenFOAM, the open hybrid fictitious domain-immersed boundary solver coupled with the discrete element method, openHFDIB-DEM [3]. In this solver, the particle-fluid interaction is fully resolved with the particles projected into the computational domain via the indicator field $\lambda$, $\lambda \in [0, 1]$, where $\lambda = 0$ for cells inside the fluid, $\lambda = 1$ for cells inside the solid body and $\lambda \in (0, 1)$ for those containing the solid-fluid boundary. The resulting set of Navier-Stokes equations for an incompressible flow of a Newtonian fluid with the solid-induced direct forcing term $f_{\text{ib}}$ is,

$$\begin{align*}
\partial_t \mathbf{u} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) - \nabla \cdot (\nu \nabla \mathbf{u}) &= -\nabla \bar{p} + f_{\text{ib}}, \\
\nabla \cdot \mathbf{u} &= 0,
\end{align*} \quad (11)$$

where $\mathbf{u}$ is the fluid velocity, $\nu$ the kinematic viscosity, $\bar{p}$ the kinematic pressure.
The movement of solid particles is solved using DEM. Hence, each solid body carries its own set of Newton equations of motion. For the $i$-th body, the considered equations are,

$$m_i \frac{d^2 \mathbf{x}_i}{dt^2} = \mathbf{f}_i^g + \mathbf{f}_i^d + \mathbf{f}_i^c, \quad I_i \frac{d\omega_i}{dt} = \mathbf{t}_i^g + \mathbf{t}_i^d + \mathbf{t}_i^c,$$

where $m_i$ is the mass of the particle $i$ and $\mathbf{x}_i$ its position. The considered forces acting on particle $i$ are the gravity $\mathbf{f}_i^g$, drag $\mathbf{f}_i^d$, and contact $\mathbf{f}_i^c$. The matrix of the inertial moments of the body $i$ is denoted by $I_i$, its angular velocity by $\omega_i$, and by $\mathbf{t}$ we mark the torques corresponding to forces $\mathbf{f}$.

As stated in the Introduction, we are interested purely in MOR of the system (11). Furthermore, for both the selected example cases, the DEM part of the solver is not required as the solids are either fixed (von Kármán vortex street) or move with prescribed velocities independently of the acting forces (Travelling discs).

**Von Kármán vortex street** The canonical case of two-dimensional laminar von Kármán vortex street is not a transport-dominated one; therefore, POD was sufficient for the construction of the reduced basis. However, the case was chosen to illustrate the benefits of interpolation via ANNs compared to the computationally cheaper piecewise linear interpolation. The full order model (FOM) was prepared using parameter values $Re = [50, 55, 60, \ldots, 110]$, that is, $P = 13$, and the number of used temporal snapshots was $N = 751$. We have chosen the velocity field for the analysis, i.e., the dimensionality of the variable was 2 and the used FVM mesh consisted of 36,000 FVM cells, which gave $m = 72000$.

Both FOM and tested ROMs were evaluated for a previously unseen parameter $Re = 81$. The values of $\eta_{\mu=81}^r, r = 1 \ldots \ell$, were obtained either by a neural network prediction (PODIANN) or by piecewise linear interpolation between the known values (PODI), that is by

$$\eta_{\mu=81}^r \approx (1 - \delta) \eta_{\mu_i}^r + \delta \eta_{\mu_{i+1}}^r, \quad \delta = \frac{\mu - \mu_i}{\mu_{i+1} - \mu_i}, \quad i = 1, \ldots, P - 1, \quad \mu \in (\mu_i, \mu_{i+1}).$$

In Fig. 1a, see that the singular value decay, which corresponds to the decay of the Kolmogorov $n$-width, is sufficiently fast. Ignoring the first mean mode, the modes 2 and 3 represent 98.1% of total fluctuation energy, calculated as $\sqrt{\frac{\sum_{r=2}^3 \sigma_r^2}{\sum_{r=2}^N \sigma_r^2}}$. The modes 1, 2 and 3 were chosen for the ROM construction, i.e., $\ell = 3$. In Fig. 1, see that the relative a-posteriori reconstruction error, calculated as

$$\varepsilon_R(t) = \frac{1}{M} \max_{(i,t)}(\|u\|) - \min_{(i,t)}(\|u\|) \sum_{i=1}^M \|u_i(t) - \bar{u}_i(t)\|,$$

Figure 1: Parameterized von Kármán vortex street, velocity field. (a) Singular value decay for matrix $Y$, (b) time evolution of global relative error between FOM and ROM for unseen parameter value $Re = 81$, (c) FOM for $Re = 81$ at $t = 0.5$, (d) PODI approximation of (c), (e) PODIANN approximation of (c). ROM dimension $\ell = 3$ for both PODI and PODIANN.
The second case considered is a two-dimensional system with two discs traveling through a rectangular domain filled with fluid and endowed with periodic boundary conditions. The discs move in parallel with prescribed velocities $c_1 = 0.01\mu$ and $c_2 = 0.02\mu$, respectively. The ROM was prepared from $\mu = [1, 1.5, 2]$, i.e., $P = 3$. The particle Reynolds number for these values ranges from 10 to 40; therefore, the flow is laminar with no vortex shedding observed. The case comprises 45000 FVM cells; 201 temporal snapshots were used for ROM preparation. The ROM was then evaluated for an unseen parameter value $\mu = 1.25$.

In Fig. 2 we present the analysis of the $\lambda$ field, that is, the indicator field for solid/fluid. In Fig. 2a see that the singular value decay for this system is extremely slow; however, shifted POD is able to sort the data into their optimal frames of reference and quickly hits the machine precision. The total amount of information in the first mode, calculated as $
abla = \sum_{r=1}^{NP} \sigma_r^2 / \sigma_1^2$, is 99.97 % for both sPOD frames; therefore in each frame, one mode was chosen for the ROM construction. The $\lambda$ field for $\mu$ values used for the ROM preparation is shown in Fig. 2c–e. In Fig. 2f, we present the FOM at the unseen parameter value; in Fig. 2g its sPODIANN approximation. A comparative slice along the red line in Fig. 2f can be seen in Fig. 2b.

In Fig. 3, see the ROM results for the velocity field generated by the discs. The singular value decay for POD is again slow. However, when using sPOD, it is significantly faster for both co-moving frames considered. The total amount of information contained in the first two modes, which were used for the ROM construction, is 99.5 % and 99.7 %, respectively. Similarly to the $\lambda$ field, we present the qualitative view of the velocity field for the $\mu$ values used for ROM preparation in Fig. 3c–e. The FOM for the unseen parameter value is shown in Fig. 2f and the sPODIANN approximation in Fig. 2g.
Figure 3: Two moving discs, velocity field. (a) singular value decay for POD and both sPOD frames, (b) evolution of global relative error for sPODIANN reconstruction vs. FOM, (c) – (e) velocity field for $\mu$ values used for ROM construction, (f) velocity field for unseen parameter value $\mu = 1.25$, (g) sPODIANN reconstruction. The $\mathbf{u}$ field snapshots at $t = 1$ are shown in (c)–(g).

prediction in Fig. 2g. Slight discrepancies are visible, especially in the upper part of the fields; however, the general trends hold. The global a posteriori reconstruction error (14) ranges from 8 to 11 %.

The performances of non-parameterized PODIANN and sPODIANN were compared in our previous contributions, where sPODIANN outperformed PODIANN for all the discussed transport-dominated systems [14, 15]. For the parameterized sPODIANN, further tests need to be performed on more complex systems, especially on those, where $\Delta_k$ depends on $\mu$ nonlinearly.

4 Conclusion

In this paper, we have built on our framework sPODIANN, a method tailored for model order reduction of transport-dominated systems, such as particle-laden flows, and extended it to parameterized systems. The method combines shifted POD, an algorithm that utilizes transport reversal to build an accurate reduced basis, with interpolation via artificial neural networks used to construct the reduced-order model itself. First, ANN-based interpolation was shown to outperform linear interpolation for the parameterized von Kármán vortex street, where the shifted POD was not needed and the reduced basis was extracted using the standard POD. Next, the complete sPODIANN framework was tested on a simple parameterized case with two traveling particles simulated using CFD-DEM, where it showed promising results, with the relative error between the FOM and the sPODIANN estimate being around 9 %. However, further tests are needed to examine the framework behavior when treating more complex systems.

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References


