CFD motivated applications of model order reduction

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1 Introduction

The ongoing advances in numerical mathematics and available computing power combined with the industrial needs promote a development of more and more complex models. However, such models are, due to their complexity, expensive from the point of view of the data storage and the time necessary for their evaluation. The model order reduction (MOR) seeks to reduce the computational complexity of large scale models. We present an approach to MOR based on the proper orthogonal decomposition (POD) with Galerking projection, which is well described for example by Pinnau [4] or Volkwein [5]. The problems arising from the nonlinearities present in the original model are adressed within the framework of the discrete empirical interpolation method (DEIM) of Chaturantabut and Sorensen [1].

The main contribution of this work consists in providing a link between the POD-DEIM based MOR and OpenFOAM[3]. OpenFOAM is an open-source CFD toolbox capable of solving even industrial scale processes. Hence, the availability of a link between OpenFOAM and POD-DEIM based MOR enables a direct order reduction for large scale systems originating in the industrial practice.

2 Model order reduction based on proper orthogonal decomposition and discrete empirical interpolation

The proper orthogonal decomposition is a projection method for reducing the dimensions of general large-scale ODE systems regardless of their origin[4]. However, within our work we will restrict our interest to the systems obtained from the semi-discretization of time dependent or parameter dependent partial differential equations (PDEs). Furthermore, given our interest in OpenFOAM, which is a finite volume method (FVM) based solver for the problems of the computational fluid dynamics (CFD), we will take a special interest in ROM of the large-scales ODE systems generated by the FV discretization of the Navier-Stokes equations.

A scalar nonlinear PDE for an unknown function $y : \mathbb{R} \times \mathbb{R}^3 \to \mathbb{R}$ may be rewritten as

$$\dot{y} + \mathcal{L}(t, y) = 0\,, \tag{1}$$

where the operator $\mathcal{L}$ represents all the terms of the original PDE apart from the temporal derivative. After the FV semi-discretization of the equation (1) one obtains the system

$$\Delta\Omega^h \dot{y} + \mathcal{L}^h(t, y) = 0\,, \tag{2}$$

where $\mathcal{L}^h(t, y)$ is the FV spatial discretization operator corresponding to the operator $\mathcal{L}$ and $\Delta\Omega^h := \mathrm{diag}(\delta\Omega_i^h) \in \mathbb{R}^{m\times m}$ is a diagonal matrix in which the symbol $\delta\Omega_i^h$ represents a volume of one element of the computational domain discretization.

In the OpenFOAM software, the operator $\mathcal{L}^h(t,y)$ has the structure $\mathcal{L}^h(t,y) = -\tilde{A}(t)y - \tilde{b}(t,y)$, where the linear, implicitly discretized, members are lumped in the term $\tilde{A}(t)y$ and the explicitly discretized nonlinearities are used for the construction of the vector $\tilde{b}(t,y)$. The size of the matrix $\tilde{A}$ and of the vector $\tilde{b}$ is determined by the number of the cells in the FV discretization mesh, m. Because the matrix $\Delta\Omega^h$ is diagonal, its inversion is cheap and one can rewrite the equation (2) as a (large) system of ODEs,

$$\dot{y} = A(t)y + b(t,y), \quad y(0) = y_0, \quad A(t) = (\Delta\Omega^h)^{-1}\tilde{A}(t),\, b(t,y) = (\Delta\Omega^h)^{-1}\tilde{b}(t,y)\,. \tag{3}$$

As POD is a projection method, its main objective is to find a subspace approximating a given set of data in an optimal least-square sense. In our case, the data is generated by sampling the solution of the full order model (3) at given times, $\{y_j := y(t_j)\}_{j=1}^n$, $t_j \in (0,T]$. These samples are called snapshots. The details on the theory of POD may be found for example in[4]. We will restrict our description to a sketch of the process of the reduced order model construction.

Let us denote the space containing the solution of the system (3) and its orthogonal basis as $V = \text{span}\{\psi_j\}_{j=1}^d$. Then it is possible to rewrite the solution of (3) as

$$y(t) = \sum_{j=1}^{d} \eta_j\, \psi_j,\, \forall t \in [0,T], \quad \eta_j(t) := \langle y(t), \psi_j\rangle_W, \quad d = \dim(V)\,, \tag{4}$$

where by $\langle\cdot,\cdot\rangle_W$ we denote a W-weighted inner product in the L^2 space. The Fourier coefficients η_j, $j = 1,\ldots,d$, are functions that map $[0,T]$ into $\mathbb{R}$.

We arrange the members of the sum in (4) in descending order by the amount of information on the original system they carry, take the first $l \leq d$ members of and introduce the ansatz

$$y^\ell(t) = \sum_{j=1}^{\ell} \eta_j^\ell\, \psi_j,\, \forall t \in [0,T], \quad \eta_j^\ell(t) := \langle y^\ell(t), \psi_j\rangle_W, \quad l \leq d\,, \tag{5}$$

which is an approximation of $y(t)$ provided $\ell < d$. Inserting (5) into (3) and assuming that the equality holds after projection of V on the ℓ-dimensional subspace $V^\ell = \text{span}\{\psi_j\}_{j=1}^\ell$ we obtain the following system,

$$\dot{\eta}^\ell = A^\ell\eta^\ell + f^\ell(t,\eta^\ell),\, \forall\, t \in (0,T], \quad \eta^\ell(0) = \eta_0^\ell\,, \tag{6}$$

where we defined the reduced system matrix

$$A^\ell := (a_{ij}^\ell) \in \mathbb{R}^{l\times l}, \quad a_{ij}^\ell = \langle A\psi_j, \psi_i\rangle_W\,, \tag{7}$$

the ROM nonlinearities $f^\ell = (f_i^\ell)^{\mathrm{T}} : [0,T] \to \mathbb{R}^\ell$, $f_i^\ell(t,\eta) = \left\langle f\left(t, \sum_{j=1}^\ell \eta_j\psi_j\right), \psi_i\right\rangle_W$, and the initial condition $\eta^\ell(0) = \eta_0^\ell = (\langle y_0,\psi_1\rangle_W, \ldots, \langle y_0, \psi_l\rangle_W)^{\mathrm{T}}$. The dimension of the newly defined system (6) is $\ell \leq d \leq m$.

The quality of the approximation is largely dependent on the choice of basis functions $\{\psi_j\}_{j=1}^\ell$. For the sake of brevity, let us only state (the proof may be found in[5]) that the columns of the matrix $\Psi \in \mathbb{R}^{m\times\ell}$ calculated via the Algorithm 1 are a suitable basis for the discrete representation of the space V^ℓ.

Furthermore, to make ROM completely independent of the full system dimension, it is necessary to address two issues. The first issue is the time dependence of the matrix A, which would cause the need to recalculate the matrix A^ℓ for each ROM evaluation.

A way to resolve the time dependence of the matrix A is to sample the system matrices the same way as the full system solution and to interpolate between the full system matrix snapshots. If one uses the linear interpolation, it is possible to write the approximate system matrix as

$$\hat{A}(t) := \varpi(t)A_{i-1} + (1 - \varpi(t))A_i, \quad \varpi(t) = \frac{t - t_{i-1}}{t_i - t_{i-1}}, \quad i = 1, \ldots, n\,. \tag{8}$$

Substituting the approximation (8) of the matrix A into A^ℓ matrix definition (7), one may define an approximate time dependent matrix of the reduced system as

$$\hat{A}^\ell(t) := \Psi^{\mathrm{T}} W \hat{A}(t) \Psi = \varpi(t)\Psi^{\mathrm{T}} W A_{i-1}\Psi + (1-\varpi(t))\Psi^{\mathrm{T}} W A_i \Psi = \varpi(t)A^\ell_{i-1} + (1 - \varpi(t))A^\ell_i \tag{9}$$

and the reduced order model, once it is created, stays fully independent on the full system dimension.

The second problem arises when you look closely at the nonlinearities in (6). One may notice that to evaluate the non-linearity in the reduced order model $f^\ell(t, \eta^\ell)$, it is necessary to evaluate the function f at (t, y^ℓ) and $y^\ell(t) = \sum_{j=1}^{\ell} \eta^\ell_j(t)\psi_j \in \mathbb{R}^m$. This significantly increases the cost of the evaluation of ROM. In this work, we address this problem via the discrete empirical interpolation method of Chaturantabut and Sorensen [1].

Algorithm 1 POD basis of rank ℓ

Require: Snapshots $\{y_j\}_{j=1}^n$, POD rank $\ell \leq d$, symmetric positive-definite matrix of weights $W \in \mathbb{R}^{m\times m}$

- Set $Y = [y_1, \ldots, y_n] \in \mathbb{R}^{m\times n}$;
- Determine $\bar{Y} = W^{1/2} Y \in \mathbb{R}^{m\times n}$;
- Compute SVD, $[\bar{\Psi}, \Sigma, \bar{V}] = \mathrm{svd}(\bar{Y})$;
- Set $\sigma = \mathrm{diag}(\Sigma)$;
- Compute $\varepsilon(l) = \sum_{i=1}^{\ell} \sigma_i / \sum_{i=1}^{d} \sigma_i$;
- Truncate $\bar{\Psi} \leftarrow [\bar{\psi}_1, \ldots, \bar{\psi}_\ell] \in \mathbb{R}^{m\times \ell}$;
- Compute $\Psi = W^{-1/2}\bar{\Psi} \in \mathbb{R}^{m\times\ell}$;
- **return** POD basis, Ψ, and ratio $\varepsilon(\ell)$

Algorithm 2 DEIM

Require: p and $F = [f_1, \ldots, f_n] \in \mathbb{R}^{m\times n}$

- Compute POD basis $\Phi = [\phi_1, \ldots, \phi_p]$ for F
- idx $\leftarrow \arg\max_{j=1,\ldots,m} |(\phi_1)_{\{j\}}|$;
- $U = [\phi_1]$ and $\vec{i} =$ idx;
- **for** $i = 2$ **to** p **do**
  - $u \leftarrow \phi_i$;
  - Solve $U_{\vec{i}}\, c = u_{\vec{i}}$;
  - $r \leftarrow u - Uc$;
  - idx $\leftarrow \arg\max_{j=1,\ldots,m} |(r)_{\{j\}}|$;
  - $U \leftarrow [U, u]$ and $\vec{i} \leftarrow [\vec{i}, \mathrm{idx}]$;
- **end for**
- **return** $\Phi \in \mathbb{R}^{m\times p}$ and index vector, $\vec{i} \in \mathbb{R}^p$

DEIM is a combination of the greedy algorithm and POD. The reduction of the computational cost of the system nonlinearity evaluation is achieved by reducing the size of the argument of the function f (assuming it is point-wise evaluable). The details of the procedure may be found for example in the aforementioned article by Chaturantabut and Sorensen. We give only the method algorithm summarized in the Algorithm 2. The outputs of the Algorithm 2 may be used to approximate the nonlinearity in ROM by

$$f^\ell(t, \eta^\ell) \approx \tilde{f}(t, \eta^\ell) := \Psi^{\mathrm{T}} W \Phi (P^{\mathrm{T}}\Phi)^{-1} f(t, P^{\mathrm{T}}\Psi\eta^\ell)\,, \tag{10}$$

where the nonlinearity argument $P^{\mathrm{T}}\Psi\eta^\ell$ is in $\mathbb{R}^p$, $p \leq m$. We would like also to emphasize that using DEIM, the nonlinearity samples $\{f_j := f(t_j, y_j)\}_{j=1}^n$ need to be included in the solution snapshots.

3 Reduced order model construction for incompressible Navier-Stokes equations

The application of the POD-DEIM based model order reduction to the systems originating in the FV discretization of the incompressible Navier-Stokes equations is not completely straightforward. In the incompressible Navier-Stokes equations,

$$\begin{aligned} u_t + \nabla\cdot(u\otimes u) - \nabla\cdot(\nu\nabla u) + \nabla p &= f\,, \\ \nabla\cdot u &= 0\,, \end{aligned} \tag{11}$$

the continuity equation $\nabla \cdot u = 0$ is pressure free. Thus, their discretization ultimately leads to a system of linear algebraic equations of the form,

$$\begin{pmatrix} M & N^T \\ N & 0 \end{pmatrix} \begin{pmatrix} u^h \\ p^h \end{pmatrix} = \begin{pmatrix} f^h \\ 0 \end{pmatrix}, \tag{12}$$

where we denoted the discrete representations of the considered functions by the superscript h. The matrix N coincides with a discrete representation of the ∇ operator. The matrix M is slightly more difficult. The Navier-Stokes equations for an incompresible isothermal flow (11) are nonlinear. Hence, the nonlinear convective term $\nabla \cdot u \otimes u$, needs to be linearized during the construction of the matrix M. If we apply the Newton linearization to the nonlinear convective term,

$$\nabla \cdot u^j \otimes u^j \approx u^{j-1} \nabla u^j + u^j \nabla u^{j-1}, \quad j \ldots \text{current time step/iteration}\,, \tag{13}$$

we can define a linear operator

$$\mathcal{M}(u^{j-1}, u^j) := \dot{u}^j + \nabla \cdot (\nu \nabla u^j) + \mathcal{P}(u^{j-1}, u^j)\,, \tag{14}$$

where $\mathcal{P}$ represents the Newton linearization operator. Then, the matrix M is a discrete representation of the operator $\mathcal{M}$.

The matrices M and N are, as results of the FV discretization, large and sparse. The system (12) is a so called saddle point problem and as such, it cannot be directly solved by the available methods of numerical linear algebra.

However, if one assumes the matrix M to be regular, it is possible to explicitly express the velocity from the first row of the system (12) and to substitute for it in the second one. Doing so, the following system for one unknown $p^h \in \mathbb{R}^m$ is obtained

$$N M^{-1} N^{\mathrm{T}} p^h = N M^{-1} f, \quad u^{\mathrm{h}} = M^{-1} \left(f - N^{\mathrm{T}} p^h \right). \tag{15}$$

Nevertheless, as M is a large sparse matrix, its inverse is usually not obtainable and the system (15) needs to be solved iteratively by alternatively updating the values of p^h and u^h (see e.g. [2] or any description of SIMPLE or PISO algorithms).

The natural variable for the solution techniques for the incompressible Navier-Stokes equations based on the solution of the system (15) is the pressure. Thus, it would seem reasonable to base the reduced order model directly on the equation (15). Unfortunately, the pressure time derivative is not explicitly present in the Navier-Stokes equations and as a consequence neither in the system (15). Hence, it is not possible to rewrite the equation (15) in the form of the equation (1) directly.

To define the base system for the construction of ROM for the pressure we propose to split the operator $\mathcal{M}$ as

$$\mathcal{M} = \mathcal{M}_t + \mathcal{M}_x, \quad \mathcal{M}_t(u^j) := \dot{u}^j, \quad \mathcal{M}_x(u^{j-1}, u^j) = \nabla \cdot (\nu \nabla u^j) + \mathcal{P}(u^{j-1}, u^j)\,. \tag{16}$$

Moreover, we will denote the implicitly discretized part of the operator $\mathcal{M}$ as $\mathcal{M}^{\mathrm{fvm}}$ and the explicitly evaluated part of the operator $\mathcal{M}$ as $\mathcal{M}^{\mathrm{fvc}}$. Finally, the base system for the construction of ROM for the pressure is defined as

$$\dot{p} \approx A(t)p + b(t,p), \quad A(t) := N^{\mathrm{fvm}} \left(M_x^{\mathrm{fvm}} \right)^{-1} \left(N^{\mathrm{fvm}} \right)^{\mathrm{T}}, \, b(t,p) := N^{\mathrm{fvc}} \left(M_x^{\mathrm{fvc}} \right)^{-1} f\,. \tag{17}$$

Please note, that the pressure derivative is defined only approximately as, at the moment, we do not have the proof of equality. Also let us emphasize that because of the linearization, the coefficients of the matrix M_x^{fvm} are dependent on the current velocity field and as a consequence, the matrix A is time dependent.

4 Numerical examples

In order to validate the proposed method, we performed a series of numerical tests. The first presented test is a creation of the reduced order model for a transient laminar flow in the vicinity of a cylindrical obstacle. Such a flow develops an instability that leads to the formation of the famous von Kármán vortex street. A comparison of the results of the full model (FVM simulation of the full Navier-Stokes equations on approximately 18000 cells) and the created ROM (system of 12 ODEs) is depicted in the Figure 1.

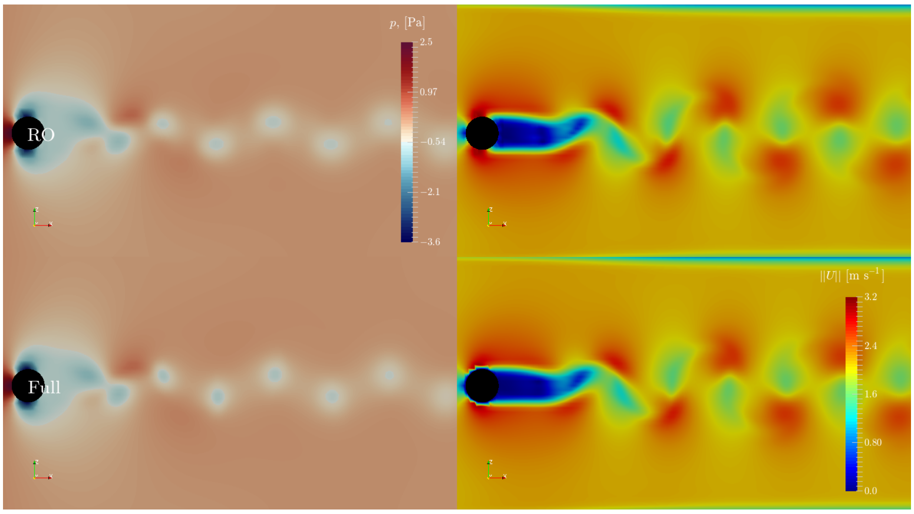

Figure 1: Qualitative comparison of the results of the CFD simulation and ROM results for the case of the flow around a cylindrical obstacle (von Kármán vortex street). Results of the ROM are depicted in the top part of the figure, results of the full model are depicted in the bottom. The left part of the image is colored according to the pressure field, the right part according to the velocity magnitude.

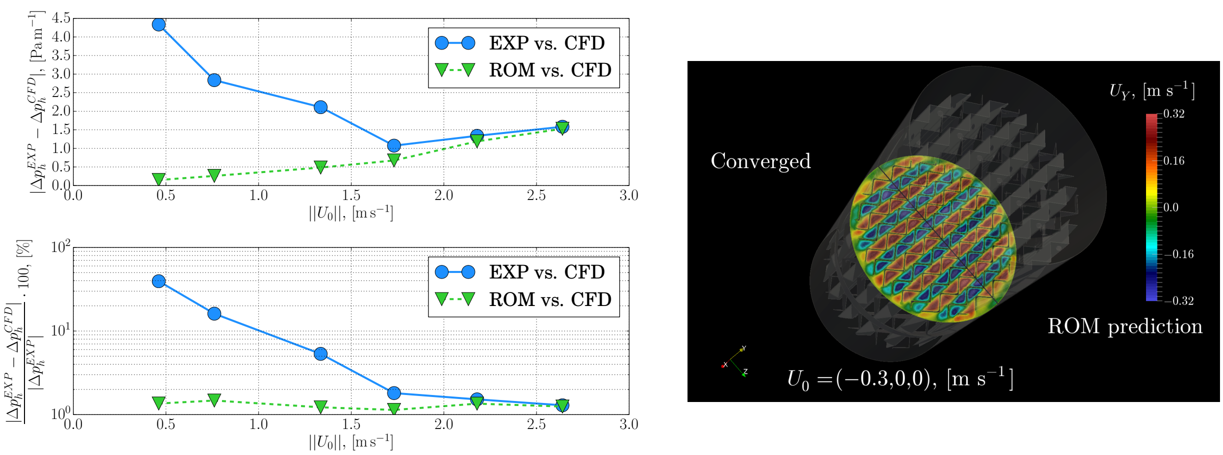

Figure 2: Comparison of the difference between the experimental data, CFD simulation and ROM estimate is depicted on the left side of the figure. On the right side, it is shown the qualitative comparison between the CFD result and ROM estimate for the velocity field.

The second selected test was a creation of ROM for a parametric study of the gas flow in a structured packing of the distillation columns. In this case, we assumed the flow to be at steady state and we studied the difference in pressure above and bellow the structured packing relative to the height of the packing, Δp_h in dependence on the gas inlet velocity.

The results of the test are depicted in Figure 2. The full model corresponds to a FVM simulation of Reynolds-averaged Navier-Stokes equations on approximately $5 \cdot 10^6$ cells. The created ROM consisted of 11 linear algebraic equations.

5 Conclusions

We proposed and validated an approach to use the proper orthogonal decomposition and the discrete empirical interpolation for the model order reduction of systems arising from the finite volume spatial discretization of the incompressible Navier-Stokes equations. The presented approach is specifically designed for the pressure-based Navier-Stokes equations solution methods (e.g. SIMPLE, SIMPLEC or PISO algorithms). We were able to link the proposed method with the OpenFOAM software whereby the method could have been tested even on systems with millions of cells and unstructured meshes. In the future, we plan to improve the mathematical background of the proposed approach to the model order reduction of the Navier-Stokes equations. Also, we would like to concentrate on the model order reduction for multiparametric systems.

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