CONVERGENCE OF POD MODES FOR CYLINDER WAKE FLOW

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Abstract

Proper orthogonal decomposition (POD) is a popular technique for both flow analysis and model order reduction. However, its applicability is strongly dependent on the amount of input data. In the present contribution, we investigate the convergence of numerical POD modes for the canonical case of turbulent flow in the wake behind a circular cylinder. In particular, the cylinder placed at a crossflow at Reynolds number of 4815 was simulated using detached eddy simulation (DES) with sufficient mesh resolution to achieve a large eddy simulation (LES) and direct numerical simulation (DNS) blend in the region of interest located directly behind the examined cylinder. The convergence of POD modes with respect to (i) the number of temporal snapshots used, (ii) the enforcement of the assumed symmetries, and (iii) spatial resolution of the CFD results was examined. Only the first eleven modes can be assumed converged when using standard POD and 12000 snapshots sampled at 2 kHz. However, the results may be significantly improved by enforcing symmetries in the data, which enables to converge even the fifteenth mode with a significantly lower number of snapshots. Finally, simple norm-based techniques did not proved to be a sufficient tool for POD toposes comparison. Therefore the quantitative evaluation of the modes convergence remains an open question.

Keywords: POD, CFD, turbulent cylinder wake flow.

1 Introduction

Modern flow analysis methods such as particle image velocimetry (PIV) or computational fluid dynamics (CFD) generate vast and complex high-dimensional data. The amount of raw information on the problem studied evokes the need for a methodology allowing one to sort the data in such a manner that the experimental and numerical results can be easily and consistently interpreted. One of the most commonly used purely data-driven techniques for analyzing flow fields is proper orthogonal decomposition (POD) [1] also known as Karhunen-Loeve decomposition [2] or empirical orthogonal functions [3]. For a given dataset, POD selects an orthonormal basis that is optimally ordered by least squares, based on the variance in the original data it represents [4]. Specifically, when the dataset pertains to the velocity fluctuations, POD captures the kinetic energy \( k \) associated with the flow turbulence and the obtained basis vectors are organized according to the magnitude of the captured kinetic energy [5].

The theory of POD was derived for infinite continuous domains. Apparently, such are not available in practice, and POD is commonly used in finite discrete domains. In such cases, POD is a statistical method equivalent to the principal component analysis, i.e., singular value decomposition (SVD) [6]. Regrettably, finite space and time discretizations bring the dependence of the POD analysis results on both space and time resolution and the length of the sampling interval, \( T \). Consequently, for a successful POD application, \( T \) has to be sufficiently long to capture all the slow system dynamics, and the space and the temporal resolutions have to allow for a statistical representation of the smallest spatial and temporal scales of interest.

In this work, we focus on POD analysis of flow field data obtained for a crossflow around a circular cylinder at Reynolds number of 4815. We build on our previous work [7], where the computational fluid dynamics (CFD) model of this case was presented and validated against the particle image velocimetry (PIV) experiment. Here, we leverage the available CFD results, for which we further extended the sampling interval \( T \), and attempt to evaluate the discrete POD convergence towards time-continuous results. First, we briefly present the CFD model as the data source. Afterwards, fundamentals of POD with a special emphasis on processing flow data are given. In the Results section, a qualitative comparison of selected POD modes differing in number.
of system temporal snapshots used for their computation is presented. Furthermore, the effects of employing a priori assumptions on the POD results and of changing input data spatial resolution on the POD modes are evaluated.

2 Mathematical model

A numerical simulation of the cross flow around a circular cylinder was performed utilizing the OpenFOAM open-source CFD library [8], which is based on the finite volume method (FVM). The model itself and its validation on experimental data are described in detail in [7]. The fluid density, \( \rho \), fluctuations are neglected, and the flow is assumed to be governed by the Navier-Stokes equations for an incompressible and isothermal flow of a Newtonian fluid,

\[
\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) - \nabla \cdot \mathbf{T} = -\nabla \tilde{p},
\]

\[
\nabla \cdot \mathbf{u} = 0,
\]

(1)

where \( \mathbf{u} \) is the fluid velocity, \( \tilde{p} = p/\rho \) is the kinematic pressure, and \( \mathbf{T} \) is the viscous stress tensor. The effects of turbulence are taken into account via the large eddy simulation (LES) framework, where \( \mathbf{T} \) is split between the resolved part, \( \mathbf{\sigma} \), and the unresolved subgrid scale (SGS) part, \( \mathbf{\tau} \) as \( \mathbf{T} = \mathbf{\sigma} + \mathbf{\tau} \).

The geometry of the model is inspired by an experimental device, which is significantly larger than the region of interest behind the cylinder, see [7]. To efficiently handle flow in the entire spatial computational domain, we employ a hybrid LES-RANS turbulence model introduced by Strelets [9] and known as the detached eddy simulation (DES), which utilizes a single turbulence model serving as SGS model in regions with high grid resolution and as an (U)RANS model in the remainder of the computational domain. In the specific DES formulation applied in this study, the turbulence model is the \( k-\omega \) shear stress transport (\( k-\omega_{SST} \)) one, developed by Menter [10] and reformulated by Hellsten [11]. Closure of the viscous stress term is achieved through two additional transport equations for the modeled turbulence kinetic energy (\( k \)) and the specific dissipation rate (\( \omega \)) (equations (1) in Menter et al. [12]). In this work, we use the OpenFOAM implementation of the \( k-\omega_{SST} \) DES turbulent model, using the default values for the associated constants.

The used boundary conditions are mostly standard for a turbulent flow past a bluff body. The flow field at the inlet is well defined with \( u_{in} = 5 \text{ m s}^{-1} \) and turbulence intensity \( I = 0.2\% \). Still, in the simulation, the inlet needed to be moved upstream of the bluff body to resolve the increased pressure in front of the cylinder. To achieve this, the spatial domain is expanded in front of the cylinder, see the red walls in Figure 1, and the boundary condition for the velocity at the test section walls in front of the cylinder is prescribed as slip, i.e.

\[
\mathbf{u} \cdot \mathbf{n} = 0 \quad \text{and} \quad \mathbf{t}_{w,t} = \mathbf{t}_w - (\mathbf{n} \cdot \mathbf{t}_w) \mathbf{n} = 0,
\]

(2)

where \( \mathbf{t}_w \) is the wall stress vector. Moreover, note that although the wall functions are prescribed for the turbulence variables (\( k \) and \( \omega \)) at the test section walls and cylinder, the mesh resolution

Figure 1: Sketch of the computational domain. Red – slip boundary condition on the test-section walls, cyan – plane of interest, yellow – plane of the symmetry for POD data preprocessing.
is high enough so they are effectively turned off for most of the test-section and affect the flow solution only downstream from the region of interest. For additional information on the full CFD model geometry, used computational mesh, and validation on PIV experimental data, the reader is referred to our previous work [7].

3 Proper orthogonal decomposition

Proper orthogonal decomposition (POD) is a purely data-driven modal decomposition technique. An arbitrary field \( q : \Omega \subset \mathbb{R}^d \times [0, T] \to \mathbb{R}^p \), where \( d = 1, 2, 3 \), \( p \) is the field dimensionality, and \([0, T]\) is the time interval of interest, is decomposed into a sum of dyadic pairs,

\[
q(x, t) = \sum_{k=1}^{n} \eta_k(t) \psi_k(x), \quad x \in \Omega, \ t \in [0, T],
\]

where \( \psi_k(x) \) are orthonormal spatial *toposes*, and \( \eta_k(t) \) are temporal coefficients, *chronoses* [13]. For a discrete representation of the field \( q \), \( Y = (y_{ij}) = [q_1(x_i, t_j), \ldots, q_p(x_i, t_j)]^T \in \mathbb{R}^{m \times n} \), where \( m \) is the number of spatial discretization points multiplied by \( p \) and \( n \) is the number of saved temporal solutions (snapshots), POD technically reduces to the thin singular value decomposition of the matrix of snapshots,

\[
Y = \Psi \Sigma \Phi^T = [\psi_1, \ldots, \psi_r] [\eta_1, \ldots, \eta_r]^T, \ \Psi \in \mathbb{R}^{m \times r}, \ \Sigma = \text{diag}(\sigma_1, \ldots, \sigma_r), \ \Phi \in \mathbb{R}^{n \times r},
\]

where \( r \) denotes the rank of \( Y \). Then, the singular values, \( \sigma_1, \ldots, \sigma_r \), correspond to the 2-norm associated with each dyadic pair \( (\psi_k, \eta_k) \), \( k = 1, \ldots, r \) (POD mode), and the decomposition (3) is optimal with respect to the 2-norm [14].

Due to the simplicity of its implementation for both the experimental and numerical data, POD became a popular tool for flow field analysis in fluid mechanics. In the analysis of dynamic flow fields, it is common to use the Reynolds decomposition to split an arbitrary field \( y(x, t) \) between a mean part, \( \bar{y}(x) \), which does not change over time, and time-dependent fluctuations, \( y'(x, t) \), \( y(x, t) = \bar{y}(x) + y'(x, t) \). Then, POD may be used to decompose and analyze the fluctuations. In the present work, we concentrate on the velocity fluctuations \( u' \) as the variable of interest. For such a selection, POD modes are optimal with respect to the total fluctuations’ kinetic energy and the energy represented by \( k \)-th mode corresponds to \( \sigma_k^2 \).

The main goal of the present work is to investigate POD convergence with an increasing number of snapshots. In many cases, this may be improved by an application of a priori assumptions on the modes structure. Particularly, in the studied case of POD for the flow in the wake behind a circular cylinder, it can be shown that the converged modes are either symmetric or anti-symmetric with respect to the plane \( x = -z \), see yellow plane in Figure 1. Following the approach of Bourgeois et al. [15], each velocity fluctuation can be decomposed into a symmetric \( u'_s \) and anti-symmetric \( u'_a \) part. For both parts, an independent POD can be performed yielding symmetric and anti-symmetric modes, \((\psi_k, \eta_k)_s\) and \((\psi_k, \eta_k)_a\), respectively. The corresponding procedure is as follows,

\[
\begin{align*}
 u'(x, t) \xrightarrow{\text{sptl.disc.}} u'^s_m(t) = u'^s_m(t) + u'^a_m(t) & \xrightarrow{\text{2 indpndnt. POD}} (\psi_k, \eta_k)_s, (\psi_k, \eta_k)_a,
\end{align*}
\]

where subscripts \( s \) and \( a \) denotes symmetric and anti-symmetric modes, respectively.

4 Results

In this section, the convergence of the POD analysis of the velocity data from the plane of interest behind a cylinder (cyan plane in Figure 1) is investigated. For simplicity, only the streamwise velocity component of the resulting toposes, \( \psi^x \), is investigated. Note that the transverse mode component, \( \psi^y \), exhibits a qualitatively similar behavior. Four representative modes were selected for the comparison, three modes with chronos spectra oscillating on the whole multiples of the vortex shedding frequency, \( f_{sh} \); the first, eleventh, and fifteenth mode with frequencies \( 2 f_{sh} \), and \( 3 f_{sh} \), respectively; and the third so-called slow-drift mode [13]. Note that the first fifteen modes were selected as they capture 70% of the flow fluctuating kinetic energy while the fifteenth mode alone captures 0.7% of the energy. The physical relevance of the higher modes drops as the influence of the stochastic errors caused by turbulence increases. The flow was sampled at

\[
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\]

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the frequency $f_{smp} \approx 28.5 f_{sh}$. Altogether, 12 000 snapshots of the numerical solution were saved, which corresponds to $\approx 420$ vortex shedding cycles.

First, the results of the raw POD (no enforced symmetries, original mesh) are discussed. Next, the influence of (i) enforcing the symmetries in the data, and (ii) changing the mesh resolution is studied. The section is concluded with a comparison of the development of the squared norm of error between the modes with an increasing number of snapshots.

Figure 2: Raw POD utilizing velocity fluctuations without enforcing the symmetries in the data. Comparison of the streamwise topos component contours, $\psi_x$, for modes 1, 3, 11, and 15 (rows), and 2 000, 4 000, 8 000, and 12 000 snapshots (columns).

### 4.1 Convergence of POD without enforced symmetries

Comparison of the topos streamwise component contours, $\psi_x$, for the selected representative modes (1, 3, 11, 15), and for the increasing number of snapshots (2 000–12 000) is depicted in Figure 2. Taking into account the first row in Figure 2, note that the convergence of the first mode is relatively fast. Even 2 000-snapshots-POD provides similar (and similarly located) coherent structures to those with a longer sampling interval and more input information. Furthermore, all presented first modes are anti-symmetric without enforcing the (anti-)symmetry during data preprocessing.

On the other hand, the convergence of the third slow-drift mode is much more problematic, see the second row in Figure 2. The resulting observed coherent structures change with the number of snapshots increasing even from 8 000 to 12 000. Moreover, the resulting modes are not symmetric as would be expected. This behavior is probably caused by the fact that the slow-drift modes oscillate with a low frequency, $f_{\psi_3} \approx 0.2 f_{sh}$, and consequently need a very long sampling interval for the correct convergence.

The results for the eleventh mode (the third row in Figure 2) are better than those for the third slow-drift mode, but worse than for the first mode. Two and four thousand snapshots are not enough to obtain consistent coherent structures, but the difference between eight and twelve thousand is not significant. Using all the 12 000 snapshots, we were also able to obtain an almost symmetric mode as expected.
Finally, studying the fifteenth mode (the last row in Figure 2), note that the convergence is similar as in the case of the eleventh mode, i.e., neither 2000 nor 4000 snapshots are sufficient. Again the difference between 8 and 12 thousands is not very large and the mode seems to be converged. However, the mode is not anti-symmetric as would be expected.

\[
\begin{array}{cccc}
\psi_1 & \psi_3 & \psi_{11} & \psi_{15} \\
2000\text{ snapshots} & 4000\text{ snapshots} & 8000\text{ snapshots} & 12000\text{ snapshots}
\end{array}
\]

Figure 3: POD utilizing (anti-)symmetrized velocity fluctuations. Comparison of the streamwise topos component contours, $\psi^x$, for modes 1, 3, 11, and 15 (rows), and 2000, 4000, 8000, and 12000 snapshots (columns).

4.2 Enforcing the symmetries in the data

Utilizing the approach proposed by Bourgeois et al. [15] described in the last paragraph of Section 3, it is possible to split velocity fluctuations into symmetric and anti-symmetric parts, and to perform two independent PODs with the symmetric and anti-symmetric data separately. The resulting symmetric and anti-symmetric modes can be then ordered based on the singular values. For example, the previously analyzed mode 3 corresponds to the first symmetric mode, $\psi_3 = \psi_{1,s}$, or mode 15 corresponds to the seventh anti-symmetric mode, $\psi_{15} = \psi_{7,a}$.

Similarly as in the previous subsection, the comparison of the studied representative modes with the increasing number of snapshots used is given in the individual rows of Figure 3. Overall, the (anti-)symmetry enforcement enhances the POD convergence significantly. Again, a converged most energetic mode is achieved even with the low number of snapshots. On the contrary, the convergence of the third slow-drift mode does not seem sufficient as there is a significant difference between 8000 and 12000 snapshots-POD. Moreover, 12000 snapshot results are more similar to 4000 than 8000 snapshots-POD results. Finally, the eleventh and fifteenth modes with enforced (anti-)symmetry provide mutually similar convergence behavior. Even with 2000 snapshots, the topology of the coherent structures is similar as in the 12000 snapshots case, but with the increasing number of snapshots, the structures are more pronounced.
4.3 Influence of the mesh resolution

Three different meshes were prepared to test the POD sensitivity to the resolution of the mesh; see the first column in Figure 4. All meshes are structured and uniform and consist of square cells. The finest mesh cell size corresponds to the computational mesh cell size, $\Delta$. The second and third meshes are constructed with the mesh cell size $2\Delta$, and $4\Delta$, respectively, and the velocity is interpolated during preprocessing. Note that the cell size $4\Delta$ (mesh in the first row in Figure 4) conforms to the experimental PIV resolution used in [7].

The convergence of the least energetic fifteenth mode in dependence on the mesh used is studied in Figure 4. The resulting streamwise topos contours, $\psi_{x15}$, are depicted, in order, for 2 000, 8 000, and 12 000 snapshots-POD. In general, it can be said that the influence of the used mesh is low. All the studied meshes provide the same coherent structures, and the coarsening of the mesh does not seem to enhance POD convergence.

4.4 Convergence in squared norm of the error

At last, the convergence of POD is quantitatively investigated. In particular, we compare the squared norm of the error (ESN) between the modes computed from 2 000–11 000 snapshots and the reference mode (ref) based on all the 12 000 snapshots,

$$\text{ESN} = \| \psi^i_{x} - \psi^i_{x,\text{ref}} \|^2 .$$

The development of the error is compared for the (i) raw POD without enforcing the symmetries (Figure 5a), (ii) raw POD with the reference results from the symmetrized 12 000 snapshots-POD (Figure 5b), and (iii) symmetrized POD (Figure 5c). Furthermore, ESN for all three previously described meshes is compared.

In general, the quantitative results mostly comply with the qualitative ones;

(i) ESN for the first mode is by order or two lower than for other studied modes, i.e., the similarity between the first modes, obtained with the different number of snapshots, is very high and the first mode is well converged,

(ii) the mesh resolution does not seem to influence the POD results much, that is, solid, dashed, and dotted lines in Figure 5 are very close for all the studied modes, and

(iii) the convergence of the third slow-drift mode is the worst from all the studied ones.
However, focusing on the ESN convergence results in more detail, several problems with the applied quantitative methodology can be found. Consider Figure 5b and the difference between the red and magenta lines (modes 11 and 15) for 8,000 snapshots-POD (orange circle). Note that the fifteenth mode seems to be more converged than the eleventh one. On the other hand, inspecting the corresponding qualitative results in Figures 2 and 3, it find out by naked eye that the eleventh mode contours from raw 8,000 snapshots-POD are qualitatively closer to the symmetrized 12,000 snapshots-POD results than the same in the case of the fifteenth mode. Hence, the simple norm of the error, and, consequently, also the mean squared error and similar approaches, are not sufficient measures of the difference between toposes structure. Thus, for a true quantitative evaluation of POD toposes convergence, a better methodology has to be developed.

5 Conclusions

The convergence of POD for the case of a crossflow around a circular cylinder at Re = 4815 was studied. The main focus of the work lied in evaluating the length of sampling interval required to obtain 15 converged POD modes while using the sampling frequency corresponding to 28 times the vortex shedding frequency. When no a priori assumptions on the resulting topos structure were made, the 15th mode did not converge even for the 12,000 snapshot \( \approx 420 \) shedding cycles, regardless of the spatial resolution of the data. However, when assumptions on POD results (anti-)symmetry are enforced during data preprocessing, coherent structures in 15th topos are resolved even when 2,000 snapshots \( \approx 70 \) shedding cycles are used. However, quantitative evaluation of the POD topos convergence remains an open question as insufficiency of simple comparison methods, such as error norm, was shown.

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References


