Zonal Reduced-Order Modelling Toward Prediction of Transitional Flow Fields

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Abstract. The utilization of measurement data is becoming attractive in various fields due to the massive growth of sensing and networking technologies. It is expected to utilize such a data-rich environment to improve engineering simulations in computer-aided engineering (CAE). Data assimilation is one of methodologies to statistically integrate a numerical model and measurement data, and it is expected to be a key technology to take advantage of measured data in CAE. However, the additional cost of data assimilation is not always affordable in CAE simulations. In this study, we consider the cost reduction of numerical flow simulation by the help of a reduced-order model. Since the prediction accuracy of existing ROMs are limited in transitional flow problems such as two- to three-dimensional flow transition, we investigate here a zonal hybrid approach of a full-order model and a reduced-order model.

1. Introduction

Computer-aided engineering (CAE) represented by numerical simulation play an indispensable role in modern research and development (R&D) processes. CAE realizes the reduction of design and development lead-time and enables design optimization for realizing better performance of products. Increase of computing power further improves the accuracy and ability of CAE, however, it also exposes the importance of the treatment of uncertainties contained in a CAE model, computational conditions and measurement data. On the other hand, downsizing and commoditization of sensors with the help of micro-electro-mechanical system (MEMS) technology are now making easy to gather measured data to a computing server. The movement of the internet of things (IoT) would make the collection of measurement data easier. One of the approaches to utilize measurement data for the improvement CAE simulation is the use of a data assimilation method. Modern data assimilation methods such as ensemble Kalman filter, particle filter and four-dimensional variational method demand several to several tens more computational resources than the original CAE simulation, therefore, there exists a wall that prevents the implementation of statistical methods such as data assimilation in the real-world R&D process.

To alleviate the above-mentioned difficulty, two major approaches can be considered, i.e., the development of efficient data assimilation techniques or the cost reduction of the original simulation model. We consider here the latter approach, which is so-called reduced-order model (ROM) approach [1,2]. The reduced-order modelling would be considered as the interpolation of a state vector in time or in a parameter space, therefore, it is not possible to predict/extrapolate a field which is not included in a learning data set such as spatial bases. In fluid problems, proper orthogonal decomposition
(POD)-based ROM is often used, where a flow field is reconstructed by using the POD spatial bases. Fast and accurate prediction is possible especially in the case of periodic flows if the pre-constructed spatial bases are appropriate. However, it is difficult to represent a transitional field without having appropriate bases before/after the transition. To overcome this, a hybrid approach, where a full-order model (FOM) and a ROM are switched to track the transition of a state, was proposed in a relatively simple problem [3]. In their research, FOM and ROM are switched in time for a whole domain. In the case of a complex flow field, the modelling fidelity can be switch in space using the framework of multi-block computational infrastructure [4].

In this study, we consider a simple flow around a square cylinder, where the flow field can be two- or three-dimensional depending on a Reynolds number. More specifically, the flow field changes from two-dimensional vortex shedding to three-dimensional complex vortical structure by increasing Reynolds number from approximately 100 to 1000. There also exists a major transition phenomenon in fluid dynamics called laminar to turbulent transition, which goes well beyond the scope of this research. First, a zonal ROM is considered. The accuracy of a ROM is then assessed by evaluating the error of full-order Navier-Stokes and the ROM predictions in the wake of the square cylinder.

2. Numerical methods
In this section, we briefly explain computational fluid dynamics simulation of a flow around a square cylinder. It is also discussed about the POD and a ROM using POD bases.

2.1. Computation flow simulation
For flow simulation, we employ the incompressible Navier-Stokes equations:

\[ \frac{\partial u_j}{\partial t} + u_k \frac{\partial u_j}{\partial x_k} = -\frac{1}{\rho} \frac{\partial p'}{\partial x_j} + 2\nu \frac{\partial S_{jk}}{\partial x_k}, \]  
\[ \frac{\partial u_j}{\partial x_j} = 0, \]  

where \( u_j \) and \( p' \) represent the velocity components in three spatial directions \( (j, k = 1, 2, 3) \), the pressure deviation from the reference state \( p = p_0 + p' \), respectively. \( S_{jk} = (\frac{\partial u_j}{\partial x_k} + \frac{\partial u_k}{\partial x_j})/2 \) denotes the strain rate tensor. The summation convention is used for the velocity components \( u_j \). \( \rho \) and \( \nu \) denote density and kinematic viscosity, respectively. Equation (1) can be normalized by introducing the Reynolds number: \( \text{Re} = U L / \nu \), which represents the ratio of inertial and viscous effects in a flow field and governs the flow structure including the onset of flow transition.

A computational domain is composed of a parallelepiped domain with a square cylinder of unit sides inside as in figure 1. The longitudinal length of the square cylinder is set to two and periodic boundary condition is employed in the longitudinal direction. A uniform flow is specified in the inlet boundary (the left boundary in figure 1) and the convection boundary condition is used on the outlet boundary (the right boundary). The Neumann boundary condition is applied to the top and bottom boundaries in figure 1. The wall boundary of the square cylinder is represented by specifying the opposite velocity vector inside the wall, which realizes the non-slip boundary condition on the wall with the linear velocity distribution near the wall.

Figure 2 shows flow fields with the Reynolds number of 100 and 1000, where the flow field has two-dimensional structure in the former case and the flow field shows three-dimensional structure with small disturbances in crossflow direction in the latter. This is one of flow transition phenomena occurs in a small Reynolds number regime. There is also an important flow transition phenomenon which is taken place in relatively high Reynolds numbers: \( \text{Re} = 2.5 \times 10^4 \) for a flow around a sphere. This type of flow transition is often due to the laminar-turbulent transition and it plays important roles
in many industrial applications. It is because skin friction and heat transfer on the wall becomes several times larger in a turbulent boundary layer than those of a laminar boundary layer.

![Figure 1. Computational domain and the region of interest for reduced-order modelling.](image)

![Figure 2. Flow fields obtained by Navier-Stokes equations for Reynolds numbers of (a) Re = 100 and (b) Re = 1000 visualized by a streamwise velocity.](image)

2.2. Proper orthogonal decomposition (POD)

The proper orthogonal decomposition (POD) is a methodology similar to the principal component analysis [5]. The POD decomposes a flow field based on the variance of deviation, that is,

\[
\arg \min \|X - \Phi \Phi^T X\|, \tag{3}
\]

where \(X\) contains a certain data set and \(\Phi\) is a POD basis vector. In the case of a flow simulation data set, the matrix \(X\) tends to be very large, therefore, a snapshot-based approach is employed. During an unsteady flow simulation, a flow field is extracted every several time steps as a snapshot. The matrix \(X\) is composed as,

\[
X = \begin{bmatrix}
  u_1^1 & \cdots & u_1^m \\
  \vdots & & \vdots \\
  u_n^1 & \cdots & u_n^m
\end{bmatrix}, \tag{4}
\]

where a superscript \(m\) indicates the number of snapshots and \(n\) is the number of variables (number of grid points multiplied by the number of variables) in the case of flow simulation. The minimization in equation (3) results in an eigenvalue problem in equation (5).
\[
X^TX\varphi_i = \lambda_i \varphi_i,
\]  
(5)

Using \(m\) snapshots of a flow field, we have \(m\) eigenvalues \(\lambda_i\) and eigenvectors \(\varphi_i\). The POD basis vector which has the same size as the original field variable is defined as,

\[
\Psi_i = X\varphi_i / \sqrt{\lambda_i}.
\]  
(6)

This POD basis vector can be used to construct the reduced-order model as described in the following section. Using the basis vectors, the original velocity field can be reproduced by,

\[
u(x, t) = \bar{u}(x) + \sum_{i=1}^{r} a_i(t) \Psi_i(x).
\]  
(7)

where \(\bar{u}(x)\) is the average field subtracted from the matrix \(X\) before composing the matrix \(X^TX\) and \(r\) denotes the number of POD modes used for reconstructing the flow field. The temporal coefficients \(a_i(t)\) can be obtained from the original snapshots by the inner-product of the velocity vector and the POD basis vector as,

\[
a_i(t) = (\nu(x, t) - \bar{u}(x)) \cdot \Psi_i(x).
\]  
(8)

The temporal coefficients obtained from the original snapshots are used to construct surrogate-based reduced-order models as described in the following section.

### 2.3. Reduced-order model (ROM)

A well-known approach to construct a reduced-order model from an unsteady flow field is the Galerkin projection method. The inner product of the POD bases and governing equations is calculated to generate a set of ordinary equations, which can be in the form of,

\[
\frac{d a_i}{dt} = f(a_1, a_2, \ldots, a_r).
\]  
(9)

Due to the orthogonality of POD bases, the derived ordinary equations are easy to solve and the number of equations corresponds to that of POD bases considered. Using the obtained time-varying coefficients \(a_i\), a velocity field is reproduced by equation (7). The Galerkin projection approach is attractive since the mathematical background is well established, however, there exist several drawbacks such as a computational cost for calculating inner products, a stability problem for high Reynolds number flows. One alternative would be the use of surrogate models for the time development of the time coefficients. A radial basis function (RBF) is one of such surrogate models to develop the temporal coefficients in time [6], i.e., the temporal coefficients of POD mode \(i\) can be represented as a linear combination of \(r\) radial basis functions \(\phi\),

\[
a^n_i = f_i(a^{n-1}_i) = \sum_{j=1}^{r} w_{i,j} \cdot \phi(r_j).
\]  
(10)

where \(w_{i,j}\) are weight coefficients and \(r_j\) is a distance \(r_j = \|a^{n-1}_i - \hat{a}_j\|\) from a set of data points \(\hat{a}_j\) calculated from the snapshots by equation (8). The temporal coefficient of mode \(i\) at time level \(n - 1\), \(a^{n-1}_i\) is advanced to that at time \(n\) with equation (10). In this study, we adopted a multi-quadratic
function is employed: $\phi(r_j) = \sqrt{r_j^2 + r_0^2}$, where $r_0$ is a parameter which can be determined, for example, by the leave-one-out cross-validation. Ensuring that the interpolated value matches the given $r + 1$ data points from the snapshots, equation (10) can be rewritten in the matrix form as,

$$A_i w_i = y_i,$$

where

$$A_i = \begin{bmatrix}
\phi(\|a^1_i - \tilde{a}^1_i\|) & \cdots & \phi(\|a^r_i - \tilde{a}^r_i\|) \\
\vdots & \ddots & \vdots \\
\phi(\|a^r_i - \tilde{a}^r_i\|) & \cdots & \phi(\|a^1_i - \tilde{a}^1_i\|)
\end{bmatrix},$$

$$w_i = [w_{i,1}, w_{i,2}, \cdots, w_{i,r}]^T,$$

$$y_i = [a^1_i, a^2_i, \cdots, a^r_i]^T.$$  

Equation (11) is solved by a matrix solver using the singular value decomposition (SVD). The resulting weights $w_{i,j}$ determine the equations for temporal coefficients.

### 3. Zonal mode analyses

In this section, we compare POD bases by changing a domain of the decomposition. Figure 3 shows the first POD mode for a flow field with Re = 100, where a Karman vortex street is formed behind a square cylinder. Using the same flow field, the POD analysis is conducted in the whole domain as shown in figure 3(a), a top-half domain in (b), a downstream half domain in (c), and the one-fourth domain in (d). Since each POD basis is normalized so that the magnitude of a POD basis is equal to one, a time coefficient is multiplied to a corresponding POD basis for comparison in those figures. The result shows that the distributions appear similarly, and the magnitude is slightly different in figures 3(c) and (d). The difference may come from the accuracy of the matrix computation related equation (5). The phase and period of the vortices are very similar for all the cases. This tendency was confirmed for other POD bases, however, the difference related to the accuracy of the matrix computation becomes more noticeable in high frequency (low energy) POD modes.
**Figure 3.** A POD mode obtained by limited domains, (a) whole domain, (b) top-half domain, (c) downstream half domain, and (d) one-fourth domain.

4. **Zonal hybrid flow prediction**

In this section, we conduct a zonal hybrid flow prediction, where a downstream part of the domain is predicted by the POD-RBF-ROM and the upstream part is simulated by the full-order Navier-Stokes equations (FOM, hereafter). The error of the hybrid flow prediction is evaluated by root mean square error (RMSE) and by visualized flow fields. To simplify the evaluation of the hybrid approach, we update the flow field in an offline manner, i.e., we prepare a set of snapshots by the FOM simulation. The evolution of the flow field is then represented simply by switching the snapshots. The POD-RBF-ROM prediction replaces the downstream half domain of the snapshot and RMSE is evaluated.

4.1. **Two-dimensional flow field for Re = 100**

We here evaluate the RMSE of the velocity field between full-order Navier-Stokes prediction and the POD-RBF-ROM prediction in the downstream half of the domain. Figure 4 shows the RMSE for cases with different values of POD energies, $E_{\text{ROM}} = 99.99$, 99.0 and 95.0%. In addition, the RMSE evaluated on the boundary between an upstream FOM domain and a downstream ROM domain. The error on the domain boundaries can be utilized in actual applications where the FOM results is not available in the ROM domain. The results show that the RMSE decreases as the POD energy increases, which corresponds to the more number of ROM equations. The RMSE on the boundary has similar magnitude as the RMSE of the downstream half domain, therefore, it can be used to evaluate the error of the ROM prediction by the comparison of FOM and ROM results on the boundary.

Figure 5 shows the streamwise velocity distribution for three different POD energy thresholds, (a) $E_{\text{ROM}} = 99.99%$, (b) $E_{\text{ROM}} = 99.0%$, and (c) $E_{\text{ROM}} = 95.0%$. The distribution is smoothly connected in the case of $E_{\text{ROM}} = 99.99%$, while discontinuity of the distribution is seen in $E_{\text{ROM}} = 95.0%$. Small distortion of the contour lines can be observed in the case of $E_{\text{ROM}} = 99.0%$. The number of POD bases (ROM equation) are 11, 6 and 3 for the cases of $E_{\text{ROM}} = 99.99$, 99.0 and 95%, respectively. For the POD, 40 snapshots are used as input.

**Figure 4.** Error of a reconstructed flow field for different energy thresholds for Re = 100.
Figure 5. A reconstructed flow field for different energy thresholds, (a) $E_{\text{rom}} = 99.99\%$, (b) $E_{\text{rom}} = 99.0\%$, and (c) $E_{\text{rom}} = 95.0\%$.

4.2. Three-dimensional flow field for $Re = 1000$

Figure 6 shows the same plot as figure 4, but for the cases with $Re = 1000$. Again, we consider cases of $E_{\text{rom}} = 99.99$, 99.0 and 95.0%. The RMSE exhibits larger values compared to the cases of $Re = 100$, which indicates that the accuracy of the ROM prediction is degraded regardless of the same energy thresholds. The number of POD bases used here are 78, 34 and 18 modes for $E_{\text{rom}} = 99.99$, 99.0 and 95.0%, respectively, which is much larger than the cases of $Re = 100$. Even so, the accuracy of the ROM prediction is not satisfactory to zonally replace the FOM prediction by the ROM. For the POD, 100 snapshots are considered as input.

Figure 7 shows the streamwise velocity distributions for (a) the FOM prediction, and (b) the ROM prediction with $E_{\text{rom}} = 99.99\%$. The ROM reproduced flow field is significantly different from the FOM results. This is because the time history of temporal coefficients predicted by equation (10) becomes slightly complex for $Re = 1000$ as shown in figure 8. In the case of $Re = 100$, the temporal coefficients varies sinusoidally and it is accurately predicted by the POD-RBF-ROM. On the other hand, the sinusoidal variation of the temporal coefficients is distorted in the case of $Re = 1000$, and this causes the difficulty in predicting using the POD-RBF-ROM. It is known that the projection-based ROM is often unstable [1]. The possibility to overcome this difficulty is to improve ROM or to use the other spatial basis which realizes the sinusoidal variation of temporal coefficients. The dynamic mode decomposition (DMD) would be used to improve the ROM prediction [7].
**Figure 6.** Error of a reconstructed flow field for different energy thresholds for Re = 1000.

**Figure 7.** (a) A reconstructed flow field for the energy threshold of $E_{\text{ROM}} = 99.99\%$, and (b) a flow field obtained by a full-order Navier-Stokes equations.

**Figure 8.** Temporal coefficients of first and second modes for (a) Re =100, and (b) Re =1000

5. **Conclusions**

In this study, we considered a simple flow field around a square cylinder, where the flow field can be two- or three-dimensional depending Reynolds numbers. First, we showed that the POD analysis can be applied to an arbitrary sub-domain of the flow field. The accuracy of the POD-RBF-ROM was then assessed by evaluating the RMSE of full-order Navier-Stokes and the POD-RBF-ROM predictions in the wake of the square cylinder. The accuracy of the POD-RBF-ROM for Re = 1000 was much degraded compared to the case with Re = 100, because the prediction of temporal coefficients became difficult by increasing Reynolds number. In the future work, we investigate the possibility of zonal model switching to reduce the cost of numerical simulation while retaining the accuracy.
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