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Letter

The performance of proper orthogonal decomposition in discontinuous flows

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HIGHLIGHTS

- The proper orthogonal decomposition (POD) modes have special pattern for flow existing shock wave.
- The reason why reconstructing transonic flow needs more POD modes is explained.
- POD combined with interpolation has good prediction ability for transonic flow.
- POD combined with extrapolation does not have prediction ability for transonic flow.

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ABSTRACT

In this paper, flow reconstruction accuracy and flow prediction capability of discontinuous transonic flow field by means of proper orthogonal decomposition (POD) method is studied. Although linear superposition of "high frequency waves" in different POD modes can achieve the reconstruction of the shock wave, the smoothness of the solution near the shock wave cannot be guaranteed. The modal coefficients are interpolated or extrapolated and different modal components are superposed to realize the prediction of the flow field beyond the snapshot sets. Results show that compared with the subsonic flow, the transonic flow with shock wave requires more POD modes to reach a comparative reconstruction accuracy. When a shock wave exists, the interpolation prediction ability is acceptable. However, large errors exist in extrapolation, and increasing the number of POD modes cannot effectively improve the prediction accuracy of the flow field.

The proper orthogonal decomposition (POD), also known as Karhunen–Loeve (K–L) expansion or principle components analysis, has been widely used in many areas, such as image processing [1], pattern recognition [2], reduced order model [3] (ROM), flow dynamics analysis [4,5], and airfoil design optimization [6], and so on. POD method is a powerful statistical tool which can extract the significant structure or pattern from a large data set. POD method is also an effective reduction tool which can use the minimum number of POD modes to present a large data ensemble with the given accuracy. Lumley [7] firstly introduced the POD method into the turbulent flow. Then, Sirovich [8] introduced snapshots as a way to efficiently determine the POD modes, which made POD method applied to a wider range of problems, especially to computational fluid dynamics (CFD).

Numerical simulation of fluid flows is a very computationally intensive endeavor. In addition, reaching a physical understanding from numerical simulation data is another challenge. Faced with these two challenges, ROM is a good choice that retains the essential physics and dynamics of the fluid flows, but has a much lower computational cost. This can enable uncertainty quantification [9], on-the-spot decision-making [10], optimization [11], and control [12]. There are two approaches in constructing an efficient ROM based on POD by integrating with Galerkin method [13–16] or surrogate technique [17,18]. One approach is based on Galerkin projection of the physical model on a reduced-dimension basis determined by POD. Xie et al. [19] employed this scheme to solve the nonlinear aeroelastic oscillations of a fluttering plate in both two and three dimensions. Pla et al. [20] described a flexible Galerkin method based on POD to construct the bifurcation diagram. Furthermore, Kim [21] developed the ROM in frequency form using a set of discrete snapshots in frequency domain instead of time domain. However, the POD-Galerkin ROM is non-robust and structurally unstable [22]. Therefore, some new approaches are developed to improve the stability and reliability of the POD-Galerkin ROM. Xiao et al. [23] applied a new non-linear Petrov–Galerkin method to the reduced order Navier–Stokes

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equations, thus improving the stability of ROM. Romain et al. [24] investigated sequential data assimilation techniques to improve the stability of POD-Galerkin ROM for fluid flows. Leblond and Allery [25] obtained a priori low-dimensional space–time separated representation of the fluid fields, which is based on the use of space–time proper generalized decomposition (PGD) definitions. PGD may be seen as a generalization of the POD for a priori construction of a separated representation of the solution. This allows ensuring the accuracy of a ROM as the parameter varies. The other approach to construct the POD-based ROM is to utilize a surrogate model as a function of the measurement POD coefficients. Mainini and Willcox [10] combined POD and a local polynomial response surface model to realize a fast mapping from measured quantities to system capabilities. This assists online rapid decision making for an unmanned aerial vehicle. Fossati [26] integrated POD and multi-dimensional interpolation for the parametric evaluation of steady aerodynamic loads. Kato and Funazaki [27] combined POD and radial basis function network (RBFN) for adaptively sampling a design parameter space using an error estimate through the reconstruction of flow field.

However, because of shock waves, boundary-layer separation, and control-surface deflection in the transonic flow regime, additional complexities of the nonlinear aerodynamic system may be introduced. Especially, shock waves involve jumps in the flow variables, which bring great difficulties in POD-based ROM [28–30]. This results in either a quite poor approximation between ROM and CFD or a huge number of POD modes [31,32]. And some special treatments are needed to avoid that problem. Iuliano and Quagliarella [11] presented a zonal approach to better solve the shock wave region and improve the ROM prediction in transonic flow. Malouin et al. [33] proposed an idea that is to use POD to interpolate the difference between the CFD solution obtained on two different grids, a coarse one and a fine one. This allows some nonlinearities associated with the flow to be introduced and gets good improvement over the classical approach. Taeibi-Rahni et al. [34] proposed the filtered and reprojection POD for transonic flow and better results were obtained than the conventional POD method. But there are no explanations why POD method results in poor approximation when dealing with shock waves and needs more POD modes to improve the behavior. Thus, this paper conducts research on this question. The performances of POD method for flow reconstruction in both subsonic and transonic flows are tested. Results show that different from subsonic flow, there are "high frequency waves" in the POD modes of transonic flow. This is the reason why reconstructing shock waves with satisfactory accuracy needs more POD modes. Furthermore, this will result in the prediction failure of the flow field beyond snapshot sets.

POD can be applied efficiently to large systems using the method of snapshots [6] as follows. $\left\{\boldsymbol{U}^k\right\}_{k=1}^m$ is a collection of m flow snapshots, where $\boldsymbol{U}^k$ is a vector containing the flow solution at a time or a parameter, such as the angle of attack (AOA) or Mach number. And usually these solutions are expressed as the sum of average values and fluctuation values.

$$\boldsymbol{U}^k = \bar{\boldsymbol{U}} + \tilde{\boldsymbol{U}}^k. \quad (1)$$

The correlation matrix $\boldsymbol{R}$ is formed by computing the inner product between every pair of snapshots,

$$\boldsymbol{R}_{ik} = \left(\boldsymbol{U}^i, \boldsymbol{U}^k\right), \quad (2)$$

where $\left(\boldsymbol{U}^i, \boldsymbol{U}^k\right)$ denotes the inner product between $\boldsymbol{U}^i$ and $\boldsymbol{U}^k$. And then compute the eigenvalues λ_i and eigenvectors $\boldsymbol{\Psi}^i$. The orthonormal POD modes can be obtained by the following formula:

$$\left\{\boldsymbol{\Phi}^i\right\}_{i=1}^m = \frac{1}{\sqrt{\lambda_i}} \left\{\boldsymbol{U}^i\right\}_{i=1}^m \left\{\boldsymbol{\Psi}^i\right\}_{i=1}^m. \quad (3)$$

The magnitude of the ith eigenvalue, λ_i, describes the relative importance of the ith POD mode, also known as the relative energy contained in the ith POD mode.

The approximate reconstruction of the flow solutions can be given by the sum of average values and a linear combination of the POD modes:

$$\boldsymbol{U}^k \approx \bar{\boldsymbol{U}} + \sum_{i=1}^{p} \alpha_i^k \boldsymbol{\Phi}^i, \quad (4)$$

where $p \ll m$ and p is chosen to capture the desired level of energy. α_i^k is the modal coefficient, corresponding to the ith POD mode, which can be obtained by projecting the kth snapshot to the ith POD mode.

$$\alpha_i^k = \left(\boldsymbol{\Phi}^i, \boldsymbol{U}^k\right). \quad (5)$$

POD method combined with interpolation and extrapolation can realize the fast prediction of flow solutions which are not contained in the snapshots [26]. The main steps are as follows:

(1) $\left\{\boldsymbol{U}^{\delta_k}\right\}_{k=1}^m$ is the set of snapshots varying with time or the flow parameter, which is described by δ.
(2) Perform the basic POD procedure described above to get the truncated orthonormal POD modes $\left\{\boldsymbol{\Phi}^i\right\}_{i=1}^p$ and the corresponding POD coefficients $\alpha_i^{\delta_k}$.
(3) $\left\{\alpha_i^{\delta_k}\right\}_{k=1}^m$ is a function of δ, and interpolation or extrapolation can be used to determine the POD coefficients of δ that are not included in the original ensemble. We choose the cubic spline interpolation as the interpolation and extrapolation method in this paper and the prediction flow solution at any δ value is given by

$$\boldsymbol{U}^\delta \approx \bar{\boldsymbol{U}} + \sum_{i=1}^{p} \alpha_i^\delta \boldsymbol{\Phi}^i. \quad (6)$$

In this paper, the steady flow solutions to a NACA 0012 airfoil with varying AOA are used as snapshots. CFD solver adopts advection upstream splitting method (AUSM) + UP scheme to solve the Euler equation. Unstructured grid is used. The number of nodes is 6916 and the number of cells is 13490, as shown in Fig. 1. A detailed description of the solver and its verification can be referred to in Ref. [35].

The snapshots set of case 1 is composed of 100 flow solutions ensemble at the fixed Mach number of 0.8, with AOA range of [0.25°, 2.23°], uniformly spaced with an interval of 0.02°. Among them, two shock waves are separately located on the upper surface and the lower surface of the airfoil in the first 70 snapshots, while there is only one shock wave on the upper surface in the last 30 snapshots. With the increase of AOA, the position of the shock wave gradually moves downstream. And the range of the shock wave on the upper surface corresponding to the x-axis is 0.53–0.71. Figure 2 shows the distribution of pressure coefficients on the upper surface at different AOAs, which illustrates the position change of the shock wave with the AOA rang. Based on this snapshots set, reconstruction of the flow solution is conducted by the POD method. For a distinct demonstration, POD method is applied only to the pressure field and the pressure is dimensionless. The procedure of the other flow fields is straightforward.

In order to better illustrate the impact of shock waves on the reconstruction result of the flow field based on POD method, a subsonic case 2 is tested. The snapshots set of case 2 is composed of a steady flow solution ensemble at the fixed Mach number of 0.5 and the AOA range, spacing and the number of snapshots are all the same as in case 1.

Figure 3 shows the first to the third POD modes of the above two cases. As can be seen from Fig. 3(d) to (f), the contour of the upper airfoil surface displays a ribbon pattern. And the value distribution of these ribbons alternates in a positive and negative way. We