Chinese Journal of Aeronautics, (2015),**28**(1): 44–56

Chinese Society of Aeronautics and Astronautics
& Beihang University

Chinese Journal of Aeronautics

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Stationary flow fields prediction of variable physical domain based on proper orthogonal decomposition and kriging surrogate model

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Received 18 February 2014; revised 23 March 2014; accepted 16 April 2014
Available online 26 December 2014

KEYWORDS

Compressible-viscous flows;
Kriging surrogate model;
Proper orthogonal decomposition;
Shock wave;
Variable physical domain

Abstract In this paper a new flow field prediction method which is independent of the governing equations, is developed to predict stationary flow fields of variable physical domain. Predicted flow fields come from linear superposition of selected basis modes generated by proper orthogonal decomposition (POD). Instead of traditional projection methods, kriging surrogate model is used to calculate the superposition coefficients through building approximate function relationships between profile geometry parameters of physical domain and these coefficients. In this context, the problem which troubles the traditional POD-projection method due to viscosity and compressibility has been avoided in the whole process. Moreover, there are no constraints for the inner product form, so two forms of simple ones are applied to improving computational efficiency and cope with variable physical domain problem. An iterative algorithm is developed to determine how many basis modes ranking front should be used in the prediction. Testing results prove the feasibility of this new method for subsonic flow field, but also prove that it is not proper for transonic flow field because of the poor predicted shock waves.

1. Introduction

For some systems governed by complex equations, a reduced order model (ROM) which approximates the high-fidelity (HF) models well with rather fewer states can be generated by some certain methods. So, developing efficient ROMs to improve computational efficiency is a hot issue in computational physics now. The combination of proper orthogonal decomposition (POD)[1–3] and projection methods (POD-projection) is such a research direction in the area of fluid dynamics. This strategy approximates the HF result by the linier superposition of some selected basis modes, and the coefficients of these selected basis modes are determined by solving ordinary differential equations (ODEs) generated from projecting the governing equations onto the selected basis modes.

In the past decades, many problems in fluid dynamics have got corresponding ROMs through POD-projection approach. Two projection methods for applying this strategy in problems governed by Euler equations are presented in Ref.[4] ROMs about aeroelasticity of airfoil[5,6] and turbine engine[7] have also

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Peer review under responsibility of Editorial Committee of CJA.

ELSEVIER Production and hosting by Elsevier

http://dx.doi.org/10.1016/j.cja.2014.12.017

been derived. But all these applications above ignored the fluid viscosity. It is true that problems which concern viscosity could also be handled by this approach. For example, Ma and Karniadakis[8] investigated the stability and dynamics of three-dimensional limit-cycle states inflow past a circular cylinder using ROM generated by POD-projection strategy. Other similar literature includes laminar, transitional and turbulent flows simulation,[9–13] flow field calculation and control in chemical process[14] and free surface shallow water flows.[15] However, these problems all ignored the compressibility of fluid.

Not many researches have been conducted concerning the problems that concern compressible viscous flows by POD-projection strategy. Rowley et al.[16] got the ROM for compressible Navier–Stokes equations, but the flow must be isentropic. Bourguet et al.[17] extended the application to transonic flows around airfoil, which are governed by Navier–Stokes equations. While, the flow fields are constrained under constant viscosity assumption. It is worth noting that all the constraints above come from the projection process. For realizing the projection process, the governing equations should be modified into some forms to lead quadratic fluxes, and the inner product should make dimensional sense.[16] Besides compressibility and viscosity, variable physical domain, which means that the domain occupied by the flow field is variable, also causes troubles for the application of POD-projection, because the projection process requires a fixed physical domain in principle. Of course, this problem has been solved in some cases. For the physical domain discretized by structured meshes, index-based POD[6,18,19] could be used to eliminate this problem. In addition, Hadamard formulation could also be used to cope with small deformations of physical domain in POD-projection process.[17]

All the drawbacks presented above can be summarized as the so-called intrusive feature: starting from an existing computational code, additional derivations and programming efforts required to develop a ROM.[20] Bui-Thanh et al.[21] combined POD with cubic spline interpolation to predict inviscid flow field of fixed airfoil when a single parameter, such as the angle of attack or inflow Mach number, is changed. This method gets over the intrusive feature, but can just treat single parameter problems, and the physical domain should still be fixed because of the constraint from inner product. Qiu et al.[22] presented a new strategy to predict flow field by the combination of surrogate model and POD. Compared with the combination of cubic spline interpolation and POD, multi-parameters problems could be handled easily by this method.

Following the work presented in Ref.[22], this paper is devoted to develop a simpler and more precise ROM method for stationary flow field prediction. For that, the combination of POD and kirging surrogate model[23] is used to build ROM system. Two simple forms of index-based inner product are applied into the POD process, which improve the computational efficiency and make the physical domain variation problems very easy. Meanwhile, an efficient algorithm, which is used to determine how many basis modes ranking front should be used, is proposed in this paper.

Brief introductions of POD and kriging surrogate model are presented in Sections 2 and 3 respectively. Section 4.1 introduces flow field prediction method based on the combination of POD and kriging surrogate model in detail. The algorithm used to determine the basis modes number is presented out in Section 4.2. Following that, the applying of different forms of inner product is discussed. Section 5 presents two sets of prediction results and the corresponding analysis under different flow conditions. A brief summary is concluded in Section 6.

2. Proper orthogonal decomposition and POD-projection system

To use POD method, the data set should be pre-treated. Normally, there are two forms,[24] covariance form and correlation form, to pre-treat the data set from the perspective of statistics. The first one is the most common method, and the second method is more suited to data with mixed units and significant magnitude difference. Since the results generated by the CFD code in present work are dimensionless, the covariance method is adopted here.

Let $\{\boldsymbol{U}^{(i)}(x) : 1 \le i \le N, x \in \Omega\}$ represent a set of N sample flow fields (called snapshots commonly), Ω is the physical domain of flow field, and we deem each snapshot as a vector. With covariance method, each snapshot should be rewritten in the form of $\boldsymbol{U}^{(i)}(x) = \tilde{\boldsymbol{U}}^{(i)}(x) + \overline{\boldsymbol{U}}(x)$, and $\overline{\boldsymbol{U}}(x)$ is the average of all snapshots. Then the vector set $\{\tilde{\boldsymbol{U}}^{(i)}(x) : 1 \le i \le N, x \in \Omega\}$ can span a linear space $\boldsymbol{\Psi}$. POD method is used to decompose space $\boldsymbol{\Psi}$ into a set of orthogonal basis $\{\boldsymbol{\Phi}^{(i)}(x) : 1 \le i \le N, x \in \Omega\}$ (called basis modes) which has the maximum mean square projection on all snapshots. This leads to such a constrained maximization problem:

$$\begin{aligned} &\max \ \frac{1}{N}\sum_{i=1}^{N}\left|\left(\tilde{\boldsymbol{U}}^{(i)}, \boldsymbol{\Phi}\right)\right|^2 \\ &\text{s.t.} \quad (\boldsymbol{\Phi}, \boldsymbol{\Phi}) = 1 \end{aligned} \tag{1}$$

where $(\cdot\,,\,\cdot)$ and $|\cdot|$ are inner product operation and norm defined on $\boldsymbol{L}^2$ (square integrable space, SIS) respectively. Since $\left\{\boldsymbol{\Phi}^{(i)}(x) : 1 \le i \le N, x \in \Omega\right\}$ is a set of orthogonal basis of space $\boldsymbol{\Psi}$ which is spanned by $\left\{\tilde{\boldsymbol{U}}^{(i)}(x) : 1 \le i \le N, x \in \Omega\right\}$, then each basis mode $\boldsymbol{\Phi}$ can be represented by the linear superposition of $\tilde{\boldsymbol{U}}^{(i)}(x)$ as

$$\boldsymbol{\Phi} = \sum_{i=1}^{N} a^{(i)}\tilde{\boldsymbol{U}}^{(i)} \tag{2}$$

If all the coefficients $a^{(i)}$ are solved out, then the basis modes are known. The so-called Rayleigh-Rita method[25] could be used to solve this problem above. Literature[14] presents the process for the most common solution. First it defines a core function

$$\boldsymbol{K}(x, x') = \frac{1}{N}\sum_{i=1}^{N}\tilde{\boldsymbol{U}}^{(i)}(x)\tilde{\boldsymbol{U}}^{(i)}(x') \tag{3}$$

and an operator

$$\boldsymbol{R\Phi} = \int_{\Omega}\boldsymbol{K}(x, x')\boldsymbol{\Phi}(x')\mathrm{d}x' \tag{4}$$

where $\boldsymbol{R} : \boldsymbol{L}^2(\Omega) \to \boldsymbol{L}^2(\Omega)$. Inner product operation between $\boldsymbol{R\Phi}$ and $\boldsymbol{\Phi}$ leads

$$(\boldsymbol{R\Phi}, \boldsymbol{\Phi}) = \int_{\Omega}\boldsymbol{R\Phi}(x)\boldsymbol{\Phi}(x)\mathrm{d}x = \frac{1}{N}\sum_{i=1}^{N}\left|\left(\tilde{\boldsymbol{U}}^{(i)}, \boldsymbol{\Phi}\right)\right| \tag{5}$$

The right side of this equation is equal to the target of Eq. (1). So, the maximization problem then transforms into finding the maximum eigenvalue of