Proper orthogonal decomposition closure models for Burgers and Navier-Stokes Equations

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Proper orthogonal decomposition closure models for Burgers and Navier-Stokes Equations

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Proper orthogonal decomposition based reduced-order models hold importance in fluid dynamics due to their utilization in flow control, design, and optimization. The reduced-ordered models have shown promising results for laminar flows, however, lack accuracy for complex and turbulent flows. In this study, we consider Burgers and Navier-Stokes equations and develop their reduced order models. Burgers equation is considered with homogenous boundary condition and Navier-Stokes equations are used for simulating the incompressible fluid flow past a circular cylinder. The literature shows that the conventional reduced-order models do not perform well in case of less number of modes and require closure model for the discarded modes. We investigate the effect of closure modeling on the accuracy of the reduced-order model for 1D Burgers equation and 2D Navier-Stokes equations. We consider three mode-dependent closure models, based on eddy viscosity model. This study compares the performance of all considered closure models for wide range of mathematical parameter ν_e and choose the best closure approach for the reduced-order model of Navier-Stokes equations. The numerical results show that the selected closure model greatly improves the accuracy of the reduced-order model for both Burgers and Navier-Stokes equations.

I. Introduction

Full order simulations (FOS) such as Direct numerical simulation, Large eddy simulation (LES), and Reynolds-averaged Navier-Stokes equations are used to numerically simulate complex and turbulent flows. FOS techniques are useful for designing complex and nonlinear systems, where accuracy is the key requirement. However, these techniques are computationally expensive as they require large set of degrees of freedom, therefore these techniques are infeasible for control design that requires many quick simulations of nonlinear systems.[1] Generally, in many practical problems, much of the information lies in subspace having very low dimension as compared to dimension used in discretization of FOS techniques. Reduced order modeling is an effective technique for engineering applications,[2,3] which are based on low dimensional model and contain a large percentage of FOS information. Proper orthogonal decomposition (POD) provides optimal basis for the reduced-order model (ROM) and has many industrial applications, which includes climate modeling of atmospheric and oceanic flows.[2,4–9] Its other applications are structural vibrations,[3,10,11] ecosystems,[12] low-dimensional dynamics modeling,[13–17] stochastic partial-differential equations,[18–20] and optimization.[21–23] The conventional ROM is developed by Galerkin projection of POD modes onto the governing equations that include heat equation, Burgers equation, and Navier-Stokes equations. The conventional POD-ROM with enough degrees of freedom provides good approximation of simple and laminar flows, whereas accuracy and stability is a limitation for complex and turbulent flows,[24–27] even in the presence of sufficient modes.[28]

In FOS, an approach that has gained considerable attention in the modeling of turbulent flows is LES.[29–32] In LES, large-scale eddies are solved directly, while small-scale eddies are modeled by a subgrid- scale (SGS) model. Mathematically, it can be done by averaging the Navier-Stokes equations, however, an extra closure term is required to model for small scale eddies. This closure term is replaced by Reynolds stresses, which are modeled through Boussinesq hypothesis.[33] The hypothesis relates the Reynolds stresses and the velocity

gradients through eddy viscosity. Figure 1 shows a schematic of energy distribution of turbulence modeling using FOS and its analogy for ROM. It can be deduced from the schematic that there exists resemblance between turbulence modeling of FOS and POD-ROM. Figure 1a presents energy distribution in turbulence modeling using FOS in which the shaded area shows high wave number disturbances in the flow being unresolved by averaging of Navier-Stokes equations. The effect of high wave number disturbances is modeled using different LES techniques such as Smagorinsky model, Dynamic subgrid scale model etc., which enables realistic estimation of the flow field. Figure 1b presents the energy distribution in the POD-ROM, where shaded region represents the discarded energy due to M selected modes containing relatively high energy as compared to discarded modes. The higher modes, despite having low energy, play a vital in the overall dynamics of complex and turbulent flows.[25,26] Therefore, we incorporate the effect of discarded modes into the POD-ROM for improved performance through different closure modeling techniques, which are inspired from FOS technique of turbulence modeling using LES. Closure models in the POD-ROM improve its performance with low computational cost, but still remains a challenging task for complex and turbulent flows.[27,34–37]
In this paper, we discuss the closure modeling in the POD-ROM based on constant eddy viscosity model. We consider three closure models, which are based on the mode dependent constant eddy viscosity model (POD-R) proposed by Rempfer.[38] San and Iliescu[24] compared these models for simple case of 1D Burgers equation with homogenous boundary condition. Burgers equation is simple and contains a nonlinear term similar to Navier-Stokes equations. In this work, we will further investigate these models for Navier-Stokes equations along with Burgers equation. For Burgers equation, we consider homogenous boundary condition, whereas for Navier-Stokes equations, we consider the 2D flow past a circular cylinder at Reynolds number of 200. This study also compares the effectiveness of the closure models for considered cases of governing equations. This work adds to the existing knowledge of the POD closure modeling with special focus on Burgers equation and Navier-Stokes equations.
The rest of this paper is organized as follows. Sec. II covers the POD method employed for computation of modes, numerical methodology for FOS and ROM of Burgers equation and Navier-Stokes equations. It also includes two closure models for Burgers equation and Navier-Stokes equation. Section III includes the results and discussion for considered cases of governing equations and comparison between conventional and closure model based POD-ROM.

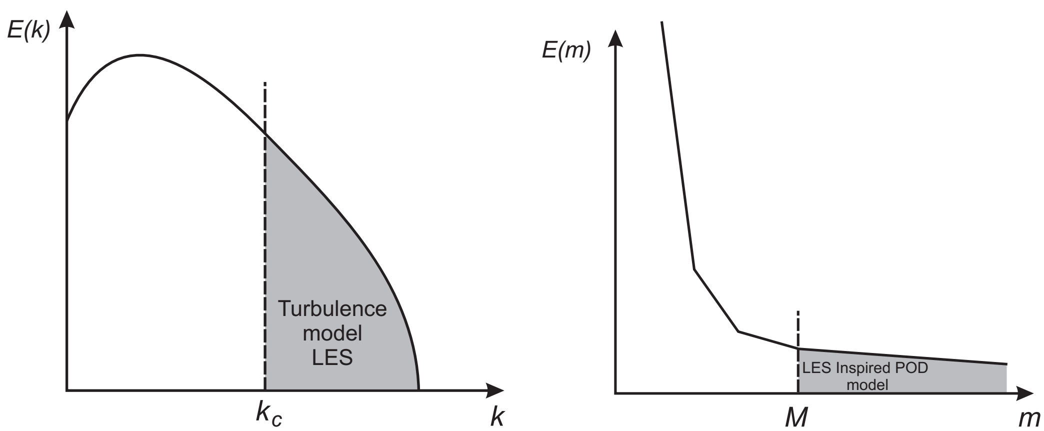


Figure 1. Schematic of energy distribution versus (a) wave number (turbulence modeling using LES approach) and (b) POD modes for conventional POD-ROM (closure modeling in POD-ROM).

II. Reduced-Order Models

II.A. Proper Orthogonal Decomposition Modes

We develop the POD-ROM by computing the POD modes and then projecting the governing equations onto the POD modes. Let $\mathbf{u}(.,t)$ be the state variable, which are evaluated on Hilbert space $\mathcal{H}$. Mathematically, it can be written as $\mathbf{u}(.,t) \in \mathcal{H}$ for $t \in [0,T]$, where the $\mathbf{u}(.,t)$ is computed using Burgers and Navier-Stokes equations. We obtain the solution for Burgers and Navier-Stokes equations using FOS and then use this solution for development of the ROM.
We take snapshots at different time instances $t_1,\ t_2\ ,...,\ t_N \in [0,T]$ and ensemble these snapshots into a

larger matrix. We consider ensemble of snapshots as

$$\mathbf{W} := \text{span}\{\mathbf{u}(t_1, .),\ \mathbf{u}(t_2, .),\ ...,\ \mathbf{u}(t_N, .)\}. \tag{1}$$

The dimensions of $\mathbf{W}$ is d_s. The POD seeks a low dimensional modes $\{\Phi_1,\ \Phi_2,\ ...,\ \Phi_M\}$, with $M << d_s$, which optimally approximates the input matrix $\mathbf{W}$ as

$$\min_{\Phi_j} \frac{1}{N} \sum_{i=1}^{N} \| \mathbf{u}(t_i, .) - \sum_{j=1}^{M} (\mathbf{u}(t_i, .), \Phi_j(.))_{\mathcal{H}} \Phi_j(.)\|_{\mathcal{H}}^2, \tag{2}$$

where equation (2) is subjected to condition that $(\Phi_i, \Phi_j)_{\mathcal{H}} = \delta_{ij}, 1 \leq i, j \leq M$. Let the time step $\delta t = \frac{T}{N-1}$ and the time instances $t_k = k\delta t,\ k$=1, 2, ..., N. The correlation matrix can be defined as

$$\mathbf{K}_{ij} = \frac{1}{N} (\mathbf{u}(t_i, .), \mathbf{u}(t_j, .))_{\mathcal{H}}, \tag{3}$$

where inner product can be defined as $(a, b) = \int_{\Omega} a.b \, d\Omega$

$$\mathbf{K}\nu = \lambda\nu, \tag{4}$$

where $\mathbf{K}$, ν, and λ are snapshot correlation matrix, eigenvectors and positive eigenvalues, respectively. It can then be shown,[28] that the solution of equation (2) is given by

$$\Phi_k(.) = \frac{1}{\sqrt{\lambda_k}} \sum_{j=1}^{N} (\nu_k)_j \mathbf{u}(t_j, .), \qquad 1 \leq k \leq M. \tag{5}$$

II.B. Burgers Equation

The Burgers equation can be written as

$$\begin{cases} \partial_t u - \nu \partial_{xx} u + u \partial_x u = f & \text{in } \Omega, \\ u(x, 0) = u_0 & \text{in } \Omega, \\ u(x, t) = f_{app}(x, t) & \text{in } \partial\Omega. \end{cases} \tag{6}$$

where $\Omega \subseteq \mathbb{R}$ is the computational domain for Burgers equation and f_{app} is considered as zeros at the domain boundaries $\partial\Omega$ for homogenous boundary. Following the Galerkin expansion, u can be approximated as $\sum_{i=1}^{M} \phi_i(x) q_i(t)$. POD-ROM for Burgers equation is developed by projecting Burgers equation onto the POD modes as follows:

$$\big\{(\partial_t u, \phi) - (\nu \partial_{xx} u, \phi) + (u \partial_x u, \phi) = (f, \phi)\big\}, \qquad \forall \phi \in S^M \tag{7}$$

Equation (7) results in the following M-dimensional model:

$$\dot{q}_k(t) = \mathcal{A}_k + \sum_{m=1}^{M} \mathcal{B}_{km} q_m(t) + \sum_{m=1}^{M} \sum_{n=1}^{M} \mathcal{C}_{kmn} q_m(t) q_n(t), \tag{8}$$

where

$$\begin{aligned} \mathcal{A}_k &= (f, \phi_k), \\ \mathcal{B}_{km} &= \nu(\partial_{xx}\phi_m, \phi_k), \\ \mathcal{C}_{kmn} &= -\phi_m(\partial_x \phi_n, \phi_k). \end{aligned}$$

The conventional reduced-order model in equation (8) is termed as POD-G for Burgers equation, where G stands for Galerkin projections of the POD mode onto the governing equations. Boussinesq[33] related the turbulent stresses to the mean flow and lumped the effects of turbulence into a turbulent viscosity. This approach equates the dissipation of kinetic energy at the sub-grid scales as molecular diffusion. In this study, we consider the same approach in the POD-ROMs for development of the closure model that is based on eddy viscosity mode-dependent model. The POD-ROM along with the closure model can be written as

$$\dot{q}_k(t) = \mathcal{A}_k + \sum_{m=1}^{M} \Big(\mathcal{B}_{km} + \tilde{\mathcal{B}}_{km}\Big) q_m(t) + \sum_{m=1}^{M}\sum_{n=1}^{M} \mathcal{C}_{kmn} q_m(t) q_n(t), \tag{9}$$

The model contains $\tilde{B}_{km}$ (k, m = 1, 2, ..., M) that can be defined for POD-R as

$$\tilde{B}_{km} = \nu_e \left(\frac{k}{M}\right) (\partial_{xx}\phi_m, \phi_k).$$

where ν_e is constant eddy viscosity whose magnitude can be adjusted for better accuracy of the POD-ROM. We consider two more closure models in this study, which are variation of POD-R. These models are named as POD-RQ and POD-RS[24] and contain $\tilde{B}_{km}$ as

$$\tilde{B}_{km} = \nu_e \left(\frac{k}{M}\right)^2 (\partial_{xx}\phi_m, \phi_k) \qquad \text{for POD} - \text{RQ}.$$
$$\tilde{B}_{km} = \nu_e \left(\frac{k}{M}\right)^{0.5} (\partial_{xx}\phi_m, \phi_k) \qquad \text{for POD} - \text{RS}.$$

II.C. Navier-Stokes Equations

We consider following governing equations for numerical solution of 2D incompressible flow past a circular cylinder

$$\left.\begin{aligned} &\mathbf{u}_t - \mathrm{Re}^{-1}\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\,\mathbf{u} + \nabla p = 0 \\ &\nabla\cdot\mathbf{u} = 0 \end{aligned}\right\} \tag{10}$$

where $\mathbf{u}$ is the velocity, p is the pressure, and Reynolds number is defined as $\mathrm{Re} = U_\infty D/\nu_s$. U_∞ is the velocity scale, and ν_s shows kinematic viscosity of the fluid. A POD basis enables a reduced representation of the FOS data as

$$\mathbf{u}(\mathbf{x}, t) = \bar{\mathbf{u}}(\mathbf{x}) + \sum_{i=1}^{M} q_i\,(t)\Phi_k\,(\mathbf{x}) \tag{11}$$

A POD-G is developed by projecting the Navier-Stokes equations onto the POD modes as follows

$$(\mathbf{u}_t, \Phi_k) - \big(\mathrm{Re}^{-1}\Delta\mathbf{u}, \Phi_k\big) + ((\mathbf{u}\cdot\nabla)\,\mathbf{u}, \Phi_k) + (\nabla p, \Phi_k) = 0 \tag{12}$$

We consider a large computational domain for the study, thus ignore the pressure term in the POD-ROM (for details, see Akhtar et al.;[39] Noack et al.[40]). POD-G yields the following autonomous dynamical system for the vector of time coefficients, $q(t)$:

$$\dot{q}_k(t) = \mathcal{A}_k + \sum_{m=1}^{M} \mathcal{B}_{km} q_m(t) + \sum_{m=1}^{M}\sum_{n=1}^{M} \mathcal{C}_{kmn} q_m(t) q_n(t), \tag{13}$$

where

$$\begin{aligned} \mathcal{A}_k &= \frac{1}{\mathrm{Re}} (\Delta\bar{\mathbf{u}}, \Phi_k) - ((\bar{\mathbf{u}}\cdot\nabla)\,\bar{\mathbf{u}}, \Phi_k)\,, \\ \mathcal{B}_{km} &= -\,(\bar{\mathbf{u}}\cdot\nabla\Phi_m, \Phi_k) - (\Phi_m\cdot\bar{\mathbf{u}}, \Phi_k) + \frac{1}{\mathrm{Re}} (\Delta\Phi_m, \Phi_k)\,, \\ \mathcal{C}_{kmn} &= -\,(\Phi_m\cdot\nabla\Phi_n, \Phi_k)\,. \end{aligned}$$

Similar to Burgers equation, we incorporate the closure term in the conventional POD-ROM of Navier-Stokes equations as

$$\dot{q}_k(t) = \mathcal{A}_k + \tilde{\mathcal{A}}_k + \sum_{m=1}^{M} \Big(\mathcal{B}_{km} + \tilde{\mathcal{B}}_{km}\Big) q_m(t) + \sum_{m=1}^{M}\sum_{n=1}^{M} \mathcal{C}_{kmn} q_m(t) q_n(t), \tag{14}$$

where

$$\tilde{\mathcal{A}}_k = \nu_e \left(\frac{k}{M}\right)(\Delta\bar{\mathbf{u}}, \Phi_k),$$
$$\tilde{\mathcal{B}}_{km} = \nu_e \left(\frac{k}{M}\right)(\Delta\Phi_m, \Phi_k),$$

The closure model is named as POD-R for Navier-Stokes equations. Similar to Burgers equation, we use the variation of k/M and develop POD-RS and POD-RQ for Navier-Stokes equation.

III. Results and Discussion

In this section, we investigate the POD-G and the closure models in the POD-ROM by making a comparison of these models. The simulations are preformed for the two test cases: Burgers equation with a small diffusion coefficient, and Navier-Stokes equations for 2D incompressible flow past a circular cylinder.

III.A. Burgers Equation

For 1D Burgers equation, we use computational setting that is similar to Kunisch and Volkwein[41] and consider following initial condition

$$u(x,0) = \begin{cases} 1, & \text{if } \ x \in (\ 0 \quad \frac{1}{2}\ ] \\ 0, & \text{otherwise} \end{cases}$$

The boundary conditions which we have considered are homogeneous Dirichlet. First, we obtain the results using FOS technique and use these results as benchmark for the POD-ROM. We use the following input parameters for FOS: $\Delta x = \frac{1}{8193}$, $\Delta t = \frac{1}{999}$ and $\nu = 10^{-3}$. We employ the Euler's method for temporal discretization, the second order central difference scheme for spatial discretization, and Newton's method for solving the nonlinear term in Burgers equation. We perform the validation study for the present results by comparing them with the results in literature. Figure 2 shows a good agreement between the present work and the results obtained by Kunisch and Volkwein[41] at $t = 1$.

Table 1. Cumulative energy distribution in percentage.

M	1D Burgers equation	2D Navier-Stokes equations
2	91.01	96.72
4	96.82	98.47
6	98.17	99.85
8	98.80	99.95
10	99.14	99.98

For generation of the POD modes, we record the data for 1000 snapshots as the solution is marched from $t = 0$ to 1 and ensemble them in the matrix $\mathbf{W}$ as given in equation (1). Using eigenvalues, we compute the energy associated with the POD modes as shown in Table 1. It shows that first 10 POD modes capture over 99% of system's energy, whereas first two modes capture only 91.01% of energy.
We obtain POD-G by numerically solving equation (8), which uses the POD modes for computation of temporal coefficients q_i (i=1, 2, ..., 10) that are used along with the POD modes for reconstruction of u. The accuracy of these reduced-order models are assessed through the relative error that is defined as

$$\text{Relative error} = \frac{\frac{1}{N} * \sum_{k=1}^{N} \|u^{POD-ROM}(x,t_k) - u^{FOS}(x,t_k)\|_0^2}{\frac{1}{N}\sum_{k=1}^{N} \|u^{FOS}(x,t_k)\|_o^2}. \tag{15}$$

The relative errors are 0.16 and 0.07 at $M = 2$ and $M = 10$, respectively. The relative error decreases for POD-G with increase in the POD modes, whereas computation time for POD-G increases with increase in the number of modes. Aubry et al.[28] also discussed that POD-G produces erroneous results, even when the POD modes capture most of the system's energy. Therefore they used a Heisenberg type of closure model

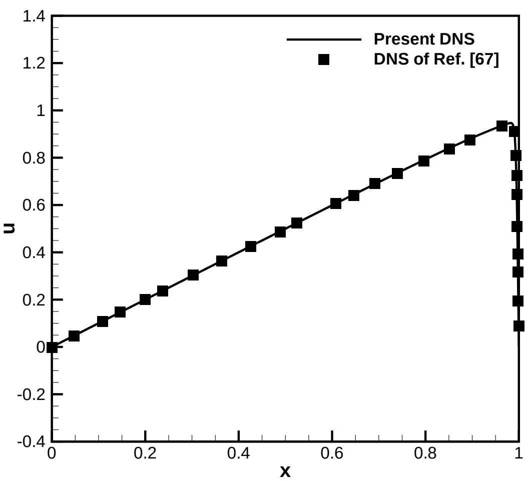


Figure 2. Validation study for 1D Burgers equation.

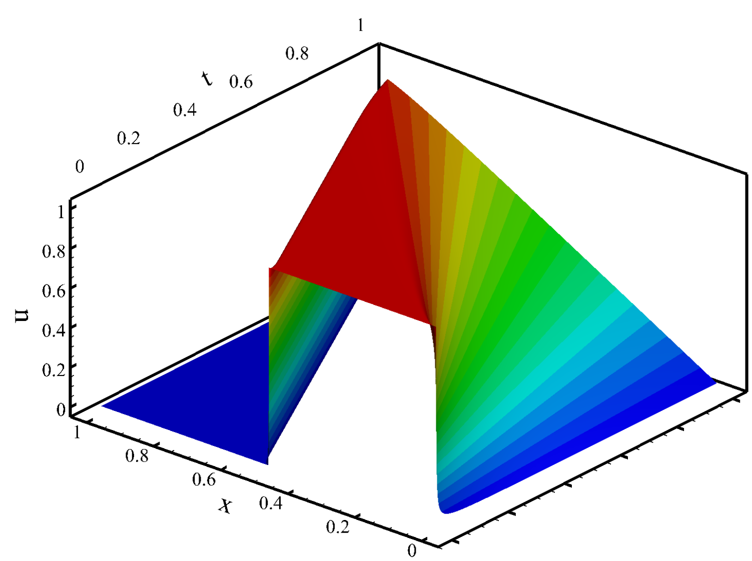


Figure 3. Data for 1D Burgers equation using FOS.

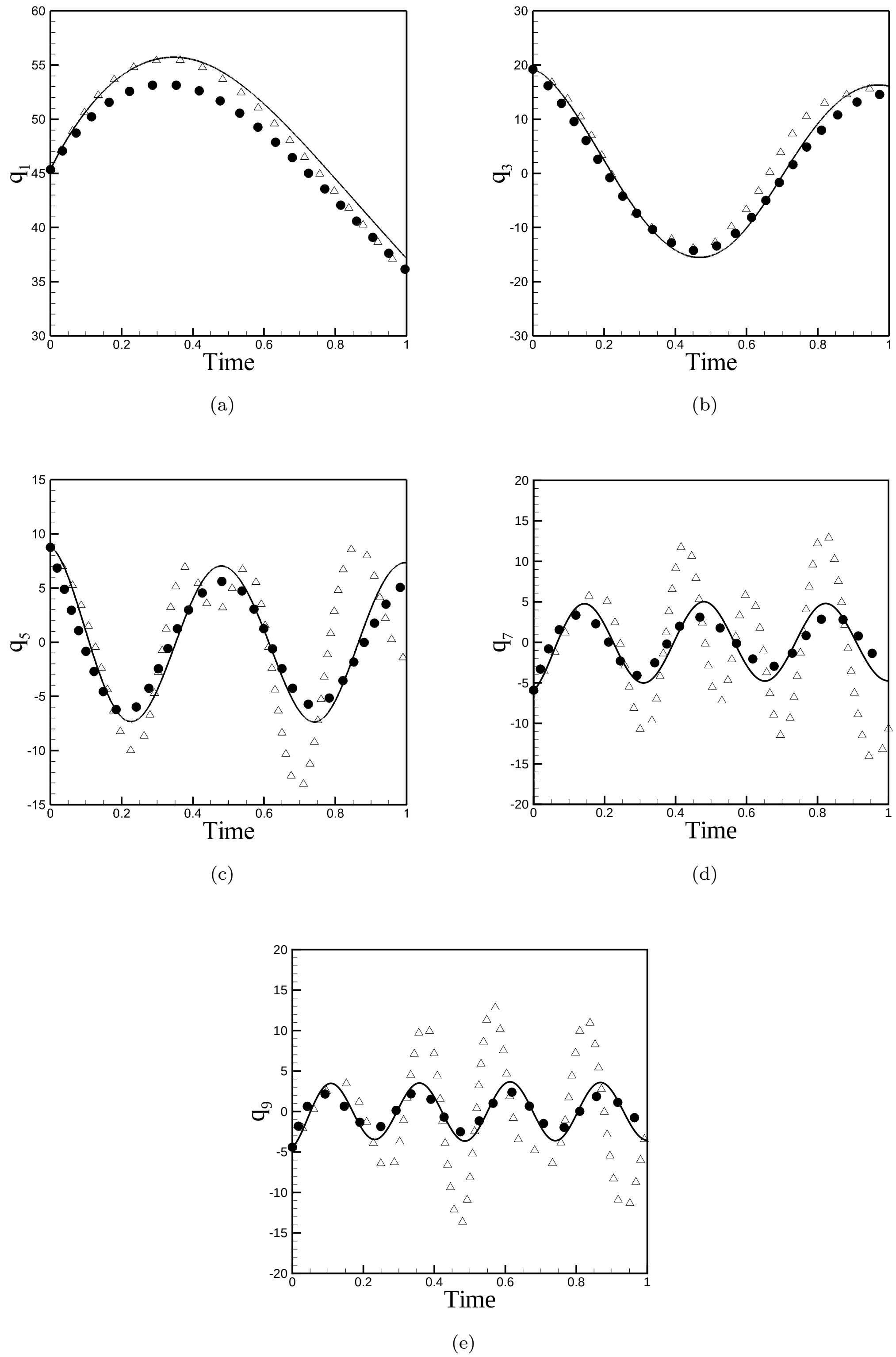
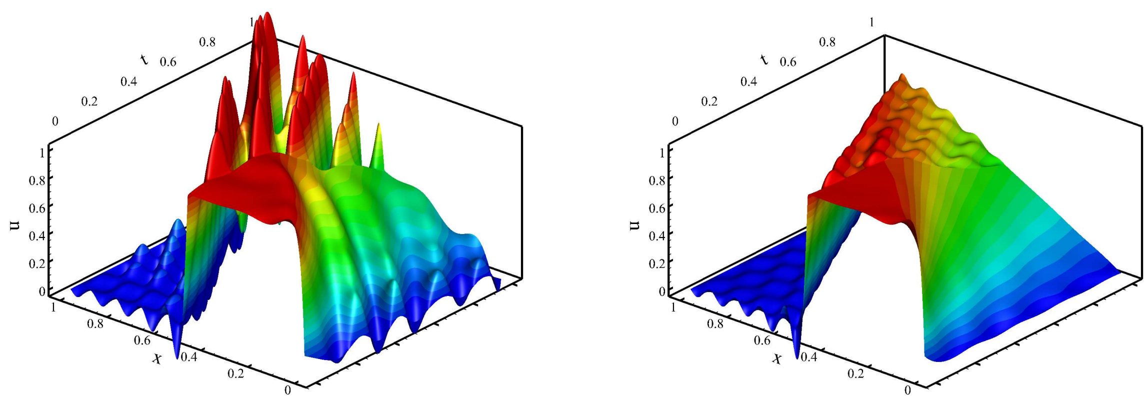


Figure 4. Time evolution of temporal coefficient q_i for 1D Burgers equation. Projection of FOS onto POD modes (solid line), POD-G (delta), and POD-R (circle).

in the wall region of turbulent boundary layer that yielded good qualitative results.
For better accuracy of the reduced-order model, we use closure models presented in equation (9). We employ 10 POD modes and set the mathematical parameter ν_e to 4.5×10^{-3} for the closure models. We compute q_i using POD-R for Burgers equation and plot them in Fig. 4. The figure shows q_i (i = 1, 3, ..., 9) of 1D Burgers using POD-G and POD-R. It also presents q_i obtained from projection of snapshot data onto the POD modes that are used as benchmark for comparison purposes with the POD-G and POD-R. The values of q_i associated with modes 5, 7 and 9 of POD-G show larger divergence from q_i obtained by projection of FOS data. Figure 4 also shows that the closure model in POD-R improves the accuracy of the POD-ROM, however, it is more effective for higher modes.
We reconstruct u using the POD modes and q_i obtained from equations (8) and (9). Figure 5 shows a qualitative comparison between POD-G and POD-R. It can be inferred from Figures 3 and 5 that u obtained from POD-R is closer to FOS than POD-G. We also compute percentage error for quantitative assessment of improvement in the ROM. We find that relative error for POD-R is 0.01 at M=10, while percentage error for POD-G is 0.07. For Burgers equation, qualitative and quantitative results show that POD-R performs better than POD-G.
We also compute the relative errors for POD-RQ and POD-RS using the same modeling parameter ν_e. The relative error for both closure models is 0.01, which is same as in case of POD-R. We investigate the effectiveness of these closure models across a wide range of ν_e as shown in Fig. 6. It shows that ν_e=4.5×10^{-3} is optimal value ν_{ep} for all three closure models as the relative error for all considered cases of the closure models is lowest. The accuracy of closure models is approximately same for $\nu_e \leq \nu_{ep}$ as relative error is same for all cases of closure models. POD-RS does not perform well for $\nu_e > \nu_{ep}$ as dissipation added into the POD-ROM becomes large with increase in ν_e as compared to other closure models. POD-RQ is more accurate than other closure models for $\nu_e > \nu_{ep}$ as it adds low amount of dissipation into the POD-ROM with increase in ν_e. Therefore POD-RQ is employed for next case of Navier-Stokes equations and compared with results of POD-G.



(a) (b)

Figure 5. Data for 1D Burgers equation (a) POD-G and (b) POD-R.

III.B. Navier-Stokes Equations

For Navier-Stokes equation, we employ an O-type grid to simulate the flow over a circular body. Details of the numerical algorithm, validation and verification can be found in Akhtar et al.[1,37] We simulate a two-dimensional flow past a cylinder at Re = 200 by employing a 193×257 grid in radial and circumferential directions, respectively over a domain size of 30D; a planar view is shown in Fig. 7. In this case, we collect 130 snapshots of the flow field over one vortex shedding cycle and ensemble them into the snapshots matrix $\mathbf{W}$ as given in equation (1). We compute the mean streamwise and crossflow component of velocity over a shedding cycle and plot them in Fig. 8. We subtract the mean velocity components from the snapshots

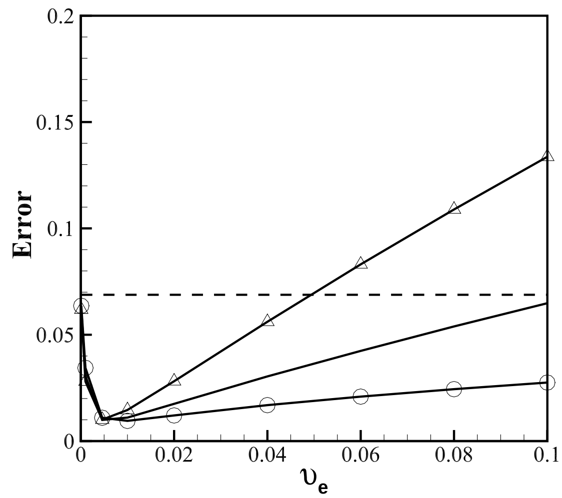


Figure 6. Relative errors for POD-ROMs: POD-G (dashed line), POD-R (solid line), POD-RQ (solid line with circle), and POD-RS (solid line with delta).

matrix and compute POD modes using the method of snapshots. We use eigenvalues to compute the energy associated with each POD mode as shown in Table 1. It shows that first 2 modes capture 96.72% of energy and first 10 modes capture 99.98% of energy. Figures 9 and 10 show the first four POD modes of the streamwise and crossflow velocity components, respectively. We observe that first two POD modes of the streamwise component are antisymmetric, whereas third and fourth POD modes are symmetric with respect to x-axis. On the other hand, first 2 POD modes of the crossflow velocity component are symmetric and third and fourth POD modes are antisymmetric with respect to x-axis.
We use 10 modes to develop the POD-ROMs for the current flow configuration. We perform Galerkin projection and compute $\mathcal{A}_k$, $\mathcal{B}_{km}$, and $\mathcal{C}_{kmn}$, where k, m, and n = 1, 2, ..., 10. We obtain q_i (i = 1, 2, ..., 10) for POD-G using equation (13). For better accuracy of the POD-ROM, we compute $\tilde{\mathcal{B}}_{km}$ and compute q_i using POD-RQ. The value of ν_e used for POD-RQ is set to 0.01. Figure 11 shows the q_i (i = 5, 6,..., 10) for POD-G, POD-RQ and the q_i obtained from projection of the snapshot data onto the POD modes. We observe that the POD-RQ improves the accuracy of POD-ROM as compared to POD-G. It can also be noted from the Fig. 11 that the POD-RQ is more effective for the values of q_i associated with higher modes. The closure model discussed in the study can also be used in future to investigate 3D turbulent flows, which provides the realistic implementation of this closure model.

IV. Conclusion

This paper investigates the effect of closure modeling on accuracy of the POD-ROM for Burgers and Navier-Stokes equations. The POD-ROM for Burgers equations are examined with homogenous boundary conditions and for Navier-Stokes equations we consider 2D incompressible flow past a circular cylinder. The study considers three mode-dependent eddy viscosity closure models for Burgers equation and investigate it over a wide range of the mathematical parameter ν_e for Burgers equation. We found that POD-RQ is more accurate than other closure models over a wide range of ν_e. Burgers equation is simple and can act as surrogate for Navier-Stokes equations. Therefore, we have selected POD-RQ and have developed it for Navier-Stokes equations. The study concludes that POD-RQ gives better accuracy not only with Burgers, but also with Navier-Stokes equations.

V. Acknowledgment

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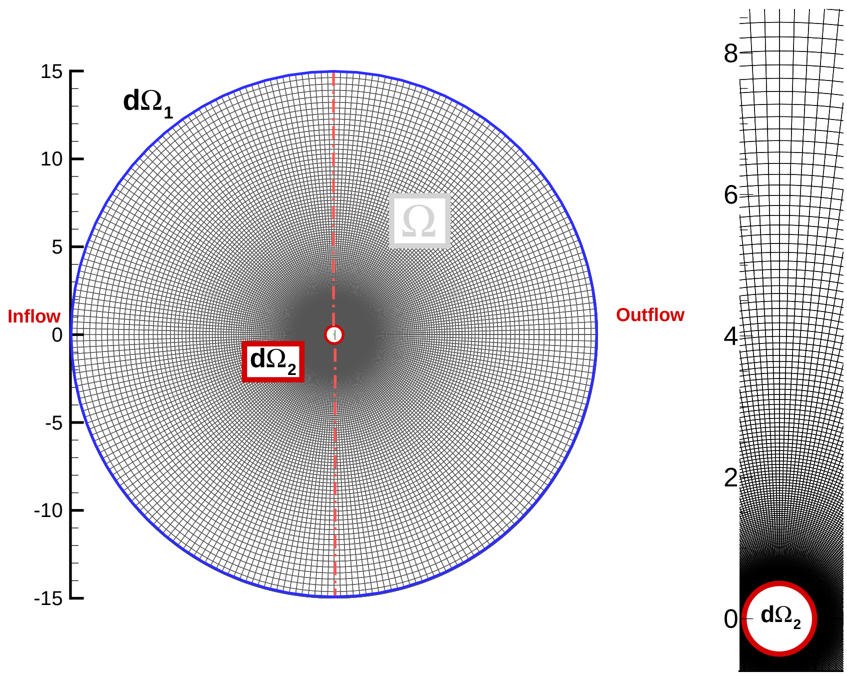
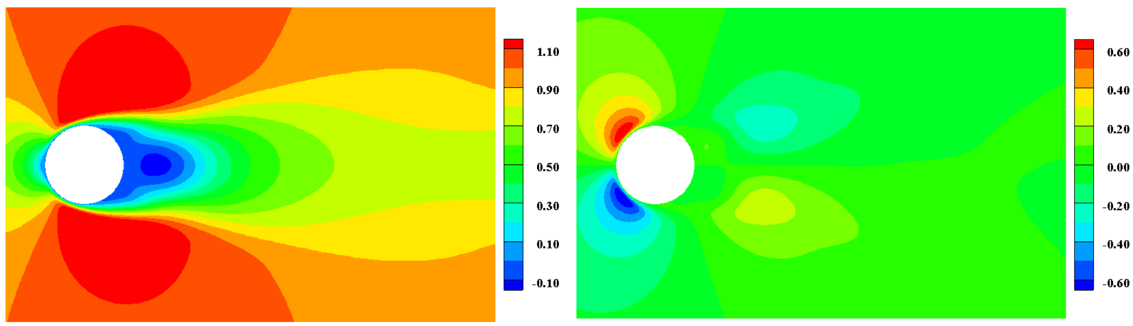


Figure 7. 2D grid layout over a circular cylinder.



(a) (b)

Figure 8. Average flow fields: a) streamwise and b) crossflow velocity components at $\mathrm{Re} = 200$

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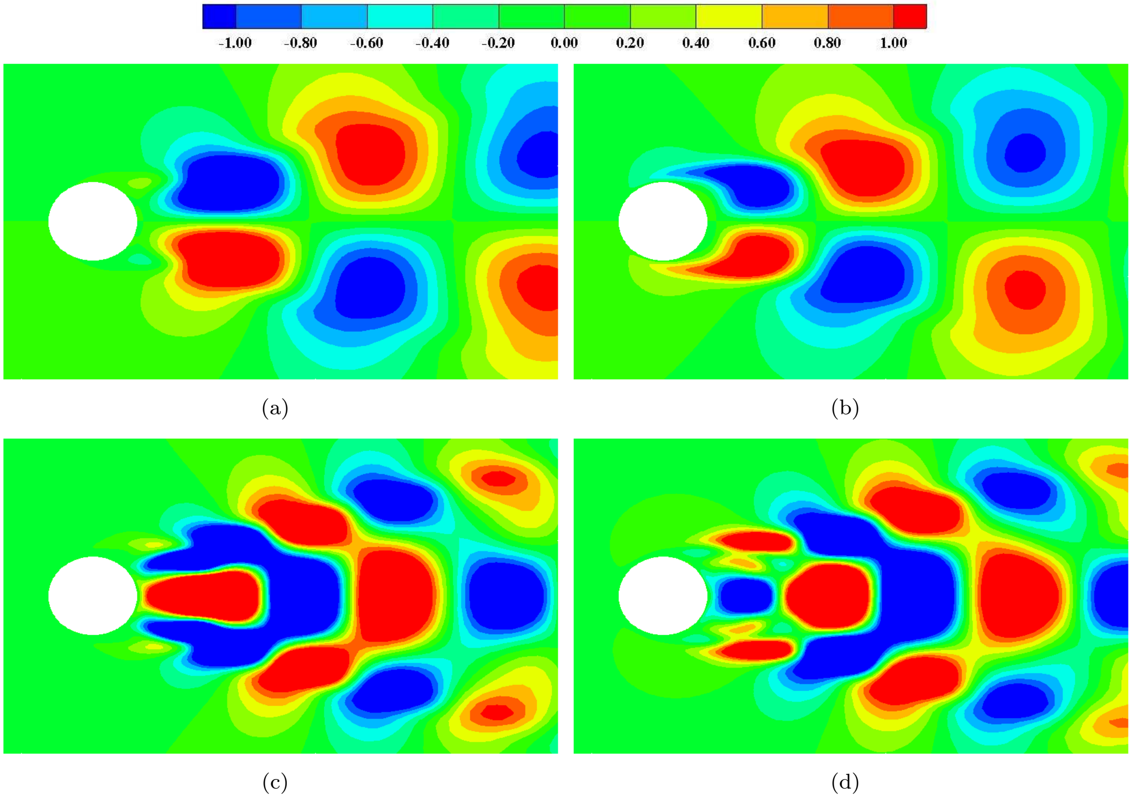

Figure 9. The streamwise velocity modes (ϕ_i^u, i = 1, 2, 3, 4.) at Re = 200.

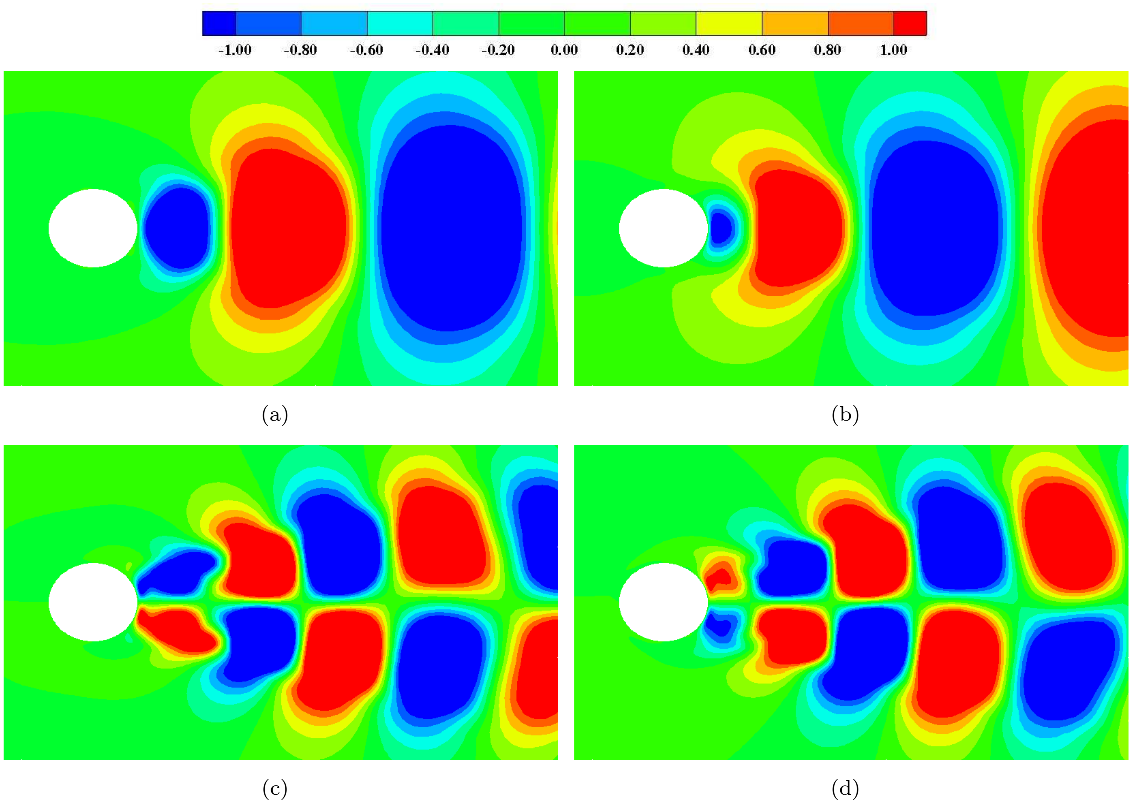

Figure 10. The crossflow velocity modes (ϕ_i^v, i = 1, 2, 3, 4.) at Re = 200.

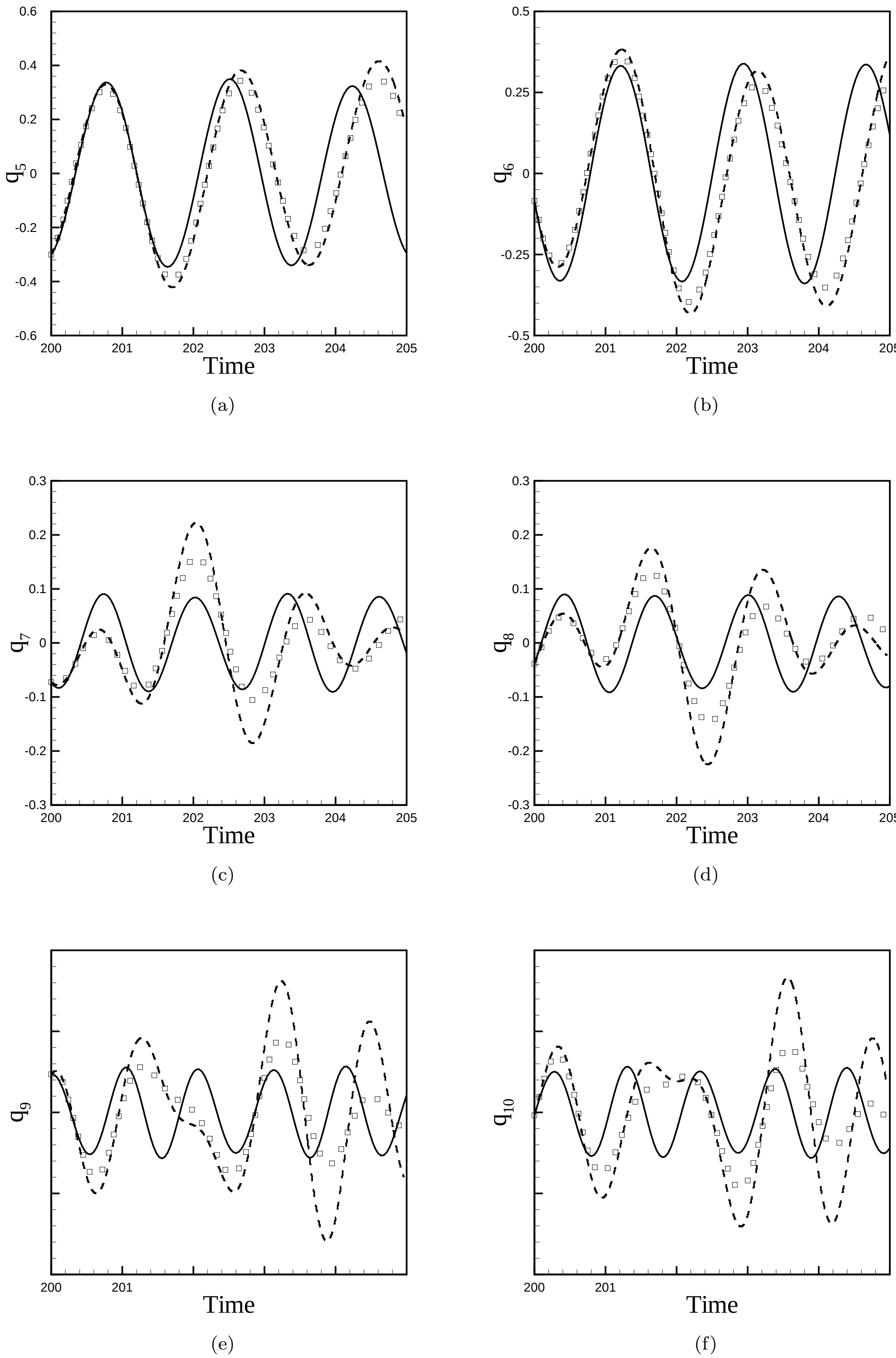

Figure 11. Time evolution of temporal coefficient q_i (i = 5, 6, ..., 10) for Navier-Stokes equations. Projection of FOS onto POD modes (solid line), POD-G (dashed line), and POD-RQ (square).

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