An iterative algorithm for POD basis adaptation in solving parametric convection-diffusion equations

Zhizhang Wu^a, Zhiwen Zhang^{a,*}

^aDepartment of Mathematics, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China.

Abstract

In this paper, we develop an iterative algorithm for proper orthogonal decomposition (POD) basis adaptation in solving linear parametric PDEs. Specifically, we consider the convectiondiffusion equations with the diffusivity as a parameter. To construct POD basis functions for the convection-diffusion equation with a small diffusivity, we need a fine-grid solver to obtain accurate solution snapshots, which leads to a large amount of computation and memory costs. Meanwhile, a coarse-grid solver is sufficient for obtaining high-resolution snapshots of a large diffusivity. We aim to adapt the POD basis functions extracted from the solution snapshots of a large diffusivity for the construction of a reduced-order model at a small diffusivity without resorting to a fine-grid solver. Our POD basis adaptation method exploits the implicit dependence of solutions on the diffusivity. The POD basis functions are adapted through an iterative algorithm, where the full-order model simulation at a large diffusivity and the PODbased reduced-order model simulation at a small diffusivity are implemented, alternatively. We also provide convergence analysis for our POD basis adaptation method. The algorithm and convergence analysis can be generalized to other types of linear parametric PDEs without any difficulty. Finally, we present numerical results to demonstrate the performance and accuracy of the proposed method. We find that a coarse-grid solver combined with the iterative process can achieve an accurate reduced-order model at a small diffusivity.

AMS subject classification: 35B30, 65M12, 65N50, 76R99, 78M34.

Keywords: Convection-diffusion equations; model reduction; basis adaptation; proper orthogonal decomposition (POD) method; iterative algorithm.

1. Introduction

Numerical simulations play an important role in studying complex physical phenomena which are usually modeled by parametric partial differential equations. The simulations become more computationally costly with the growing need for modeling more complicated phenomena and including more details in the models. In many applications, multiple simulations of the underlying model are needed, which leads to even greater computational burdens.

^{*}Corresponding author

Email addresses: wuzz@hku.hk (Zhizhang Wu), zhangzw@hku.hk (Zhiwen Zhang)

A powerful tool to alleviate this computational burden and enhance efficiency is model reduction [8, 9, 28]. Model reduction seeks for the original underlying system an intrinsic low-dimensional surrogate model which can be efficiently simulated but still yields high accuracy. During the past few decades, model reduction has been widely applied in different fields [6, 15, 17, 20, 22, 27, 29, 33]. Many basis generation techniques of model reduction have been developed, including rational interpolation methods [6, 23], balanced truncation methods [4, 7], proper orthogonal decomposition methods [44, 47], etc.

The proper orthogonal decomposition (POD) method is one of the most commonly used techniques of model reduction and has been applied in many problems [1, 5, 10, 11, 31, 34]. For parametric evolutionary PDEs, the POD method takes solutions of some certain parameters at a series of time instances and their finite difference quotients as inputs and returns an ordered set of orthogonal basis functions that best approximates the input data in the least square sense. The reduced-order model is obtained by truncating the optimal basis functions. The error estimate of the POD methods for the parabolic equation is shown in [32] and the high accuracy of the method can be obtained if an adequate number of basis functions are selected. However, if the parameter changes into a different value in the subsequent simulations, a direct application of the pre-constructed reduced-order model would probably result in a totally wrong solution. Hence the study of basis adaptation has been one of the most important problems in model reduction, which is also our focal point in this paper.

A natural idea of adaptive model reduction is interpolation between the pre-constructed reduced-order models to construct a reduced-order model for the new parameter [2, 16, 37, 49]. The localization approaches [3, 12, 18, 19, 40] pre-build a number of reducedorder models and select one of them in the online stage, depending on the current state of the system. We also have dictionary approaches [35], which pre-compute many basis vectors and then construct a reduced space online from a subset of them. All of the above mentioned methods rely on pre-computed quantities. Another way of basis adaptation is to incorporate observations of the new parameter. The updates of the reduced-order model based on new data are usually low-rank [41]. In [42], an adaptive DEIM using the sparse data from nonlinear terms is derived for nonlinear problems. The adaptation can also be done by updating the reduced subspace from a geometric perspective [50] with new information that is unavailable in the offline phase. There are also a class of adaptive methods that aims to improve the reduced-order model in an iterative manner, in which one may update the reduced bases by subspace iteration [43], enrich the bases using a greedy search with a posterior error estimate [36, 39], or improve the bases by *h*-refinement [13]. This type of methods has been widely applied in inverse problems [14, 24], optimization [25, 48], etc.

In this paper, we propose a new idea of POD basis adaptation for the computation of linear parametric PDEs, where we exploit the implicit dependence of the solutions on the parameter. To demonstrate the idea, we consider the following convection-diffusion equation with the diffusivity as the parameter

$$\partial_t u + \mathbf{b} \cdot \nabla u - \kappa \Delta u = f, \quad \mathbf{x} \in \Omega \subset \mathbb{R}^d, \quad t \in [0, T].$$
 (1)

It is well known that the interior layer or the boundary layer would appear in the solution and become sharper as the diffusivity becomes small [38]. Hence more complicated schemes and finer meshes are needed to obtain an accurate solution at a small diffusivity. In other words, the full-order model simulation at a small diffusivity is more computationally expensive than that at a large diffusivity. We consider the case where the full-order model simulation at a small diffusivity is too costly to perform and no new observation data are available. Thus we aim to adapt the POD basis functions constructed from solution snapshots of a large diffusivity κ_1 for the construction of an accurate reduced-order model at a small diffusivity κ_2 without resorting to the full-order model simulation at κ_2 .

We find that the difference of solutions of these two parameters satisfies a convectiondiffusion equation with κ_1 as the diffusivity. Hence the adaptation proceeds by iteratively applying the full-order model simulation at κ_1 and the POD reduced-order model simulation at κ_2 . We also study the convergence analysis of the proposed iterative algorithm. The algorithm and its corresponding convergence analysis can be generalized to other types of linear parametric evolutionary problems without any difficulty. This idea of POD basis adaptation is particularly useful for constructing a reduced-order model for singularly perturbed problems when the full-order model simulation at a small parameter is prohibitively costly. Several numerical experiments are presented and show that our algorithm is effective. And convergence to an accurate reduced-order model is observed. Hence the combination of a coarse-grid solver and the iterative algorithm is able to construct an accurate reduced-order model at a small diffusivity, the direct construction of which needs a fine-grid solver for the computation of snapshots.

The rest of this paper is organized as follows. In Section 2, we introduce some preliminaries on the POD method. Then we propose the iterative algorithm for POD basis adaptation in Section 3. We provide the convergence analysis of our iterative algorithm in Section 4. Several numerical experiments are presented in Section 5. Finally, concluding remarks are given in Section 6.

2. Preliminaries

To make this paper self-contained, in this section we give a brief review of the POD method, including the construction of the POD basis functions and POD-based Galerkin method for solving evolutionary problems.

2.1. POD method

Let X be a real Hilbert space endowed with the inner product $(\cdot, \cdot)_X$ and norm $\|\cdot\|_X$. Throughout the rest of this paper, (\cdot, \cdot) denotes the L^2 inner product. Given the snapshots $y_1, y_2, \ldots, y_m \in X$, the POD method aims to find an set of orthogonal basis functions $\{\psi_i\}_{i=1}^{\ell}$ that optimally approximates the snapshots $\{y_i\}_{i=1}^m$ in the X-norm sense. That is, $\{\psi_i\}_{i=1}^{\ell}$ is the solution to the following constrained optimization problem:

$$\min_{\{\psi_k\}_{k=1}^{\ell}} \sum_{j=1}^{m} \|y_j - \sum_{k=1}^{\ell} (y_j, \psi_k)_X \psi_k\|_X^2, \\
\text{s.t. } (\psi_i, \psi_j)_X = \delta_{ij}, \quad i, j = 1, \dots, \ell.$$
(2)

To solve the problem (2), the method of snapshots [45] introduces a correlation matrix K corresponding to the snapshots with entries

$$K_{i,j} = (y_i, y_j)_X, \quad i, j = 1, \dots, m.$$
 (3)

Then K is semi-positive-definite. Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_m \geq 0$ be the sorted eigenvalues of K in the descending order and $\varphi_1, \ldots, \varphi_m$ be the associated eigenvectors. Assume that $\lambda_{\ell} > 0$. Then the basis can be constructed as

$$\psi_k = \frac{1}{\sqrt{\lambda_k}} \sum_{j=1}^m (\varphi_k)_j y_j,\tag{4}$$

where $(\varphi_k)_j$ is the *j*-th element of φ_k and $k = 1, \ldots, \ell$. Moreover, the approximation error is

$$\sum_{j=1}^{m} \|y_j - \sum_{k=1}^{\ell} (y_j, \psi_k)_X \psi_k\|_X^2 = \sum_{k=\ell+1}^{m} \lambda_k.$$
 (5)

In practice, the number of basis functions ℓ is usually not pre-chosen. A typical way to determine ℓ is to choose the smallest ℓ such that

$$\frac{\sum_{k=1}^{\ell} \lambda_k}{\sum_{k=1}^{m} \lambda_k} \ge 1 - \varepsilon \tag{6}$$

for some small $\varepsilon > 0$.

2.2. POD approximations of evolutionary problems

Assume that $u \in H_0^1(\Omega)$ is the solution to the following weak formulation of an evolutionary problem

$$(\partial_t u, \psi) - a(u, \psi) = (f, \psi), \quad \forall \psi \in H^1_0(\Omega), \quad t \in [0, T],$$

$$u|_{t=0} = g,$$
(7)

where $\Omega \subset \mathbb{R}^d$ and $a(\cdot, \cdot)$ is a bilinear form on $H_0^1(\Omega) \times H_0^1(\Omega)$. Given a set of solutions at different time instances $\{u(\cdot, t_0), u(\cdot, t_1), \ldots, u(\cdot, t_m)\}$ where $t_k = k\Delta t$ with $\Delta t = \frac{T}{m}$, the POD basis functions $\{\psi_k\}_{k=1}^{\ell}$ are built from the ensemble $\{y_1, \ldots, y_{m+1}, y_{m+2}, \ldots, y_{2m+1}\}$, where

$$y_k = u(\cdot, t_{k-1}), \quad k = 1, \dots, m+1,$$
(8)

$$y_k = \overline{\partial} u(\cdot, t_{k-m-1}), \quad k = m+2, \dots, 2m+1, \tag{9}$$

with

$$\overline{\partial}u(\cdot, t_k) = \frac{u(\cdot, t_k) - u(\cdot, t_{k-1})}{\Delta t}, \quad k = 1, \dots, m.$$
(10)

The POD basis functions are obtained by choosing $X = H^1(\Omega)$ and the approximation errors are

$$\sum_{j=0}^{m} \|u(t_j) - \sum_{k=1}^{\ell} (u(t_j), \psi_k)_{H^1} \psi_k\|_{H^1}^2 \le \sum_{k=\ell+1}^{2m+1} \lambda_k,$$
(11)

and

$$\sum_{j=1}^{m} \|\overline{\partial}u(t_j) - \sum_{k=1}^{\ell} (\overline{\partial}u(t_j), \psi_k)_{H^1} \psi_k\|_{H^1}^2 \le \sum_{k=\ell+1}^{2m+1} \lambda_k,$$
(12)

where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{2m+1} \geq 0$ are the sorted eigenvalues of the correlation matrix K corresponding to the input data $\{y_1, \ldots, y_{m+1}, y_{m+2}, \ldots, y_{2m+1}\}$ with entries

$$K_{ij} = (y_i, y_j)_{H^1}, \quad i, j = 1, \dots, 2m + 1.$$

Let $\Psi = \text{span}\{\psi_1, \ldots, \psi_\ell\}$. The semi-discrete scheme of the POD-based Galerkin method seeks a solution $\tilde{u}(t)$ such that $\tilde{u}(t) \in \Psi, \forall t \in [0, T]$ and

$$(\partial_t \tilde{u}, \psi) - a(\tilde{u}, \psi) = (f, \psi), \quad \forall \psi \in \Psi, \quad t \in [0, T],$$

$$\tilde{u}|_{t=0} = \tilde{g},$$
(13)

where \tilde{g} is some projection of g in Ψ . The fully discrete scheme of the POD-based Galerkin method can be obtained by combining (13) with a finite difference scheme in temporal discretization, e.g. the Backward Euler scheme or the Crank-Nicolson scheme.

3. An iterative algorithm for POD basis adaptation

3.1. Problem formulation

We consider the convection-diffusion equation with zero boundary conditions

$$\partial_t u + \mathbf{b} \cdot \nabla u - \kappa \Delta u = f, \quad \mathbf{x} \in \Omega \subset \mathbb{R}^d, \quad t \in [0, T],$$

$$u|_{\partial\Omega} = 0, \quad u|_{t=0} = g,$$
 (14)

where the velocity field **b** is divergence-free, i.e. $\nabla \cdot \mathbf{b} = 0$ and **b**, f, and g are sufficiently smooth. We define the bilinear form $a(\varphi, \psi; \kappa) = (\mathbf{b} \cdot \nabla \varphi, \psi) + \kappa(\nabla \varphi, \nabla \psi)$ for any $\varphi, \psi \in$ $H_0^1(\Omega)$. Let $\kappa_1 > \kappa_2 > 0$ be fixed. Without loss of generality, we assume that $1 \ge \kappa_1 > \kappa_2 > 0$. Then let u_j be the solution to (14) with $\kappa = \kappa_j$ for j = 1, 2. Let m be a fixed integer and $\Delta t = T/m, t_k = k\Delta t$ for $k = 0, 1, \ldots, m$. For any ordered set $\{c_0, c_1, \ldots, c_m\}$, we define the finite difference quotient operator $\overline{\partial}$ as

$$\overline{\partial}c_k = \frac{c_k - c_{k-1}}{\Delta t},$$

where k = 1, ..., m. Assume that $V_h \subset H_0^1(\Omega)$ is the first-order conforming finite element space associated with a quasi-uniform and shape-regular simplicial finite element mesh \mathcal{T}_h of Ω with mesh size h. Then let $\{\hat{u}_{j,0}, \hat{u}_{j,1}, \ldots, \hat{u}_{j,m}\} \subset V_h$ be the backward-Euler-type approximation of u_j in V_h , i.e. $\hat{u}_{j,k} \in V_h$ satisfies

$$(\overline{\partial}\hat{u}_{j,k},\psi) + a(\hat{u}_{j,k},\psi;\kappa_j) = (f(t_k),\psi), \quad \forall \psi \in V_h, \\ \hat{u}_{j,0} = \tilde{g},$$
(15)

for j = 1, 2 and k = 1, ..., m, where \tilde{g} is some projection of g in V_h . Using standard arguments of FEM [46], we can prove that there exists a constant C independent of Δt and h such that for j = 1, 2,

$$\frac{1}{m} \sum_{k=1}^{m} \|\hat{u}_{j,k} - u_j(t_k)\|_{H^1}^2 \le C(\Delta t^2 + h^2).$$
(16)

Our goal is to adapt the POD basis functions built from $\{\hat{u}_{1,0},\ldots,\hat{u}_{1,m},\overline{\partial}\hat{u}_{1,1},\ldots,\overline{\partial}\hat{u}_{1,m}\}$ to a set of POD basis functions that are able to approximate $\{\hat{u}_{2,0},\ldots,\hat{u}_{2,m}\}$ and hence $\{u_2(t_0),\ldots,u_2(t_m)\}$ well. The adaptation will be based on the dependence of the solution on the diffusivity κ , without resorting to a fine-grid solver for the small diffusivity κ_2 .

3.2. The implementation of the iterative algorithm Let $w = u_1 - u_2$. Then w satisfies

$$\partial_t w + \mathbf{b} \cdot \nabla w - \kappa_1 \Delta w = (\kappa_1 - \kappa_2) \Delta u_2, \quad \mathbf{x} \in \Omega, \quad t \in [0, T],$$

$$w|_{\partial\Omega} = 0, \quad w|_{t=0} = 0.$$
 (17)

Hence if an approximation for u_2 from the current reduced-order model is available, an approximation for w can be computed using the full-order model simulation of (17) with the diffusivity $\kappa = \kappa_1$. Then a new set of POD basis functions can be constructed from $v = u_1 - w$. The new POD basis functions are expected to yield better approximations for u_2 . Therefore, it is expected that the POD approximation computed by the newest POD basis functions can approximate u_2 with progressively higher accuracy through an iterative process.

We propose the following iterative algorithm of POD basis adaptation. Let $U_k^{(i)}$ be the POD approximation for $\hat{u}_{2,k}$ at iteration *i* and $U^{(i)} = [U_0^{(i)}, \ldots, U_m^{(i)}]$. The algorithm can be summarized as follows:

Algorithm 1 Iterative POD basis adaptation

- 1: Step 1: Set i = 1 and $U_k^{(0)} = 0$ for k = 0, 1, ..., m.
- 2: Step 2: Solve the full-order model simulation at κ_1 for the Galerkin approximation $w_k^{(i)} \in V_h$ that satisfies

$$(\overline{\partial}w_k^{(i)},\psi) + a(w_k^{(i)},\psi;\kappa_1) = -(\kappa_1 - \kappa_2)(\nabla U_k^{(i-1)},\nabla\psi), \quad \forall \psi \in V_h,$$

$$w_0^{(i)} = 0,$$
(18)

for k = 1, ..., m. 3: **Step 3**: Set $v_k^{(i)} = \hat{u}_{1,k} - w_k^{(i)}$ and extract POD basis functions $\{\psi_k^{(i)}\}_{k=1}^{\ell^{(i)}}$ from $\{y_1^{(i)}, ..., y_{m+1}^{(i)}, y_{m+2}^{(i)}, ..., y_{2m+1}^{(i)}\}$, where

$$y_k^{(i)} = v_{k-1}^{(i)}, \quad k = 1, \dots, m+1,$$
 (19)

$$y_k^{(i)} = \overline{\partial} v_{k-m-1}^{(i)}, \quad k = m+2, \dots, 2m+1.$$
 (20)

The number of POD basis functions $\ell^{(i)}$ is determined by choosing the smallest $\ell^{(i)}$ such that

$$\frac{\sum_{k=1}^{\ell^{(i)}} \lambda_k^{(i)}}{\sum_{k=1}^{2m+1} \lambda_k^{(i)}} \ge 1 - \varepsilon$$

for some $\varepsilon > 0$, where $\lambda_1^{(i)} \ge \lambda_2^{(i)} \ge \ldots \ge \lambda_{2m+1}^{(i)} \ge 0$ are the sorted eigenvalues of the correlation matrix $K^{(i)}$ corresponding to the input data $\{y_1^{(i)}, \ldots, y_{m+1}^{(i)}, y_{m+2}^{(i)}, \ldots, y_{2m+1}^{(i)}\}$ with entries

$$K_{j,k}^{(i)} = (y_j^{(i)}, y_k^{(i)})_{H^1}, \quad j,k = 1,\dots, 2m+1.$$
 (21)

4: Step 4: Set $V^{(i)} = \operatorname{span}\{\psi_1^{(i)}, \ldots, \psi_{\ell^{(i)}}^{(i)}\} \subset V_h$ and solve the reduced-order model simulation at κ_2 for the POD-Galerkin approximation $U_k^{(i)} \in V^{(i)}$ that satisfies

$$(\overline{\partial}U_{k}^{(i)},\psi) + a(U_{k}^{(i)},\psi;\kappa_{2}) = (f(t_{k}),\psi), \quad \forall \psi \in V^{(i)}, U_{0}^{(i)} = U_{0}^{(i)},$$
(22)

for k = 1, ..., m.

5: Step 5: Set i = i + 1 and go back to Step 2 until a certain criterion is reached.

Remark 3.1. In Step 4, the choice of initial data $U_0^{(i)}$ will be discussed later.

Remark 3.2. In our numerical experiment, we stop the iteration when the number of iterations reaches a pre-set value.

4. Convergence analysis of the algorithm

4.1. Some preparations

We begin by fixing some notations. Throughout this section, we still use all the notations and quantities that are introduced in Section 3. We let $\mathbb{N}^+ = \mathbb{N} \setminus \{0\}$. We also define a Ritz projection at each iteration *i*, denoted by $P^{(i)}$, such that $\forall \varphi \in H_0^1(\Omega), P^{(i)}\varphi \in V^{(i)}$ and

$$a(\varphi,\psi;\kappa_2) = a(P^{(i)}\varphi,\psi;\kappa_2), \quad \forall \psi \in V^{(i)}.$$
(23)

For any $\varphi \in H_0^1(\Omega)$, we have by the Poincaré inequality

$$\|\varphi\|_{L^2}^2 \le C_P \|\nabla\varphi\|_{L^2}^2,\tag{24}$$

where the constant C_P is dependent on the region Ω and the dimension d. The notation C_P is reserved for the constant of Poincaré inequality throughout this section. And we have the following lemma.

Lemma 4.1. For $1 \ge \kappa_1 > \kappa_2 > 0$ fixed and any $\varphi, \psi \in H_0^1(\Omega)$, there exist a constant $\beta > 0$ independent of κ_1, κ_2 such that for j = 1, 2,

$$|a(\varphi,\psi;\kappa_j)| \le \beta \|\varphi\|_{H^1} \|\psi\|_{H^1}.$$
(25)

Let $\alpha_j = \frac{\kappa_j}{1+C_P}$. Then it holds true for any $\varphi \in H^1_0(\Omega)$ that

$$|a(\varphi,\varphi;\kappa_j)| \ge \alpha_j \|\varphi\|_{H^1}^2.$$
(26)

Proof. For $1 \ge \kappa_1 > \kappa_2 > 0$ and any $\varphi, \psi \in H_0^1(\Omega)$, by the smoothness assumption of **b**, there exists $\beta > 0$ independent of κ_1, κ_2 such that for j = 1, 2,

$$|a(\varphi,\psi;\kappa_j)| \le \beta \|\varphi\|_{H^1} \|\psi\|_{H^1}.$$
(27)

By the Poincaré inequality and the fact that $\nabla \cdot \mathbf{b} = 0$, we obtain that

$$|a(\varphi,\varphi;\kappa_j)| = \kappa_j \|\nabla\varphi\|_{L^2}^2 \ge \frac{\kappa_j}{1+C_P} \|\varphi\|_{H^1}^2, \quad j = 1, 2.$$

$$(28)$$

The proof is completed.

The constants β , α_1 , α_2 are also fixed for this section.

4.2. Convergence of the algorithm

We study the convergence analysis of the iterative algorithm by estimating $\frac{1}{m} \sum_{k=1}^{m} ||U_k^{(i)} - u_2(t_k)||_{H^1}^2$. To do so, we decompose it as

$$\frac{1}{m}\sum_{k=1}^{m} \|U_k^{(i)} - u_2(t_k)\|_{H^1}^2 \le \frac{2}{m}\sum_{k=1}^{m} \|U_k^{(i)} - \hat{u}_{2,k}\|_{H^1}^2 + \frac{2}{m}\sum_{k=1}^{m} \|\hat{u}_{2,k} - u_2(t_k)\|_{H^1}^2.$$
(29)

We only need to estimate the iteration error $\frac{1}{m}\sum_{k=1}^{m} \|U_k^{(i)} - \hat{u}_{2,k}\|_{H^1}^2$, since the estimate of $\frac{1}{m}\sum_{k=1}^{m} \|\hat{u}_{2,k} - u_2(t_k)\|_{H^1}^2$ has been given in (16). We decompose the term $\frac{1}{m}\sum_{k=1}^{m} \|U_k^{(i)} - \hat{u}_{2,k}\|_{H^1}^2$ as

$$\frac{1}{m}\sum_{k=1}^{m} \|U_{k}^{(i)} - \hat{u}_{2,k}\|_{H^{1}}^{2} \leq \frac{3}{m}\sum_{k=1}^{m} \left(\|U_{k}^{(i)} - P^{(i)}v_{k}^{(i)}\|_{H^{1}}^{2} + \|P^{(i)}v_{k}^{(i)} - v_{k}^{(i)}\|_{H^{1}}^{2} + \|v_{k}^{(i)} - \hat{u}_{2,k}\|_{H^{1}}^{2} \right).$$

$$(30)$$

The estimation of $\frac{1}{m} \sum_{k=1}^{m} \|U_k^{(i)} - \hat{u}_{2,k}\|_{H^1}^2$ will be done by analysing each term in (30), separately.

From the result by Kunisch and Volkwein [32], we have the following lemma for the second term in (30).

Lemma 4.2. It holds true for every $i \in \mathbb{N}^+$ that

$$\frac{1}{m}\sum_{k=1}^{m} \|P^{(i)}v_k^{(i)} - v_k^{(i)}\|_{H^1}^2 \le \frac{3\beta}{m\alpha_2}\sum_{k=\ell^{(i)}+1}^{2m+1}\lambda_k^{(i)} = \frac{3\beta(1+C_P)}{m\kappa_2}\sum_{k=\ell^{(i)}+1}^{2m+1}\lambda_k^{(i)}.$$
(31)

The following corollary of Lemma 4.2 is also given in [32].

Corollary 4.1. It holds true for every $i \in \mathbb{N}^+$ that

$$\frac{1}{m}\sum_{k=1}^{m} \|P^{(i)}\overline{\partial}v_{k}^{(i)} - \overline{\partial}v_{k}^{(i)}\|_{H^{1}}^{2} \le \frac{3\beta}{m\alpha_{2}}\sum_{k=\ell^{(i)}+1}^{2m+1}\lambda_{k}^{(i)} = \frac{3\beta(1+C_{P})}{m\kappa_{2}}\sum_{k=\ell^{(i)}+1}^{2m+1}\lambda_{k}^{(i)}.$$
(32)

For the third term in (30), we have the following estimate.

Lemma 4.3. It holds true for every $i \in \mathbb{N}^+$ that

$$\frac{1}{m}\sum_{k=1}^{m}\|v_{k}^{(i)}-\hat{u}_{2,k}\|_{H^{1}}^{2} \leq (1+C_{P})\frac{(\kappa_{1}-\kappa_{2})^{2}}{\kappa_{1}^{2}}\frac{1}{m}\sum_{k=1}^{m}\|U_{k}^{(i-1)}-\hat{u}_{2,k}\|_{H^{1}}^{2}.$$
(33)

Proof. Let $r_k^{(i)} = v_k^{(i)} - \hat{u}_{2,k}$. Then by (15), (18) and (22), $r_0^{(i)} = 0$ and $r_k^{(i)}$ satisfies

$$(\overline{\partial}r_k^{(i)},\psi) + a(r_k^{(i)},\psi;\kappa_1) = (\kappa_1 - \kappa_2)(\nabla(U_k^{(i-1)} - \hat{u}_{2,k}),\nabla\psi), \quad \forall \psi \in V_h,$$
(34)

for k = 1, ..., m. Taking $\psi = r_k^{(i)}$, we have by the proof of Lemma 4.1

$$(\overline{\partial}r_k^{(i)}, r_k^{(i)}) + \kappa_1(\nabla r_k^{(i)}, \nabla r_k^{(i)}) = (\kappa_1 - \kappa_2)(\nabla (U_k^{(i-1)} - \hat{u}_{2,k}), \nabla r_k^{(i)}).$$
(35)

Since

$$\Delta t(\overline{\partial}r_k^{(i)}, r_k^{(i)}) = \frac{1}{2} \left(\|r_k^{(i)}\|_{L^2}^2 - \|r_{k-1}^{(i)}\|_{L^2}^2 + \|r_k^{(i)} - r_{k-1}^{(i)}\|_{L^2}^2 \right) \ge \frac{1}{2} \left(\|r_k^{(i)}\|_{L^2}^2 - \|r_{k-1}^{(i)}\|_{L^2}^2 \right)$$
(36)

and by Young's inequality

$$(\kappa_1 - \kappa_2) \left(\nabla (U_k^{(i-1)} - \hat{u}_{2,k}), \nabla r_k^{(i)} \right) \le \frac{\kappa_1}{2} \| \nabla r_k^{(i)} \|_{L^2}^2 + \frac{(\kappa_1 - \kappa_2)^2}{2\kappa_1} \| \nabla (U_k^{(i-1)} - \hat{u}_{2,k}) \|_{L^2}^2, \quad (37)$$

then

$$\|r_k^{(i)}\|_{L^2}^2 - \|r_{k-1}^{(i)}\|_{L^2}^2 + \Delta t \kappa_1 \|\nabla r_k^{(i)}\|_{L^2}^2 \le \Delta t \frac{(\kappa_1 - \kappa_2)^2}{\kappa_1} \|\nabla (U_k^{(i-1)} - \hat{u}_{2,k})\|_{L^2}^2.$$
(38)

Summation over $k = 1, \ldots, m$ gives

$$\kappa_1 \frac{1}{m} \sum_{k=1}^m \|\nabla r_k^{(i)}\|_{L^2}^2 \le \frac{(\kappa_1 - \kappa_2)^2}{\kappa_1} \frac{1}{m} \sum_{k=1}^m \|\nabla (U_k^{(i-1)} - \hat{u}_{2,k})\|_{L^2}^2.$$
(39)

The Poincaré inequality indicates that

$$\frac{1}{m} \sum_{k=1}^{m} \|r_{k}^{(i)}\|_{H^{1}}^{2} \leq (1+C_{P}) \frac{(\kappa_{1}-\kappa_{2})^{2}}{\kappa_{1}^{2}} \frac{1}{m} \sum_{k=1}^{m} \|\nabla(U_{k}^{(i-1)}-\hat{u}_{2,k})\|_{L^{2}}^{2} \\
\leq (1+C_{P}) \frac{(\kappa_{1}-\kappa_{2})^{2}}{\kappa_{1}^{2}} \frac{1}{m} \sum_{k=1}^{m} \|U_{k}^{(i-1)}-\hat{u}_{2,k}\|_{H^{1}}^{2}.$$
(40)

Now we turn to the remaining term in
$$(30)$$
.

Lemma 4.4. It holds true for every $i \in \mathbb{N}^+$ that

$$\frac{1}{m}\sum_{k=1}^{m} \|U_{k}^{(i)} - P^{(i)}v_{k}^{(i)}\|_{H^{1}}^{2} \leq \frac{1+C_{P}}{\kappa_{2}T} \|U_{0}^{(i)} - P^{(i)}\tilde{g}\|_{L^{2}}^{2} + \frac{3\beta(1+C_{P})^{3}}{m\kappa_{2}^{3}}\sum_{k=\ell^{(i)}+1}^{2m+1}\lambda_{k}^{(i)} + M(\kappa_{1}-\kappa_{2})^{2}\frac{1}{m}\sum_{k=1}^{m} \|U_{k}^{(i-1)} - \hat{u}_{2,k}\|_{H^{1}}^{2},$$
(41)

where

$$M = \frac{2(1+C_P)^2}{\kappa_2^2} \left((1+C_P) \frac{(\kappa_1 - \kappa_2)^2}{\kappa_1^2} + 1 \right).$$
(42)

Proof. Let $\rho_k^{(i)} = U_k^{(i)} - P^{(i)}v_k^{(i)}$. Then by (15), (18), (22) and the definition of $P^{(i)}$ (23), for any $\psi \in V^{(i)}$,

$$(\overline{\partial}\rho_{k}^{(i)},\psi) + a(\rho_{k}^{(i)},\psi;\kappa_{2}) = (\overline{\partial}U_{k}^{(i)},\psi) + a(U_{k}^{(i)},\psi;\kappa_{2}) - (\overline{\partial}P^{(i)}v_{k}^{(i)},\psi) - a(P^{(i)}v_{k}^{(i)},\psi;\kappa_{2}) = (f(t_{k}),\psi) - (\overline{\partial}P^{(i)}v_{k}^{(i)},\psi) - a(v_{k}^{(i)},\psi;\kappa_{1}) + a(v_{k}^{(i)},\psi;\kappa_{1}) - a(v_{k}^{(i)},\psi;\kappa_{2}) = (\xi_{k}^{(i)},\psi) + (\kappa_{1} - \kappa_{2})(z_{k}^{(i)},\nabla\psi),$$
(43)

where $\xi_k^{(i)} = \overline{\partial} v_k^{(i)} - \overline{\partial} P^{(i)} v_k^{(i)}$ and $z_k^{(i)} = \nabla v_k^{(i)} - \nabla U_k^{(i-1)}$. Let $\psi = \rho_k^{(i)}$ and by the Young's inequality, we have

$$(\kappa_1 - \kappa_2)(z_k^{(i)}, \nabla \rho_k^{(i)}) \le \frac{\kappa_2}{2(1 + C_P)} \|\nabla \rho_k^{(i)}\|_{L^2}^2 + \frac{(\kappa_1 - \kappa_2)^2 (1 + C_P)}{2\kappa_2} \|z_k^{(i)}\|_{L^2}^2,$$
(44)

$$(\xi_k^{(i)}, \rho_k^{(i)}) \le \frac{\kappa_2}{2(1+C_P)} \|\rho_k^{(i)}\|_{L^2}^2 + \frac{1+C_P}{2\kappa_2} \|\xi_k^{(i)}\|_{L^2}^2.$$
(45)

Hence by Lemma 4.1, we have

$$\|\rho_k^{(i)}\|_{L^2}^2 - \|\rho_{k-1}^{(i)}\|_{L^2}^2 + \Delta t \frac{\kappa_2}{1+C_P} \|\rho_k^{(i)}\|_{H^1}^2 \le \Delta t \frac{1+C_P}{\kappa_2} \left(\|\xi_k^{(i)}\|_{L^2}^2 + (\kappa_1 - \kappa_2)^2 \|z_k^{(i)}\|_{L^2}^2 \right).$$
(46)

Summation over $k = 1, \ldots, m$ gives

$$\Delta t \frac{\kappa_2}{1+C_P} \sum_{k=1}^m \|\rho_k^{(i)}\|_{H^1}^2 \le \|\rho_0^{(i)}\|_{L^2}^2 + \Delta t \frac{1+C_P}{\kappa_2} \sum_{k=1}^m \left(\|\xi_k^{(i)}\|_{L^2}^2 + (\kappa_1 - \kappa_2)^2 \|z_k^{(i)}\|_{L^2}^2 \right).$$
(47)

By Corollary 4.1,

$$\frac{1}{m}\sum_{k=1}^{m} \|\xi_k^{(i)}\|_{L^2}^2 = \frac{1}{m}\sum_{k=1}^{m} \|\overline{\partial}v_k^{(i)} - \overline{\partial}P^{(i)}v_k^{(i)}\|_{L^2}^2 \le \frac{3\beta(1+C_P)}{m\kappa_2}\sum_{k=\ell^{(i)}+1}^{2m+1}\lambda_k^{(i)}.$$
(48)

Furthermore by Lemma 4.3,

$$\frac{1}{m} \sum_{k=1}^{m} \|z_{k}^{(i)}\|_{L^{2}}^{2} = \frac{1}{m} \sum_{k=1}^{m} \|\nabla v_{k}^{(i)} - \nabla U_{k}^{(i-1)}\|_{L^{2}}^{2}
\leq \frac{2}{m} \sum_{k=1}^{m} (\|\nabla v_{k}^{(i)} - \nabla \hat{u}_{2,k}\|_{L^{2}}^{2} + \|\nabla U_{k}^{(i-1)} - \nabla \hat{u}_{2,k}\|_{L^{2}}^{2})
\leq 2 \left((1+C_{P}) \frac{(\kappa_{1}-\kappa_{2})^{2}}{\kappa_{1}^{2}} + 1 \right) \frac{1}{m} \sum_{k=1}^{m} \|U_{k}^{(i-1)} - \hat{u}_{2,k}\|_{H^{1}}^{2}.$$
(49)

Hence we obtain the lemma by combining (47), (48) and (49).

To sum up, we have

Theorem 4.1. It holds true for every $i \in \mathbb{N}^+$ that

$$\frac{1}{m}\sum_{k=1}^{m} \|U_{k}^{(i)} - \hat{u}_{2,k}\|_{H^{1}}^{2} \leq \gamma_{1} \|U_{0}^{(i)} - P^{(i)}\tilde{g}\|_{L^{2}}^{2} + \gamma_{2}\sum_{k=\ell^{(i)}+1}^{2m+1} \lambda_{k}^{(i)} + \gamma_{3}\frac{1}{m}\sum_{k=1}^{m} \|U_{k}^{(i-1)} - \hat{u}_{2,k}\|_{H^{1}}^{2},$$
(50)

where

$$\gamma_1 = \frac{3(1+C_P)}{\kappa_2 T},\tag{51}$$

$$\gamma_2 = \frac{9\beta(1+C_P)^3}{m\kappa_2^3} + \frac{9\beta(1+C_P)}{m\kappa_2},\tag{52}$$

$$\gamma_3 = 3(1+C_P)\frac{(\kappa_1-\kappa_2)^2}{\kappa_1^2} + 6\left((1+C_P)\frac{(\kappa_1-\kappa_2)^2}{\kappa_1^2} + 1\right)\frac{(1+C_P)^2(\kappa_1-\kappa_2)^2}{\kappa_2^2}.$$
 (53)

Proof. The proof can be easily done by using (30) and Lemmas 4.2, 4.3 and 4.4.

By combining Theorem 4.1 and the estimate (16), we have the following convergence result.

Theorem 4.2. Let u_2 be the solution to (14) with $\kappa = \kappa_2$ and $t_k = k\Delta t$ with $\Delta t = T/m$ for $k = 1, \ldots, m$. Assume that in each iteration *i* of Algorithm 1, we choose $U_0^{(i)} = P^{(i)}\tilde{g}$ and $\frac{1}{m}\sum_{k=\ell(i)}^{2m+1}\lambda_k^{(i)} < \delta$ for some small $\delta > 0$, and obtain $U_k^{(i)}$ as the numerical approximation of $u_2(t_k)$ for $k = 1, \ldots, m$. Let $\gamma_1, \gamma_2, \gamma_3$ be defined as in Theorem 4.1. Then if $\gamma_3 < 1$, there exists a constant *C* independent of $\Delta t, h, \delta$ such that

$$\lim_{k \to \infty} \frac{1}{m} \sum_{k=1}^{m} \|U_k^{(i)} - u_2(t_k)\|_{H^1}^2 \le C(\Delta t^2 + h^2 + \delta).$$
(54)

Proof. We have the decomposition (29)

$$\frac{1}{m}\sum_{k=1}^{m} \|U_k^{(i)} - u_2(t_k)\|_{H^1}^2 \le \frac{2}{m}\sum_{k=1}^{m} \|U_k^{(i)} - \hat{u}_{2,k}\|_{H^1}^2 + \frac{2}{m}\sum_{k=1}^{m} \|\hat{u}_{2,k} - u_2(t_k)\|_{H^1}^2$$

and the estimate (16)

$$\frac{1}{m}\sum_{k=1}^{m} \|\hat{u}_{2,k} - u_2(t_k)\|_{H^1}^2 \le C(\Delta t^2 + h^2),$$

where C is independent of $\Delta t, h, \delta$. For $\frac{1}{m} \sum_{k=1}^{m} \|U_k^{(i)} - u_2(t_k)\|_{H^1}^2$, if the conditions are satisfied,

$$\frac{1}{m} \sum_{k=1}^{m} \|U_{k}^{(i)} - u_{2}(t_{k})\|_{H^{1}}^{2} \leq \gamma_{2}\delta + \gamma_{3} \frac{1}{m} \sum_{k=1}^{m} \|U_{k}^{(i-1)} - \hat{u}_{2,k}\|_{H^{1}}^{2} \\
\leq \gamma_{2} \frac{1 - \gamma_{3}^{i}}{1 - \gamma_{3}}\delta + \gamma_{3}^{i} \frac{1}{m} \sum_{k=1}^{m} \|U_{k}^{(0)} - \hat{u}_{2,k}\|_{H^{1}}^{2}.$$
(55)

Hence if $\gamma_3 < 1$, there exists a constant C independent of $\Delta t, h, \delta$ such that

$$\lim_{k \to \infty} \frac{1}{m} \sum_{k=1}^{m} \|U_k^{(i)} - u_2(t_k)\|_{H^1}^2 \le C(\Delta t^2 + h^2 + \delta).$$
(56)

We choose the initial data $U_0^{(i)} = P^{(i)}\tilde{g}$ at Step 4 in Algorithm 1 as the error arising from the approximation of initial data would disappear.

Remark 4.1. To ensure $\gamma_3 < 1$, $|\kappa_1 - \kappa_2|$ needs to be small. However, our numerical experiments show that the algorithm still converges when $\frac{\kappa_1 - \kappa_2}{\kappa_2}$ is large. The derivation of a sharper error bound for this iterative algorithm is our focal point in the near future.

If we consider the convection-diffusion equation (14) with periodic boundary conditions and a spatially periodic velocity field **b**, then we consider $\hat{u} = u - \bar{u}$, where \bar{u} is the spatial mean

$$\bar{u}(t) = \frac{1}{|\Omega|} \int_{\Omega} u(t, x) dx.$$
(57)

The Poincaré inequality still applies to \hat{u} and hence the subsequent convergence analysis also applies. A similar treatment can be found in [26]. Therefore, we can still obtain the convergence result for the iterative algorithm of POD basis adaptation in solving the convectiondiffusion equation (14) with periodic boundary conditions. We will show numerical results to confirm this case in the next section.

5. Numerical experiments

In this section, we show several numerical examples to demonstrate the convergence of our iterative algorithm. The relative errors at final time T are considered. We consider the L^2 relative error

$$e_{L^2} = \frac{\|U^{(N)}(T) - u_2(T)\|_{L^2}}{\|u_2(T)\|_{L^2}}$$
(58)

and the H^1 relative error

$$e_{H^1} = \frac{\|U^{(N)}(T) - u_2(T)\|_{H^1}}{\|u_2(T)\|_{H^1}},$$
(59)

where u_2 is the reference solution of the small diffusivity κ_2 and $U^{(N)}$ is the numerical solution with N as the number of iteration.

5.1. Verification of the convergence

Example 5.1. Consider a one-dimensional convection-diffusion equation

$$\frac{\partial}{\partial t}u + \frac{\partial}{\partial x}u - \kappa \frac{\partial^2}{\partial x^2}u = 0, \quad x \in (0,1), \quad t \in [0,T],$$

$$u(t,0) = u(t,1) = 0, \quad u(0,x) = -x^2 + x$$
(60)

where we choose T = 1 and $\kappa_1 = 0.1$, $\kappa_2 = 0.01$.

Let Solver 1 be the Crank-Nicolson finite volume method with $\Delta x = 1/400$ and $\Delta t = 1/1000$, Solver 2 be the combination of fifth-order WENO scheme [30] for first-order spatial derivatives, central difference scheme for the spatial laplacian and third-order Runge-Kutta method in temporal discretization with $\Delta x = 1/800$ and $\Delta t = 1/16000$. The reference solution u_1 of κ_1 is computed using Solver 1 and the reference solution u_2 of κ_2 is computed using Solver 2.

For the iterative POD basis adaptation algorithm, 1001 solution snapshots at $t_j = \frac{j}{1000}$, $j = 0, 1, \ldots, 1000$ and their finite difference quotients are used in each iteration. The number of POD basis functions is chosen according to the smallest $\ell^{(i)}$ such that $\frac{\sum_{k=1}^{\ell^{(i)}} \lambda_k^{(i)}}{\sum_{k=1}^{2m+1} \lambda_k^{(i)}} > 1 - \varepsilon$ with m = 1000 and $\varepsilon = 10^{-7}$. In each iteration, backward-Euler POD Galerkin method with $\Delta t = 1/1000$ is applied for POD approximation and Solver 1 is applied for the full-order model simulation. The iteration is stopped when the iteration number reaches N = 50.

The solutions at different iterations are shown in Figure 1 and the relative errors at T = 1 in the iteration process are shown in Figure 2. The relative errors of $U^{(50)}$ at T = 1 are $e_{L^2} = 3.679e - 2$ and $e_{H^1} = 2.951e - 2$. It can be seen from Figure 1 that the reduced-order model approximation using basis functions extracted from u_1 , i.e. $U^{(1)}$, does not recover u_2 and hence a direct application of the pre-constructed reduced-order model can probably lead to an incorrect approximation if the parameter changes into a different value in the simulation. And we can also see from Figures 1 and 2 that our method can adapt the reduced-order model to the new small diffusivity κ_2 since the iterated solution approximates u_2 with progressively higher accuracy as N increases.



Figure 1: $U^{(N)}$ and u_2 at T = 1 of Example 5.1



Figure 2: Relative errors of $U^{(N)}$ at T = 1 of Example 5.1

We also show the first three basis functions at several iterations in Figure 3. It can be seen from Figure 3 that the iterated POD basis functions are gradually adapted to the basis functions extracted from u_2 as N increases. The basis functions extracted in the 25-th iteration are almost the same as those extracted from u_2 .



Figure 3: First 3 POD modes extracted in the N-th iteration and from u_2 of Example 5.1

Let u_2^{FVM} be the FVM solution at κ_2 using Solver 1. The comparison between u_2^{FVM} and $U^{(50)}$ is given in Table 1 and Figure 4. It can be seen that the relative errors of $U^{(50)}$ at T = 1 are smaller than those of u_2^{FVM} at T = 1, which implies that the combination of a coarse-grid solver and our iteration process leads to a better approximation than the direct simulation using the coarse-grid solver in this case.

Table 1: Relative errors of	u_2^{FVM}	and $U^{(50)}$	at T	= 1 of	Example 5.1
-----------------------------	----------------------	----------------	--------	---------	-------------

	L^2 relative error	H^1 relative error
$u_2^{\rm FVM}$	8.704e-2	6.928e-2
$U^{(50)}$	3.679e-2	2.951e-2



Figure 4: Solutions at T = 1 of Example 5.1

Example 5.2. Consider a two-dimensional convection-diffusion equation

$$\partial_t u + \mathbf{b} \cdot \nabla u - \kappa \Delta u = 0, \quad (x, y) \in \Omega = (0, 1)^2, \quad t \in [0, T], \\ u|_{\partial\Omega} = 0, \quad u(0, x) = (x^2 - x)(y^2 - y)$$
(61)

with

$$\mathbf{b} = (\cos(2\pi y), \cos(2\pi x)), \tag{62}$$

where we choose T = 1 and $\kappa_1 = 0.1$, $\kappa_2 = 0.005$.

Let Solver 1 be the Crank-Nicolson finite volume method with $\Delta x = \Delta y = 1/400$ and $\Delta t = 1/1000$, Solver 2 be the combination of fifth-order WENO scheme for first-order spatial derivatives, central difference scheme for the spatial laplacian and third-order Runge-Kutta method in temporal discretization with $\Delta x = \Delta y = 1/800$ and $\Delta t = 1/16000$. The reference solution u_1 of κ_1 is computed using Solver 1 and the reference solution u_2 of κ_2 is computed using Solver 2.

For the iterative POD basis adaptation algorithm, 1001 solution snapshots at $t_j = \frac{j}{1000}$, $j = 0, 1, \ldots, 1000$ and their finite difference quotients are used in each iteration. The number of POD basis functions is chosen according to the smallest $\ell^{(i)}$ such that $\frac{\sum_{k=1}^{\ell^{(i)}} \lambda_k^{(i)}}{\sum_{k=1}^{2m+1} \lambda_k^{(i)}} > 1 - \varepsilon$ with m = 1000 and $\varepsilon = 10^{-9}$. In each iteration, backward-Euler POD Galerkin method with $\Delta t = 1/1000$ is applied for POD approximation and Solver 1 is applied for the full-order model simulation. We stop the iteration at N = 100.

The solutions at different iterations and the relative errors at T = 1 are shown in Figures 5 and 6 respectively. The relative errors of $U^{(100)}$ at T = 1 are $e_{L^2} = 1.097e - 2$ and $e_{H^1} = 3.258e - 2$. Similar phenomena to the one-dimensional case in Example 5.1 are observed. $U^{(1)}$ is not a good approximation for u_2 and the iterated solution also approximates u_2 with progressively higher accuracy as N increases.



Figure 5: $U^{(N)}$ and u_2 at T = 1 of Example 5.2



Figure 6: Relative errors of $U^{(N)}$ at T = 1 of Example 5.2

We also show the basis functions of the first mode at several iterations in Figure 7. The iterated POD basis function is also gradually adapted to the basis function extracted from u_2 as N increases. The basis function extracted in the 35-th iteration is almost the same as that extracted from u_2 .



Figure 7: The first POD mode extracted in the N-th iteration and from u_2 of Example 5.2

Let u_2^{FVM} be the FVM solution at κ_2 using Solver 1. We still compare u_2^{FVM} with $U^{(100)}$ in Table 2 and Figure 8. We can still observe that the relative errors of $U^{(100)}$ at T = 1 are smaller than those of u_2^{FVM} at T = 1 in this case. This observation shows that a coarse-grid solver combined with our iteration process is able to construct a reduced-order model that yields an approximation of higher accuracy than the full-order model simulation barely using the coarse-grid solver.

Table 2: Relative errors of u_2^{FVM} and $U^{(50)}$ at T = 1 of Example 5.2

	L^2 relative error	H^1 relative error
$u_2^{\rm FVM}$	3.761e-2	9.016e-2
$U^{(100)}$	1.097e-2	3.258e-2



Figure 8: Solutions at T = 1 of Example 5.2

Example 5.3. Consider the following two-dimensional convection-diffusion equation with periodic boundary conditions

$$\partial_t u + \mathbf{b} \cdot \nabla u - \kappa \Delta u = 0, \quad (x, y) \in \Omega = (0, 1)^2, \quad t \in [0, T],$$

u periodic, $u(0, x) = \sin(2\pi x) \sin(2\pi y),$
(63)

with a time dependent velocity field

$$\mathbf{b} = \left(\cos(2\pi y) + 0.5\cos(2\pi t)\sin(2\pi y), \ \cos(2\pi x) + 0.5\cos(2\pi t)\sin(2\pi x)\right), \tag{64}$$

where we choose T = 1 and $\kappa_1 = 0.08$, $\kappa_2 = 0.002$.

Let Solver 1 be the Crank-Nicolson finite volume method with $\Delta x = \Delta y = 1/200$ and $\Delta t = 1/1000$, Solver 2 be the combination of fifth-order WENO scheme for first-order spatial derivatives, central difference scheme for the spatial laplacian and third-order Runge-Kutta method in temporal discretization with $\Delta x = \Delta y = 1/400$ and $\Delta t = 1/4000$. The reference solution u_1 of κ_1 is computed using Solver 1 and the reference solution u_2 of κ_2 is computed using Solver 2.

For the iterative POD basis adaptation algorithm, 1001 solution snapshots at $t_j = \frac{j}{1000}$, $j = 0, 1, \ldots, 1000$ and their finite difference quotients are used in each iteration. The number of POD basis functions is chosen according to the smallest $\ell^{(i)}$ such that $\frac{\sum_{k=1}^{\ell^{(i)}} \lambda_k^{(i)}}{\sum_{k=1}^{2m+1} \lambda_k^{(i)}} > 1 - \varepsilon$ with m = 1000 and $\varepsilon = 10^{-9}$. In each iteration, backward-Euler POD Galerkin method with $\Delta t = 1/1000$ is applied for POD approximation and Solver 1 is applied for the full-order model simulation. We still stop the iteration at N = 100.

We still have solutions at different iterations shown in Figure 9 and relative errors at T = 1 shown in Figure 10. The relative errors of $U^{(100)}$ at T = 1 are $e_{L^2} = 1.639e - 2$ and $e_{H^1} = 4.113e - 2$. Again, similar phenomena to Examples 5.1 and 5.2 are observed. $U^{(1)}$ is not a good approximation for u_2 . And the iterated solution can approximate u_2 with progressively higher accuracy as N increases.

The basis functions of the first mode at several iterations are shown in Figure 11. It can still be seen that the iterated POD basis function is gradually adapted to the basis function extracted from u_2 as N increases. The basis function extracted in the 25-th iteration is almost the same as that extracted from u_2 .









Figure 9: $U^{(N)}$ and u_2 at T = 1 of Example 5.3



Figure 10: Relative errors of $U^{(N)}$ at T = 1 of Example 5.3



Figure 11: The first POD mode extracted in the N-th iteration and from u_2 of Example 5.3

As we can see from Examples 5.1, 5.2 and 5.3, the reduced-order model for the convectiondiffusion equation is sensitive the diffusivity and hence a direct application of the preconstructed reduced-order model will possibly lead to an incorrect approximation if the diffusivity changes into a different value in the simulation. And we can also see that our method can adapt the POD basis functions and the reduced-order model to a new small diffusivity in the iteration process. Moreover, our iterative POD basis adaptation method combined with a coarse-grid solver can construct an accurate reduced-order model for the convection-diffusion model with a small diffusivity.

5.2. Computing the effective diffusivity in passive tracer models

Example 5.4. We apply our iterative POD basis adaptation method in computing the effective diffusivity for the stream function

$$H(x,y) = \frac{1}{4\pi^2} \sin(2\pi x) \sin(2\pi y).$$
(65)

We solve

$$\partial_t u + \mathbf{b} \cdot \nabla u - \kappa \Delta u = 0, \quad (x, y) \in \Omega = (0, 1)^2, \quad t > 0,$$

u periodic, $u(0, x) = u_0(x, y),$
(66)

where

$$\mathbf{b}(x,y) = \frac{1}{\theta} \nabla^{\perp} H(\frac{x}{\theta}, \frac{y}{\theta}) = \frac{1}{\theta} \Big(-H_y(\frac{x}{\theta}, \frac{y}{\theta}), H_x(\frac{x}{\theta}, \frac{y}{\theta}) \Big)$$
$$= \frac{1}{2\pi\theta} \Big(-\sin(\frac{2\pi x}{\theta})\cos(\frac{2\pi y}{\theta}), \cos(\frac{2\pi x}{\theta})\sin(\frac{2\pi y}{\theta}) \Big)$$
(67)

and

$$u_0(x,y) = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{(x-0.5)^2 + (y-0.5)^2}{2\sigma^2}\right)$$
(68)

with $\theta = 0.05$ and $\sigma = 0.01$. If we define the quantity

$$\phi_{\kappa}(t) = \frac{1}{4t} \int \int (x^2 + y^2) u(t, x, y) dx dy,$$
(69)

then the effective diffusivity [21, 38] can be defined as $\phi_{\kappa}^{\text{Eff}} = \lim_{t \to \infty} \phi_{\kappa}(t)$. We solve equation (66) using our iterative POD basis adaptation method. We start at $\kappa_1 = 0.1$ and adapt the reduced-order model for solutions of $\kappa_2 = 0.08$, $\kappa_3 = 0.04$ and $\kappa_4 = 0.02$. Each adaptation is stopped at the 50-th iteration.

The result is shown in Figure 12.



Figure 12: Temporal behavior of $\phi_{\kappa}(t)$

6. Conclusion

In this paper, we propose an iterative algorithm for the POD basis adaptation in solving linear parametric PDEs. The idea exploits the dependence of the solution on the parameter. The algorithm and its corresponding convergence analysis are presented for the convectiondiffusion equation with the diffusivity as the parameter, where we adapt the POD basis functions constructed at the large diffusivity κ_1 for the construction of an accurate reducedorder model at the small diffusivity κ_2 without resorting to a fine-grid solver at κ_2 . It is found that the difference of the solutions of two different parameters would satisfy a convection-diffusion equation with κ_1 as the diffusivity, which can be efficiently simulated using a coarse-grid full-order model solver. Hence the algorithm iteratively performs the full-order model simulation at κ_1 and the reduced-order model simulation at κ_2 . We also provide convergence analysis for the proposed method. The algorithm and analysis can also be easily generalized to other types of linear parametric PDEs without any difficulty. This idea of POD basis adaptation is particularly useful for constructing a reduced-order model for singularly perturbed problems with a small parameter. Numerical results show that a coarse-grid solver combined with the iterative process can achieve an accurate reduced-order model at a small diffusivity. In the future, we will derive sharper error bounds for the iterative algorithm. In addition, we will study the basis adaptation for solving nonlinear parametric PDEs.

Acknowledgement

The research of Z. Zhang is supported by Hong Kong RGC grants (Projects 17300817 and 17300318), Seed Funding Programme for Basic Research (HKU), and Basic Research Programme (JCYJ20180307151603959) of The Science, Technology and Innovation Commission of Shenzhen Municipality. The computations were performed using research computing facilities offered by Information Technology Services, the University of Hong Kong.

References

References

- [1] A. ALLA AND L. SALUZZI, A hjb-pod approach for the control of nonlinear pdes on a tree structure, Appl. Numer. Math., 155 (2020), pp. 192–207.
- [2] D. AMSALLEM AND C. FARHAT, An online method for interpolating linear parametric reduced-order models, SIAM J. Sci. Comput., 33 (2011), pp. 2169–2198.
- [3] D. AMSALLEM, M. J. ZAHR, AND C. FARHAT, Nonlinear model order reduction based on local reduced-order bases, Int. J. Numer. Methods Eng., 92 (2012), pp. 891–916.
- [4] A. C. ANTOULAS, Approximation of large-scale dynamical systems, SIAM, 2005.
- [5] J. A. ATWELL AND B. B. KING, Reduced order controllers for spatially distributed systems via proper orthogonal decomposition, SIAM J. Sci. Comput., 26 (2004), pp. 128– 151.
- [6] U. BAUR, C. BEATTIE, P. BENNER, AND S. GUGERCIN, Interpolatory projection methods for parameterized model reduction, SIAM J. Sci. Comput., 33 (2011), pp. 2489– 2518.

- [7] U. BAUR AND P. BENNER, Model reduction for parametric systems using balanced truncation and interpolation, at-Automatisierungstechnik, 57 (2009), pp. 411–419.
- [8] P. BENNER, S. GUGERCIN, AND K. WILLCOX, A survey of projection-based model reduction methods for parametric dynamical systems, SIAM Rev., 57 (2015), pp. 483– 531.
- [9] P. BENNER, M. OHLBERGER, A. COHEN, AND K. WILLCOX, Model reduction and approximation: theory and algorithms, SIAM, 2017.
- [10] G. BERKOOZ, P. HOLMES, AND J. L. LUMLEY, The proper orthogonal decomposition in the analysis of turbulent flows, Ann. Rev. Fluid Mech., 25 (1993), pp. 539–575.
- [11] J. BORGGAARD, T. ILIESCU, AND Z. WANG, Artificial viscosity proper orthogonal decomposition, Math. Comput. Model., 53 (2011), pp. 269–279.
- [12] J. BURKARDT, M. GUNZBURGER, AND H.-C. LEE, Pod and cvt-based reduced-order modeling of navier-stokes flows, Comput. Methods Appl. Mech. Engrg., 196 (2006), pp. 337–355.
- [13] K. CARLBERG, Adaptive h-refinement for reduced-order models, Int. J. Numer. Methods Eng., 102 (2015), pp. 1192–1210.
- [14] T. CUI, Y. M. MARZOUK, AND K. WILLCOX, Data-driven model reduction for the bayesian solution of inverse problems, Int. J. Numer. Methods Eng., 102 (2015), pp. 966– 990.
- [15] E. DE STURLER, S. GUGERCIN, M. E. KILMER, S. CHATURANTABUT, C. BEAT-TIE, AND M. O'CONNELL, Nonlinear parametric inversion using interpolatory model reduction, SIAM J. Sci. Comput., 37 (2015), pp. B495–B517.
- [16] J. DEGROOTE, J. VIERENDEELS, AND K. WILLCOX, Interpolation among reducedorder matrices to obtain parameterized models for design, optimization and probabilistic analysis, Int. J. Numer. Methods Fluids, 63 (2010), pp. 207–230.
- [17] V. DRUSKIN, V. SIMONCINI, AND M. ZASLAVSKY, Solution of the time-domain inverse resistivity problem in the model reduction framework part i. one-dimensional problem with siso data, SIAM J. Sci. Comput., 35 (2013), pp. A1621–A1640.
- [18] J. L. EFTANG AND A. T. PATERA, Port reduction in parametrized component static condensation: approximation and a posteriori error estimation, Int. J. Numer. Methods Eng., 96 (2013), pp. 269–302.
- [19] J. L. EFTANG AND B. STAMM, Parameter multi-domain hp empirical interpolation, Int. J. Numer. Methods Eng., 90 (2012), pp. 412–428.

- [20] H. C. ELMAN AND Q. LIAO, Reduced basis collocation methods for partial differential equations with random coefficients, SIAM/ASA J. Uncertain. Quantif., 1 (2013), pp. 192–217.
- [21] A. FANNJIANG AND G. PAPANICOLAOU, Convection enhanced diffusion for periodic flows, SIAM J. Appl. Math., 54 (1994), pp. 333–408.
- [22] L. FENG, D. KOZIOL, E. B. RUDNYI, AND J. G. KORVINK, Parametric model reduction for fast simulation of cyclic voltammograms, Sensor Lett., 4 (2006), pp. 165–173.
- [23] R. W. FREUND, Model reduction methods based on krylov subspaces, Acta Numer., 12 (2003), pp. 267–319.
- [24] D. GARMATTER, B. HAASDONK, AND B. HARRACH, A reduced basis landweber method for nonlinear inverse problems, Inverse Probl., 32 (2016), p. 035001.
- [25] C. GOGU, Improving the efficiency of large scale topology optimization through on-the-fly reduced order model construction, Int. J. Numer. Methods Eng., 101 (2015), pp. 281–304.
- [26] H. GU, J. XIN, AND Z. ZHANG, Error estimates for a pod method for solving viscous g-equations in incompressible cellular flows, SIAM J. Sci. Comput., (to appear).
- [27] M. W. HESS AND P. BENNER, A reduced basis method for microwave semiconductor devices with geometric variations, COMPEL, (2014).
- [28] J. S. HESTHAVEN, G. ROZZA, AND B. STAMM, Certified reduced basis methods for parametrized partial differential equations, vol. 590, Springer, 2016.
- [29] S. HOVLAND, J. T. GRAVDAHL, AND K. WILLCOX, Explicit model predictive control for large-scale systems via model reduction, J. Guidance Control Dynam., 31 (2008), pp. 918–926.
- [30] G.-S. JIANG AND D. PENG, Weighted eno schemes for hamilton-jacobi equations, SIAM J. Sci. Comput., 21 (2000), pp. 2126–2143.
- [31] D. KALISE AND K. KUNISCH, Polynomial approximation of high-dimensional hamiltonjacobi-bellman equations and applications to feedback control of semilinear parabolic pdes, SIAM J. Sci. Comput., 40 (2018), pp. A629–A652.
- [32] K. KUNISCH AND S. VOLKWEIN, Galerkin proper orthogonal decomposition methods for parabolic problems, Numer. Math., 90 (2001), pp. 117–148.
- [33] C. LIEBERMAN, K. WILLCOX, AND O. GHATTAS, Parameter and state model reduction for large-scale statistical inverse problems, SIAM J. Sci. Comput., 32 (2010), pp. 2523– 2542.

- [34] D. MA, W.-K. CHING, AND Z. ZHANG, Proper orthogonal decomposition method for multiscale elliptic pdes with random coefficients, J. Comput. Appl. Math., 370 (2020), p. 112635.
- [35] Y. MADAY AND B. STAMM, Locally adaptive greedy approximations for anisotropic parameter reduced basis spaces, SIAM J. Sci. Comput., 35 (2013), pp. A2417–A2441.
- [36] M. OHLBERGER AND F. SCHINDLER, Error control for the localized reduced basis multiscale method with adaptive on-line enrichment, SIAM J. Sci. Comput., 37 (2015), pp. A2865–A2895.
- [37] H. PANZER, J. MOHRING, R. EID, AND B. LOHMANN, Parametric model order reduction by matrix interpolation, at-Automatisierungstechnik, 58 (2010), pp. 475–484.
- [38] P. J. PARK, Multiscale numerical methods for the singularly perturbed convectiondiffusion equation, PhD thesis, California Institute of Technology, 2000.
- [39] A. PAUL-DUBOIS-TAINE AND D. AMSALLEM, An adaptive and efficient greedy procedure for the optimal training of parametric reduced-order models, Int. J. Numer. Methods Eng., 102 (2015), pp. 1262–1292.
- [40] B. PEHERSTORFER, D. BUTNARU, K. WILLCOX, AND H.-J. BUNGARTZ, Localized discrete empirical interpolation method, SIAM J. Sci. Comput., 36 (2014), pp. A168– A192.
- [41] B. PEHERSTORFER AND K. WILLCOX, Dynamic data-driven reduced-order models, Comput. Methods Appl. Mech. Engrg., 291 (2015), pp. 21–41.
- [42] —, Online adaptive model reduction for nonlinear systems via low-rank updates, SIAM J. Sci. Comput., 37 (2015), pp. A2123–A2150.
- [43] L. PENG AND K. MOHSENI, An online manifold learning approach for model reduction of dynamical systems, SIAM J. Numer. Anal., 52 (2014), pp. 1928–1952.
- [44] M. RATHINAM AND L. R. PETZOLD, A new look at proper orthogonal decomposition, SIAM J. Numer. Anal., 41 (2003), pp. 1893–1925.
- [45] L. SIEOVICH, Turbulence and the dynamics of coherent structures. part 1: Coherent structures, Quart. Appl. Math., 45 (1987), pp. 561–571.
- [46] V. THOMÉE, Galerkin finite element methods for parabolic problems, Lecture notes in mathematics, 1054 (1984).
- [47] S. VOLKWEIN, Proper orthogonal decomposition: Theory and reduced-order modelling, Lecture Notes, University of Konstanz, 4 (2013), pp. 1–29.

- [48] M. J. ZAHR AND C. FARHAT, Progressive construction of a parametric reduced-order model for pde-constrained optimization, Int. J. Numer. Methods Eng., 102 (2015), pp. 1111–1135.
- [49] R. ZIMMERMANN, A locally parametrized reduced-order model for the linear frequency domain approach to time-accurate computational fluid dynamics, SIAM J. Sci. Comput., 36 (2014), pp. B508–B537.
- [50] R. ZIMMERMANN, B. PEHERSTORFER, AND K. WILLCOX, Geometric subspace updates with applications to online adaptive nonlinear model reduction, SIAM J. Matrix Anal. Appl., 39 (2018), pp. 234–261.