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RESEARCH ARTICLE

Reduced-order extrapolation spectral-finite difference scheme based on POD method and error estimation for three-dimensional parabolic equation

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Abstract In this study, a classical spectral-finite difference scheme (SFDS) for the three-dimensional (3D) parabolic equation is reduced by using proper orthogonal decomposition (POD) and singular value decomposition (SVD). First, the 3D parabolic equation is discretized in spatial variables by using spectral collocation method and the discrete scheme is transformed into matrix formulation by tensor product. Second, the classical SFDS is obtained by difference discretization in time-direction. The ensemble of data are comprised with the first few transient solutions of the classical SFDS for the 3D parabolic equation and the POD bases of ensemble of data are generated by using POD technique and SVD. The unknown quantities of the classical SFDS are replaced with the linear combination of POD bases and a reduced-order extrapolation SFDS with lower dimensions and sufficiently high accuracy for the 3D parabolic equation is established. Third, the error estimates between the classical SFDS solutions and the reduced-order extrapolation SFDS solutions and the implementation for solving the reduced-order extrapolation SFDS are provided. Finally, a numerical example shows that the errors of numerical computations are consistent with the theoretical results. Moreover, it is shown that the reduced-order extrapolation SFDS is effective and feasible to find the numerical solutions for the 3D parabolic equation.

Keywords Singular value decomposition (SVD), proper orthogonal decomposition (POD) bases, spectral-finite difference scheme (SFDS), error estimation, parabolic equation

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1 Introduction

The three-dimensional (3D) parabolic equation has been an extremely vital significance in the field of physics. For example, it is widely applied to describe many physical phenomenon such as process of heat conduction and spread of electromagnetic field. It is not easy to find their exact solutions for the 3D parabolic equation describing practical engineering problems which include generally many complex physical nature or irregular computing field. On the contrary, an efficient approach is to find their numerical solutions. The spectral-finite difference scheme (SFDS) is one of the most important and efficient numerical methods to solve 3D parabolic equation due to SFDS with high precision in spatial directions. However, SFDS includes many degrees of freedom and is a large-scale system of linear equations at each time level so that solving such system of linear equations needs a lot of computational load. Thus, an essential problem is how to alleviate the computational load and save time-consuming calculations and resource demands in the computational process in a way that guarantees sufficiently accurate numerical solutions.

Proper orthogonal decomposition (POD) combined with some numerical methods can reduce infinite-dimensional partial differential equations (PDEs) into some adequate approximate models with fewer degrees of freedom and sufficiently high accuracy so as to alleviate the computational load and memory requirements savings (see [10]). POD is also known as Karhunen-Loève expansions in signal analysis and pattern recognition (see [8]), or principal component analysis in statistics (see [11]), or the method of empirical orthogonal functions in geophysical fluid dynamics and meteorology (see [34]).

POD method has been successfully applied in many fields. In fluid dynamics, Lumley [18] first employed the POD technique to capture the large eddy coherent structures in a turbulent boundary layer. This technique was further extended in [4], where a link between the turbulent structure and the dynamics of a chaotic system was investigated. The method of snapshot was introduced by Sirovich [36] and was widely used in applications to reduce the order of the POD eigenvalue problem. Examples of these were applications to optimal flow control problems [12] and turbulence [33]. POD method was also applied to data compression, signal analysis (see [2]), simulation, and control in chemistry reaction system (see [9,35]). Until resent ten years, some researches that POD method was used to reduce some Galerkin methods of PDEs have not been presented (see [13,14]). More recently, some reduced finite difference models and finite element formulations have been studied (see [5,6,17,19–32,37]). Moreover, there are related works available for POD applications in optimization, for instance, adaptive POD [1], trust-region-POD [3], optimality systems-POD [15], and POD-a-posteriori error estimates [39].

However, almost all existing reduced-order numerical computational methods (see, e.g., [1–3,5,6,13–15,17,19–32,37]) based on POD technique utilize numerical solutions obtained from classical numerical methods on the total time span $[0, T]$ to construct POD bases and reduced-order models, and then recompute the solutions on the same time span $[0, T]$, which actually belongs to re-computations on the same time span $[0, T]$. Especially, to the best of our knowledge, there are no published results addressing that POD method is used to reduce SFDS for the 3D parabolic equation or providing error estimates between the classical SFDS solutions and the reduced SFDS solutions based on POD method. In this work, we establish a reduced-order extrapolation SFDS based on POD method and singular value decomposition (SVD) for the 3D parabolic equation. It is different existing some works. First, the 3D parabolic equation is discretized in spatial directions by using spectral collocation method and the discrete scheme is transformed into matrix formulation by tensor product. Second, a classical SFDS is obtained by difference discretization in time-direction. The ensemble of data are comprised with the first few transient solutions of the classical SFDS for the 3D parabolic equation and the POD bases of ensemble of data are generated by using POD technique and SVD. The unknown quantities of SFDS are replaced with the linear combination of POD bases and a reduced-order extrapolation model, i.e., a reduced-order extrapolation SFDS with lower dimensions and sufficiently high accuracy for the 3D parabolic equation is established. Third, the error estimates between the classical SFDS solutions and the reduced-order extrapolation SFDS solutions and the implementation for solving the reduced-order extrapolation SFDS are provided. Finally, a numerical example has shown that the errors of numerical computations are consistent with the theoretical results. Moreover, it is shown that the reduced-order extrapolation SFDS is effective and feasible to find the numerical solutions for the 3D parabolic equation.

2 Classical SFDS for 3D parabolic equation and generation of snapshots

Spectral method is one of the ‘big three’ technologies for the numerical solution of PDEs (see [38]). Naturally, the origins of each technology can be traced further back. For spectral method, some of the ideas are as old as interpolation and expansion, and more specifically algorithmic developments arrived with Lanczos as early as 1938 (see [16]) and with Clenshaw et al. and others in the 1960s (see [7]). Then, in the 1970s, a transformation of the field took place initiated by work by Orszag and others on problems in fluid dynamics and meteorology, and spectral method became famous. In particular, collocation method is the most popular form of the spectral methods among practitioners. It is very easy to implement and generally leads to satisfactory results as long as the problems possess sufficient smoothness. Collocation method is derived by asking that the approximation solutions satisfy exactly the boundary conditions and the equation at the interior collocation points. In this work, we mainly take the following 3D parabolic equation into account by use of collocation method.

$$\begin{cases} \dfrac{\partial u}{\partial t} - \alpha\Delta u = f, & (x,y,z,t) \in \Omega \times (0,T), \\ u|_{\partial\Omega} = 0, & t \in (0,T), \\ u(x,y,z,0) = u_0(x,y,z), & (x,y,z) \in \Omega, \end{cases} \tag{1}$$

where $u = u(x,y,z,t)$ is unknown function, $\alpha > 0$ is a given positive parameter, $f(x,y,z,t)$ and $u_0(x,y,z)$ are two given functions, T is the total time, and for the sake of convenience, without loss of generality, we may as well suppose $\Omega = (-1,1)^3$.

First, the 3D parabolic equation is discretized in spatial directions by using spectral collocation method. For the sake of simplicity, we shall use the same number of points N at the x, y, and z directions, although in practical applications, one may wish to use different numbers of points at each direction. Let P_N denote the space of all algebraic polynomials of degree less than or equal to N, let

$$X_N = \{p \in P_N \times P_N \times P_N \colon p|_{\partial\Omega} = 0\},$$

and let $\{\xi_i\}_{i=0}^N$ be Legendre Gauss-Lobatto points. Then the Legendre collocation method is to look for $u_N \in C^1(0,T;X_N)$ such that, for any $t \in (0,T)$,

$$\begin{cases} \dfrac{\partial u_N(\xi_i,\xi_j,\xi_k,t)}{\partial t} - \alpha\Delta u_N(\xi_i,\xi_j,\xi_k,t) = f(\xi_i,\xi_j,\xi_k,t), & 1 \leqslant i,j,k \leqslant N-1, \\ u_N(\xi_i,\xi_j,\xi_k,0) = u_0(\xi_i,\xi_j,\xi_k), & 0 \leqslant i,j,k \leqslant N. \end{cases} \tag{2}$$

Let

$$\begin{aligned} U(t) &= (u_N(\xi_1,\xi_1,\xi_1,t),\ldots,u_N(\xi_{N-1},\xi_1,\xi_1,t),\xi_1,t),\ldots, \\ &\quad u_N(\xi_{N-1},\xi_{N-1},\xi_{N-1},t))^{\mathrm{T}}, \\ U^0 &= (u_0(\xi_1,\xi_1,\xi_1),\ldots,u_0(\xi_{N-1},\xi_1,\xi_1),\ldots,u_0(\xi_{N-1},\xi_{N-1},\xi_1),\ldots, \\ &\quad u_0(\xi_{N-1},\xi_{N-1},\xi_{N-1}))^{\mathrm{T}}, \\ F(t) &= (f(\xi_1,\xi_1,\xi_1,t),\ldots,f(\xi_{N-1},\xi_1,\xi_1,t),\ldots,f(\xi_{N-1},\xi_{N-1},\xi_{N-1},t))^{\mathrm{T}}. \end{aligned}$$

Then (2) can be transformed into following matrix form by tensor product

$$\begin{cases} \dfrac{\partial U(t)}{\partial t} - \alpha(I \otimes I \otimes D2 + I \otimes D2 \otimes I + D2 \otimes I \otimes I)U(t) = F(t), \\ U(0) = U^0, \end{cases} \tag{3}$$

where $D2$ is the second-order differentiation matrix of order $N-1$ for Chebyshev case (see [40]), I is the unit matrix of order $N-1$, and $\otimes$ denotes the tensor product of matrixes, i.e.,

$$A \otimes B = (Ab_{i,j})_{i,j=1}^{N-1}.$$

Now, a classical SFDS will be obtained by difference discretization in time-direction. Let τ be the time step increment, $t_n = n\tau$ $(n = 0, 1, \dots, M, M = [T/\tau])$. The implicit difference scheme of (3) is as follows:

$$\frac{U^{n+1} - U^n}{\tau} - \alpha(I \otimes I \otimes D2 + I \otimes D2 \otimes I + D2 \otimes I \otimes I)U^{n+1} = F^{n+1}, \quad (4)$$

where

$$\begin{aligned} U^n = (&u_N(\xi_1, \xi_1, \xi_1, t_n), \dots, u_N(\xi_{N-1}, \xi_1, \xi_1, t_n), \dots, \\ &u_N(\xi_{N-1}, \xi_{N-1}, \xi_{N-1}, t_n))^{\mathrm{T}}, \end{aligned}$$

$$\begin{aligned} F^n = (&f(\xi_1, \xi_1, \xi_1, t_n), \dots, f(\xi_{N-1}, \xi_1, \xi_1, t_n), \dots, f(\xi_{N-1}, \xi_{N-1}, \xi_1, t_n), \dots, \\ &f(\xi_{N-1}, \xi_{N-1}, \xi_{N-1}, t_n))^{\mathrm{T}}. \end{aligned}$$

Then, we get by simplifying (4) that

$$AU^{n+1} = U^n + \tau F^{n+1}, \quad (5)$$

where

$$A = I_1 - \alpha\tau(I \otimes I \otimes D2 + I \otimes D2 \otimes I + D2 \otimes I \otimes I),$$

I_1 is the unit matrix of order $(N-1)^3$. Thus, if $\alpha > 0$, f, and τ are given, then we can get the set of SFDS solutions, i.e., $\{U^0, U^1, \dots, U^M\}$ by solving (5). A subset, i.e., $\{U^i\}_{i=0}^{L}$ (usually, $L \ll M$), known as snapshots which are useful and of interest to us, is chosen from first L elements of $\{U^0, U^1, \dots, U^M\}$.

It is well known (see [40]) that the errors between the solution $U(x, y, z, t)$ to equation (1) and the solutions u^n to equation (4) are as follows:

$$\|U(t_n) - U^n\|_0 = O(\tau, N^{-3}), \quad (6)$$

where $\|\cdot\|_0$ is the standard norm of vector.

Remark 1 When one computes actual problems, one may obtain the ensemble of snapshots from physical system trajectories by drawing samples from experiments and interpolation (or date assimilation). For example, when one finds numerical solutions to PDEs representing weather forecast, one can use the previous weather result, then restructure the optimal basis for the ensemble of snapshots by following POD technique, and finally combine it with spectral method to derive a reduced order dynamical system. Thus, the forecast of future weather change can be quickly simulated, which is of major importance for actual real-life applications.

3 Formulate POD bases

Let $A_u = (U^0, U^1, \dots, U^L)$. For matrix A_u, there exists the SVD as follows:

$$A_u = U_u \begin{pmatrix} S_u & O \\ O & O \end{pmatrix} V_u^{\mathrm{T}},$$

where $U_u \in \mathbb{R}^{(N-1)^3}$, $V_u \in \mathbb{R}^{(L+1)\times(L+1)}$ are all orthogonal matrices. $S_u = \mathrm{diag}(\sigma_1, \sigma_2, \dots, \sigma_r) \in \mathbb{R}^{r\times r}$ is the diagonal matrix correspondent to A_u. $\sigma_i > 0$ $(i = 1, 2, \dots, r)$ are the positive singular values. The matrices $U_u = (\phi_1, \phi_2, \dots, \phi_{(N-1)^3})$ and $V_u = (\varphi_1, \varphi_2, \dots, \varphi_{L+1})$ consist of the orthogonal eigenvectors to the $A_u A_u^{\mathrm{T}}$ and $A_u^{\mathrm{T}} A_u$, respectively. The columns of these eigenvector matrices are organized so as to correspond to the singular values σ_i comprised in S_u in a non-increasing order. And the singular values of the decomposition are connected to the eigenvalues of the matrices $A_u A_u^{\mathrm{T}}$ and $A_u^{\mathrm{T}} A_u$ in a manner such that $\lambda_i = \sigma_i^2$ $(i = 1, 2, \dots, r)$. Since the number of mesh points is far larger than that of transient moment points, i.e.,

$$(N-1)^3 \gg L+1,$$

that is also that the order $(N-1)^3$ for matrix $A_u A_u^{\mathrm{T}}$ is far larger than the order $L+1$ for matrix $A_u^{\mathrm{T}} A_u$, however, their non-zero eigenvalues are identical, therefore, we may first solve the eigenequation corresponding to matrix $A_u^{\mathrm{T}} A_u$ to find the eigenvectors φ_j $(j = 1, 2, \dots, L+1)$, and then by relationship

$$\phi_j = \frac{A_u \varphi_j}{\sigma_j}, \quad j = 1, 2, \dots, r,$$

we may obtain r $(r \leqslant L+1)$ eigenvectors corresponding to the non-zero eigenvalues for matrix $A_u A_u^{\mathrm{T}}$.

Define matrix norm

$$\|A\|_{a,\beta} = \sup_{x\neq 0} \frac{\|Ax\|_\alpha}{\|x\|_\beta}.$$

Let

$$A_{M_u} = \sum_{i=1}^{M_u} \sigma_i \phi_i \varphi_i^{\mathrm{T}},$$

where σ_i $(i = 1, 2, \dots, M_u)$ are the first M_u diagonal elements of matrix S_u, ϕ_i and φ_i $(i = 1, 2, \dots, M_u)$ be the first M_u column vectors of matrices U_u and V_u, respectively. According the relationship properties of spectral radius and $\|\cdot\|_{2,2}$ for matrix, if

$$M_u < r = \mathrm{rank}(A_u),$$

then there holds the following formula (see [26,27]):

$$\min_{\mathrm{rank}(B)\leqslant M_u} \|A_u - B\|_{2,2} = \|A_u - A_{M_u}\|_{2,2} = \sigma_{(M_u+1)} = \sqrt{\lambda_{(M_u+1)}}, \qquad (7)$$

which shows that A_{M_u} is an optimal representation of A_u. Denote the $L+1$ column vectors of matrices A_u by

$$a_u^l = (u_1^l, u_2^l, \dots, u_{(N-1)^2}^l)^{\mathrm{T}}, \quad l = 0, 1, \dots, L,$$

by ε_l $(l = 1, 2, \ldots, L{+}1)$ the unit column vectors except that a vector component is 1, while the other components are 0. Then, by the compatibility of the norm for matrixes and vectors, we obtain

$$\begin{aligned}\|a_u^l - P_{Mu}(a_u^l)\|_2 &= \|(A_u - A_{M_u})\varepsilon_l\|_2 \\ &\leqslant \|(A_u - A_{M_u})\|_{2,2}\,\|\varepsilon_l\|_2 \\ &= \sigma_{(M_u+1)} \\ &= \sqrt{\lambda_{(M_u+1)}}\,,\end{aligned} \tag{8}$$

where

$$P_{M_u}(a_u^l) = \sum_{j=1}^{M_u} (\phi_j, a_u^l)\phi_j,$$

and (ϕ_j, a_u^l) is the canonical inner product for vectors ϕ_j and a_u^l. Inequality (8) shows that $P_{M_u}(a_u^l)$ is the optimal approximation to a_u^l. It follows that a group of optimal base $\Phi_u = (\phi_1, \phi_2, \ldots, \phi_{M_u})$ is obtained from (7) and (8), which is known as a group of POD base.

4 Reduced-order extrapolation SFDS

If we approximate U^n with $\Phi_u \alpha_{Mu}^n$, i.e.,

$$U^n \approx \Phi_u \alpha_{Mu}^n, \tag{9}$$

where α_{Mu}^n is a constant vector, then, by inserting (9) into (5), we could obtain an approximating formula of (5) as follows:

$$\Phi_u \alpha_{Mu}^{n+1} \approx A^{-1}\Phi_u \alpha_{Mu}^n + \tau A^{-1} F^{n+1}. \tag{10}$$

Then we may obtain an iterative scheme of least square approximation of (10) by multiplying Φ_u^{T} as follows:

$$\beta_{Mu}^n = \Phi_u^{\mathrm{T}} U^n, \quad 0 \leqslant n \leqslant L, \tag{11}$$

$$\Phi_u^{\mathrm{T}} A \Phi_u \beta_{Mu}^{n+1} = \beta_{Mu}^n + \Phi_u^{\mathrm{T}} \tau F^{n+1}, \quad L \leqslant n \leqslant M-1, \tag{12}$$

$$U_{M_u}^{*n} = \Phi_u \beta_{Mu}^n, \quad 1 \leqslant n \leqslant M. \tag{13}$$

The system of equations (11)–(13) is known as a reduced-order extrapolation SFDS based on POD technique, $U_{M_u}^{*n}$ is known as the reduced-order solution of SFDS based on POD technique, it has no repeating computations. Especially, the method here is totally different from the existing reduced-order numerical methods based on POD technique, whose snapshots are taken from total transient solutions at all time instances t_n $(1 \leqslant n \leqslant M)$ or taken one from every ten transient solutions at uniform intervals (see, e.g., [1–3,5,6,13–15,17,19–32,37]), while snapshots here are taken from the first $L+1$ transient solutions ($L \ll M \ll (N-1)^3$), it is used existing data (the first $L+1$ transient solutions) to simulate future development and change of natural phenomenon (all M solutions, $L \ll M$), which is an important computational method. Since the classical SFDS (5) includes $(N-1)^3$ linear equations on each time level, while the reduced-order extrapolation SFDS (11)–(13) based on POD technique includes only M_u unknowns ($M_u \ll (N-1)^3$). Thus, the reduced-order extrapolation SFDS (11)–(13) could greatly save the computing time in the computational process.

5 Error estimates of reduced-order SFDS solutions and implementation for solving reduced-order extrapolation SFDS

5.1 Error estimates of reduced-order SFDS solutions

In this subsection, we devote to deriving the error estimates for the reduced-order SFDS solutions above section. To this end, we first introduce two lemmas.

Lemma 1 $A_{Mu} = \Phi_u \Phi_u^{\mathrm{T}} A_u$.

Proof Owing to

$$A_{Mu} = \sum_{i=1}^{Mu} \sigma_i \phi_i \varphi_i^{\mathrm{T}} = (\phi_1, \phi_2, \ldots, \phi_{M_u}) \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_{Mu})(\varphi_1, \varphi_2, \ldots, \varphi_{Mu})^{\mathrm{T}},$$

$$A_u = (\phi_1, \phi_2, \ldots, \phi_r) \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_r)(\varphi_1, \varphi_2, \ldots, \varphi_r)^{\mathrm{T}},$$

we have

$$\begin{aligned}
\Phi_u \Phi_u^{\mathrm{T}} A_u &= \Phi_u \begin{pmatrix} \phi_1^{\mathrm{T}} \\ \vdots \\ \phi_{Mu}^{\mathrm{T}} \end{pmatrix} (\phi_1, \phi_2, \ldots, \phi_r) \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_r)(\varphi_1, \varphi_2, \ldots, \varphi_r)^{\mathrm{T}} \\
&= \Phi_u (I_{Mu}\ O) \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_r)(\varphi_1, \varphi_2, \ldots, \varphi_r)^{\mathrm{T}} \\
&= \Phi_u (\mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_{Mu})\ O)(\varphi_1, \varphi_2, \ldots, \varphi_r)^{\mathrm{T}} \\
&= (\phi_1, \phi_2, \ldots, \phi_{M_u}) \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_{Mu})(\varphi_1, \varphi_2, \ldots, \varphi_{Mu})^{\mathrm{T}} \\
&= A_{Mu},
\end{aligned}$$

which completes the proof. □

Lemma 2 $\|a_u^l - \Phi_u \Phi_u^{\mathrm{T}} a_u^l\|_2 \leqslant \sigma_{(Mu+1)} = \sqrt{\lambda_{(M_u+1)}}$ $\quad (l = 0, 1, \ldots, L)$.

Proof By using Lemma 1, we obtain $A_{Mu} = \Phi_u \Phi_u^{\mathrm{T}} A_u$. Then, we have

$$\Phi_u \Phi_u^{\mathrm{T}} a_u^l = A_{Mu} \varepsilon_l = P_{Mu}(a_u^l).$$

We derive from (8) that

$$\|a_u^l - \Phi_u \Phi_u^{\mathrm{T}} a_u^l\|_2 = \|a_u^l - P_{Mu}(a_u^l)\|_2 \leqslant \sigma_{(Mu+1)} = \sqrt{\lambda_{(M_u+1)}}, \quad l = 0, 1, \ldots, L,$$

which completes the proof. □

We have the following main result for the reduced-order extrapolation SFDS (11)–(13).

Theorem 1 *Let U^n $(n = 0, 1, \ldots, M)$ be classical SFDS solutions, and let $U^{*n}_{M_u}$ $(n = 0, 1, \ldots, M)$ be the reduced SFDS solutions. Then we have*

$$\|U^n - U^{*n}_{M_u}\|_\infty \leqslant C(n)\sqrt{\lambda_{(M_u+1)}}\,, \tag{14}$$

where

$$C(n) = \begin{cases} 1, & 1 \leqslant n \leqslant L, \\ \|A^{-1}\|_\infty^{n-L}, & L+1 \leqslant n \leqslant M. \end{cases}$$

Proof By using (5), we have

$$U^{n+1} = A^{-1}U^n + \tau A^{-1}F^{n+1}.$$

While, by using (12), we have

$$U^{*n+1}_{M_u} = A^{-1}U^{*n}_{M_u} + \tau A^{-1}F^{n+1}.$$

Let

$$e_n = U^n - U^{*n}_{M_u}.$$

Then we have

$$\|e_{n+1}\|_\infty = \|A^{-1}e_n\|_\infty \leqslant \|A^{-1}\|_\infty\,\|e_n\|_\infty \quad (L+1 \leqslant n \leqslant M-1).$$

Thus, we obtain that

$$\|e_n\|_\infty \leqslant \|A^{-1}\|_\infty^{n-L}\,\|e_L\|_\infty \quad (L \leqslant n \leqslant M). \tag{15}$$

Using Lemma 2, we obtain that

$$\begin{aligned} \|e_n\|_\infty &= \|U^n - U^{*n}_{M_u}\|_\infty \\ &= \|U^n - \Phi_u\Phi_u^{\mathrm{T}}U^n\|_\infty \\ &\leqslant \|U^n - \Phi_u\Phi_u^{\mathrm{T}}U^n\|_2 \\ &\leqslant \sqrt{\lambda_{(M_u+1)}}\,, \quad 1 \leqslant n \leqslant L. \end{aligned} \tag{16}$$

Then it follows from (15) and (16) that

$$\|e_n\|_\infty \leqslant \|A^{-1}\|_\infty^{n-L}\sqrt{\lambda_{(M_u+1)}}\,, \quad L+1 \leqslant n \leqslant M, \tag{17}$$

which completes the proof. □

Combining (6) with Theorem 1 yields the following result.

Theorem 2 *Let U be the solution to equation* (1), *and let $U^{*n}_{M_u}$ ($n = 0, 1, \ldots, M$) be the reduced SFDS solutions. Then we have*

$$\|U(t_n) - U^{*n}_{M_u}\|_\infty = O\big(\tau, N^{-3}, C(n)\sqrt{\lambda_{(M_u+1)}}\,\big), \tag{18}$$

where

$$C(n) = \begin{cases} 1, & 1 \leqslant n \leqslant L, \\ \|A^{-1}\|_\infty^{n-L}, & L + 1 \leqslant n \leqslant M. \end{cases}$$

Remark 2 The error estimates of Theorems 1 and 2 have given the guides to determine the number M_u of POD basic satisfying

$$\sqrt{\lambda_{(M_u+1)}} = O(\tau, N^{-3})$$

and whether or not need to renew POD bases in the computational process, i.e., if

$$\|A^{-1}\|_\infty^{n-L}\sqrt{\lambda_{(M_u+1)}} = O(\tau, N^{-3}) \quad (L + 1 \leqslant n \leqslant M),$$

then we do not need to renew POD bases, otherwise, we need.

5.2 Implementation for solving reduced-order extrapolation SFDS

In this subsection, we provide the implementation for solving the reduced-order extrapolation SFDS, which consists of the following 5 steps.

Step 1 For given positive parameter $\alpha > 0$, source term $f(x, y, z, t)$, initial value function $u_0(x, y, z)$, the time step increment τ, the space of all algebraic polynomials of degree no more than N:

$$X_N = \{p \in P_N \times P_N \times P_N \colon p|_{\partial\Omega} = 0\},$$

and Legendre Gauss-Lobatto points $\{\xi_i\}_{i=0}^N$, solving the classical FD scheme at the first fewer L steps (in usually, take $L = 20$):

$$AU^{n+1} = U^n + \tau F^{n+1}, \quad 0 \leqslant n \leqslant L - 1,$$

where

$$A = I_1 - \alpha\tau(I \otimes I \otimes D2 + I \otimes D2 \otimes I + D2 \otimes I \otimes I),$$

I_1 is the unit matrix of order $(N-1)^3$, $D2$ the second-order differentiation matrix of order $N - 1$ for Chebyshev case (see [40]), I the unit matrix of order $N - 1$,

$$A \otimes B = (Ab_{i,j})_{i,j=1}^{N-1},$$

$$\begin{aligned} U^n = {} & (u_N(\xi_1, \xi_1, \xi_1, t_n), \ldots, u_N(\xi_{N-1}, \xi_1, \xi_1, t_n), \ldots, u_N(\xi_{N-1}, \xi_{N-1}, \xi_1, t_n), \\ & \ldots, u_N(\xi_{N-1}, \xi_{N-1}, \xi_{N-1}, t_n))^{\mathrm{T}}, \\ F^n = {} & (f(\xi_1, \xi_1, \xi_1, t_n), \ldots, f(\xi_{N-1}, \xi_1, \xi_1, t_n), \ldots, f(\xi_{N-1}, \xi_{N-1}, \xi_1, t_n), \ldots, \\ & f(\xi_{N-1}, \xi_{N-1}, \xi_{N-1}, t_n))^{\mathrm{T}}, \end{aligned}$$

yields the set of classical SFDS solutions, i.e., $\{U^i\}_{i=0}^{L}$ (usually, $L \ll M$).

Step 2 Formulate the snapshot matrixes

$$A_u = (U^0, U^1, \ldots, U^L)$$

and solve the linear system of equation

$$(A_u^{\mathrm{T}} A_u - \lambda_u I_{L+1})\varphi_u = 0$$

obtaining, respectively, the eigenvalues

$$\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_{\widetilde{M}_u} > 0$$

($\widetilde{M}_u = \mathrm{rank} A_u$) and corresponding eigenvectors φ_{uj} ($j = 1, 2, \ldots, \widetilde{M}_u$).

Step 3 For the error $\mu = O(\tau, N^{-3})$ needed, determine the number M_u ($M_u \leqslant \widetilde{M}_u$) of POD bases such that $\sqrt{\lambda_{u(M_u+1)}} \leqslant \mu$ and formulate the POD bases $\Phi_u = (\phi_{u1}, \phi_{u2}, \ldots, \phi_{uM_u})$ (where $\phi_{uj} = A_u \varphi_{uj}/\sqrt{\lambda_{uj}}$, $j = 1, 2, \ldots, M_u$).

Step 4 Solve the reduced-order extrapolation SFDS

$$\begin{aligned}
\beta_{Mu}^{n} &= \Phi_u^{\mathrm{T}} U^n, \quad 0 \leqslant n \leqslant L,\\
\Phi_u^{\mathrm{T}} A \Phi_u \beta_{M_u}^{n+1} &= \beta_{M_u}^{n} + \Phi_u^{\mathrm{T}} \tau F^{n+1}, \quad L \leqslant n \leqslant M-1,\\
U_{M_u}^{*n} &= \Phi_u \beta_{M_u}^{n}, \quad 1 \leqslant n \leqslant M.
\end{aligned}$$

obtaining the reduced-order solution vectors

$$\begin{aligned}
U_{M_u}^{*n} = {} & (u_N^*(\xi_1, \xi_1, \xi_1, t_n), \ldots, u_N^*(\xi_{N-1}, \xi_1, \xi_1, t_n), \ldots, u_N^*(\xi_{N-1}, \xi_{N-1}, \xi_1, t_n),\\
& \ldots, u_N^*(\xi_{N-1}, \xi_{N-1}, \xi_{N-1}, t_n))^{\mathrm{T}} \quad (0 \leqslant n \leqslant M).
\end{aligned}$$

Step 5 If

$$C(n)\sqrt{\lambda_{u(M_u+1)}} \leqslant \mu,$$

then $U_{M_u}^{*n}$ ($n = 1, 2, \ldots, M$) are just solutions satisfying accuracy needed. Else, i.e., if

$$C(n)\sqrt{\lambda_{u(M_u+1)}} > \mu,$$

then put $U^l = U_{M_u}^{*l}$ ($l = n-L-1, n-L, \ldots, n-1$), return Step 2.

6 Numerical example

To verify the efficiency of the method, we take

$$\begin{aligned}
u_0(x, y, z) &= \sin \pi x \sin \pi y \sin \pi z,\\
f(x, y, z, t) &= (3\pi^2 - 1) \sin \pi x \sin \pi y \sin \pi z \, \mathrm{e}^{-t},\\
(x, y, z) &\in [-1, 1]^3, \quad t \in [0, 10], \quad \alpha = 1,
\end{aligned}$$

in equation (1). It is easy to obtain the accurate solution as follows:

$$u(x,y,z,t)=\sin\pi x\sin\pi y\sin\pi z\,\mathrm{e}^{-t}.$$

Let us denote the accurate solution at discrete points by

$$\widetilde{u}=(\widetilde{U}^1,\widetilde{U}^2,\ldots,\widetilde{U}^M),$$

where

$$\begin{aligned}\widetilde{U}^i=&(u(\xi_1,\xi_1,\xi_1,t_i),\ldots,u(\xi_{N-1},\xi_1,\xi_1,t_i),\ldots,u(\xi_{N-1},\xi_{N-1},\xi_1,t_i),\ldots,\\&u(\xi_{N-1},\xi_{N-1},\xi_{N-1},t_i))^{\mathrm{T}}.\end{aligned}$$

Denote

$$u_1=(U^1,U^2,\ldots,U^M)$$

the classical SFDS solution at the same discrete points and

$$u_2^{M_u}=(U^{*1}_{M_u},U^{*2}_{M_u},\ldots,U^{*M}_{M_u})$$

the reduced-order extrapolation SFDS solution based on POD method at the same discrete points, which is found with the reduced-order extrapolation SFDS according five steps of implementation of algorithm in Section 5.2 with the first $L=10$ snapshots. Let

$$\begin{aligned}e(\widetilde{u},u_1)&=\max_{1\leqslant i,j,k\leqslant N-1,\,1\leqslant n\leqslant M}|(\widetilde{u}-u_1)^n_{i,j,k}|,\\e(\widetilde{u},u_2^{M_u})&=\max_{1\leqslant i,j,k\leqslant N-1,\,1\leqslant n\leqslant M}|(\widetilde{u}-u_2^{M_u})^n_{i,j,k}|,\\e(\widetilde{u}_1,u_2^{M_u})&=\max_{1\leqslant i,j,k\leqslant N-1,1\leqslant n\leqslant M}|(\widetilde{u}_1-u_2^{M_u})^n_{i,j,k}|.\end{aligned}$$

Let t_1 be the computing time of classical SFDS solution, and let t_2 be the computing time of the reduced-order SFDS solution based on POD method. When $\tau=0.0001$ and $N=15$, the errors between accurate solution $\widetilde{u}$ and the reduced-order SFDS solution u_2 at the same discrete points for different numbers of POD bases are

$$e(\widetilde{u},u_2^{M_u})=1.48\times10^{-4},\quad M_u=1,2,3.\tag{19}$$

Since the error

$$e(\widetilde{u},u_1)=1.48\times10^{-4}$$

between accurate solution and classical SFDS solution which is obtained by computing, it follows that the error between accurate solution and classical SFDS solution is very proximate to the errors between accurate solution and the reduced-order SFDS solutions based on POD method with $M_u=1,2,3$.

Table 1 shows the errors between the classical SFDS solution u_1 and the reduced-order SFDS solutions u_2 based on POD method with $M_u=1,2,3$ and their computing time.

Table 1 Error between SFDS solutions and reduced SFDS solutions and computing time

	M_u		
	1	2	3
$e(u_1, u_2^{M_u})$	2.96×10^{-12}	2.08×10^{-12}	2.53×10^{-13}
t_2/s	3.43	3.62	3.7606

Since the computing time $t_1 = 553.2\,\mathrm{s}$ of classical SFDS solution when $T = 10$, it follows from Table 1 that the computing time finding the reduced-order SFDS solution based on POD method can be saved greatly and since the reduced-order extrapolation SFDS only includes M_u degrees of freedom at every time level, the computational load can be alleviated greatly, too.

(19) and Table 1 show that the numerical results are consistent with the theoretical result (10^{-4}), and the error between the accurate solution and the classical SFDS solution and the error between the accurate solution and the reduced-order SFDS solutions based on POD method are all very small, while the errors between the classical SFDS solution and the reduced-order SFDS solution based on POD method is smaller, but the computing time of the reduced-order SFDS solutions based on POD method can be saved greatly. Therefore, the reduced-order SFDS solution based on POD method is effective and feasible to solve high dimensional problems.

7 Conclusions and perspective

In this study, we have employed POD method and SVD to study the classical SFDS for the 3D parabolic equation. First, the ensemble of data is obtained by using the classical SFDS of 3D parabolic equation. Then the POD bases of the ensemble of data are generated by using SVD and POD technique. The unknown quantities of the classical SFDS are replaced with the linear combination of POD bases and the reduced-order extrapolation model, i.e., the reduced-order extrapolation SFDS with lower dimensions and sufficiently high accuracy for the 3D parabolic equation is established. Finally, the error estimates of the reduced-order extrapolation SFDS solutions based on POD method is provided, which can be used to determine the number M_u of POD basic and whether or not to renew POD bases in the computational process. The numerical example has shown that the numerical errors between the classical SFDS solutions and the reduced-order SFDS solutions based on POD method are consistent with the theoretical results. Moreover, it is also shown that the reduced-order extrapolation SFDS based on POD method is effective and feasible to find the numerical solutions for 3D parabolic equation. Especially, we here thoroughly improve the existing methods, where we do only use the first fewer given numerical solutions on very short time span $[0, T_0]$ ($T_0 \ll T$) as snapshots to formulate the POD basis and establish the reduced-order extrapolation SFDS based on POD technique for finding the numerical solutions on total time span $[0, T]$. Thus, we sufficiently adopt the advantage of POD method, namely, sufficiently utilize the given data (on very short time span $[0, T_0]$ and $T_0 \ll T$) to forecast future physic phenomenons (on time span $[T_0, T]$). For some practical problems, such as in order to simulate numerical weather forecast corresponding to weather forecast PDEs, it is only necessary to structure the POD bases by using the previous data information as snapshots, and then solve the reduced-order extrapolation SFDS without solving the classical SFDS. Thus, we can forecast quite precisely the future natural phenomena with existing information and can greatly save the computing time solving the reduced-order extrapolation SFDS.

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