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EDITORIAL

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Editorial for Journal of Numerical Simulations in Physics and Mathematics

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Abstract

This editorial mainly states the meanings for creating the *Journal of Numerical Simulations in Physics and Mathematics*, and the significance and foreground for the numerical simulations. In particular, the significance and foreground for the three most commonly used numerical methods: the finite element (FE) method, the finite difference (FD) scheme, and the finite volume element (FVE) method, as well as their reduced-dimension methods in the numerical simulations in physics and mathematics will be emphatically introduced and reviewed.

Keywords: numerical simulations, finite element method, finite difference scheme, finite volume element method.

1 Introduction

The numerical simulation, also known as computer simulation, is one of most effective technique that uses electronic computers in combination with some numerical methods such as the FE method, the FD scheme, and the FVE method, and through numerical calculation and image display methods, to study engineering problems, physical problems, and various problems in nature. Numerical simulation technology was first introduced in 1953 by Bruce et al. [1] to simulate one-dimensional (1D) gas-phase unsteady radial and linear flows. Due to the limited computational capabilities at the time, it was initially applied only to single-phase 1D problems. In 1954, West et al. [2] extended the approach to two-dimensional (2D) problems, presenting a method to simulate unsteady two-phase flow in oil reservoirs.

With the development of computer technology, the numerical simulation has made significant progress and has been applied in more fields. For example, in the field of aerospace, the numerical simulation can be used as an alternative to wind tunnel tests, thereby saving a significant amount of costs; in nuclear test field, by using the numerical simulation to conduct the tests on a computer, nuclear pollution can be avoided and more reliable data can be obtained.

The *Journal of Numerical Simulations in Physics and Mathematics* serves mainly as a platform for numerical simulation scholars to showcase their numerical calculation and simulation results.

Of course, the development for the numerical

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simulations technology is inseparable from the progress of the calculation methods such as the FE method, the FD scheme, and the FVE method. In other words, the progress of the calculation methods such as the FE method, the FD scheme, and the FVE method is the source for the development for the numerical simulations technology. Therefore, promoting the development and advancement of computational methods is the main central task, which is main purpose for the *Journal of Numerical Simulations in Physics and Mathematics*.

Hence, in the next Section 2, we will review the development of the FE method, the FD scheme, and the FVE method as well as their merit and demerit. Then, in Section 3, we will introduce some reduced-dimension approaches for the FE method, the FD scheme, and the FVE method. Finally, we summary main conclusions for this editorial in Section 4.

2 The merit and demerit of the FE method, the FD scheme, and the FVE method

The FE method, originally proposed by Turner et al. [3], has been widely used to solve structural problems. It has found extensive applications in real-world engineering computations and has become an effective approach for solving various steady and unsteady partial differential equations (PDEs), including hydrokinetic equations.

The FD method has a longer history than the FE method, which is originated from the work of Newton, Euler, and others. They once used the difference quotient instead of the derivative to simplify the calculation. In 1928, Courant et al. [4] proved the convergence theorem of the typical FD schemes of the three typical PDEs, providing a foundation for modern FD theory. Meanwhile, they also applied the FD method to find the numerical solutions of PDEs and developed the FD method. Because the FD method is universal and easy to implement numerical calculations and numerical simulations in electronic computers, it has developed greatly and been widely applied in scientific engineering computing.

The FVE method was developed in Imperial College mainly to solve fluid dynamics problems in 1980, whose emergence was much later than that of the FD scheme and the FE method (see [5]). The core idea of the FVE method is based on the law of conservation. By partitioning a continuous physical domain into a series of control volumes and then applying the law of conservation to each control volume, the PDEs are transformed into systems of algebraic equations. The FVE method is not only applicable to fluid mechanics, but also gradually extends to other fields, including elastic mechanics, for solving the stress, strain, and displacement of structures.

Nevertheless, when the FE method, the FD scheme, and the FVE method are applied to solving the PDEs in the actual engineering, they all generally contain hundreds of thousands or even tens of millions of unknowns. Even when solved on advanced computers, it still takes several days or even dozens of days to calculate the FE, FD, and FVE solutions. Especially, as a result of the FE method, the FD scheme, and the FVE method in the actual engineering computations containing a large number of unknowns, the calculating errors during the actual calculations could be quickly accumulated. This leads to significant differences in the obtained FE, FD, FVE solutions and fails to achieve the expected results. Therefore, how to reduce the unknowns in the FE method, the FD scheme, and the FVE method to slow down the accumulation of computing errors in the calculation, save CPU running time, mitigate the calculation load, and improve the accuracy of the FE, FD, and FVE solutions is a key issue.

Therefore, we will review the reduced-dimension methods for the FE method, the FD scheme, and the FVE method in the next section, which can greatly reduce the unknowns in the FE method, the FD scheme, and the FVE method so as to slow down the accumulation of computing errors in the calculation, lessen CPU running time, mitigate the calculated load, and improve the accuracy of the FE, FD, and FVE solutions.

3 The reduced-dimension approaches for the FE method, the FD scheme, and the FVE method

Lots of examples for the numerical simulations, for example, those examples in [6], have shown the proper orthogonal decomposition (POD) is one of the most effective approaches to reduce the dimension for the FE, FD, and FVE equations. The POD method has a long history. It is actually principal vector analysis in optimization. Therefore, it is still applied in data mining at present. The POD method is essentially to find a set of orthogonal bases for a set of known data under a certain least squares optimality, that is, to find an optimal low-dimensional approximation for the set of known data. It was originally proposed by Pearson [7] in 1901 for extracting targeted main components from a large amount of data. Pearson's sample analysis and data processing are still used in the data mining at present. The fashionable term for this kind of data is known as "Big Data". The term for the POD method was proposed by Sirovich [8] in 1987 and is mainly used for analyzing the characteristics of fluids.

The reduced-dimension approaches for the FE method, the FD scheme, and the FVE method are first proposed by Luo's team, they are specifically introduced as follows.

3.1 The reduced-dimension for the FE method

There are two dimensionality reduction methods for the FE method. One is the dimensionality reduction of the FE subspace, and the other is the dimensionality reduction of the unknown coefficient vectors in the unknown FE solutions. They are stated as follows.

3.1.1 *The reduced-dimension for the FE subspace*

The POD-based FE subspace dimension reduction method was first gradually proposed by Luo's team internationally since 2007 (see [9]), whose basic idea is stated as follows.

Let $\Omega \subset \mathbb{R}^s$ $(s = 1, 2, 3)$ be a bounded and simply connected region, and t_e be the most maximum time limit. Consider the following unsteady PDE:

$$\frac{\partial^l u(\boldsymbol{x}, t)}{\partial t^l} = \tilde{A}u(\boldsymbol{x}, t) + f(\boldsymbol{x}, t), \quad (\boldsymbol{x}, t) \in \Omega \times (0,\ t_e), \tag{1}$$

where $l \geqslant 1$ is an integer, $\tilde{A}$ is a differential operator with respect to spatial variables, and f is a known function.

Step 1. By using the FE method to discretize spatial variables and difference quotient to discretize time derivatives, we get a fully discrete FE equation:

$$(u_h^{n+1}, v_h) = A(u_h^{n-1}, u_h^{n-2}, ..., u_h^{n-l})(u_h^n, v_h) + F^n(v_h), \forall v_h \in V_h, 1 \leqslant n \leqslant N-1, \tag{2}$$

here V_h =:span$\{\phi_1, \phi_2, ..., \phi_M\}$, ϕ_i $(1 \leqslant i \leqslant M)$ are the FE basis functions, M is related to the number of spatial nodes and the degree of the basis function ϕ_i of the piecewise interpolation polynomial, $A(u_h^{n-1}, u_h^{n-2}, ..., u_h^{n-l})$ is a positive definite bilinear functional for given $u_h^{n-1}, u_h^{n-2}, ..., u_h^{n-l}$, and $F^n(\cdot)$ is a linear continuous functional determined by f.

step 2. Find the first L $(L \ll N$, usually take $L = 20)$ FE solutions $u_h^1, u_h^2, ..., u_h^L$ from (2) and use the continuous POD method in [6, Chapter 4] to construct d (generally $d = 5 \sim 7$) POD basis functions $\boldsymbol{\Phi} = \{\varphi_1, \varphi_2, ..., \varphi_d\}$ containing the main information.

step 3. By replacing the FE space V_h in (2) with $V_d =$: span $\{\varphi_1, \varphi_2, ..., \varphi_d\}$ spanned by the POD bases $\boldsymbol{\Phi}$, the FE equation (2) with tens of millions of unknowns is simplified into the following FE POD reduction model with only d unknowns:

$$(u_d^{n+1}, v_d) = A(u_d^{n-1}, u_d^{n-2}, ..., u_d^{n-l})(u_d^n, v_d) + F^n(v_d), \ \ \forall v_d \in V_d, \ \ 1 \leqslant n \leqslant N-1. \tag{3}$$

Remark 1 *The most contribution of Luo's team is to create the basic theories of the existence, stability, and convergence for the reduced-order FE solutions by using the bounded functional extension theory in Functional Analysis to link ingeniously the classical FE method with the FE subspace reduced-dimension method. These theories are used as the theoretical criteria for the selection of POD bases and the update of POD bases, which are proposed by Luo's team for first times and are original.*

3.1.2 *The reduced-dimension for the unknown FE solution coefficient vectors*

The POD-based dimension reduction method for the unknown FE solution coefficient vectors was first gradually proposed by Luo's team internationally since 2020 (see [10]), whose basic idea is stated as follows.

Step 1. Represent the unknown FE solutions u_h^n in (2) into some linear combinations of the FE basis function vector $\hat{\boldsymbol{\Phi}} =: (\phi_1, \phi_2, ..., \phi_M)$ and the unknown solution coefficient vectors $\boldsymbol{U}^n =: (u_1^n, u_2^n, ..., u_M^n)$ as folllows:

$$u_h^n = (u_1^n, u_2^n, ..., u_M^n) \cdot (\phi_1, \phi_2, ..., \phi_M) = \boldsymbol{U}^n \cdot \hat{\boldsymbol{\Phi}}, \quad 1 \leqslant n \leqslant N. \tag{4}$$

Step 2. Substitute the linear combinations $u_h^n = \boldsymbol{U}^n \cdot \hat{\boldsymbol{\Phi}}$ into (2) to obtain the following matrix form:

$$\begin{cases} \boldsymbol{U}^{n+1} = \hat{\boldsymbol{A}}(\boldsymbol{U}^{n-1}, \boldsymbol{U}^{n-2}, ..., \boldsymbol{U}^{n-l})\boldsymbol{U}^n + \hat{\boldsymbol{F}}^n; \\ u_h^n = \boldsymbol{U}^n \cdot \hat{\boldsymbol{\Phi}}, \quad 1 \leqslant n \leqslant N-1, \end{cases} \tag{5}$$

where $\hat{\boldsymbol{A}}$ and $\hat{\boldsymbol{F}}^n$ are determined by the positive definite bilinear functional A and $F^n(\cdot)$ in (2), respectively.

Step 3. Find the first L $(L \ll N$, usually take $L = 20)$ FE solution coefficient vectors $\boldsymbol{U}^i$ $(1 \leqslant i \leqslant L)$ from (5) and construct matrix $\boldsymbol{P} = (\boldsymbol{U}^1, \boldsymbol{U}^2, ..., \boldsymbol{U}^L)$.

Step 4. Find the d (usually $d = 5 \sim 7$) standard orthogonal eigenvectors $\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, ..., \boldsymbol{\varphi}_d$ corresponding to the largest d eigenvalues for the $\boldsymbol{P}\boldsymbol{P}^T$ and form the POD basis $\boldsymbol{\Phi} = (\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, ..., \boldsymbol{\varphi}_d)$.

Step 5. Replace $\boldsymbol{U}^n$ in (5) with $\boldsymbol{U}_d^n = \boldsymbol{\Phi}\boldsymbol{\beta}^n$ to obtain a dimensionality reduction format with only

d unknowns:

$$\begin{cases} \boldsymbol{\beta}^n = \boldsymbol{\Phi}^T \boldsymbol{U}_h^n, \ 1 \leqslant n \leqslant L; \\ \boldsymbol{\beta}^{n+1} = \boldsymbol{\Phi}^T \hat{\boldsymbol{A}}(\boldsymbol{\Phi}\boldsymbol{\beta}^{n-1}, \boldsymbol{\Phi}\boldsymbol{\beta}^{n-2}, ..., \boldsymbol{\Phi}\boldsymbol{\beta}^{n-l})\boldsymbol{\Phi}\boldsymbol{\beta}^n \\ +\boldsymbol{\Phi}^T \hat{\boldsymbol{F}}^n, \ L+1 \leqslant n \leqslant N-1, \\ u_d^n = \boldsymbol{\Phi}\boldsymbol{\beta}^n \cdot \hat{\boldsymbol{\Phi}}, \ 1 \leqslant n \leqslant N, \end{cases} \tag{6}$$

where $\boldsymbol{\beta}^n = (\beta_1^n, \beta_2^n, ..., \beta_d^n)^T$ are the d-dimensional unknown vectors and $\boldsymbol{U}_h^n$ $(1 \leqslant n \leqslant L)$ are the first L solution coefficient vectors in (5).

Remark 2 *By comparing* (5) *with* (6)*, it is easy to know that the reduced-dimensional FE solutions for the solution coefficient vectors have the same basis function vectors* $\hat{\boldsymbol{\Phi}}$ *as the classical FE solutions. Therefore, the reduced-dimensional FE solutions about the solution coefficient vectors have the same accuracy as the classical FE solutions. In other words, though the unknowns of the reduced-dimensional FE format* (6) *are greatly reduced, which contain only* d *(usually* $d = 5 \sim 7$*) unknowns, the accuracy for the reduced-dimensional FE solutions keeps unchanged. Especially, it is easy to prove the existence, stability, and convergence (i.e., error estimation) of the reduced-order FE solutions by using matrix analysis. The error estimation can be used as the theoretical criterion for the selection of the POD basis vectors and the update of the POD basis vectors.*

3.2 The reduced-dimension for the FD scheme

The POD-based FD dimension reduction method was also first gradually proposed by Luo's team internationally since 2007 (see [11]), whose basic idea is stated as follows.

Step 1. The PDE (1) is discretized by difference quotient and is written into a vector form FD scheme:

$$\boldsymbol{U}^{n+1} = \boldsymbol{A}(\boldsymbol{U}^{n-1}, \boldsymbol{U}^{n-2}, ..., \boldsymbol{U}^{n-l})\boldsymbol{U}^n \\ + \boldsymbol{F}^n, \ \ 1 \leqslant n \leqslant N-1, \tag{7}$$

where $\boldsymbol{A}(\boldsymbol{U}^{n-1}, \boldsymbol{U}^{n-2}, ..., \boldsymbol{U}^{n-l})$ is a positive definite matrix for the obtained $\boldsymbol{U}^{n-1}, \boldsymbol{U}^{n-2}, ..., \boldsymbol{U}^{n-l}$ and $\boldsymbol{F}^n$ are determined by f.

Step 2. Find the first L FE solution coefficient vectors $\boldsymbol{U}^i$ $(1 \leqslant i \leqslant L \ll N$, usually take $L = 20)$ from (7) and construct matrix $\boldsymbol{P} = (\boldsymbol{U}^1, \boldsymbol{U}^2, ..., \boldsymbol{U}^L)$. The d (usually $d = 5 \sim 7$) standard orthogonal eigenvectors $\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, ..., \boldsymbol{\varphi}_d$ corresponding to the largest d eigenvalues for the $\boldsymbol{P}\boldsymbol{P}^T$ to form the POD basis $\boldsymbol{\Phi} = (\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, ..., \boldsymbol{\varphi}_d)$. Replace $\boldsymbol{U}^n$ in (5) with $\boldsymbol{U}_d^n = \boldsymbol{\Phi}\boldsymbol{\beta}^n$ to obtain a dimensionality reduction FD scheme as follows:

$$\begin{cases} \boldsymbol{\beta}^n = \boldsymbol{\Phi}^T \boldsymbol{U}_h^n, \ 1 \leqslant n \leqslant L; \\ \boldsymbol{\Phi}\boldsymbol{\beta}^{n+1} = \boldsymbol{A}(\boldsymbol{\Phi}\boldsymbol{\beta}^{n-1}, \boldsymbol{\Phi}\boldsymbol{\beta}^{n-2}, ..., \boldsymbol{\Phi}\boldsymbol{\beta}^{n-l})\boldsymbol{\Phi}\boldsymbol{\beta}^n \\ \quad + \boldsymbol{F}^n, \ \ 1 \leqslant n \leqslant N-1, \\ \boldsymbol{U}_d^n = \boldsymbol{\Phi}\boldsymbol{\beta}^n, \ \ 1 \leqslant n \leqslant N, \end{cases} \tag{8}$$

or

$$\begin{cases} \boldsymbol{\beta}^n = \boldsymbol{\Phi}^T \boldsymbol{U}_h^n, \ 1 \leqslant n \leqslant L; \\ \boldsymbol{\beta}^{n+1} = \boldsymbol{\Phi}^T \boldsymbol{A}(\boldsymbol{\Phi}\boldsymbol{\beta}^{n-1}, \boldsymbol{\Phi}\boldsymbol{\beta}^{n-2}, ..., \boldsymbol{\Phi}\boldsymbol{\beta}^{n-l})\boldsymbol{\Phi}\boldsymbol{\beta}^n, \\ \quad + \boldsymbol{\Phi}^T \boldsymbol{F}^n, \ \ 1 \leqslant n \leqslant N-1, \\ \boldsymbol{U}_d^n = \boldsymbol{\Phi}\boldsymbol{\beta}^n, \ \ 1 \leqslant n \leqslant N, \end{cases} \tag{9}$$

where $\boldsymbol{\beta}^n = (\beta_1, \beta_2, ..., \beta_d)^T$ $(1 \leqslant n \leqslant N)$ are the d-dimensional unknown vectors and $\boldsymbol{U}^n$ $(1 \leqslant n \leqslant L)$ are the first L solution coefficient vectors in (7).

Remark 3 *Similarly, the reduced-dimensional FD scheme* (9) *can not only greatly reduce the unknowns, but also easily prove the existence, stability, and convergence (i.e., error estimation) of the reduced-order FD solutions by using matrix analysis. The error estimation can also be used as the theoretical criterion for the selection of the POD basis vectors and the update of the POD basis vectors.*

3.3 The reduced-dimension for the FVE method

The POD-based FVE dimension reduction method was first gradually proposed by Luo's team internationally since 2011 (see [12]), whose basic idea is also stated as follows.

Step 1. Discretize the PDE (1) into a fully discrete FVE equation:

$$(u_h^{n+1}, \pi^* v_h) = A(u_h^{n-1}, u_h^{n-2}, ..., u_h^{n-l})(u_h^n, \pi^* v_h) \\ + F^n(\pi^* v_h), \forall v_h \in V_h, 1 \leqslant n \leqslant N-1, \tag{10}$$

where V_h, M, A, and F^n are the same as those in (2), $\pi^* : V_h \to V_h^*$ is a linear interpolation operator, and V_h^* is a piecewise polynomial space one order lower than V_h.

step 2. Find the first L $(L \ll N$, usually take $L = 20)$ FVE solutions $u_h^1, u_h^2, ..., u_h^L$ from (10) and use the continuous POD method in [6, Chapter 4] to construct d (generally $d = 5 \sim 7$) POD bases $\boldsymbol{\Phi} = \{\varphi_1, \varphi_2, ..., \varphi_d\}$ containing the main information.

step 3. Replace the FE space V_h in (10) with $V_d =:$ span $\{\varphi_1, \varphi_2, ..., \varphi_d\}$ spanned by the POD bases $\boldsymbol{\Phi}$, the FVE equation (10) with tens of millions of unknowns is simplified into the following POD-based FVE reduction formulation with only d unknowns:

$$(u_d^{n+1}, \pi^* v_d) = A(u_d^{n-1}, u_d^{n-2}, ..., u_d^{n-l})(u_d^n, \pi^* v_d) \\ + F^n(\pi^* v_d), \ \ \forall v_d \in V_d, \ \ 1 \leqslant n \leqslant N-1. \tag{11}$$

Remark 4 *The most contribution of Luo's team for the FVE reduced-dimension is to create the basic theories of the existence, stability, and convergence of the reduced-order FVE solutions by using the bounded functional extension theory in Functional Analysis to link ingeniously the classical FVE method with the FVE subspace reduced-dimension method. These theories are also used as some suggestions for the choice of POD bases and the update of POD bases, which are also proposed by Luo's team for first times and are also original.*

4 Conclusion

In this editorial, we have stated the significance for the numerical simulations and the creating the *Journal of Numerical Simulations in Physics and Mathematics*. We have also reviewed the origin and development of three commonly used computational methods: the FE method, the FD scheme, and the FVE method, as well as their dimension reduction methods, which are often used in the numerical simulations. It is worth noting that these methods, especially the dimensionality reduction methods based on the POD method, still have considerable room for development.

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Not applicable.

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Conflicts of Interest

The authors declare no conflicts of interest.

Ethical Approval and Consent to Participate

Not applicable.

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