Journal of Computational Physics 371 (2018) 152–167

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A positivity-preserving pyramid scheme for anisotropic diffusion problems on general hexahedral meshes with nonplanar cell faces ☆

Shuai Wang [a,b], Xudeng Hang [a,b,*], Guangwei Yuan [a,b]

[a] Institute of Applied Physics and Computational Mathematics, Fenghaodong Road, Haidian District, Beijing 100094, China
[b] Laboratory of Computational Physics, P.O. Box 8009, Beijing, 100088, China

A R T I C L E   I N F O

Article history:
Received 31 January 2018
Received in revised form 12 May 2018
Accepted 15 May 2018
Available online 16 May 2018

Keywords:
Positivity-preserving finite volume scheme
General hexahedrons
Nonplanar cell-faces
Three dimensional anisotropic diffusion equations

A B S T R A C T

In this paper, a new cell-centered positivity-preserving pyramid scheme (called P^3-scheme) is proposed for anisotropic diffusion problems. It can be regarded as a development of the O-scheme [31] for general hexahedral meshes with nonplanar cell-faces. In the P^3-scheme, the flux on the nonplanar cell-face is approximated by the so called effective directional flux. Compared with the O-scheme, the P^3-scheme is much more robust with respect to the distortion of the meshes, and has lower cost in computation and storage. Being different from the P-scheme [32], the P^3-scheme is positivity-preserving and can be applied to anisotropic diffusion problems. Numerical results are presented to show the performance of P^3-scheme on various kinds of distorted meshes for problems with continuous and discontinuous diffusion coefficients.

1. Introduction

In the numerical simulation of radiation hydrodynamic problems arising from some applications such as inertial confinement fusion (ICF) [17,26] and magnetic confinement fusion [28], radiation diffusion equations with strong anisotropic tensor coefficients should be solved on meshes moving with the hydrodynamics. Both the strong anisotropy and extremely distorted meshes bring significant difficulties in designing accurate and efficient discrete methods for the diffusion equations.

To give a reliable solution of the diffusion equations, the positivity-preserving character for a discrete scheme is one of the key requirements. In the context of heat conduction, a non-positivity-preserving scheme can lead to non-physical oscillation and even negative temperatures, which may cause the abnormal interruption of nonlinear iteration. In the simulation of Lagrangian radiation hydrodynamic problems, monotonicity of finite volume schemes on distorted meshes is very important in avoiding non-physical oscillations of temperatures, which in turn become a source of numerical instability of simulation.

☆ This work was partially supported by the National Science Foundation of China (11571048, 11401034) and the CAEP developing fund of science technology (2015B0202033, 2014A0202009).

* Corresponding author at: Institute of Applied Physics and Computational Mathematics, Fenghaodong Road, Haidian District, Beijing 100094, China.
E-mail addresses: wang_shuai@iapcm.ac.cn (S. Wang), hang_xudeng@iapcm.ac.cn (X. Hang), yuan_guangwei@iapcm.ac.cn (G. Yuan).

https://doi.org/10.1016/j.jcp.2018.05.026
0021-9991/

For the recent years, various numerical methods have been proposed to ensure monotonicity or discrete maximum principle for solving two dimensional diffusion problems [3,13,20,34]. The approaches to preserve positivity can be classified in three families:

- The first family is based on postprocess techniques. After numerically solving the diffusion equations, by using these techniques, the numerical results are modified directly to ensure positivity. In [30,33], a simple way is used, i.e. once the negative numerical solution is observed in a cell, a part of energy from neighboring cells is added to this cell. In [20], based on the repaired technique and the constrained optimization technique, the discrete finite element solutions are modified to satisfy the discrete maximum principle. Some delicate treatments are introduced to preserve both conservation and positivity in these papers. The repaired solutions of these methods are not solutions of certain discrete scheme consistent with the original equation. In other words, it violates the governing equation due to the modified part.
- The second family is based on nonlinear two-point flux [4,7,15,18,25,34] or nonlinear correction techniques [1,8,25], which are used to construct new schemes to achieve the positivity. A nonlinear finite volume scheme based on nonlinear two-point flux has been proposed in [25] for diffusion operators on unstructured triangular meshes. This scheme has been further developed and analyzed for elliptic problems in two dimension [7,15,18,29,34]. The three dimensional case is studied by Danilov [11], which uses one cell center value and three selected cell face values to approximate the normal flux. The scheme is generalized to convection–diffusion problems by Nikitin [23]. Moreover, in [16] a nonlinear monotone finite volume scheme for three-dimensional diffusion equation on tetrahedral meshes is constructed as a generalization of two-dimensional case in [34]. At each step of nonlinear iteration, the solution of positivity-preserving scheme is conservative since the normal flux across the cell face has a unique expression.
- The third family uses a nonlinear combination technique to construct new schemes preserving the discrete maximum principle [3,12,19,27]. Positivity-preserving is the special case of discrete maximum principle, hence, a scheme satisfying discrete maximum principle must be monotone. All of these schemes satisfying the maximum principle are nonlinear. However, in each step of nonlinear iteration, there are two discrete flux expressions on each cell face, which can not preserve exact conservation during the nonlinear iteration process. The two flux expressions converge to the same one if the nonlinear iteration converges. The conservation is achieved only after the nonlinear iteration is converged.

There are some other approaches to ensure the positivity of numerical solutions, such as a non-negative mixed finite element methods (MFE) [22] and a variational inequality approach [9]. The purpose of this paper is to construct a positivity-preserving finite volume method based on the combination of effective planar face approach [32] with nonlinear two-point flux technique [34] on hexahedral meshes with nonplanar faces. The new scheme should be capable to manage anisotropic and discontinuous diffusion coefficients problems. As mentioned above, there are numerous works on this issue in two dimensional (2D) cases. However, many 2D diffusion schemes on convex or star-shaped polygonal cells can not be directly extended to 3D cases because of the complex geometry. In this paper, the star-shaped cells are always understood as being star-shaped with respect to the cell centers, which is used in the construction of discrete schemes. The appearance of nonplanar cell-faces is one of the distinct characteristics in 3D, which brings extra difficulties in discretizing the normal flux on cell faces. For example, general three dimensional meshes are inclined to violate the star-shaped condition, i.e., a 3D cell is not star-shaped with respect to its cell center. Moreover, in the simulation of Lagrangian radiation hydrodynamic flow problems on hexahedral meshes, even if the cell-faces are initially planar (i.e., all vertices of a cell-face are on one plane), with the movement of the fluid, the cell faces would become nonplanar. A common treatment is to decompose each nonplanar face into triangles by adding an additional point on the face (see [31] e.g.). Then the total flux on the nonplanar face is approximated by the sum of the normal fluxes on these triangles. However, in the applications, there are two drawbacks for this treatment:

- The computation and storage cost are expensive. The flux on a nonplanar face is the sum of fluxes on triangles. Hence, the discrete fluxes are computed on every triangular sub-faces instead of on the whole original nonplanar face. This fact makes 3D diffusion scheme a complex combination of many geometric quantities and diffusion coefficients. One has to update both the geometric quantities and the diffusion coefficients at each time step in simulating nonlinear diffusion equations for Lagrangian radiation hydrodynamics problems. Moreover, one has to store various geometric quantities on all sub-faces (triangles), which makes the scheme expensive.
- The treatment may lead to numerical instability. The additional point on the cell face should be carefully defined, in order that the cell is star-shaped with respect to the cell center. In some special cases, the point defined by a simple average of face vertices may cause the cell being not star-shaped with respect to its center. If it occurs, there will be a near zero or even negative volume of one tetrahedron, which is formed by connecting the cell center, two cell vertices and the additional face point, as shown in Fig. 4. If the volume of certain tetrahedron approximates to zero, the scheme may break down because of an overflow error from a division operation. When a negative volume occurs, the sign of the discrete flux is wrong, and so is the diffusion direction.

In this paper, based on nonlinear two-point flux technique, a new positivity-preserving pyramid scheme (called P^3-scheme in short) is proposed on general hexahedral meshes. Moreover, the effective face technique [32] is applied,