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A pyramid scheme for three-dimensional diffusion equations on polyhedral meshes ☆

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

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ABSTRACT

In this paper, a new cell-centered finite volume scheme is proposed for three-dimensional diffusion equations on polyhedral meshes, which is called as pyramid scheme (P-scheme). The scheme is designed for polyhedral cells with nonplanar cell-faces. The normal flux on a nonplanar cell-face is discretized on a planar face, which is determined by a simple optimization procedure. The resulted discrete form of the normal flux involves only cell-centered and cell-vertex unknowns, and is free from face-centered unknowns. In the case of hexahedral meshes with skewed nonplanar cell-faces, a quite simple expression is obtained for the discrete normal flux. Compared with the second order accurate O-scheme [31], the P-scheme is more robust and the discretization cost is reduced remarkably. Numerical results are presented to show the performance of the P-scheme on various kinds of distorted meshes. In particular, the P-scheme is shown to be second order accurate.

1. Introduction

In the numerical simulation of Lagrangian hydrodynamic problems arising from some applications such as inertial confinement fusion (ICF), energy diffusion equations should be solved on meshes moving with the hydrodynamics. The discretization of energy diffusion equation usually uses the cell-centered finite volume schemes in order to adapt to Lagrangian distorted meshes and to assure total energy conservation.

It is a challenging task to obtain an accurate and efficient numerical solution of three-dimensional (3D) diffusion equations on distorted meshes. Obviously, the design of 3D diffusion scheme is more complicated than two-dimensional (2D) case especially on distorted polyhedral meshes. There are numerous achievements on diffusion schemes, e.g., [1,2,20,5,7,10,14,25,28,32,33] for two dimensional diffusion problems. The finite volume methods of diffusion equations lead to many kinds of schemes. Aavatsmark [1,2] introduces the multi-point flux approximation (MPFA) methods, which are constructed by the unknowns on cell centers and cell-faces. And each unknown on the faces is related to the surrounding cell unknowns by a small linear system. So the scheme is a cell-centered scheme, and the solution of the MPFA scheme requires many solutions of small linear systems. The mimetic finite difference methods (MFD) introduced by Shashkov [25] is constructed based on the unknowns defined on the cell centers and the fluxes one the cell-faces. Eymard in [15] introduced the hybrid finite volume method (HFV), and Droniou in [12] introduced the mixed finite volume method (MFV). These three methods

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* Corresponding author.
E-mail addresses: wang_shuai@iapcm.ac.cn (S. Wang), hang_xudeng@iapcm.ac.cn (X. Hang), yuan_guangwei@iapcm.ac.cn (G. Yuan).

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are constructed by the unknowns defined on the cells and the cell-faces. Droniou [14] showed that any one of the three kinds of schemes can be constructed by each of the frameworks of MFD, HFV or MFV, and the theoretical analysis can be carried out for them. The further functional analysis results on the compatible discrete operator schemes are given, and links with existing schemes (finite elements, finite volumes, mimetic finite differences) are discussed by Bonelle and Ern in [6]. The hybrid mimetic mixed (HMM) scheme, defined in [13], is a family of methods that includes mixed-hybrid mimetic finite difference schemes [25], mixed finite volume schemes [12] and hybrid finite volume (SUSHI) schemes [15]. The vertex approximate gradient (VAG) scheme which has only cell vertices unknowns is described in [16,17,19]. Another scheme is the discrete duality finite volume scheme (DDFV) proposed by Andreianov [3] etc. It is constructed by the unknowns defined both on the cells and the dual cells centered on the vertices. Then the scheme consists of two systems, i.e., one for the (primary) cells and the other for the dual cells, which are fully coupled.

Moreover, a kind of "diamond" method is firstly proposed by Li [22], and studied later by Yuan [33], Sheng [28], Wu [32] for two-dimensional problems, and Lai [21] for three-dimensional problems, etc. This method is similar to DDFV except that it gives an explicit interpolation for the cell-vertex unknowns. It is a cell-centered scheme, and has an explicit expression for the normal fluxes on the cell faces, which makes the scheme different from those introduced above.

The scheme to be introduced in this paper can be seen as a special extension of Li's method [22] to three dimensional problems, though many 2D diffusion schemes can not be directly extended to 3D because of the complex geometry, see for example [18]. In 2D case, the edges of the cells are usually straight segments other than curved lines, and then the normal vectors on the edge are parallel. But it is not true for general polyhedrons. Nonplanar cell-faces appear usually in polyhedral meshes, and bring distinctive difficulties in discretizing the normal flux on cell faces. In some applications, it is inevitable to use polyhedral meshes with nonplanar cell-faces. As an example, 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 the same plane), with the movement of the fluid, the cell faces would become nonplanar. In the case of hexahedral cells, a common treatment is to split each face into four triangles by setting an auxiliary point on the face, and then hexahedral cells are refined to be icositetrahedron cells. In the case of general polyhedral cells, the faces have to be split into triangles more than 4. The diffusion schemes on such polyhedral meshes are complicated, and the coding work becomes very tedious and less efficient. It is interesting and necessary to give a scheme based on original hexahedrons rather than on icositetrahedrons. So do the general polyhedral cases.

Some diffusion schemes have explicit expressions for discrete normal flux, e.g., the 2D nine-point scheme in [22], while some others do not have, e.g., Kershaw's scheme in [20], and MFD scheme in [24]. The explicit expression of the discrete normal flux is helpful in two aspects. The first is that it is convenient to write codes, especially 3D codes. The second is that it is convenient to compute the energy flux across cell-face. Recently there are some papers on 3D diffusion schemes [8,9,11,16,27,26,21]. In [26] the 2D Kershaw's scheme in [20] is extended to 3D case, which is based on discrete coordinates transform. The 3D extensions of MFD and MPFA method are presented in [8,9] and [27].

General polyhedral meshes with nonplanar cell-faces are considered in [27,31], where the nonplanar faces are decomposed into triangles by introducing auxiliary face points. Then the normal flux is discretized on each triangle formed by connecting 3 points, i.e., the segment extreme points and the auxiliary point. To get a cell-centered scheme, the unknowns at face-centered points must be eliminated by certain interpolation of cell-centered unknowns around. Note that the discrete normal flux on a cell-face is a summation of fluxes on these triangles. This fact makes a 3D diffusion scheme a complex combination of many geometric quantities and diffusion coefficients. One has to update the geometric quantities and the diffusion coefficients at the same time in simulating nonlinear diffusion problems. Otherwise, one has to store many geometric quantities on all sub-faces, which makes the scheme expensive. Besides, the star-shaped assumption is needed for every skewed polyhedral cell. The assumption is essential to ensure the positive volume of each tetrahedron on the split faces.

In [9] Brezzi and Lipnikov noticed that the curved faces affect the performance of MFD. They propose a new method which makes use of the average normal vector of the curved face. It is not discussed in detail, that how to compute the average normal vector in practice on a curved face precisely. Here we will further study the average normal vector on polyhedral curved faces and give a way to compute it, so that we can simplify the design of 3D diffusion schemes. Moreover the new scheme will be more efficient and stable.

In the Lagrangian hydrodynamical simulation with finite volume methods, mass-cell moving with the fluids is enclosed within nonplanar faces. For the O-scheme [31], the different definitions of face-centers lead to different diffusion schemes. In this paper, we propose a new efficient cell-centered finite volume scheme (named as pyramid scheme, or P-scheme) for 3D diffusion equations on polyhedral meshes with nonplanar cell faces. Under some weak assumptions, a unique discrete normal flux is determined by the boundary of curved face. In the construction of P-scheme, the cell vertices are required to be connected by segments, while the shape formation of cell-faces is not obligatory. And then the flux expression of the P-scheme can be free from the face-center unknowns. Because of the large number of degrees of freedom, the computational cost for solving 3D diffusion equation is huge. In order to increase the efficiency of 3D simulation, diffusion schemes should be as accurate as possible on Lagrangian distorted meshes. Moreover, diffusion schemes should also be as simple and efficient as possible. The discrete normal flux on each nonplanar face of the P-scheme only need 5 geometric quantities, which can be reused when solving nonlinear problems or diffusion system of equations, e.g., the non-equilibrium radiation diffusion equations and multi-group radiation diffusion equations [29,30].