A Decoupled and Positivity-Preserving DDFV Scheme for Diffusion Problems on Polyhedral Meshes

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\textbf{Abstract.} We propose a decoupled and positivity-preserving discrete duality finite volume (DDFV) scheme for anisotropic diffusion problems on polyhedral meshes with star-shaped cells and planar faces. Under the generalized DDFV framework, two sets of finite volume (FV) equations are respectively constructed on the dual and primary meshes, where the ones on the dual mesh are derived from the ingenious combination of a geometric relationship with the construction of the cell matrix. The resulting system on the dual mesh is symmetric and positive definite, while the one on the primary mesh possesses an M-matrix structure. To guarantee the positivity of the two categories of unknowns, a cutoff technique is introduced. As for the local conservation, it is conditionally maintained on the dual mesh while strictly preserved on the primary mesh. More interesting is that the FV equations on the dual mesh can be solved independently, so that the two sets of FV equations are decoupled. As a result, no nonlinear iteration is required for linear problems and a general nonlinear solver could be used for nonlinear problems. In addition, we analyze the well-posedness of numerical solutions for linear problems. The properties of the presented scheme are examined by numerical experiments. The efficiency of the Newton method is also demonstrated by comparison with those of the fixed-point iteration method and its Anderson acceleration.

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\textbf{Key words:} DDFV, decoupled algorithm, diffusion problems, positivity-preserving, polyhedral meshes.
1 Introduction

Consider a steady-state diffusion problem on the bounded connected polyhedral domain $\Omega \subset \mathbb{R}^3$

$$-\text{div}(\Lambda \nabla u) = f \quad \text{in } \Omega,$$

$$u = g_D \quad \text{on } \partial \Omega,$$

(1.1)

where $f$ and $g_D$ denote the source term and the Dirichlet boundary data, respectively. The $3 \times 3$ diffusion tensor $\Lambda$ is assumed to be symmetric and there exist two positive constants $\kappa$ and $\kappa'$, such that

$$\kappa \|\xi\|^2 \leq \xi^T \Lambda \xi \leq \kappa' \|\xi\|^2, \quad \forall \xi \in \mathbb{R}^3,$$

where $\|\cdot\|$ denotes the Euclidean norm. For simplicity of exposition, a pure Dirichlet boundary condition is considered in this article. Construction and analysis of the scheme can be discussed analogously for other types of boundary conditions. Furthermore, if $f \geq 0$, $g_D \geq 0$, the nonnegativity of the solution is guaranteed by the maximum principle.

Diffusion equations have a wide range of practical applications, such as reservoir simulation, radiation hydrodynamics, semiconductor modeling and groundwater flow. In these applications, the media is usually highly anisotropic and the meshes are generally severely distorted, which may cause the numerical solutions to violate the positivity-preserving property. Finite volume (FV) methods have been widely applied to the discretization of diffusion operators due to its simplicity and local conservation. It is interesting and meaningful to construct a FV scheme with both good accuracy and positivity-preserving property for anisotropic problems on general polyhedral meshes.

In recent years, many literatures have been published about positivity-preserving FV schemes for two-dimensional diffusion problems, such as [3, 16, 31, 39, 46]. However, most of those schemes can not be directly extended to 3D grids due to the complex geometry. So far, several positivity-preserving works for 3D diffusion problems have been suggested. Inspired by [39], the authors in [25] proposed a monotone scheme on unstructured tetrahedral meshes. Based on the original idea in [32], an interpolation-free positivity-preserving FV scheme was developed in [10] on unstructured conformal polyhedral meshes with planar faces, and it was further extended to advection-diffusion equations [38] and multiphase flow model [37]. A 3D positivity-preserving interpolation algorithm was proposed in [48] and then used in [49] to design a FV scheme that preserves the solution positivity in discontinuous anisotropic environment. A positivity-preserving FV scheme was constructed in [29] on tetrahedral meshes where a nonlinear interpolation algorithm was given for auxiliary unknowns defined at vertices. Combined with optimization techniques, a nonlinear two-point flux approximation (TPFA) was suggested in [41] to simulate the subsurface flow on some challenging grids. Recently, the authors in [50] studied positivity-preserving schemes based on the interpolation of vertex unknowns via the harmonic averaging points [1, 15]. The authors in [54] presented a positivity-preserving cell-centered scheme for the three-dimensional heat