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Piecewise linear transformation in diffusive flux discretization

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ABSTRACT

To ensure the discrete maximum principle or solution positivity in finite volume schemes, diffusive flux is sometimes discretized as a conical combination of finite differences. Such a combination may be impossible to construct along material discontinuities using only cell concentration values. This is often resolved by introducing auxiliary node, edge, or face concentration values that are explicitly interpolated from the surrounding cell concentrations. We propose to discretize the diffusive flux after applying a local piecewise linear coordinate transformation that effectively removes the discontinuities. The resulting scheme does not need any auxiliary concentrations and is therefore remarkably simpler, while being second-order accurate under the assumption that the structure of the domain is locally layered.

1. Introduction

Diffusion in an anisotropic discontinuous environment plays a role in various fields of engineering, such as subsurface flows. Steady state diffusion of a solute with concentration C in a bounded domain $\Omega \subset \mathbb{R}^3$ is modeled by the following boundary problem:

$$\nabla \cdot \mathbf{u} = g, \tag{1}$$

$$\mathbf{u} = -\mathbb{D}\nabla C, \tag{2}$$

$$C = g_{\mathrm{D}} \quad \text{on } \Gamma_{\mathrm{D}}, \tag{3}$$

$$\mathbf{u} \cdot \mathbf{n} = g_{\mathrm{N}} \quad \text{on } \Gamma_{\mathrm{N}}, \tag{4}$$

$$\mathbf{u} \cdot \mathbf{n} = \Psi (C - g_{\mathrm{R}}) \quad \text{on } \Gamma_{\mathrm{R}}, \tag{5}$$

where $\mathbf{u}$ is the velocity, g is the volumetric source term, $\mathbf{n}$ is the unit vector normal to $\partial\Omega$ pointing outwards, Ψ is the transfer coefficient, $\Gamma_{\mathrm{D}} \cup \Gamma_{\mathrm{R}} = \overline{\Gamma_{\mathrm{D}} \cup \Gamma_{\mathrm{R}}}$, $\Gamma_{\mathrm{D}} \cup \Gamma_{\mathrm{N}} \cup \Gamma_{\mathrm{R}} = \partial\Omega$, $\Gamma_{\mathrm{D}} \cup \Gamma_{\mathrm{R}} \neq \emptyset$, and Γ_{D}, Γ_{N}, and Γ_{R} are mutually disjoint. Diffusion tensor $\mathbb{D}$ is symmetric, positive definite, and piecewise continuous. Connected subsets of Ω in which $\mathbb{D}$ is continuous are called *material zones*, and the interfaces between them are referred to as *material interfaces*. Presumably, mesh faces coincide with material interfaces, i.e. $\mathbb{D}$ is continuous within mesh cells.

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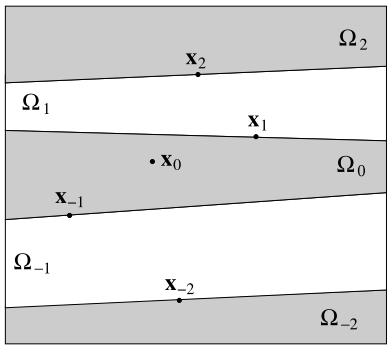

Fig. 1. It is assumed that the structure of the domain is locally layered.

Various numerical schemes are used to solve this problem. Most of them produce non-physical oscillations and negative concentration values in particular cases. Nevertheless, certain schemes are specifically designed to address these issues. One such finite volume scheme appeared in [1] and was further developed in [2–9]. These schemes do not satisfy the maximum principle, but they guarantee that the concentration does not become negative. A recent review of linear and non-linear finite volume schemes for diffusion is found in [10].

In addition to the primary concentration unknowns associated with mesh cells, these schemes use auxiliary concentration values located in faces and elsewhere. Face concentration values are easily determined from the continuity, but some kind of interpolation must be used to determine other auxiliary values. The interpolation method presented in [7] performs this task using piecewise linear interpolation and convex combinations. It satisfies the maximum principle and is second order accurate even when it uses interpolation nodes at the opposite sides of a material discontinuity. Since a simple brute force search for collocation points that form a convex combination can result in a combinatorial explosion, in [7] we proposed a complex but efficient alternative search algorithm based on Delaunay triangulations.

In this paper we deploy the piecewise linear transformation introduced in [7] directly in the velocity decomposition, without any auxiliary concentration variables. Such a scheme is simpler than [7] because the complicated construction of convex combinations is avoided. In addition, fluxes over discontinuities do not need special treatment, resulting in further simplification.

The paper is organized as follows: in Section 2 we explain how to use the piecewise linear transformation to obtain a one-side flux approximation. In Section 3 the one-side fluxes are combined in the usual fashion to obtain a two-point scheme. Euler implicit temporal discretization of the time-dependent problem is presented in Section 4. Numerical tests presented in Section 5 show that the accuracy and the convergence rate do not change much in comparison to [7], and thus the simpler scheme should be the method of choice. Moreover, it is shown that a single iteration is sufficient to maintain the second order accuracy in a time-dependent problem.

2. Fluxes and piecewise linear transformation

The piecewise linear transformation used here to approximate the flux was constructed in [7]. The main steps are repeated for convenience.

We assume that some neighborhood of point $\mathbf{x}_0 \in \Omega$ consists of layers $\Omega_{-m}, \ldots, \Omega_n$, $m \geq 0$, $n \geq 0$, with interfaces that are smooth so that they can be locally approximated by planes (see Fig. 1). This assumption was used in [7] in order to derive the piecewise linear transformation used in this paper. As shown by an example in [7], if this assumption does not hold then the accuracy is reduced. Even though other authors do not usually state the interface smoothness requirement explicitly, it is implied by the solution smoothness assumption. A non-smooth material interface introduces singularities with respect to the solution differentiability. Unless these singularities are explicitly treated, the accuracy of this or any other numerical scheme is reduced. Thus the interface smoothness assumption is not a limitation of our scheme in comparison with other methods.

The diffusion tensor is allowed to have discontinuities between layers, but it is assumed to be constant or almost constant within each layer, thus $\mathbb{D}|_{\Omega_i} = \mathbb{D}_i$. This assumption needs to hold only locally — the diffusion tensor is allowed to vary smoothly within layers on a larger scale. We assume that the concentration changes linearly in each layer

$$C(\mathbf{x}) = C_i + \mathbf{G}_i \cdot (\mathbf{x} - \mathbf{x}_0), \quad \mathbf{x} \in \overline{\Omega}_i. \tag{6}$$

This function must satisfy two conditions:

1. It must be continuous, and
2. The flux through each interface must be continuous.