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Second-order accurate interface- and discontinuity-aware diffusion solvers in two and three dimensions

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ABSTRACT

A numerical scheme is developed for two- and three-dimensional time-dependent diffusion equations in numerical simulations involving mixed cells. The focus of the development is on the formulations for both transient and steady states, the property for large time steps, second-order accuracy in both space and time, the correct treatment of the discontinuity in material properties, and the handling of mixed cells. For a mixed cell, interfaces between materials are reconstructed within the cell so that each of resulting sub-cells contains only one material and the material properties of each sub-cell are known. Diffusion equations are solved on the resulting polyhedral mesh even if the original mesh is structured. The discontinuity of material properties between different materials is correctly treated based on governing physics principles. The treatment is exact for arbitrarily strong discontinuity. The formulae for effective diffusion coefficients across interfaces between materials are derived for general polyhedral meshes. The scheme is general in two and three dimensions. Since the scheme to be developed in this paper is intended for multi-physics code with adaptive mesh refinement (AMR), we present the scheme on mesh generated from AMR. The correctness and features of the scheme are demonstrated for transient problems and steady states in one-, two-, and three-dimensional simulations for heat conduction and radiation heat transfer. The test problems involve dramatically different materials.

1. Introduction

In multi-physics simulations, for example, hydrodynamics and radiation diffusion, mixed cells are often generated no matter how fine the resolution of a simulation is. In many simulations there is more than one material in one cell, such as melting metal and gas. Mesh refinement only can reduce the number of materials within a cell, but cannot eliminate mixed cells in simulations. Treatment of mixed cells is critical for many applications, but material property of mixture of materials is often unknown.

Numerical techniques for diffusion equations [1–3,6] may be divided into explicit and implicit methods. An explicit scheme, for example, the forward Euler method, is simple, but the size of time step is limited by a stability condition that is normally much smaller than the required accuracy of physics problems. On the other hand, in implicit methods the size of time step is not limited by numerical stability conditions, and therefore it may be changed according to the requirement of physics problems.

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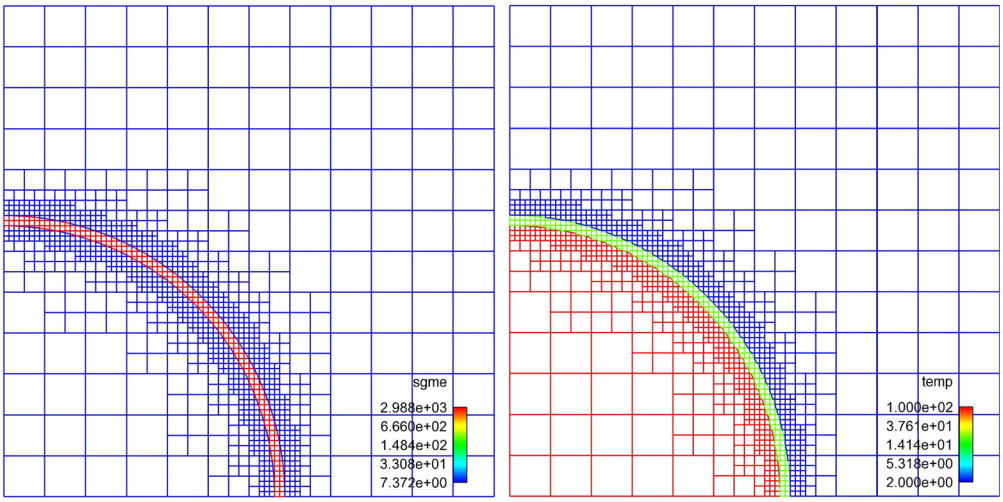

Fig. 1. The heat conduction coefficients of three materials (left image) and the initial temperature in a mesh (right image).

Two typical implicit methods are the backward Euler method and Crank–Nicolson method. The backward Euler method is first-order accurate in time, but numerical errors in the method undergo quick damping for large time steps. Therefore the method is very useful for large time steps and steady states. Although Crank–Nicolson method is second-order accurate, numerical errors do not damp out for large time steps, and significant numerical errors will be introduced when time steps are large. This is the reason Crank–Nicolson method cannot be used for steady states. The formulation for steady states is very important for problems involving dramatically different materials even for transient problems. A given time step may be considered so large for some material that the formulation for steady state is more appropriate for the material than the formulation with the second order of accuracy, but the time step is so small for some other material that accuracy in time is more important, as illustrated in Fig. 1 in which there are three materials. The left image in the figure is the diffusion coefficients of the three materials, and right image is temperature of each material. If we are not interested in how temperature changes with time in the material in the thin layer, we can give a very large time step relative to the material in the thin layer.

For systems of multi-materials with dramatically different material properties, the correct treatment for the discontinuity of material properties is important. A typical approach for the flux calculation near material interfaces on unstructured meshes is to use mathematical approximations, for example, Taylor expansion or some weighted average of two adjacent materials, but not governing physics laws. This approach would introduce numerical errors when thermal properties of two materials are very different.

There are many investigations on numerical methods for diffusion equations [4,8,9,11–15,17–22,24,25,27,28,30–33,35]. Some work on unstructured meshes but is only first-order accurate in time. Some are second-order accurate but cannot give correct steady states for large time steps. Some work well for clean cells (i.e., cells with single material), but do not deal with mixed cells. Some are designed for mixed cells, but lack special consideration for the discontinuity at material interfaces. In this paper, we will develop a numerical method for two- and three-dimensional diffusion equations for systems of multi-materials with arbitrarily different thermal properties. We will focus on the case in which there are mixed cells, although the resulting scheme is perfectly appropriate for general polyhedral meshes and structured meshes with and without adaptive mesh refinement (AMR). We will give formula for effective diffusion coefficient across a material interface for flux calculations on polyhedral meshes. The scheme is formally second-order accurate in both space and time, works for any size of time steps, and will give exact steady states when time steps are very large.

Although AMR, implicit diffusion, and the treatment of mixed cells increase the complexity of numerical algorithms, AMR has gradually become common practice in many institutions. Even with AMR and implicit treatment of diffusion, it is still a challenge to effectively simulate some physics problems through Eulerian methods. Recently, in these institutions efforts are put on interface reconstruction for hydrodynamics and diffusion. The sub-cell structure within mixed cells is considered necessary for Eulerian methods to solve some problems, particularly those problems that are traditionally solved through Lagrangian methods. In many institutions, the sub-cell structure becomes increasingly important, for example see presentations in 2013 Multi-material Hydrodynamics Conference [36,37]. The work reported in this paper is one of the efforts, which was reported in the conference.

The plan of the papers is as follows. Section 2 is for the basic equation to be solved. In Section 3 we will describe mixed cells through volume fraction of each material in cells. A procedure to reconstruct interfaces between materials within a numerical cell is presented there. In Section 4 we will present our numerical scheme, which includes the simultaneous discretization in space and time, realization of the second order of accuracy in time, consideration of large time steps and steady states, and correct treatment for the discontinuity of material properties. The scheme may apply to two-, and