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A Cartesian grid embedded boundary method for solving the Poisson and heat equations with discontinuous coefficients in three dimensions

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ABSTRACT

We present a method for solving Poisson and heat equations with discontinuous coefficients in two- and three-dimensions. It uses a Cartesian cut-cell/embedded boundary method to represent the interface between materials, as described in Johansen and Colella (1998). Matching conditions across the interface are enforced using an approximation to fluxes at the boundary. Overall second order accuracy is achieved, as indicated by an array of tests using non-trivial interface geometries. Both the elliptic and heat solvers are shown to remain stable and efficient for material coefficient contrasts up to 10^6, thanks in part to the use of geometric multigrid. A test of accuracy when adaptive mesh refinement capabilities are utilized is also performed. An example problem relevant to nuclear reactor core simulation is presented, demonstrating the ability of the method to solve problems with realistic physical parameters.

1. Introduction

We consider elliptic and parabolic problems in regions with two materials, each of which occupies a bounded subset Ω^p, $p = +, -$, of the overall domain $\Omega = \bigcup_p \Omega^p$. One region usually encloses the other; in that case we refer to the inclusion, or interior region, by Ω^- and the exterior region by Ω^+. At the boundary $\delta\Omega^{\pm}$ between materials, jump conditions on the solution φ and flux $\mathbf{F}^B$ are specified

$$\begin{aligned} [\varphi^B] &= \varphi^{B,+} - \varphi^{B,-} = g_D(\mathbf{x}, t), \\ \left[\mathbf{F}^B \cdot \hat{\mathbf{n}}^B\right] &= \mathbf{F}^{B,+} \cdot \hat{\mathbf{n}}^B - \mathbf{F}^{B,-} \cdot \hat{\mathbf{n}}^B = g_N(\mathbf{x}, t). \end{aligned} \tag{1}$$

Here $\hat{\mathbf{n}}^B$ is the normal to the boundary, and the functions g_D and g_N describe the magnitude of the jump at each point in time and space. For many problems $g_D = g_N = 0$. However, this method can be used when more general jump conditions are required, for instance when sources are present at the interface. The method can handle material domains Ω^p that consist of any number of spatially distinct sub-domains. It may be applied to domains consisting of more than two materials as well, so long as the interfaces between materials remain spatially distinct. For the present work, we restrict the scope to two materials.

Our method solves the heat equation in two materials,

$$\partial_t \varphi = \kappa^p \Delta \varphi + f \text{ on } \Omega^p, \quad \varphi(\mathbf{x}, 0) = \varphi_0(\mathbf{x}), \tag{2}$$

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subject to the above jump conditions at the interface. In this case, as well as in the elliptic equations to which the method is applied, the flux $\mathbf{F}^B$ is proportional to the material coefficient. While this coefficient is constant within each material, it is discontinuous across the interface.

A number of schemes for handling elliptic and parabolic problems of this type exist in the literature. Finite difference schemes for fixed boundaries, of the type pioneered by Shortley and Weller [1], have been greatly improved upon in the intervening years. Most importantly in the context of this work, they have been extended to handle discontinuous jumps in the form of Eq. (1). Immersed boundary methods, modifications of the method first presented by Peskin [2], discretize a delta-function source term on the boundary, retaining the symmetric form of the linear system. Immersed interface methods [3] use analytic continuation of the solution across the interface to explicitly incorporate the jump condition into the underlying finite difference stencil coefficients. This results in a scheme that more accurately represents the jump conditions, at the expense of considerable additional complexity and the loss of symmetry in the underlying linear system for non-constant coefficients. Finally in the context of finite difference schemes, ghost fluid methods [4] also use analytic continuation of the solution. A ghost fluid, residing in the regions outside the solution domain, is used to explicitly enforce the matching conditions. As originally formulated, the method was first order accurate. It has been extended to second order accuracy for boundaries with continuous second derivatives [5]. They have the advantage of retaining a symmetric system, allowing the use of a wider range of fast linear solvers. More recently, another symmetry-preserving method developed by Chen and Strain [6] couple a polynomial reconstruction of the solution at the interface with a multigrid-preconditioned Krylov solver that improves efficiency for large material coefficient contrasts.

Outside the realm of finite difference methods, integral methods recast the elliptic PDE via potential theory as integral equations. Fast integral solvers can often be utilized against this class of problem; these generally fall into two categories. One method involves the use of a fast Poisson solver on a simple (e.g. Cartesian) enclosing domain, plus the application of a suitable correction at the boundary [7]. The second combines a fast (e.g. multipole or FFT) method and an iterative solver. In either case, conditioning issues can arise in problems with large discontinuities in the material coefficient [8], necessitating a modification of the underlying integral equation representation. Nevertheless, these methods are efficient in a wide variety of problems.

Our method is based on a finite volume approach to the spatial discretization of elliptic equations. The method is conservative, a distinct advantage in certain classes of problems. For low-Mach flows with heat transfer, for instance, conservative schemes avoid unphysical results arising in marginally resolved or under-resolved situations [9,10].

Finite volume methods for interface problems encompass a variety of approaches. In the context of conjugate heat transfer in complex geometries, the overlapping grid method of Henshaw and Chand [11] decomposes the domain into a number of sub-domains. The grid on each sub-domain is boundary fitting, an advantage that comes at the expense of the loss of conservation. Each sub-domain uses a solver specific to the relevant physics in it.

Oevermann et al. [12,13] present a hybrid finite volume method for variable and discontinuous coefficient elliptic problems in two- and three-dimensions. In 3-D, it relies on tri-linear approximations to the solution within each Cartesian control volume to discretize the integral form of the divergence theorem in a finite element fashion. Small volume cells are handled via an asymptotic approach. The method exhibits local and global second order accuracy on this class of problems.

Our work follows in the steps of the work in [14–16] in using pure finite-volume schemes for elliptic and parabolic equations with embedded boundaries (EB). The first step in using Cartesian EB methods is grid generation, which has been studied extensively using a number of different representations of the geometry. Surface triangulations [17] are widely used, particularly in engineering contexts involving extremely complex geometries. Our method uses an implicit function representation [18] that provides discretizations of complex geometries accurate to arbitrary order in a straightforward manner.

The main shortcoming in previous Cartesian EB methods, insofar as their application to multi-material problems, lies in their use of prescribed boundary conditions at the EB. A Neumann interface gave boundary fluxes directly, while Dirichlet boundary conditions at the EB necessitated defining a stencil for calculating fluxes at the boundary using data at neighboring cells. In the multi-material context boundary conditions at the interface are not directly prescribed, but instead constrained by matching conditions on the jump in the solution and flux across it. The present work extends the EB methodology to handle such jump conditions, and thereby solve multi-material Poisson and heat equations with a discontinuity in the material coefficient at the interface between the two. Like previous work, it maintains global second order accuracy. By treating special cases related to under-resolved geometries, like the presence of multiple interfaces within a single Cartesian control volume, we are able to use geometric multigrid methods for efficient solution of elliptic equations. Moreover, our use of the Chombo software infrastructure provides important capabilities from a computational efficiency standpoint. The primary one is adaptive mesh refinement, which is crucial in many problems involving widely separated spatial scales.

Our time discretization of this equation necessitates solving a set of elliptic equations during each step forward in time. Specifically, we solve the Helmholtz equation

$$(\alpha^p + \beta^p \Delta)\varphi = \rho, \tag{3}$$

where α^p and β^p are the material coefficients, subject to jump conditions across the boundary $\delta\Omega^{\pm}$. We first describe the elliptic algorithm, starting with the spatial discretization in Section 2. This is followed by a treatment of special considerations for the use of geometric multigrid, in Section 3. The stability of the spatial discretization and time integration are explored in Section 4. An outline of the overall algorithm is given in Section 5.