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A second order virtual node method for elliptic problems with interfaces and irregular domains in three dimensions

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ABSTRACT

We present a numerical method for the variable coefficient Poisson equation in three-dimensional irregular domains and with interfacial discontinuities. The discretization embeds the domain and interface into a uniform Cartesian grid augmented with virtual degrees of freedom to provide accurate treatment of jump and boundary conditions. The matrix associated with the discretization is symmetric positive definite and equal to the standard 7-point finite difference Poisson stencil away from embedded interfaces and boundaries. Numerical evidence suggests second order accuracy in the L^∞-norm. Our approach improves the treatment of Dirichlet and jump constraints in the recent work of Bedrossian et al. [1] and introduces innovations necessary in three dimensions. Specifically, we construct new constraint-based Lagrange multiplier spaces that significantly improve the conditioning of the associated linear system of equations; we provide a method for cell-local polyhedral approximation to the zero isocontour surface of a level set needed for three-dimensional embedding; and we show that the new Lagrange multiplier spaces naturally lead to a class of easy-to-implement multigrid methods that achieve near optimal efficiency, as shown by numerical examples. For the specific case of a continuous Poisson coefficient in interface problems, we provide an expansive treatment of the construction of a particular solution that satisfies the value jump and flux jump constraints. As in [1], this is used in a discontinuity removal technique that yields the standard 7-point stencil across the interface and only requires a modification to the right-hand side of the linear system.

1. Introduction

Elliptic interface problems such as

$$-\nabla\cdot(\beta(\mathbf{x})\nabla u(\mathbf{x})) = f(\mathbf{x}), \quad \mathbf{x}\in\Omega\setminus\Gamma; \tag{1}$$
$$[u] = a(\mathbf{x}), \quad \mathbf{x}\in\Gamma; \tag{2}$$
$$[\beta\nabla u\cdot\hat{\mathbf{n}}] = b(\mathbf{x}), \quad \mathbf{x}\in\Gamma; \tag{3}$$
$$u = p(\mathbf{x}), \quad \mathbf{x}\in\partial\Omega_d; \tag{4}$$
$$\beta\nabla u\cdot\hat{\mathbf{n}} = q(\mathbf{x}), \quad \mathbf{x}\in\partial\Omega_n; \tag{5}$$

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have a wide variety of applications in physics and engineering, and naturally arise when two dissimilar materials interact across a thin interface. Common examples include immiscible, incompressible fluids in contact and phase change problems. The interface Γ is generally a co-dimension one closed curve (dimension 2) or surface (dimension 3) that divides the domain into an interior region Ω^- and an exterior region Ω^+ such that $\Omega = \Omega^- \sqcup \Omega^+ \sqcup \Gamma \subset \mathbb{R}^d$ ($d = 2$ or 3, typically). The scalar coefficient field β and the source term f can exhibit discontinuities across Γ, but have smooth restrictions β^σ, f^σ to Ω^σ, $\sigma \in \{-,+\}$. We let $\hat{\mathbf{n}}(\mathbf{x})$ denote the outward unit normal, whether to Ω^- at a point $\mathbf{x} \in \Gamma$ or to Ω at a point $\mathbf{x} \in \partial\Omega$; and define $[v](\mathbf{x}) := v^+(\mathbf{x}) - v^-(\mathbf{x}) := \lim_{\epsilon \to 0^+} v(\mathbf{x} + \epsilon\hat{\mathbf{n}}(\mathbf{x})) - \lim_{\epsilon \to 0^+} v(\mathbf{x} - \epsilon\hat{\mathbf{n}}(\mathbf{x}))$ as the *jump* of the quantity v across the interface Γ. The relevant physics generally determine the jumps in the solution (2) and in the flux (3), as well as the boundary conditions on $\partial\Omega$. Unless stated otherwise, we assume the surfaces Γ, $\partial\Omega$ are smooth.

Due to irregular geometry of the boundary and/or interface in many physical phenomena, a natural approach to the numerical approximation is the *finite element method* (FEM) with unstructured meshes that conform to the geometry of Γ and $\partial\Omega$ [2–9]. However, meshing complex interface geometries can prove difficult and time-consuming when the interface frequently changes shape, especially in 3 dimensions. Also, many numerical methods, such as geometric multigrid methods, do not naturally apply to unstructured meshes. These concerns are largely circumvented with the use of *embedded* (or *immersed*) methods that approximate solutions to (1)–(3) on Cartesian grids or structured meshes that do not conform to the interface. Despite advances in this direction, embedded methods that retain higher order accuracy in L^∞ often are limited to 2 dimensions and introduce relatively difficult linear algebra problems and complex implementations that sometimes require significant effort to adapt to general applications.

Recently, however, Bedrossian et al. [1] introduced a second order virtual node method for solving the elliptic interface problem (1)–(5) in 2 dimensions. The discretization presented in [1] is easy to implement and yields a symmetric positive definite sparse linear system for both interface problems and boundary value problems on irregular domains. In summary, this virtual node method employs a uniform Cartesian grid with duplicated Cartesian bilinear elements along the interface. These duplicated elements introduce additional *virtual* nodes or degrees of freedom to accurately capture the lack of regularity in the solution. The method is variational to define stencils symmetrically, and a different discretization is used depending on proximity to embedded features, allowing for the retention of the standard 5-point finite difference stencil away from embedded boundaries and interfaces. Langrange multipliers are used to enforce embedded Dirichlet conditions (4) and embedded jump conditions (2), and the choice of Lagrange multiplier space admits a symmetric positive definite discretization. In the special case when β is smooth, a discontinuity removal technique allows the use of the standard 5-point Poisson stencil even across the embedded interface.

The feature set of this virtual node approach is very powerful. In the present work, we improve many aspects of [1] and provide key modifications necessary to extend the method to 3 dimensions. Within the context of embedded Dirichlet and embedded interface discretizations, we present a novel and flexible algorithm to define the discrete Lagrange multiplier space. This algorithm gives more control on the conditioning of the resulting linear system and specifically addresses the conditioning issues (see Appendix C) we found in the straightforward extension of [1] to 3 dimensions. We also give an expanded treatment of the discontinuity removal technique, detailing an algorithm for the construction of a scalar function satisfying the jump conditions (2) and (3). Specific to the 3-dimensional implementation, we describe an algorithm for creating a polyhedral representation of cell-local interface/boundary geometry and quadrature rules suitable for these polyhedral surfaces. Finally, we present a family of multigrid algorithms that solve (1)–(5) with near-optimal multigrid efficiency.

The remainder of the paper proceeds as follows. We review existing embedded methods and related multigrid algorithms in Section 2. Section 3 presents our numerical discretizations for embedded Neumann (Section 3.2), embedded Dirichlet (Section 3.3), and embedded interface problems (Section 3.4). We outline our new constraint aggregation algorithm as it applies to our embedded Dirichlet discretization in Section 3.3.2, and detail the special case in embedded interface problems of smooth β in Section 3.4.1. Section 4 explains the components of our multigrid algorithms for all discretization types. We use numerical examples to demonstrate the accuracy of our discretization and the performance of our multigrid solvers in Section 5, and we conclude with a short summary and discussion in Section 6. We include an appendix with some additional miscellaneous details.

2. Existing methods

The *Immersed Interfaced Method* (IIM) is perhaps the most popular finite difference method for approximating (1)–(3) to second order accuracy. LeVeque and Li first proposed the IIM for approximating elliptic interface problems in [10] and the term now applies to a widely researched and extensively applied class of finite difference methods [11–17]. See [18] and the references therein for a complete exposition of the method and its numerous applications, and [19] for justification of the general IIM approach. Using generalized Taylor expansions, the original IIM adaptively modifies the stencil to obtain $\mathcal{O}(h)$ truncation error along the interface. For smooth β, this reduces to the standard 5-point or 7-point finite difference stencil, but otherwise results in an asymmetric discretization that follows from locally solving constrained optimization problems that enforce a discrete maximum principle [20]. The IIM also generally requires the evaluation of higher order jump conditions and surface derivatives along the interface. This can lead to difficulty in implementation, especially in 3 dimensions [21,18,15,17]. Chen and Strain described a new approach to the IIM, called the *Piecewise-polynomial Interface*