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Short note

Poisson equations in irregular domains with Robin boundary conditions — Solver with second-order accurate gradients

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ABSTRACT

We present a conservative method for solving the Poisson equation in irregular domains with Robin boundary conditions. Second-order accurate solutions and gradients in the L^∞ norm are obtained.

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1. Introduction

The simulation of many diffusion-dominated phenomena require the solution of Poisson-type equations in irregular domains subject to Robin boundary conditions. Examples include the solidification of multicomponent alloys [14] and epitaxial growth [25,19,20], where Robin boundary conditions model solute-rejection relations in the case of solidification and the Ehrlich–Schwoebel step-edge energy barrier in the case of epitaxy. Moreover, both examples are free boundary problems, in which the evolution of the free boundary depends on the *gradients* of the solution. Thus, it is important to develop schemes for solving Poisson-type equations with Robin boundary conditions on irregular domains that produce not only accurate solutions, but also accurate gradients.

In last few decades special interest has been given to the development of Cartesian grid methods in conjunction with the Level-Set method, due to their versatility. Perhaps the most popular methods for solving Poisson-type equations in irregular domains subject to Dirichlet boundary conditions are [9,7,23], in which the arms of the standard discrete Laplacian are adjusted near the irregular boundary. They produce solutions with second to fourth order accuracy and gradients from first to third order accuracy. These methods are straightforward to implement in a dimension-by-dimension approach and lead to symmetric or nonsymmetric linear systems depending on whether the accuracy of their gradients is required to be at least second-order accurate. Neumann and Robin boundary conditions require different methodology, since the value of the solution is not immediately available at the domain's boundary. Both finite-difference [10,2,24,1,12,13,4,6] and finite-volume methods [20] for discretizing Robin boundary conditions have been proposed. Only [4,6] obtain second-order convergence in gradients. Both methods are finite-difference based and necessitate a relatively large stencil to approximate the normal derivative of the solution at the boundary. In [11], finite-volume methods for Dirichlet and Neumann boundary conditions

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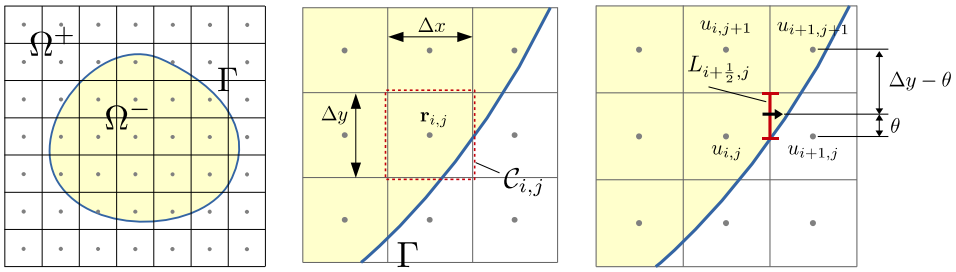

Fig. 1. Spatial discretization Ω (left), definition of a grid cell (center) and flux between cells (right).

producing second-order accurate gradients were proposed. Compared to the finite-difference methods, [11] uses only nearest neighbors in case of Neumann boundary conditions, which is important for adaptive grids and parallel computations since access to farther regions imply additional difficulties and message passing. Robin boundary conditions were not considered in [11]. A symmetric finite-volume method for Robin boundary conditions was proposed in [20], however gradients are only first-order accurate.

We propose an improvement of the method of [20] using ideas of [11] to obtain a numerical method with second-order accurate gradients for Poisson-type equations subject to Robin boundary conditions. We discretize the Poisson equation using a combination of a first-order finite-volume discretization for grid points near the irregular boundary and a classical second-order central discretization for the other grid points. We illustrate numerically that this method is second-order-accurate in the L^∞ norm for both the solution and its gradients. Compared to existing finite-difference methods the new method uses only nearest neighbor grid points.

2. Numerical method

Consider a physical domain Ω separated into two regions Ω^- and Ω^+ by an interface Γ with outward normal $\boldsymbol{n}$. We solve the system:

$$\begin{cases} -\nabla\cdot(D\nabla u) = f & \text{in } \Omega, \quad \text{(a)} \\ D\dfrac{\partial u}{\partial \boldsymbol{n}} + \alpha u = g & \text{on } \Gamma, \quad \text{(b)} \end{cases} \tag{1}$$

where D is the diffusion constant that is bounded from below by a positive constant, α is a scalar, f and g are given integrable functions and u is the solution we seek to solve numerically.

Referring to Fig. 1 (left), we discretize the domain Ω into a uniform grid of rectangular cells and represent the interface as the zero level-set of a Lipschitz continuous function ϕ, i.e. $\Gamma = \{\boldsymbol{x}\in\mathbb{R}^2 : \phi(\boldsymbol{x}) = 0\}$, $\Omega^- = \{\boldsymbol{x}\in\mathbb{R}^2 : \phi(\boldsymbol{x}) < 0\}$ and $\Omega^+ = \{\boldsymbol{x}\in\mathbb{R}^2 : \phi(\boldsymbol{x}) > 0\}$ [18]. In what follows, we present a numerical scheme for solving (1) in Ω^-; Ω^+ is treated similarly.

Let us consider a grid cell $\mathcal{C}_{i,j}$ with the center located at $\boldsymbol{r}_{i,j}$ and crossed by the irregular interface Γ (see Fig. 1 center). The integration of equation (1a) over $\Omega^-\cap\mathcal{C}_{i,j}$ yields

$$-\int_{\mathcal{C}_{i,j}\cap\Omega^-} \nabla\cdot(D\nabla u)\, d\boldsymbol{r} = \int_{\mathcal{C}_{i,j}\cap\Omega^-} f(\boldsymbol{r})\, d\boldsymbol{r}. \tag{2}$$

We approximate the domain integral on the right-hand side of (2) by the integrand value at the cell center multiplied by the area of the domain of integration, i.e.,

$$\int_{\mathcal{C}_{i,j}\cap\Omega^-} f(\boldsymbol{r})\, d\boldsymbol{r} = \int_{\mathcal{C}_{i,j}\cap\Omega^-} \Big(f(\boldsymbol{r}_{i,j}) + \underbrace{\nabla f(\boldsymbol{r}_{i,j})\cdot(\boldsymbol{r}-\boldsymbol{r}_{i,j})}_{\sim h} + \mathcal{O}\left(h^2\right)\Big)\, d\boldsymbol{r} = A_{i,j} f(\boldsymbol{r}_{i,j}) + \mathcal{O}\left(h^3\right),$$

where $A_{i,j} = \int_{\mathcal{C}_{i,j}\cap\Omega^-} d\boldsymbol{r}$ is the area of $\mathcal{C}_{i,j}\cap\Omega^-$ and $h = \max(\Delta x, \Delta y)$.

Applying the divergence theorem on the left-hand side of (2) gives:

$$\int_{\mathcal{C}_{i,j}\cap\Omega^-} \nabla\cdot(D\nabla u)\, d\boldsymbol{r} = \int_{\partial(\mathcal{C}_{i,j}\cap\Omega^-)} D\frac{\partial u}{\partial \boldsymbol{n}}\, d\Gamma = \int_{\partial\mathcal{C}_{i,j}\cap\Omega^-} D\frac{\partial u}{\partial \boldsymbol{n}}\, d\Gamma + \int_{\mathcal{C}_{i,j}\cap\Gamma} D\frac{\partial u}{\partial \boldsymbol{n}}\, d\Gamma. \tag{3}$$