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A simple weak formulation for solving two-dimensional diffusion equation with local reaction on the interface

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ABSTRACT

In this paper, we propose a numerical method for solving two-dimensional diffusion equation with nonhomogeneous jump condition and nonlinear flux jump condition located at the interface. We use finite element method coupled with Newton's method to deal with the jump conditions and to linearize the system. It is easy to implement. The grid used here is body-fitting grids based on the idea of semi-Cartesian grid. Numerical experiments show that this method is nearly second order accurate in the L^∞ norm.

1. Introduction

In some chemical reaction–diffusion processes, the reaction only takes place at some local sites because of the existence of the catalyst [1]. In [2,3], a mathematical model was introduced to describe the phenomena in which the concentration is continuous in a bounded domain and the gradient of the concentration has a jump at the local sites. In [2], some one-dimensional numerical results were given by using the immersed interface method to solve this reaction–diffusion equation numerically. However, in practical settings, the geometry is much more complicated. The model we consider in this paper is a more realistic one. It illustrates the practical problem much more closely. It is a two dimensional diffusion equation with nonhomogeneous solution jump condition and nonlinear flux jump condition at the local sites. Mathematically, it is an interface problem. More advanced methods are required to achieve efficient computations due to the challenges that arise from the jump conditions.

The importance of interface problems is well established because of its wide application in a variety of disciplines, such as fluid mechanics, material science, electromagnetic wave propagation, and so on. It is rather nontrivial to get highly accurate numerical solutions to these problems with standard numerical methods because of the low global regularity of the solutions due to the interface jumps, especially when there are arbitrarily complex interfaces with sharp geometric singularities. For this reason, various numerical methods have been developed for interface problems since the 1970s in order to achieve numerical results with high accuracy.

One of the pioneering works in this field was proposed by Peskin in modeling blood flows in heart. The Immersed Boundary Method (IBM) proposed by Peskin [4] uses a numerical approximation of the δ-function, which smears out the

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solution on a thin finite band around the interface Γ. In [5], the IBM was combined with the level set method, resulting in a first order numerical method that is simple to implement, even in multiple spatial dimensions. In [6–8], efforts were made to achieve higher order accuracy of the IBM. This method has been extensively used in engineering computations due to its simplicity, efficiency and robustness [9–11]. Some other pioneering works are summarized in a review paper [12].

The construction of higher order interface schemes is a big challenge in the numerical solution of interface problems. The Immersed Interface Method (IIM) constructed by LeVeque and Li [13] was a major advance in the field after Peskin's contribution. It incorporates the interface conditions into the finite difference scheme near the interface to achieve second-order accuracy based on a Taylor expansion in a local coordinate system. The second order convergence of the IIM for smooth interfaces was proved by Beale and Layton [14].

The Boundary Condition Capturing Method(BCCM) [15] uses the idea of Ghost Fluid Method(GFM) [16] to capture the boundary conditions. The method extends the solution from one side across the interface using the jump conditions. The GFM is robust and simple to implement, and so is the resulting BCCM. In [17], the BCCM has been sped up by a multi-grid method. The method can solve the elliptic equation with interface conditions $[u] \neq 0$ and $[\beta u_n] \neq 0$ in two and three dimensions.

In [18], the Matched Interface and Boundary method (MIB) was proposed to solve elliptical problems with smooth interfaces. In [19], the MIB method was generalized for problems involving sharp-edged interfaces. In [20], the MIB method was generalized for methods involving triple point junctions. Upon refinement, this method has achieved 2nd order accuracy.

Finite element methods (FEMs) are another class of important approaches for elliptic interface problems. Examples of finite element methods for interface problems are Extended Finite Element Method [21–23], Immersed Finite Element Method [24,25], and Penalty Finite Element Method [26,27]. Chen and Zou [28] studied the convergence of the finite element method for elliptic and parabolic interface problems, sub-optimal error estimates can be achieved for smooth interfaces. The convergence of Immersed Finite Element Method for semi-linear parabolic interface problems was analyzed in [29], which proved that the convergence rates for the semi-discrete and fully discrete schemes based on the backward Euler method are in the optimal order.

In [30], a non-traditional finite element (NTFEM) formulation for solving elliptic equations with smooth or sharp-edged interfaces was proposed with non-body-fitting grids for $[u] \neq 0$ and $[\beta u_{\boldsymbol{n}}] \neq 0$. It achieved second order accuracy in the L^∞ norm for smooth interfaces and about 0.8th order for sharp-edged interfaces. In [31,32], the method is modified and improved to close to 2nd order accurate for sharp-edged interfaces, and it is extended to handle general elliptic equations with matrix coefficient and lower order terms. The resulting linear system is non-symmetric but positive definite. Extension to problems with imperfect contact conditions are discussed in [33].

Also, there has been a large body of work from the finite volume perspective for developing high order methods for elliptic and parabolic interface problems. Colella and collaborators proposed the Embedded Boundary Method (EBM) [34–36] from the finite volume perspective, which embeds the domain into a regular Cartesian grid. In [37], this method was extended to parabolic problems with fixed or moving interfaces in domains with complex geometry. This method can achieve second-order accuracy in both space and time.

Because of the nonlinear flux jump condition, the diffusion equation with local reaction on the interface is much harder to be solved by the normal interface solver.

In this paper, inspired by the finite element method for solving elliptic interface problem we proposed in [38], we propose a simple numerical method for solving the two-dimensional diffusion equation with nonhomogeneous flux jump condition and nonlinear jump condition. We use traditional finite element method coupled with Newton's method to deal with these two special kinds of jump conditions. The reason we did not use the NTFEM [31,32,39–45] is because the nonlinear term of this problem comes from the jump condition. It is effective to use Newton's method to linearize the nonlinear system. However, when the nonlinearity comes from the jump condition along the interface, we need to solve the nonlinear system at the local cell if we use the NTFEM, and the result of this system will be a linear combination of the unknown solution located at the vertices of the element cell. Newton's method need to have an initial entry at every iteration step. However, the NTFEM can only provide an unknown linear combination, which will cause a serious problem at the linearization step. That is why we choose to use the traditional finite element method, rather than NTFEM. The nonlinear jump condition is the main new challenge of this problem compared with some other well-studied interface problems. To save the cost of mesh generation, we use semi-Cartesian grid so that the grid is independent of the interface away from the interface. Several numerical examples with various flux jump conditions on different interface geometry are considered. Numerical results show that our method is robust and can achieve nearly second order accuracy.

Although we obtained promising results, there are also some existing work in the literature that generates semi-structured mesh with better quality of the triangles, for example [46,47]. It could be interesting future work to implement such methods to solve similar problems.

2. Mathematical formulation

Consider an open bounded domain $\Omega \subset R^2$. Let Γ be a fixed interface of co-dimension 1, which divides Ω into disjoint open subdomains, Ω^- and Ω^+, hence $\Omega = \Omega^- \bigcup \Omega^+ \bigcup \Gamma$. Assume that the boundary $\partial\Omega$ and the boundary of each subdomain $\partial\Omega^\pm$ are Lipschitz continuous.