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An Interface-Fitted Finite Element Level Set Method with Application to Solidification and Solvation

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Abstract. A new finite element level set method is developed to simulate the interface motion. The normal velocity of the moving interface can depend on both the local geometry, such as the curvature, and the external force such as that due to the flux from both sides of the interface of a material whose concentration is governed by a diffusion equation. The key idea of the method is to use an interface-fitted finite element mesh. Such an approximation of the interface allows an accurate calculation of the solution to the diffusion equation. The interface-fitted mesh is constructed from a base mesh, a uniform finite element mesh, at each time step to explicitly locate the interface and separate regions defined by the interface. Several new level set techniques are developed in the framework of finite element methods. These include a simple finite element method for approximating the curvature, a new method for the extension of normal velocity, and a finite element least-squares method for the reinitialization of level set functions. Application of the method to the classical solidification problem captures the dendrites. The method is also applied to the molecular solvation to determine optimal solute-solvent interfaces of solvation systems.

AMS subject classifications: 65M

Key words: Level set method, finite element, interface-fitted mesh, curvature approximation, velocity extension, reinitialization, solidification, dendrites, molecular solvation, variational implicit-solvent models.

1 Introduction

Consider a moving interface $\Gamma = \Gamma(t)$ that separates two regions $\Omega_- = \Omega_-(t)$ and $\Omega_+ = \Omega_+(t)$, respectively, where t denotes time. The interface Γ can have multiple connected

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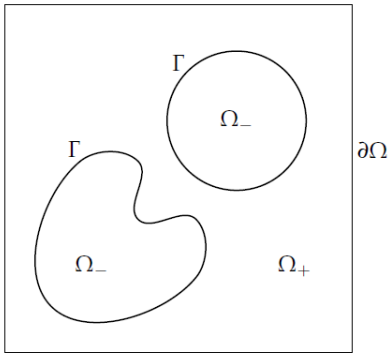

Figure 1: The geometry of interface motion.

components. We assume all Γ, Ω_-, and Ω_+ are inside a large computational domain Ω whose boundary is denoted by $\partial\Omega$, cf. Fig. 1.

The motion of the interface $\Gamma(t)$ is completely determined by its normal velocity, $v_n = v_n(x,t)$, at each point $x \in \Gamma(t)$ at each time t. For many physical systems, such a normal velocity consists of two parts. One is the local geometry, such as the curvature or mean curvature. The other is the external force such as flux of certain diffusive material. The concentration of such material is governed by a one-sided or two-sided diffusion equation, together with suitable boundary conditions on the moving interface $\Gamma(t)$. A typical system of a moving interface can thus be described by the following equations:

$$v_n = F_{geo}(H,K) + F_{ext}(u,\nabla u), \qquad \text{on } \Gamma(t), \tag{1.1a}$$
$$A_-(u) = f_-, \qquad \text{in } \Omega_-(t), \tag{1.1b}$$
$$A_+(u) = f_+, \qquad \text{in } \Omega_+(t), \tag{1.1c}$$
$$\text{boundary conditions for } u, \qquad \text{on } \Gamma(t). \tag{1.1d}$$

Here, $F_{geo}(H,K)$ is a function of the mean curvature H and Gaussian curvature K, $F_{ext}(u,\nabla u)$ is a function of a field variable u and its gradient ∇u, and $A_-(u)$ and $A_+(u)$ are partial differential operators of u, and f_- and f_+ are known functions on Ω_- and Ω_+, respectively. We shall call (1.1b) and (1.1c) the field equations for u. We also call (1.1d) the interface conditions.

There are many examples of moving interfaces that separate different media that are deforming or flowing. For instance, an ice-water boundary moves during the change of temperature, an interface separates two fluids with different viscosities and densities in a two-phase flow, phase boundaries in solid-solid phase transformations such as precipitates and martensite interfaces, domain boundaries that separate different parts of material such as grain boundaries in polycrystals, and the solute-solvent interface that separates a molecule from its surrounding solvent in a solvation system.

We use the level set method to numerically track the interface motion [12–14]. This method is perhaps one of the most popular methods due to its easy handling of topological changes, such as interface merging and breaking up. We denote by $\phi = \phi(x,t)$ a level