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A non-iterative local remeshing approach for simulating moving boundary transient diffusion problems

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ABSTRACT

A computational framework relying on a non-iterative mesh generation algorithm is introduced for modeling moving boundary transient diffusion problems, with a special focus on its application for simulating corrosion phenomena. In this approach, the Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) technique is employed to adapt the finite element mesh to the evolving morphology of the problem. CISAMR combines customized *h*-adaptivity, *r*-adaptivity, and sub-triangulation algorithms to transform a simple structured mesh into a high quality hybrid conforming mesh composed of rectangular and triangular elements. A key advantage of this method for modeling moving boundary problems is that only the elements located along the moving boundary must be modified to regenerate a conforming mesh at each step. This feature not only facilitates the remeshing process but also reduces the error associated with projecting nodal values of the solution to the new mesh. After a convergence study, we verify the accuracy of CISAMR for modeling pitting corrosion problems by comparing results with analytical solutions and phase field simulations. Additional examples are also provided to show the application of CISAMR for simulating corrosion problems with intricate morphologies.

1. Introduction

Several physical phenomena including the phase transformation are formulated as transient moving boundary problems governed by the diffusion law [1,2], which are also referred to as Stefan problems [3,4]. A major challenge toward simulating such problems using the finite element method (FEM) is the evolution of the domain morphology, which necessitates continuous updating of the mesh structure to conform to the moving boundary [5,6]. Varying robust algorithms can be employed to generate finite element (FE) meshes with proper element aspect ratios and negligible discretization error, among which we can mention the Delaunay triangulation [7–9], advancing front [10,11], quadtree/octree-based techniques [12–14], marching cubes [15], and the dual contouring method [16–18]. However, the computational cost associated with reconstructing a new conforming mesh at each time step for simulating moving boundary problems using these methods could be overwhelming. This is in part due to the iterative/optimization phase involved in such algorithms to improve the aspect ratios of elements. For example, a Laplacian smoothing is often used in quadtree-based algorithms to create elements with proper aspect ratios by iteratively relocating the mesh nodes [13,19]. Another challenge associated with the remeshing process is the requirement to project the solution between the nodes of the old (deformed) and new (reconstructed) meshes that coexist at each time step [20]. This nodal projection not only imposes an additional computational burden but also deteriorates the accuracy and convergence rate by undermining the superconvergence feature of FEM [21].

Alternative techniques such as the Arbitrary Lagrangian-Eulerian (ALE) method [22–25] can be implemented to evolve a conforming mesh during an FE simulation without remeshing the entire domain at each time step. In the ALE method, after evaluating the updated morphology of the domain at each time step, techniques such as the relocation of mesh nodes [26,27] and edge swapping [28] are employed to improve the quality of elements (i.e., their shape and aspect ratio) [29]. For problems with significant geometrical changes, a combination of smoothing algorithms and modifying the interface velocity has been used to prevent the element tangling issue [30]. Despite all these treatments, remeshing may still be required after a certain number of time steps for problems with intricate evolving geometries and/or those undergoing large deformations [26,31]. Automatic mesh moving techniques, often combined with interface-tracking and space-time methods [32,33], have also been introduced to limit the burden of remesh-

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ing for modeling moving boundary problems [34–38]. Similar to the ALE method, iterative nodal repositioning, edge/face swap, and mesh optimization techniques have been used in such methods to avoid the creation of tangling elements and improve their aspect ratios [39–41]. Recently, Gawlik and Lew [42] have introduced a robust technique for modeling 2D moving boundary problems that employs an iterative relaxation algorithm to adapt a stationary background mesh (universal mesh) to the evolving interface geometry [43,44].

To obviate the challenges associated with the remeshing process, one can implement meshfree techniques such as the smoothed particle hydrodynamics [45,46], element-free Galerkin method [47,48], exponential basis functions meshfree technique [49,50], and the Green's discrete transformation method [51]. The idea of making the solution field independent of the mesh structure can also be incorporated in the FE formulation by appropriate enrichment strategies [52–54]. The eXtended/Generalized FEM (X/GFEM) [55–59] is one of the most popular techniques in this category that relies on enrichment functions constructed using the partition of unity method to reconstruct strong/weak discontinuities in nonconforming elements. This method has successfully been implemented for modeling a variety of moving boundary problems, e.g., [60–67]. Compared to remeshing and ALE techniques, X/GFEM provides a major advantage by allowing the use of a stationary nonconforming mesh for modeling problems with evolving morphologies. XFEM has also been combined with the grid-based particle method [68] to tracks interface motion with meshless particles and handle topological changes such as boundary merging [69]. It is worth mentioning that additional treatments might be required in enriched methods such as X/GFEM to resolve implementation issues such as the high condition number of the stiffness matrix [70,71] and enforcing Dirichlet boundary conditions [72,73].

Another approach that can eliminate the need to create conforming meshes during the FE simulation of moving boundary problems is the phase field method [74,75]. In this method, a diffuse interface model is employed to approximate the strong discontinuity across the interface as a continuously varying function with a pre-defined thickness [76]. The phase field method has been employed to simulate a variety of moving boundary problems, such as the solidification [77,78], dislocation interactions [79,80], and corrosion [81–83]. While eliminating the need to generate conforming meshes, the phase field method requires a highly refined (nonconforming) mesh in the vicinity of the diffuse interface to accurately approximate the sharp gradients of the fields in this region. Further, an additional phase field variable must be incorporated in the problem formulation to implicitly track the interface location [76], which leads to a higher computational cost compared to sharp interface models. The peridynamics (PD) model introduced in Refs. [84,85] is an alternative diffuse interface model that can be employed for simulating moving boundary problems. In the PD model, the domain is discretized using a structured grid, where each node interacts with its neighboring nodes within a certain distance. The phase transformation is achieved by monitoring the concentration associated with each node, which unlike the phase field method does not use an additional variable to track the interface location.

In this manuscript, we introduce a computational framework relying on a non-iterative mesh generation algorithm named Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) [86] for simulating moving boundary transient diffusion problems. The concept behind this approach is similar to the universal meshing method [42], as we regenerate the FE model after a few time steps by transforming a background mesh into a conforming mesh. However, CISAMR performs this transformation using a non-iterative algorithm (versus the iterative relaxation approach in universal remeshing) that only affects the locations of nodes of background elements intersecting with the moving interface. This algorithm generates a hybrid conforming mesh composed of quadrilateral and triangular elements with proper aspect ratios. An *h*-adaptive refinement phase is incorporated in the CISAMR algorithm that enables reducing the geometric discretization error and approximating sharp gradients along the moving interface more accurately. This technique can handle moving boundary problems undergoing large changes in the domain morphology without compromising the mesh quality. Among a variety of transient diffusion problems with evolving geometries, in this work we focus on the application of CISAMR for simulating corrosion phenomena and in particular the pitting corrosion [87,88]. It must be noted that although the focus of the current manuscript is on modeling 2D problems, there is no inherent limitation for expanding the CISAMR non-iterative algorithm to 3D.

The remainder of this article is structured as follows. In Section 2 we introduce strong and weak forms of transient diffusion governing equations, together with the special considerations required for modeling the pitting corrosion phenomenon [89,90]. A brief overview of the CISAMR algorithm and the algorithmic aspects pertaining to its application for modeling moving boundary problems are presented in Section 3. Several numerical examples, including a detailed convergence study, are presented in Section 4 to verify the accuracy of CISAMR simulations through comparison with analytical results and phase field simulations. We also show the application of this method for simulating several geometrically elaborate corrosion problems, such as the electropolishing and pitting corrosion phenomena. Final concluding remarks are presented in Section 5.

2. Governing equations

Consider an open domain $\Omega = \Omega_s \cup \Omega_f$ consisting of solid Ω_s and fluid Ω_f phases, with the boundary $\overline{\Omega}\backslash\Omega = \Gamma$ and the outward unit normal vector $\mathbf{n}$. The domain boundary is composed of three non-overlapping partitions Γ_D, Γ_N, and Γ_R, corresponding to the Dirichlet, Neumann, and Robin boundary conditions, respectively. Also, Γ_S refers to the interface between the fluid and the solid phases, which moves with velocity $\mathbf{v}$ during the transient diffusion phenomenon. The strong form of governing equations describing this process are given by: Find the transient field $c(\mathbf{x}, t)$ such that

$$\begin{aligned}
\frac{\partial c(\mathbf{x},t)}{\partial t} &= D\nabla^2 c(\mathbf{x},t) && \text{in } \Omega_f \\
c(\mathbf{x},0) &= c_0 && \text{in } \Omega_f \\
c(\mathbf{x},t) &= c_{\text{solid}} && \text{in } \Omega_s \\
c(\mathbf{x},t) &= \overline{c} && \text{on } \Gamma_D \\
\nabla c(\mathbf{x},t)\cdot\mathbf{n} &= \overline{\mathbf{q}} && \text{on } \Gamma_N \\
-D\nabla c(\mathbf{x},t)\cdot\mathbf{n} + hc(\mathbf{x},t) &= g && \text{on } \Gamma_R,
\end{aligned} \tag{1}$$

where D is the diffusivity, c_0 is the initial distribution of the field, $\overline{c}$ is the prescribed value of the field along Γ_D, $\overline{\mathbf{q}}$ is the applied flux along Γ_N, and h and g are problem-specific constants.

While (1) can be employed for modeling a variety of moving boundary problems governed by the diffusion law, in the current manuscript we focus on the pitting corrosion phenomenon as the physical application. Pitting corrosion is the localized degradation of a metal due to the partial breakdown of the passive film protecting its surface against a corrosive environment [88,91]. Although high strength alloys such as stainless steel and 7xxx-series aluminum alloys are resistant to uniform corrosion, they are susceptible to pitting corrosion in environments with aggressive anions such as chloride. Pitting corrosion is devastating not only due to the mass loss caused by reverse metallurgical processes but also because growing pits induce significant stress concentrations that accelerates the crack nucleation and reduces the fatigue life [92]. Fig. 1 schematically illustrates the domain of a pitting corrosion prob-