Conforming to interface structured adaptive mesh refinement technique for modeling moving boundary problems

A Thesis

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This thesis introduces a new computational framework relying on a non-iterative mesh generation algorithm for modeling moving boundary transient diffusion problems. In particular, we focus on simulating the activation-diffusion-controlled pitting corrosion phenomenon, which is a specific class of such problems. In order to locally adapt the FE mesh to the evolving domain morphology, we employ the Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) technique. CISAMR combines customized versions of the $h$-adaptivity, $r$-adaptivity, and sub-triangulation algorithms to transform a structured grid into a conforming mesh. One of the key advantages of this technique for modeling problems with evolving geometries is that only the elements located along the moving boundary must be modified to regenerate a conforming mesh at each time step. This feature not only facilitates the remeshing process but also reduces the error associated with projecting the solution to the nodes of the new mesh. A detailed discussion is provided on different aspects of the CISAMR implementation for modeling moving boundary problems, including the nodal projection procedure and evaluating the moving interface velocity. After presenting a detailed convergence study, we verify the accuracy of this method for modeling pitting corrosion problems by comparing results with analytical solutions and phase field simulations. Additional example problems are also presented.
to demonstrate the application of CISAMR for simulating corrosion problems with intricate morphologies.
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Chapter 1: Introduction

1.1 Background

Several physical phenomena including the phase transformation are formulated as transient moving boundary problems governed by the diffusion law [33, 32], which are also referred to as Stefan problems [67, 27]. 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 [34, 77]. 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 [39, 13, 3], advancing front [68, 35], modified Quadtree/Octree techniques [46, 57, 50], Marching Cubes [78], and the Dual Contouring method [85, 86, 82]. However, the computational cost associated with reconstructing a new conforming mesh at each time step for simulating moving boundary problems using such methods, which involves an iterative process to improve elements aspect ratios, could be overwhelming. For example, the Laplacian smoothing technique is often used in Quadtree-based methods to obtain elements with proper aspect ratios via iterative relocation of the mesh nodes [57, 49]. Another challenge associated with the remeshing process is the
requirement to project the FE solution between the nodes of the old (deformed) and new (reconstructed) meshes that coexist at each time step [44]. This nodal projection not only imposes an additional computational burden but could also undermine the accuracy and convergence rate by taking away the superconvergence characteristic of the FEM [53].

Alternative techniques such as the Arbitrary Lagrangian-Eulerian (ALE) method [18, 9, 5] can be employed to evolve the conforming FE mesh during the simulations a moving boundary problem, without remeshing at each time step. In the ALE method, after evaluating the updated morphology of the domain at a time step, techniques such as relocation of the mesh nodes [77, 60] and edge swapping [2] are implemented to improve the elements quality (i.e., shape and aspect ratio) [38]. A combination of smoothing algorithms and modifying the interface velocity [36] has also been used to prevent element tangling. Despite all these treatments, remeshing would still be required after a certain number of time steps for simulating moving boundary problems with intricate geometries or those undergoing large deformations [55]. Other automatic mesh moving techniques, often combined with interface-tracking and space-time methods [75, 6], have also been introduced to limit the burden of remeshing for modeling moving boundary problems [74, 56, 41, 40, 19]. Similar to the ALE method, iterative nodal repositioning, edge/face swap, and mesh optimization techniques have been used in such methods to avoid the mesh tangling and create elements with proper aspect ratios [54, 71, 28]. More recently, Gawlik and Lew [24] have introduced a general framework for modeling 2D moving boundary problems, which employs an iterative relaxation algorithm to adapt a stationary background mesh (universal mesh) to the interface morphology at each time step [26, 25].
To obviate the challenges associated with the remeshing process, one can implement meshfree techniques such as the smoothed particle hydrodynamics [47, 37], element-free Galerkin method [72, 48], exponential basis functions meshfree technique [70, 11], and the Green’s discrete transformation method [80]. The idea of making the solution field independent of the mesh structure can also be incorporated in the FE formulation by appropriate enrichment strategies [76, 52, 65]. The eXtended/Generalized FEM [73, 22, 21, 10] is one of the most popular techniques in this category, which relies on enrichment functions constructed using the partition of unity method to capture strong/weak discontinuities in nonconforming elements. This method has successfully been implemented for modeling a variety of moving boundary problems, e.g., [61, 30, 31, 83, 59, 58]. While allowing the use of a stationary nonconforming mesh for discretizing the domain, additional treatments are often required in mesh-independent methods such as X/GFEM to resolve challenges such as the high condition number of the stiffness matrix [14, 7] and enforcing Dirichlet boundary conditions [51].

Another approach for eliminating the need to create conforming meshes in the FE modeling of moving boundary problems is to implement the phase field method [79, 45]. 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 [8]. The phase field method has been employed to simulate a variety of moving boundary problems, such as the solidification [4, 12], dislocation interactions [20, 15], and corrosion [84, 1, 81]. While eliminating the need for mesh generation, 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 field in
this region. Further, an additional phase field variable must be incorporated in the problem formulation to implicitly track the interface location [8], which leads to a higher computational cost compared to sharp interface models. The peridynamics (PD) model introduced in [16, 17] 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 eliminates the need for using an additional variable for tracking the interface location.

In the current manuscript, we introduce an automated computational framework relying on a non-iterative mesh generation algorithm named Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) [66] for simulating moving boundary transient diffusion problems. The concept behind this technique is similar to the universal mesh method [24], as we regenerate the FE model after a few time steps by transforming a background mesh into a conforming mesh. However, the CISAMR relies a non-iterative algorithm to perform this transformation, which only affects the nodal position of background elements intersecting with the moving boundary. In addition to facilitating the remeshing process, this feature reduces the computational cost and the loss of accuracy associated with projecting the nodal values of the new (reconstructed) mesh. Further, an $h$-adaptive refinement phase is incorporated in the CISAMR algorithm, which enables reducing the geometric discretization error and more accurate approximation of sharp gradients along the moving interface. This technique can handle problems undergoing large deformations of the domain morphology with weakly-discontinuous moving boundaries without compromising the mesh
quality. While the CISAMR can be used for modeling a variety of moving boundary problems, in this work we focus on the application of this method for simulating corrosion problems and in particular the pitting corrosion phenomenon \cite{69, 29}.

1.2 Thesis structure

This thesis is structured as follows. Chapter 2 introduces the strong and weak forms of transient diffusion governing equations, together with the special considerations required for modeling the pitting corrosion phenomenon. This chapter also presents a standard FEM formulation for solving steady-state and transient diffusion problem. A brief overview of the CISAMR algorithm and the algorithmic aspects pertaining to its application for modeling moving boundary problems are presented in Chapter 3. To elucidate the accuracy of the presented algorithm, several examples are presented in Chapter 4 studying the convergence rate and accuracy of CISAMR. Chapter 5 presents the application of the model for simulating corrosion problems with complex morphologies. Final concluding remarks and anticipations for future work are presented in Chapter 6.
Chapter 2: Problem formulation

This chapter introduces the governing equation and Stefan boundary condition for simulating the activation-diffusion-controlled corrosion phenomenon in Section 2.1. Subsequently, a standard FEM approximation of the steady-state and transient diffusion problems are formulated in Section 2.2.

2.1 Pitting corrosion governing equation

In particular, this research work focuses on pitting corrosion moving boundary problem. Consider an open domain $\Omega = \Omega_s \cup \Omega_f$ consisting of solid $\Omega_s$ and fluid $\Omega_f$ phases, with the boundary $\bar{\Omega} \setminus \Omega = \Gamma$ and the outward unit normal vector $\mathbf{n}$. The domain boundary is composed of three non-overlapping partitions $\Gamma_D$, $\Gamma_N$, and $\Gamma_R$, corresponding to the Dirichlet, Neumann, and Robin boundary conditions, respectively. Also, $\Gamma_S$ 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 $c(x, t)$ such that
\[
\frac{\partial c(x, t)}{\partial t} = D \nabla^2 c(x, t) \quad \text{in } \Omega_f
\]
\[
c(x, 0) = c_0 \quad \text{in } \Omega_f
\]
\[
c(x, t) = c_{\text{solid}} \quad \text{in } \Omega_s
\]
\[
c(x, t) = \bar{c} \quad \text{on } \Gamma_D
\]
\[
\nabla c(x, t) \cdot \mathbf{n} = \bar{q} \quad \text{on } \Gamma_N
\]
\[
-D \nabla c(x, t) \cdot \mathbf{n} + hc(x, t) = g \quad \text{on } \Gamma_R,
\]
where \(D\) is the diffusivity, \(c_0\) is the initial distribution of the field, \(\bar{c}\) is the prescribed value of the field along \(\Gamma_D\), \(\bar{q}\) is the applied flux along \(\Gamma_N\), and \(h\) and \(g\) are problemspecific constants.

While (2.1) 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 [29, 23]. 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 [42]. Figure 2.1 schematically illustrates the domain of a pitting corrosion problem, consisting of the metal and electrolyte phases, together with the initial and boundary conditions assigned to each phase.

For pitting corrosion problems, the concentration of dissolved ions in the electrolyte solution and the velocity of the moving pit boundary can be described using the activation-diffusion-controlled model presented in [64]. In this model, the evolution of the corroding interface \(\Gamma_S\) is characterized using the Rankine-Hugoniot
Figure 2.1: Schematic of the domain morphology and boundary conditions for a pitting corrosion problem.

\[ \Gamma_D : c (\mathbf{x}, t) = 0 \]

\[ \frac{\partial c}{\partial n}(\mathbf{x}, t) = 0 \]

\[ v_n(\mathbf{x}, t) \]

\[ \text{Interface velocity} \]

\[ \text{Pit interface (} \Gamma_S \text{)} \]

\[ \text{Solid phase: } c(\mathbf{x}, t) = c_{\text{solid}} \]

\[ \text{Electrolyte: } c(\mathbf{x}, 0) = 0 \]

\[ \text{Passive film (} \Gamma_N \text{)} \]

\[ \text{Passive film (} \Gamma_N \text{)} \]

\[ \Gamma_N : [c_{\text{solid}} - c(\mathbf{x}, t)] v_n = 0 \text{ on } \Gamma_S, \]  

\[ (2.2) \]

where \( v_n = \mathbf{v} \cdot \mathbf{n} \) is the normal velocity of the moving pit boundary. The numerical implementation of this condition depends on the relative rates of the metal dissolution and the ions diffusion in the electrolyte. If the metal dissolution rate is relatively fast, the concentration of dissolved ions gradually increases and would eventually reach the saturation concentration \( c_{\text{sat}} \). At this stage, dissolved metal ions react with \( \text{Cl}^- \) ions in the electrolyte and precipitate a thin salt film along the pit interface, which does not allow further increase of the concentration. After the formation of the salt film, the diffusion law governs the release of the ions from the film into the electrolyte and thereby controls the pit growth rate, which is often referred to as the diffusion-controlled pitting corrosion phenomenon. For modeling this process, a Dirichlet boundary condition of \( \bar{c} = c_{\text{sat}} \) is imposed along the pit interface \( \Gamma_S \). The interface velocity is then computed by rearranging (2.2) as a function of the
concentration gradient, i.e.,

$$v_n = \frac{D \nabla c(x, t) \cdot n}{c_{\text{solid}} - c_{\text{sat}}}, \text{ if } c(x, t)|_{\Gamma} = c_{\text{sat}}. \quad (2.3)$$

Unlike the diffusion-controlled pitting corrosion, before the formation of the salt film the interface velocity is controlled by the overpotential $\eta$. At this stage, the pit interface velocity $v_n$ is evaluated based on the Tafel electrochemical kinetics and the Faraday’s second law, which is given by [62, 23]

$$v_n = \frac{i_0 e^{\frac{\eta}{b_a n F c_{\text{solid}}}}}{n F c_{\text{solid}}}, \text{ if } c(x, t)|_{\Gamma} < c_{\text{sat}}, \quad (2.4)$$

where $i_0$ is the exchange current density, $b_a$ is the anodic Tafel slope, $F$ is the Faraday’s constant, and $n$ is the average charge number. The Robin boundary condition along $\Gamma_S$ during the activation-controlled pitting is obtained by substituting (2.4) in the Rankine-Hugoniot condition given in (2.2).

After deriving the weak form of the governing equations in (2.1) and using the Backward Euler time integration scheme for the time discretization, the solution field $c_{n+1}^h$ at time $t_{n+1}$ can be approximated as

$$\int_{\Omega_f} \frac{1}{\Delta t} w c_{n+1}^h \,d\Omega + \int_{\Omega_f} D \nabla w \cdot \nabla c_{n+1}^h \,d\Omega - \int_{\Gamma_D} w c_{n+1}^h v_n \,d\Gamma = \int_{\Omega_f} \frac{1}{\Delta t} w c_n^h \,d\Omega + \int_{\Gamma_N} w \bar{q} \,d\Gamma + \int_{\Gamma_D} L w v_n \,d\Gamma, \quad \forall c_{n+1}^h \in \mathcal{V}^h, \quad (2.5)$$

where $\Delta t$ is the time increment, $c_n^h$ is the approximate solution at $t_n$, and $\mathcal{V}^h$ is a sufficiently smooth space function. In the standard Galerkin FEM, $\mathcal{V}^h$ is the space of the Lagrangian shape functions used for interpolating $c_{n+1}^h$.

One of the major challenges involved in simulating transient diffusion problems such as the pitting corrosion using the FEM is to maintain a conforming mesh with proper element aspect ratios during the evolution of the domain morphology. It
is evident that the quality of the FE mesh has a crucial impact on the fidelity of results and in particular on the accurate recovery of the gradient field. Note that in diffusion-controlled pitting corrosion problems, the concentration gradient along the pit interface is directly used in (2.3) to evaluate the moving boundary velocity \( v_n \). Thereby, the accurate approximation of the gradient in such problems, which is contingent upon creating elements with small aspect ratios at each time step, has an even more pronounced impact on the accuracy.

### 2.2 Finite element method formulation

#### 2.2.1 Steady-state field problem

For steady state heat transfer, consider an open domain \( \Omega \) and boundary domain \( \Gamma_q \) and \( \Gamma_\phi \), an essential boundary condition is specified on the boundary \( \Gamma_\phi \) and a natural boundary condition is specified on the boundary \( \Gamma_q \)

\[
\begin{align*}
Q + k \nabla^2 \phi &= 0 \quad \text{on } \Omega \\
\phi &= \phi_0 \quad \text{on } \Gamma_\phi \\
\nabla \phi(x) \cdot n &= \bar{q} \quad \text{on } \Gamma_q,
\end{align*}
\]

(2.6)

where \( k \) is heat conductivity, \( Q \) is heat source, \( \phi_0 \) is Dirichlet boundary value on \( \Gamma_\phi \). \( \bar{q} \) is heat flux normal to the boundary \( \Gamma_q \). The variational form of this governing equation is written as summation of all the domain elements

\[
\Pi = \sum_{i=0}^{e} \left[ \int_{\Omega} \left\{ \frac{1}{2} \left( \nabla \phi^T \right) D \left( \nabla \phi^e \right) - Q \phi^e \right\} dV + \int \bar{q} \phi^e d\Gamma_q \right].
\]

(2.7)

Apply Rayleigh-Ritz method to the above equation which derives the linear system equation

\[
[K] \{ \phi \} = \{ F_Q \} - \{ F_q \},
\]

(2.8)

where

\[
[K^e] = \int_{V^e} [B^e]^T [D] [B^e] dV^e,
\]

(2.9)
\{F_Q^e\} = \int_{V^e} \langle N^e \rangle^T Q dV^e, \quad (2.10)
\{F_q^e\} = \int_{\Gamma_q^e} \bar{q} \langle N^e \rangle^T d\Gamma_q^e. \quad (2.11)

2.2.2 Transient problem

For transient state heat transfer, consider an open domain \(\Omega\) and boundary domain \(\Gamma_q\) and \(\Gamma_\phi\), an essential boundary condition is specified on the boundary \(\Gamma_\phi\) and a natural boundary condition is specified on the boundary \(\Gamma_q\). There is one initial condition assigned on \(\Omega\)

\[
\begin{align*}
k \nabla^2 \phi(x, t) &= \frac{\partial \phi(x, t)}{\partial t} + Q \quad \text{on } \Omega \\
\phi &= \phi_0 \quad \text{on } \Gamma_\phi \\
\nabla \phi(x) \cdot n &= \bar{q} \quad \text{on } \Gamma_q \\
\phi(x, 0) &= \phi_i \quad \text{on } \Omega,
\end{align*}
\]

(2.12)

where \(k\) is heat conductivity, \(Q\) is heat source, \(\phi_0\) is Dirichlet boundary value on \(\Gamma_\phi\), \(\bar{q}\) is heat flux normal to the boundary \(\Gamma_q\).

The variational form of this governing equation can be written as summation of all the domain elements

\[
\sum_{e} \left[ \int_{V^e} \left\{ \nabla W^e \right\}^T \left[ \frac{\partial \phi^e(x, t)}{\partial t} \right] dV^e \right] + \sum_{e} \left[ \int_{\Gamma_{\phi}^e} W^e q_{\phi} d\Gamma_{\phi}^e \right] = 0. \quad (2.13)
\]

The derived matrix form for above governing equation is

\[
[C] \left\{ \dot{\phi} \right\} + [K] \{\phi\} = \{F_Q\} - \{F_q\}, \quad (2.14)
\]

where

\[
[C^e] = \int_{V^e} \langle N^e \rangle^T \langle N \rangle dV^e, \quad (2.15)
\]
\[
[K^e] = \int_{V^e} [B^e]^T [D] [B^e] dV^e, \quad (2.16)
\]
\[
\{F_Q^e\} = \int_{\Gamma_q} \bar{q} \langle N^e \rangle^T d\Gamma_q^e, \quad (2.17)
\]

\[
\{F_q^e\} = \int_{\Gamma_q^e} \bar{q} \langle N^e \rangle^T d\Gamma_q^e.
\]
\{F_Q^e\} = \int_{V_e} Q(N_e)^T dV_e. \quad (2.18)
Chapter 3: Automated mesh generation

This chapter presents a computational framework relying on the CISAMR technique for simulating transient moving boundary problems. Section 3.1 presents a brief overview of CISAMR algorithm. Section 3.2 presents algorithm aspects pertaining to the moving boundary and recursive mesh generation. Section 3.3 discusses two implementation aspects regarding to this work.

3.1 CISAMR algorithm

Figure 3.1 schematically illustrates the non-iterative process of transforming a structured mesh (Figure 3.1(a)) to a conforming mesh for modeling a corrosion pit using the CISAMR. This process involves three major steps: (i) $h$-adaptive refinement of the background mesh using a customized Structured Adaptive Mesh Refinement (SAMR) algorithm, as shown in Figure 3.1(b); (ii) $r$-adaptivity of the nodes of elements intersecting with the materials interfaces, as shown in Figure 3.1(c); (iii) Sub-triangulating the remaining nonconforming elements, together with elements with hanging nodes on their edges, as shown in Figure 3.1(d). The following paragraphs introduces the detail of CISAMR algorithms.
Figure 3.1: Transforming a background mesh to a high quality conforming mesh using the CISAMR: (a) Structured grid used for discretizing the domain; (b) SAMR of the background grid; (c) $r$-adaptivity phase; (d) Sub-triangulating the elements deformed during the $r$-adaptivity or having hanging nodes on their edges.

- $h$-adaptivity: As the first step, we implement a customized SAMR algorithm to achieve the desired level of refinement in the vicinity of materials interfaces (Figure 3.1(b)). At each level of refinement, the quadrilateral background elements cut by the interface and their selected neighboring elements are recursively subdivided into four sub-quadrangles. A neighboring element is subjected to refinement if one of its nodes $N_i$ is located at distance $d < 0.5h$ from the intersection point of the interface
with one of the edges connected to that \((h)\) is the length of that edge). To ensure that the confirming elements of the final conforming mesh have proper aspect ratios, any element with more than one hanging node on one of its edges, which could be created due to multiple levels of SAMR in adjacent elements, is also subjected to refinement. It is worth mentioning that the objectives of the local refinement of the mesh in the vicinity of the interface during the SAMR phase are twofold: reducing the geometric discretization error and more accurate approximation of the field and its gradient in this region. As noted previously, the accurate prediction of the gradient field is crucial for the accurate evaluation of the moving boundary velocity in diffusion-controlled pitting corrosion problems.

- **\(r\)-adaptivity:** Next, we visit the nodes of the background elements cut by the interface to determine their new locations based on their relative distance to the moving boundary interface. It must be emphasized none of the nodes of elements not intersecting with the interface are relocated during the \(r\)-adaptivity, which highly facilitates the implementation of this non-iterative step. As illustrated in Figure 3.1(c), performing the \(r\)-adaptivity leads to deforming the original nonconforming elements of the background mesh, which transforms some of them to conforming elements, while the rest are converted to elements diagonally cut by the interface. The following algorithm, which is schematically shown in Figure 3.2, is employed to determine the new location of node \(N_i\) of a nonconforming background element during this process:

1. If none of the edges connected to \(N_i\) is cut by the interface: the node is not relocated.
2. If only one of the edges connected to $N_i$ is cut by the interface: (a) If $d \geq 0.5h$ the node is not relocated. (b) If $d < 0.5h$ we snap $N_i$ to the edge/interface intersection point.

3. If two of the edges connected to $N_i$ are cut by the interface: (a) If $d_1 \geq 0.5h_1$ and $d_2 \geq 0.5h_2$ the node is not relocated. (b) If $d_1 < 0.5h_1$ and $d_2 \geq 0.5h_2$ we snap $N_i$ to the edge/interface intersection point. (c) If $d_1 < 0.5h_1$ and $d_2 < 0.5h_2$ and $d_1 < d_2$ we snap $N_i$ to the edge/interface intersection point at $d_1$ and discard the other intersection point.

![Figure 3.2](image-url)  
Figure 3.2: Different case scenarios for relocating a mesh node during the $r$-adaptivity phase of CISAMR.

It must be emphasized that none of the case scenarios outlined above contradict or interfere with one another; thus each node can be visited independently during the $r$-adaptivity process to determine its new location. Also, note that weak discontinuities
(sharp corners) in the materials interface can easily be handled via a hierarchical $r$-
adaptivity scheme, as shown in Figure 3.3(a). In this non-iterative approach, we first
apply the regular $r$-adaptivity algorithm described above to nodes of the element
holding the weak discontinuity point. We then identify the node that has the closest
distance to the gradient discontinuity point and relocate that by moving to this
point. It must be noted that in modeling pitting corrosion problems, such weak
discontinuities often occur at the intersection point of the pit interface and the metal
surface protected by the passive film, as depicted in Figure 2.1.

![Diagram](image)

Figure 3.3: (a) Hierarchical $r$-adaptivity of the nodes of an element cut by a weakly
discontinuous materials interface; (b) single- and double-diagonal rules for sub-
triangulating background elements.

- **Sub-triangulation**: The final step of the CISAMR algorithm is to sub-
triangulate the background elements that either are deformed after the $r$-adaptivity
or have hanging nodes (generated during the SAMR process) on their edges, as shown
in Figure 3.1(d). Sub-triangulating the background elements with hanging nodes is a
straightforward task, which depending on the number of hanging nodes would result
in the construction of between three to six sub-elements. For sub-triangulating the
elements with at least one re-located node after applying the $r$-adaptivity, the following simple rules ensure that the aspect ratios of resulting sub-elements are lower than three (Figure 3.3(b)):

1. **Single-diagonal rule**: If the element is not cut by the interface along the diagonal emanating from its smallest angle $\theta_{\text{min}}$, the other diagonal (corresponding to the largest angle $\theta_{\text{max}}$) is employed to cut the elements into two conforming sub-triangles.

2. **Double-diagonal rule**: Otherwise, if $\theta_{\text{min}} < 60^\circ$, the elements is sub-triangulated by cutting that along both diagonals. In this case, an additional interior node is created at the intersection point of the interface with the diagonal emanating from $\theta_{\text{max}}$, which is used for subdividing the background element into four conforming sub-triangles.

### 3.2 CISAMR modeling of moving boundary problems

One of the unique advantage that CISAMR shares with X/GFEM for modeling moving boundary problems is that only the background elements cut by the materials interface must be modified for the reconstruction of the mesh. This not only facilitates the remeshing process but also reduces the computational burden and the error associated with mapping nodal values of the solution between the deformed and updated meshes at each time step. As shown in Figure 3.4(a), the simulation begins with determining new coordinates of the interface nodes at $t_{n+1}$ as

$$x_{t_{n+1}} = x_{t_n} + v_n \Delta t.$$  \hspace{1cm} (3.1)
In an activation-controlled pitting corrosion problem, a constant velocity evaluated using (2.4) is assigned to each interface node. As the ions concentration along the interface reaches the saturation concentration or subject to a sufficiently high overpotential, the corrosion regime becomes diffusion-controlled and the interface velocity must be evaluated using (2.3), which is a function of the concentration gradient. Since CISAMR ensures that the adaptively refined conforming elements generated along the interface have proper aspect ratios, the gradient and thereby the interface velocity can accurately be approximated at this stage, without the need to use a special smoothing algorithm. Thus, we evaluate the gradient at quadrature points of the elements located along the pit interface and then project them to the interface nodes. The nodal averaging scheme is then employed to approximate the gradient used for evaluating the interface velocity in (2.3) at each node.

Figure 3.4: (a) Deformed mesh created after moving the mesh nodes located along the pit interface in the direction of their outward unit normal vectors to evaluate the solution at \( t_{n+1} \); (b) The new mesh reconstructed using CISAMR at \( t_{n+1} \), which requires projecting the nodal values at the new nodes (shown in red) generated during this process.

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After evaluating the new locations of interface nodes at \( t_{n+1} \), one can use a standard time integration scheme (in this work, the Backward Euler method) to evaluate the corresponding solution field. However, the continuation of this process in subsequent time steps could result in significant deterioration of element aspect ratios and even the formation of tangling elements. This is one of the major challenges that necessitates additional treatments (e.g., node relocation or reconstruction of the mesh) in methods such as the ALE. In addition to the computational cost associated with either of these approaches, one must re-evaluate the field values at the nodes of the new mesh based on the solution approximated using the deformed mesh at \( t_{n+1} \), which is needed as the initial values for evaluating the field at \( t_{n+2} \). Since the FE solution is super-convergent at the mesh nodes, mapping the solutions between all the nodes of the deformed and updated meshes at each time step leads to the loss of accuracy and deterioration of the convergence rate [24].

To simulate a moving boundary problem using the CISAMR, we can re-generate the mesh at each time step to avoid the deterioration of the elements quality as the solution proceeds. If the maximum distance the nodes located along the interface are relocated is small compared to the size of elements, the mesh reconstruction could happen after a few time steps. Unlike conventional mesh generation algorithms, new nodes are only created along the interface in the mesh reconstructed using the CISAMR. To generate this mesh, we employ NURBS to parameterize the moving interface geometry as an explicit function. Note that using a NURBS curve of at least second-order provides a \( C^1 \)-continuous representation of the interface geometry, which yields a unique normal vector \( \mathbf{n} \) at each interface node that in turn improves the accuracy for approximating \( v_\mathbf{n} \). A NURBS curve \( \mathbf{C}(u, t) \) is composed of \( n \) B-splines.
$M_p^p(u)$ of order $p$ with the parametric coordinate $u$ that are interpolated on a set of control points $x_i(t)$ with a given weight $w_i(t)$ as \[ C(u, t) = \sum_{i=1}^{n} x_i(t) w_i(t) M_p^p(u) \sum_{j=1}^{n} w_j(t) M_p^p(u). \] (3.2)

Note that in the equation above, $x_i(t)$ and $w_i(t)$ are considered as time-dependent parameters to take into account the evolution of the interface geometry in a moving boundary problem.

After updating the NURBS curve representing the moving boundary morphology at $t_{n+1}$, we interact this curve with the background grid to create a new conforming mesh using the CISAMR non-iterative algorithm described previously. The key advantage of this method appears during the projection of the nodal values of the field between the old (deformed) and new (reconstructed) meshes coexisting at $t_{n+1}$. Figure 3.4(b) illustrates the conforming elements in the new mesh constructed using the CISAMR at $t_{n+1}$ for the updated interface morphology shown in Figure 3.4(a). Comparing the two meshes depicted in these figures indicates that the nodal values of the field must only be interpolated at certain nodes of the elements located along the interface (shown in red in Figure 3.4(b)). All other nodes of the reconstructed mesh away from the interface directly inherit the solution values from nodes with similar coordinates in the deformed mesh depicted in Figure 3.4(a). This feature reduces both the computational burden and the loss of accuracy by restricting the projection to a minimum number of nodes, for which the nodal interpolation would be inevitable due to the evolution of the domain morphology.

In order to project the field values to the nodes of the reconstructed mesh located near the boundary, (red nodes in Figure 3.4(b)), we first locate the element in the deformed mesh that contains each node. Assuming that the global coordinates of
node $N_{\text{new}}$ that requires nodal projection is $(x_p, y_p)$, we identify node $N_{\text{old}}$ belonging to the deformed mesh that has the closest distance to $N_{\text{new}}$. We then map $(x_p, y_p)$ to local coordinates $(\xi_p, \eta_p)$ of all the element sharing node $N_{\text{old}}$ using an inverse isoparametric mapping. This can be achieved by evaluating $(\xi_p, \eta_p)$ from

\[ (x_p, y_p) = \sum_{i=1}^{n_n} N_i(\xi_p, \eta_p)(\xi_i, \eta_i), \tag{3.3} \]

where $N_i$ is the Lagrangian shape function corresponding to the $i$th node of the element, $(\xi_i, \eta_i)$ is the local coordinates of this node, and $n_n$ is the number of nodes of this element. The element in the deformed mesh for which the conditions $0 \leq \xi_p \leq 1$ and $0 \leq \eta_p \leq 1$ are satisfied is identified as the element holding node $N_{\text{new}}$. We can then easily interpolate the solution at that node based on its nodal values of the solution using the isoparametric mapping.

### 3.3 Implementation aspects

It is worthwhile to further discuss two implementation issues in the application of CISAMR for simulating moving boundary problems. The first issue pertains to the projection algorithm described above, as $N_{\text{new}}$ may fall outside the discretized boundary of the deformed mesh. As shown in Figure 3.5(a), this could happen due to the geometric discretization error associated with different discretization patterns in the old and new meshes. Although by using sufficient levels of refinement in the SAMR phase this geometric discretization error would be negligible, the conditions $0 \leq \xi_p \leq 1$ and $0 \leq \eta_p \leq 1$ may still not be satisfied in all the elements sharing $N_{\text{new}}$ during the inverse mapping. In such cases, we expand the search by introducing a small tolerance $\varepsilon > 0$ on the upper and lower bonds of these conditions (e.g., $\varepsilon \leq \xi_p \leq 1 - \varepsilon$) to locate the element closest mapped node. Note that although this
node is slightly outside the identified element in the deformed mesh, the isoparametric approach can still be employed for nodal projection with a small error provided that the geometric discretization error is negligible.

![Diagram showing deformed mesh, reconstructed mesh, and protective film](image)

Figure 3.5: (a) Lower right portion of the corrosion pit depicted in Figure 3.4, showing a new node belonging to the reconstructed mesh that falls outside the discretized domain of the old (deformed) mesh after mapping; (b) upper left portion of the pit in Figure 3.4(a), showing the moving boundary velocity at the intersection point of the pit interface and the metal surface.

The second implementation issue that worths discussing here is related to calculating the moving boundary velocity at the intersection point of the pit interface and the metal surface covered with a protective film in pitting corrosion problems (Figure 3.5(b)). The gradient discontinuity of the domain boundary at this point leads to a higher error in recovering the gradient, which in turn deteriorates the accuracy of the moving interface velocity $v_n$ evaluated using (2.3) in diffusion-controlled pitting corrosion problems. What increases the error in computing $v_n$ at this point even further is the difference between the boundary conditions imposed along the metal surface (non-corroding, $\nabla c \cdot n = 0$) and the pit interface (corroding, $\bar{c} = c_{sat}$). Hence, recovering the gradient at this point via the nodal averaging scheme and using that in (2.3) to evaluate $v_n$ leads to under-estimation of the velocity, which would deteriorate
the accuracy as the simulation proceeds. To resolve this issue, we extrapolate the velocity $v_c$ at the pit corner points based on the velocity $\bar{v}_n$ of its neighboring point as (Figure 3.5(b))

$$v_c = \frac{\bar{v}_n}{n_c \cdot e_1},$$

(3.4)

where $n_c$ is the outward unit normal vector to the interface at the corner point and $e_1$ is the basis vector of the Euclidean space in the direction of the metal surface (horizontal direction in Figure 3.5(b)). Note that the velocity $v_c$ evaluated using (3.4) at the corner point of the pit is the projection of the normal velocity on the metal surface in the direction of the tangent vector at this point.
Chapter 4: Accuracy studies

In this chapter, three example problems are approximated using the CISAMR model to verify its accuracy and convergence. The first example employs CISAMR to simulate a two-dimensional moving boundary problem with analytical solutions. Its convergence rate versus the background FE element size and the effect of the level of SAMR phase are studied. The second verification study simulates a semi-circular pitting corrosion problem, and the results are compared with those derived from the phase field model introduced in [81]. Finally, the modified pencil electrode test is employed to verify that the CISAMR corrosion model satisfies the mass conservation law.

4.1 Convergence study

In this example, we study the accuracy and convergence rate of CISAMR for modeling a moving boundary diffusion problem with the geometry and boundary condition depicted in Figure 4.1(a). The circular region located at the center of this 5 mm × 5 mm domain has an initial radius of \( R(0) = 960 \, \mu m \) and an initial concentration of \( c(x, 0) = \exp (-|x|^2/4D) \). Analytical solutions for the evolution of the field and radius of the circle can be written as

\[
c(x, t) = \frac{1}{t + 1} \exp \left( -\frac{x \cdot x}{4D(t + 1)} \right),
\]  

(4.1)
\[ R(t) = \sqrt{-4D(t+1) \ln[\bar{c}(t+1)]}, \quad (4.2) \]

where \( D = 0.05 \text{ mm}^2/\text{s} \) and \( \bar{c} = 0.01 \text{ mol/L} \) is the prescribed Dirichlet boundary condition along the perimeter of the circle.

To simulate this problem using a prescribed normal velocity \( \bar{v}_n \) along the domain boundary, we employ (4.2) to analytically evaluate the interface velocity as \( \bar{v}_n = \frac{\partial R(t)}{\partial t} \).

The CISAMR approximation of the field at \( t = 0.6 \text{ s} \) using a \( 20 \times 20 \) background mesh for discretizing the domain with two levels of SAMR is depicted in Figure 4.1(b) \((\Delta t = 0.05 \text{ s})\). The radius of the circle at this time step has approximately increased by 20\%. The other three quarters of Figure 4.1(b) characterize the quality of the conforming elements generated using the CISAMR based on three metrics: aspect ratio \( R_a \), edge ratio \( R_e \), and minimum angle \( \theta_{\text{min}} \). The first two metrics are evaluated as \([66]\)

\[ R_a = \frac{L_{\text{max}} \sum_{i=1}^{3} L_i}{4\sqrt{3}A}, \quad R_e = \frac{L_{\text{max}}}{L_{\text{min}}}, \quad (4.3) \]

where \( L_i \) and \( A \) are the edge length and area of the element, respectively. This figure confirms that CISAMR is capable of generating high-quality conforming elements with \( \max(R_a) = 1.84, \max(R_e) = 2.41, \) and \( \min(\theta_{\text{min}}) = 25.8, \) without relocating the nodes of the background mesh away from the moving interface.

The variations of the \( L_2 \) and \( H^1 \) norms of the error versus the element size \( h \) for the CISAMR approximation of this problem using a prescribed interface velocity is presented in Figure 4.2(a). In each element, the norms of the error at a given time step can be computed as

\[ E_{L_2} = \sqrt{\int_{\Omega} (c_{\text{ex}} - c^h)^2 \, d\Omega}, \quad E_{H^1} = \sqrt{\int_{\Omega} \left[ (c_{\text{ex}} - c^h)^2 + (\nabla c_{\text{ex}} - \nabla c^h)^2 \right] \, d\Omega}, \quad (4.4) \]
Figure 4.1: First example problem: (a) schematic of the domain geometry and initial/boundary conditions; (b) CISAMR approximation of the field (top left quarter) and three mesh quality metrics at $t = 0.6$ s using a $20 \times 20$ background mesh with two levels of SAMR for discretizing the domain ($\Delta t = 0.05$ s).

where $c_{ex}$ and $c^h$ are the exact and approximate fields, respectively. Five structured meshes with 10, 20, 30, 40, and 50 elements along each edge are employed to create conforming meshes with 0, 1, and 2 levels of SAMR. In the absence of the $h$-adaptive refinement, the CISAMR yields the optimal convergence rates of 2.01 and 1.03 for the $L_2$ and $H^1$ norms of the error, respectively (measured between the last two data points). Due to the creation of smaller conforming elements along the interface for meshes with one and two levels of SAMR, the improved convergence rates in the corresponding plots in Figure 4.2(a) is not meaningful. However, specially for the $L_2$-norm of the error, it can be seen that the adaptive refinement along the interface has a notable impact on improving the accuracy. For example, the $L_2$-norm of the error associated with the $50 \times 50$ background mesh with two levels of SAMR is
approximately 174\% lower than that corresponding to the same mesh with no \(h\)-adaptive refinement. Note that in this problem, increasing the number of SAMR levels has no appreciable impact on reducing \(E_{H^1}\), as the maximum curvature of \(c(x, t)\) occurs at the center of the circular-shaped domain, which is away from the refinement zone.

\begin{figure}[h]
\centering
\begin{subfigure}{0.45\textwidth}
\includegraphics[width=\textwidth]{figure4a.png}
\caption{}
\end{subfigure}
\begin{subfigure}{0.45\textwidth}
\includegraphics[width=\textwidth]{figure4b.png}
\caption{}
\end{subfigure}
\caption{First example problem: variations of the \(L_2\) and \(H_1\) norms of the error versus the element size \(h\) for three different levels of SAMR. (a) prescribed interface velocity; (b) non-prescribed interface velocity evaluated using (4.5).}
\end{figure}

In order to better demonstrate the impact of the \(h\)-adaptive refinement phase of the CISAMR algorithm on reducing local errors, we adopted a second approach for simulating this problem by removing the prescribed velocity along the moving interface. Instead, the normal velocity in the new simulations is evaluated as a function of the field gradient along the interface, which is obtained based on the temporal
derivative of (4.1) as

\[ v_n = \frac{\bar{c}}{(t + 1) \nabla c} \cdot \mathbf{n} \{\ln[\bar{c}(t + 1)] + 1\}, \quad \forall \mathbf{x} \in \Gamma_s. \] (4.5)

The resulting variations of the \( L_2 \) and \( H^1 \) norms of the error versus \( h \) for the same background meshes and SAMR levels as those of the prescribed velocity cases are depicted in Figure 4.2(b). As expected, the approximation of the normal interface velocity for evolving the domain morphology at each time increment leads to a sub-optimal convergence rate of 1.72 for the \( L_2 \)-norm of the error. This is because the velocity evaluated using (4.5) is a function of the recovered gradient of the field along the interface, which has a slower convergence rate than the field approximation. Thereby, the accumulation of the error corresponding to predicting the evolving domain morphology throughout the simulation disturbs the optimal convergence rate observed in the prescribed velocity simulations illustrated in Figure 4.2(a). However, due to the local nature of this error, the SAMR of the domain in the vicinity of the interface has a considerably more pronounced impact on reducing \( E_{L_2} \) compared to the prescribed velocity cases. For example, as shown in Figure 4.2(b), applying two levels of SAMR to the 50 × 50 background mesh leads to more than 243% decrease in the error compared to the case with no refinement. This study shows the effectiveness of the adaptive refinement in more precise evaluation of the moving interface velocity, which in turn leads to a more accurate approximation of the field. It is worth mentioning that we can still recover the optimal convergence rate for \( E_{H^1} \), although values of the error are slightly larger than those of the simulations with a prescribed interface velocity.

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4.2 Verification study: Semi-circular pitting corrosion

In this example, we implement the CISAMR to simulate the diffusion-controlled and activation-controlled growth of a semi-circular shaped corrosion pit in a stainless steel plate, as shown in Figure 4.3(a). For the diffusion-controlled case, $\bar{c} = 0$ mol/L and $\bar{c} = c_{\text{sat}}$ are assigned along the electrolyte and the corroding pit boundaries, respectively. Also, a zero flux boundary condition ($\nabla c \cdot n = 0$) is imposed along the horizontal metal surface to replicate the intact protective passive film on this surface. We assume that the initial ions concentration in the electrolyte solution is zero everywhere, i.e., $c(x,0) = 0$ mol/L. For the activation-controlled problem, we replace the Dirichlet boundary condition along the pit interface with the Robin boundary condition given in (2.2), while assuming that a uniform overpotential of $\eta = 63$ mV. This overpotential corresponds to a moving interface normal velocity of $v_n \approx 2$ nm/s, which is evaluated using (2.4).

The main objective of the current example is to verify the accuracy of CISAMR simulations of pitting corrosion problems through comparing the results with similar simulations conducted using the phase field corrosion model presented in [81]. The phase field method simulates the growth of a corrosion pit using an auxiliary phase field variable to track the evolution of the moving pit interface. In the context of the FEM, using the phase field variable allows the implementation of a nonconforming mesh for discretizing the domain, although this increases the computational cost due to the requirement to solve for this additional variable at each time step. To obtain a reference solution using the phase field model to compare with CISAMR results in this example, we use a refined mesh composed of six-node Lagrangian elements with a maximum size of 25 $\mu$m for discretizing the domain. Adaptive mesh
Figure 4.3: Second example problem: (a) schematic of the domain geometry; (b) comparison between the predicted pit depth growth versus time during the diffusion-controlled pitting corrosion using the CISAMR and phase field techniques.

Refinement is also employed in the vicinity of the pit interface to more accurately approximate the sharp gradients in this region, resulting in 350,534 degrees of freedom (DOFs) in the first time step. Note that as the pit grows, the number of DOFs constantly increases in the subsequent time steps. It is worth mentioning that the phase field simulations presented here are conducted using an adaptive time marching scheme with a maximum allowable time step of $\Delta t = 0.5$ s. However, the first few time increments needed for convergence in the phase field simulation are considerably smaller ($\Delta t \approx 10^{-7}$ s).

The comparison between the CISAMR and phase field simulations for the evolution of the pit depth versus time in the diffusion-controlled problem is presented in Figure 4.3(b). The CISAMR simulation is conducted using a $30 \times 30$ background mesh for discretizing the domain and a time increment of $\Delta t = 2.5$ s. Also, two levels
Table 4.1: Values of the parameters used in the pitting corrosion example problems.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{\text{solid}}$</td>
<td>143 mol/L</td>
<td>$c_{\text{sat}}$</td>
<td>5.1 mol/L</td>
</tr>
<tr>
<td>$D$</td>
<td>$8.5 \times 10^{-10}$ m$^2$/s</td>
<td>$n$</td>
<td>2.1 equiv/mol</td>
</tr>
<tr>
<td>$F$</td>
<td>96485 C/equiv</td>
<td>$i_0$</td>
<td>1.422 mA/cm$^2$</td>
</tr>
<tr>
<td>$b_a$</td>
<td>45.1 mV</td>
<td>$\eta$</td>
<td>63 mV</td>
</tr>
</tbody>
</table>

of adaptive refinement is applied to the mesh in the SAMR phase. The material properties used in this example and all the following examples (unless stated otherwise) are presented in Table 4.1. As shown in Figure 4.3(b), both the CISAMR and the phase field methods yield similar approximations of the pit depth at any given time, with a maximum relative error of 2.3%, which happens at $t \approx 60$ s. Note that while the CISAMR simulation starts with a prescribed concentration of $\bar{c} = c_{\text{sat}}$ along the pit interface, the phase field method does not allow prescribing this Dirichlet boundary condition. Therefore, the concentration along the pit interface in the phase field model ramps up from 0 mol/L to $c_{\text{sat}}$ in the first few time steps, which accounts for the initial discrepancy between the results shown in Figure 4.3(b). However, due to the diffusion of ions away from the pit bottom, this initial effect fades in subsequent time steps, resulting in a considerably smaller relative error of only 0.19% at the last time step ($t = 400$ s). A comparison between the morphologies of the pits obtained from the CISAMR and phase field simulations at this time step is provided in Figure 4.4(a).

Figure 4.4(b) illustrates the CISAMR approximations of the ions concentration and the pit morphology at last time step ($t = 3.89$ h) of the activation-controlled pitting problem. This figure also shows the results obtained from the corresponding
Figure 4.4: Second example problem: Comparison between the CISAMR and phase field simulations of the evolved pit morphologies at the last time step for (a) diffusion-controlled pitting, \( t = 400 \) s; (b) activation-controlled pitting, \( t = 3.89 \) h.

Phase field simulation, which predicts a similar distribution of ions concentration in the pit. Note that the maximum ions concentration in this case \( (c_{\text{max}} = 0.078 \text{ mol/L}) \) is well below \( c_{\text{sat}} \) and thereby the activation-controlled assumptions used in these simulations is valid. Further, the pit maintains its semi-circular shape, as a constant velocity obtained from (2.4) is assigned along the pit interface throughout the simulation. This velocity is considerably smaller than the diffusion-controlled velocity evaluated using (2.3) and thereby a larger time step \( (\Delta t = 100 \text{ s}) \) is used for the CISAMR simulation of this activation-controlled problem. It must be noted that during the simulation of both the diffusion-controlled and activation-controlled phenomena, the maximum aspect ratio of conforming elements generated using the CISAMR is lower than 1.70.

4.3 Verification study: Modified pencil electrode test

In this example, we present a modified pencil electrode corrosion test to verify that the CISAMR corrosion model satisfies the mass conservation law. The initial
and boundary conditions for this problem are shown in Figure 4.5(a), where the bare metal surface is exposed to an electrolyte solution. In the pencil electrode test, the metal wire and the electrolyte are surrounded by epoxy, which is equivalent to the insulated boundary condition for the concentration field on the left and right edges of the domain. Under the diffusion-controlled condition, the pit surface remains flat and only moves in the longitudinal direction. A standard pencil electrode test is designed such that the pit mouth has the same concentration as the bulk solution [81, 63]. However, in this example we assume that the pit mouth is covered (e.g., with a porous glass separator) such that the exchange of water between the bulk and pit solution is allowed but the ions cannot be transferred outside the pit. Therefore, the growing pit is always filled with the electrolyte and the average ions concentration is constantly increasing until it reaches \( c_{\text{sat}} \). Since according to (2.3) mass transfer is the rate-limiting step in diffusion-controlled pitting corrosion, after reaching \( c_{\text{sat}} \) everywhere in the pit, \( \nabla c(x, t) \cdot n = 0 \) along the interface and thereby the pit can no longer grow.

Using the mass conservation law, we can analytically determine the final depth \( d_f \) of the pit as

\[
d_f = \frac{c_{\text{solid}}d_i}{c_{\text{solid}} - c_{\text{sat}}},
\]

where \( d_i \) is the initial pit depth. In this example, the metal wire has a radius of 100 \( \mu m \) and the initial pit depth is \( d_i = 301 \mu m \). To perform the simulation, an \( 80 \times 16 \) background mesh with two levels of refinement is employed to build the FE mesh using the CISAMR (time increment: \( \Delta t = 4 \) s). We also assume \( c_{\text{solid}} = 30 \text{ mol/L} \) to allow an appreciable growth of the pit depth in this example. The simulated variation of the pit depth versus time is depicted in Figure 4.5(b), which shows that the CISAMR
predicts a similar value as the analytical solution evaluated using (4.6) for the final pit depth, with a relative error of 0.14%. This figure also shows that the growth rate of the pit is higher at the beginning of the simulation due to a higher concentration gradient along the pit interface. However, the growth rate gradually decreases and eventually stops when the electrolyte is fully saturated with dissolved ions. Three snapshots of the pit geometry in this simulation, together with the evolution of the ions concentration, are illustrated in Figure 4.5(a). Note that at the last time step \((t = 300 \text{ s})\), the ions concentration is equal to \(c_{\text{sat}} = 5 \text{ mol/L}\) everywhere inside the pit.

Figure 4.5: Third example problem: (a) schematic of the domain geometry and boundary conditions; (b) CISAMR prediction of the variation of pit depth versus time and its comparison with the analytical solution.
Chapter 5: Application

This chapter presents two example problems simulated by CISAMR. The first example presents the simulation of electropolishing process of a stainless steel specimen. The second example presents the simulation of the growth of three arbitrary-shaped corrosion pits under activation-controlled and diffusion-controlled conditions.

5.1 Electropolishing

In this example, we employ the CISAMR to simulate the electropolishing of a stainless steel specimen with the geometric features shown in Figure 5.1. The electropolishing is commonly used in industry to reduce the surface roughness of metallic parts by applying a high electric voltage that induces diffusion-controlled corrosion on the metal surface. The boundary conditions used for simulating this phenomenon is similar to the first example problem with the difference that the zero-flux boundary condition associated with the portion of the metal surface covered by the passive film is eliminated. The simulated evolution of the metal surface during the electropolishing process is depicted in Figure 5.1. As shown in this figure, this diffusion-controlled corrosion process leads to smoothening of the metal surface and removing the roughness. This is because of the smaller diffusion distance and hence the higher ions concentration gradient near the peak points, which results in a higher corrosion rate.
near these regions. Figure 5.1 also illustrates a portion of the $20 \times 20$ background mesh used for discretizing the domain, together with the conforming elements generated using the CIASMR at each snapshot. The maximum element aspect ratio recorded during this simulation is 1.69.

Figure 5.1: Fourth example: Schematic of the domain geometry and the CISAMR simulation of the evolution of the surface roughness and dissolved ions concentration during the electropolishing process.

5.2 Growth of arbitrary-shaped corrosion pits

In this final example problem, we employ the CISAMR to simulate the growth of three pits with complex initial morphologies, as shown in Figure 5.2. The simulations
are conducted under both diffusion-controlled and activation-controlled conditions. The initial and boundary conditions are similar to those described in the second example problem (Figure 2.1). A $20 \times 20$ background mesh is employed to create the FE models for all three pits using the CISAMR, with two levels of refinement in the SAMR phase.

![Pit 1, Pit 2, Pit 3](image)

Figure 5.2: Fifth example problem: Domain geometry and initial shapes of corrosion pits.

The CISAMR simulation of the evolving pits morphologies under the diffusion-controlled condition is depicted in Figure 5.3. As shown in that figure, the diffusion-controlled process leads to opening of the pit mouth, while causing a considerably less growth at the pit bottom. This is due to the lower concentration of ions near the pit mouth compared to the pit bottom, which in turn leads to a higher concentration gradient and thereby higher interface velocity according to (2.3) in the former region. Note that the low concentration of ions in the bulk electrolyte in the vicinity of the pit mouth accelerates the diffusion of ions away from the interface, which justifies the lower ions concentration observed there. Figure 5.3 also shows the evolution of the conforming meshes generated using the CISAMR in each simulation.
Figure 5.3: Fifth example problem: Diffusion-controlled CISAMR simulation of evolving shapes of three corrosion pits with different initial geometries and the corresponding approximate concentration fields.

Figure 5.4 illustrates the CISAMR approximation of the concentration field during the activation-controlled growth of the pits shown in Figure 5.2. Due to the lower velocity of the pit interface in this condition ($v_n \approx 2 \text{ nm/s}$), these simulations are conducted over a longer time period ($t_{\text{max}} \approx 10 \text{ h}$) to allow an appreciable pit growth. Note that in these simulations, the ions concentration in the electrolyte is built up at the pit bottom, with the maximum value at the deepest point of the pit. This
trend is attributed to the slow growth of the pit, which allows the dissolved ions near
the pit mouth to fully diffuse into the bulk electrolyte. However, as the pit grows,
the increase of the diffusion distance near the pit bottom leads to the increase of
the ions concentration in this region, as observed in Figure 5.4. It must noted that
the maximum element aspect ratio during the evolution of all three meshes in both
diffusion and activation controlled problems does not exceed 2.04.

Figure 5.4: Fifth example problem: Activation-controlled CISAMR simulation of
evolving shapes of three corrosion pits with different initial geometries and the cor-
responding approximate concentration fields. The values of $c_{\text{max}}$ for pits 1, 2, and 3
are 0.174 mol/L, 0.169 mol/L, and 0.257 mol/L, respectively.
Chapter 6: Conclusion and future work

In conclusion, the Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) technique was implemented to simulate moving boundary transient diffusion phenomena, with the activation-diffusion-controlled pitting corrosion selected as the main application problem. The CISAMR is a non-iterative algorithm that transforms a structured grid into a high quality conforming mesh using a combination of customized $h$-adaptivity, $r$-adaptivity, and sub-triangulation algorithms. The key feature that highly facilitates the application of this method for modeling moving boundary problems is that the background mesh is only modified in the vicinity of the materials interface. In other words, none of the nodes of elements not intersecting with the interface are relocated throughout the mesh transformation and directly inherit the nodal solution values from the old mesh, which also reduces the error associated with nodal projection process. We discussed several implementation issues pertaining to the application of CISAMR for modeling moving boundary problems and in particular the pitting corrosion phenomenon. In addition to a detailed convergence study, two benchmark problems were presented to verify the accuracy of this method for modeling corrosion problems versus analytical and phase field simulation results. We also presented two example problems to demonstrate the application of CISAMR for simulating corrosion problems with complex geometries, including the
electropolishing of stainless steel and the growth of arbitrary-shaped corrosion pits under activation-controlled and diffusion-controlled conditions.

For future work, one of the advantages of CISAMR is that it can accurately describe interface between two phases. Therefore, CISAMR can be employed for simulating moving boundary phenomenon in materials with complex micro structures, such as metallic alloys and polycrystalline materials. Besides, the current CISAMR framework is only limited in 2D cases, which does not demonstrate the full potential of this new numerical technique. Efforts will be made to expand the method to simulate three-dimensional moving boundary problem, which would provide more realistic prediction of phase transformation phenomenon.
Bibliography


