An unfitted finite element method for the numerical approximation of void electromigration

Robert Nürnberg*, Andrea Sacconi*

*Department of Mathematics, Imperial College, London, SW7 2AZ, UK

Abstract

Microelectronic circuits usually contain small voids or cracks, and if those defects are large enough to sever the line, they cause an open circuit. We present a numerical method for investigating the migration of voids in the presence of both surface diffusion and electric loading. Our mathematical model involves a bulk-interface coupled system, with a moving interface governed by a fourth-order geometric evolution equation and a bulk where the electric potential is computed. Thanks to a novel approximation of the interface, equidistribution of its vertices is guaranteed, and no remeshing is necessary. In addition, the used curvature approximation means that our method is unconditionally stable for the evolution by surface diffusion only. Various examples are performed to demonstrate the accuracy of the method.

1. Introduction

Microelectronic circuits contain thin lines of aluminium alloy, that make electric contact between neighbouring devices possible. As producers try to reduce the dimensions of microchips further and further, and since interconnects always contain small voids or cracks, it is of great interest to investigate the physical mechanisms that impede such a reduction, due to mechanical failures in the lines induced by the motion of the cracks. The problem considered in this paper involves the evolution over time of voids in a conducting metal line where two different effects contribute to the drift of the voids: the surface tension and the electric field. This phenomenon is known as electromigration; for further details see, e.g., [29, 16], and the references therein.

As the height of interconnect lines is extremely thin compared to the dimensions of the base, voids generally fully penetrate in this vertical direction. Hence in this paper we restrict ourselves to a two dimensional model of void electromigration. In addition, we idealise the interconnect line as a rectangular solid, which conducts electric current. The electric field is induced in the line by prescribing the voltage on its vertical boundaries; we assume that the electric field in the line is invariant in the direction that is normal to the plane of the figure. The initial shape of the void is assumed to be known. Surface diffusion may cause voids to change their shape. When there is no electric loading, the void will approach the shape that minimises the total surface free energy, i.e. a circle. When an electric field is present, on the other hand, it too is responsible for driving diffusion on the void surface, and this may lead the void to drift through the conductor as well as changing its shape. Overall, a complicated free boundary problem is obtained.

In this paper, we will introduce a novel front-tracking finite element method for the approximation of void electromigration. Our approximation uses two totally independent meshes, one for the parametric approximation of the moving boundary and one for the finite element approximation of the bulk quantities. An advantage of this unfitted finite element approach, compared to other direct front-tracking methods, is that costly remeshings of the bulk grid are avoided. A typical mesh for the unfitted approach is shown in Figure 1. Moreover, our novel discretisation of the moving boundary means that the vertices on the discrete interface equidistribute asymptotically. In particular, no reparameterisation of the discrete interface is necessary.

*Corresponding author

Email addresses: robert.nurnberg@imperial.ac.uk (Robert Nürnberg), a.sacconi11@imperial.ac.uk (Andrea Sacconi)
The paper is organised as follows: in Section 2 we give a mathematical description of the problem of void electromigration that we are interested in. We also give a brief overview of the different numerical methods applicable to this problem. Section 3 contains a detailed description of our proposed finite element approximation. In Section 4 we discuss possible solution methods of the algebraic system of equations arising at each time level. In addition, we present details on the mesh adaptation strategy used, as well as on the algorithm that defines the discrete approximation to the conductor regions. Finally, in Section 5 we perform a convergence experiment for a situation in which an exact solution is known, and we present various other examples of the applications of our numerical method.

2. Problem formulation

For the formulation of the governing equations we closely follow the presentation in [8]. Let \( \Omega = (-L_1, L_1) \times (-L_2, L_2) \), where \( L_1, L_2 > 0 \), be the domain that contains the conductor. We denote the boundary of \( \Omega \) with \( \partial \Omega \). At any time \( t \in [0, T] \), let \( \Gamma(t) \subset \Omega \) be the boundary of the void \( \Omega_-(t) \) inside the conductor \( \Omega \). Then \( \Gamma(t) = \partial \Omega_-(t) \) and \( \Omega_+(t) := \Omega \setminus \Omega_-(t) \) denotes the conducting region (see Figure 2). Now the evolution of the interface \( \Gamma(t) \), which represents the void boundary, is given by

\[
\dot{\nu} = -\alpha_1 \kappa_{ss} + \alpha_2 \phi_{ss},
\]

where \( \nu \) represents the velocity of \( \Gamma(t) \) in the direction \( \nu \) (the unit normal to \( \Gamma(t) \) pointing into \( \partial \Omega_-(t) \)), \( s \) is the arc-length of the curve, \( \kappa \) is the curvature of \( \Gamma(t) \) (positive when \( \Omega_-(t) \) is convex). In particular, it holds that

\[
\hat{x}_{ss} = \kappa \nu,
\]

where \( \hat{x} \) is a suitable parameterisation of \( \Gamma(t) \), i.e. \( \Gamma(t) = \hat{x}(I, t) \), with \( I = \mathbb{R} / \mathbb{Z} \) denoting the “periodic” interval \([0, 1]\). Moreover, \( \phi(t) \) is the electric potential that satisfies a Laplace equation in \( \Omega_+(t) \), i.e.:  

\[
\begin{align*}
\Delta \phi &= 0 \quad \text{in } \Omega_+(t), \\
\frac{\partial \phi}{\partial \nu} &= 0 \quad \text{on } \Gamma(t), \tag{3a}
\end{align*}
\]

\[
\begin{align*}
\frac{\partial \phi}{\partial \nu} &= 0 \quad \text{on } \partial_1 \Omega, \\
\phi &= g^\pm \quad \text{on } \partial_2 \Omega. \tag{3b}
\end{align*}
\]

In the above, \( g^\pm := \pm L_1 \) denotes the Dirichlet boundary condition on parts of \( \partial \Omega \), where \( \partial \Omega = \partial_1 \Omega \cup \partial_2 \Omega \), with \( \partial_1 \Omega \cap \partial_2 \Omega = \emptyset \) and

\[
\partial_2 \Omega = \partial_2^- \Omega \cup \partial_2^+ \Omega \quad \text{with} \quad \partial_2^\pm \Omega := \{ \pm L_1 \} \times [-L_2, L_2].
\]
The Dirichlet boundary conditions in (3b) model a uniform parallel electric field, \( \phi \approx x_1 \) as \( L_1 \to \infty \). Finally, \( \alpha_1 \in \mathbb{R}_{>0} \) and, without loss of generality (see, e.g., [16, p. 101]), \( \alpha_2 \in \mathbb{R}_{\geq 0} \) are given parameters depending on the conductor and on the strength of the electric field. The first term on the right-hand side of (1) is surface diffusion due to interfacial tension, which models atoms moving around the boundary of the void to positions of large curvature, whereas the second term is surface diffusion due to the electric field. The void electromigration model is then the coupled system of equations (1), (3a) and (3b). In the case \( \alpha_2 = 0 \), the evolution (1) is called surface diffusion, which is an example of a geometric evolution equation. A local existence result for the motion by surface diffusion can be found in [19]. Moreover, it was shown that a global solution exists if the initial curve, \( \Gamma(0) \), is close to a circle and that it converges to a circle. Numerical approximations of surface diffusion have been proposed in [2, 4, 6], and we refer to [18] for a review of possible numerical approaches for the approximation of geometric evolution equations in general. For \( \alpha_2 \geq 0 \), the motion (1) preserves the area enclosed by the closed curve \( \Gamma(t) \) since

\[
\frac{d}{dt}|\Omega_-(t)| = -\int_{\Gamma(t)} \mathcal{V} \, ds = 0,
\]

where \(|D|\) is the measure of a domain \( D \). In addition, for \( \alpha_2 = 0 \) this motion decreases the length of the interface since

\[
\frac{d}{dt}|\Gamma(t)| = -\int_{\Gamma(t)} \mathcal{V} \kappa \, ds = -\alpha_1 \int_{\Gamma(t)} (z_2)_s^2 \, ds \leq 0.
\]

For later use we recall the following true solution of a circular void, moving at constant speed through an infinite conductor. That is, for any \( \alpha_i \in \mathbb{R}_{\geq 0} \), \( R \in \mathbb{R}_{>0} \), and \( z = (z_1, z_2) \in \mathbb{R}^2 \),

\[
\Gamma(t) := \{ x \in \mathbb{R}^2 : (x_1 - z_1(t))^2 + (x_2 - z_2)^2 = R^2 \}, \quad z_1(t) := z_1 + \frac{2\alpha_2}{R} t,
\]

where the corresponding electric potential

\[
\phi(x, t) = \left[ x_1 - z_1(t) \right] \left[ 1 + \frac{R^2}{(x_1 - z_1(t))^2 + (x_2 - z_2)^2} \right]
\]

solves (1) and (3) with

\[
\Omega_+ \text{ in (3a) replaced by } \mathbb{R}^2 \setminus \Omega_-(t) \text{ and (3b) replaced by } \nabla \phi \to (1,0)^T \text{ as } |x| \to \infty.
\]
Observe that (1) reduces to $V = -\frac{2\alpha^2}{l^2} [x_1 - z_1(t)]$ on $\Gamma(t)$. The explicit solution (6a), (6b) was first noted in [20].

The void electromigration problem (1) and (3) represents a complicated free boundary problem. In general, the numerical solution of partial differential equations for systems with moving boundaries can be approached in different ways. The most direct choice is an explicit tracking of the interface. In these front tracking methods the interface is either triangulated or represented by a connected set of particles, which carry forces. The interface is then transported using the given normal velocity of the interface. Since the interface is tracked directly, these methods are also called sharp interface approximations. Examples of such methods for the approximation of void electromigration can be found in [13, 22, 29]. In this paper we propose a new front tracking method for void electromigration that will be based on a parametric description of the moving interface.

Also in the level set method, see [26], the interface is assumed to be sharp. But here the interface is represented as the zero level set of a smooth function, which means that topological changes are handled naturally. We refer to [23, 28, 1] for examples of the application of the level set method to the approximation of void electromigration.

Finally, in phase field methods, the sharp interface is replaced by a diffusive interfacial layer, in which a phase field variable rapidly changes between two different constant values that represent the void and the conductor, respectively. It can often be formally shown that if the interfacial thickness goes to zero, then the original sharp interface problem is recovered. Since the interface is only captured implicitly in the phase field method, changes of topology occur naturally. We refer to [24, 25, 12, 8, 5] for different phase field approximations of void electromigration.

In what follows, we will group the types of methods described above into either implicit or explicit methods, depending on how they represent the free boundary. Of course, implicit and explicit methods differ in the way they handle topological changes, such as pinching-off and merging. The fact that such topological changes occur naturally within the framework of implicit methods is often perceived as their main advantage over explicit methods. However, with modern tools available to incorporate topological changes into explicit methods, see e.g. [14], this advantage is diminishing. In fact, within explicit methods it is possible to draw up a list of heuristic criteria which trigger a topological change. In contrast to implicit methods, where topological changes take place automatically, this gives some active control over the topological changes, see also [21]. In addition, explicit methods have the advantage that the partial differential equation that governs the evolution of the interface can be solved with numerical methods in one dimension lower than is the case for implicit methods, where the interface is usually captured as the zero level set of an auxiliary function. Finally, in applications where geometric quantities of the interface are of interest, implicit methods face the difficulty of having to extract an explicit representation of the interface from the implicit definition, which in general is a nontrivial operation, especially in higher space dimensions.

The approach proposed in this paper belongs to the explicit front tracking category. The main difference to existing methods, see [13, 22, 29], is that our approach is based on a variational formulation of (1) and (3), that includes a novel treatment of curvature, which was first introduced in [4]. Moreover, in contrast to existing methods, we use an unfitted finite element grid for the approximation of (3). The main drawback of existing front tracking methods for the approximation of void electromigration is that a new grid for the approximation of $\Omega_+(t)$ has to be created at each time step. We avoid this remeshing, and the associated numerical effort, by maintaining a triangulation of the whole domain $\Omega$ throughout. Altogether, the main advantages of our approach can be briefly summarised as follows.

- the method is unfitted: the bulk grid and the interface grid are totally independent. This feature means that there is no need to re-mesh or deform the bulk mesh in order to preserve the correspondence with the interface;
- the method shows good properties for the interface mesh: the parametric approximation of the interface motion leads to an asymptotic equidistribution of vertices, without any necessity of refining or re-meshing the interface grid;
- a novel approximation of curvature means that the method for integrating the surface diffusion equation is unconditionally stable;
• the area enclosed by the curve is preserved for a semidiscrete variant of our scheme;
• the method can handle initial geometries, where more than one void is present, as well as topological changes that occur during the evolution.

3. Finite element approximation

As already pointed out earlier, our approach is based on a coupled bulk-interface algorithm. We begin with the finite element spaces needed for the approximation of the moving boundary \( \Gamma(t) \). To this end, let \( I := \mathbb{R} / \mathbb{Z} = \bigcup_{j=1}^{N} I_j, N \geq 3 \), be a decomposition of \( I \) into intervals given by the nodes \( q_j, I_j = [q_{j-1}, q_j] \).

Here \( I \) is the “periodic” interval \([0,1]\), which we obtain by identifying points \( q \in \mathbb{R} \) and \( q + k \) for \( k \in \mathbb{Z} \).

Let \( h_j = |I_j| \) and \( h = \max_{j=1,...,N} h_j \) be the maximal length of a grid element. Then the necessary finite element spaces are defined as follows:

\[
V^h := \{ \tilde{\chi} \in C(I, \mathbb{R}^2) : \tilde{\chi} |_{I_j} \text{ is linear } \forall j = 1,\ldots, N \} =: \{ W^h \}^2 \subset H^1(I, \mathbb{R}^2),
\]

where \( W^h \subset H^1(I, \mathbb{R}) \) is the space of scalar continuous (periodic) piecewise linear functions, with \( \{\phi_i\}_{i=1}^N \) denoting the standard basis of \( W^h \). Throughout this paper, we make use of the periodicity of \( I \), i.e. \( q_N \equiv q_0, q_{N+1} \equiv q_1 \) and so on.

In addition, let \( 0 = t_0 < t_1 < \ldots < t_{M-1} < t_M = T \) be a partitioning of \([0,T]\) into possibly variable time steps \( \tau_m := t_{m+1} - t_m, m = 0,\ldots, M-1 \). We set \( \tau := \max_{m=0,...,M-1} \tau_m \). Let \( \tilde{X}^m \in V^h \) be an approximation to \( \tilde{x}(\cdot, t_m) \), and similarly \( \kappa^m \in W^h \) to \( \kappa(\cdot, t_m) \).

For scalar and vector functions \( f, g \in L^2(I, \mathbb{R}^2) \) we introduce the \( L^2 \) inner product \( \langle \cdot, \cdot \rangle_{V^m} \) over the current polygonal curve \( \Gamma^m \), which is described by the vector function \( \tilde{X}^m \in V^h \), as follows:

\[
\langle f, g \rangle_{V^m} := \int_{\Gamma^m} f \cdot g \, ds = \int_{I} f \cdot g \, |\tilde{X}_\rho^m| \, d\rho \; , \quad (7)
\]

where \( \rho \in [0,1] \) is the parameterisation variable. In addition, if \( f, g \) are piecewise continuous, with possible jumps at the nodes \( \{q_j\}_{j=1}^N \), we define the mass lumped inner product \( \langle \cdot, \cdot \rangle_{V^h}^m \) as

\[
\langle f, g \rangle_{V^h}^m := \frac{1}{2} \sum_{j=1}^{N} \|\tilde{X}^m(q_j) - \tilde{X}^m(q_{j-1})\|^2 \left( [(f \cdot g)(q_j^-) + (f \cdot g)(q_{j-1}^+)] \right) , \quad (8)
\]

where we define \( f(q_j^+) := \lim_{\varepsilon \searrow 0} f(q_j + \varepsilon) \). Furthermore, we note that

\[
f_s \cdot g_s = \frac{f_\rho \cdot g_\rho}{|\tilde{X}_\rho^m|} \quad \text{and} \quad \kappa^m = \frac{\left(\tilde{X}_\rho^m\right)^\perp}{|\tilde{X}_\rho^m|} ,
\]

where \( \perp \) acting on \( \mathbb{R}^2 \) denotes clockwise rotation by \( \frac{\pi}{2} \).

We introduce now the finite element approximation for quantities defined over the bulk mesh. Let \( \mathcal{T}^m \) be a partitioning of \( \Omega \) into disjoint open triangles \( o \) with \( h_o := \text{diam}(o) \) and \( h := \max_{o \in \mathcal{T}^m} h_o \) so that \( \Omega = \bigcup_{o \in \mathcal{T}^m} o \). Moreover, let \( \Omega^m \) and \( \Omega^m_o \) be the interior and the exterior of \( \Gamma^m \), respectively. We can then define

\[
\mathcal{T}^m_+ := \{ o \in \mathcal{T}^m : o \cap \Omega^m_o \neq \emptyset \} \quad \text{and} \quad \Omega^m_+ := \bigcup_{o \in \mathcal{T}^m_+} o . \quad (9)
\]

\( \Omega^m_+ \) is hence given by a union of bulk elements and represents a suitable approximation of \( \Omega^m_+ \), on which the electric potential is going to be computed. Associated with \( \mathcal{T}^m_+ \) we can define the standard finite element space of piecewise linear functions

\[
S^m := \{ \chi \in C(\Omega^m_+) : \chi |_{o} \text{ is linear } \forall o \in \mathcal{T}^m_+ \} ,
\]

as well as

\[
S^m_g := \{ \chi \in S^m : \chi |_{\partial^+ \Omega} = g^+ \} \quad \text{and} \quad S^m_0 := \{ \chi \in S^m : \chi |_{\partial^0 \Omega} = 0 \} .
\]
We then propose the following finite element approximation of (1) and (3). Given \( \Gamma^0 \), a polygonal approximation of \( \Gamma_0 \), for \( m = 0, \ldots, M - 1 \) find functions \((\phi^{m+1}, \hat{X}^{m+1}, \kappa^{m+1}) \in S_g^m \times \bigcup^h \times W^h\) such that

\[
\begin{align*}
\int_{\Omega^m} \nabla \phi^{m+1} \cdot \nabla \psi \, dx &= 0 \quad \forall \psi \in S^m_0, & (10a) \\
\left( \frac{\hat{X}^{m+1} - \hat{X}^m}{\tau_m} , \chi^m \right)_{\Gamma^m}^h - \alpha_1 \left( \kappa^{m+1} , \chi_s \right)_{\Gamma^m} &= -\alpha_2 \left( (\pi^h \phi^{m+1})_s , \chi_s \right)_{\Gamma^m} \quad \forall \chi \in W^h, & (10b) \\
\left( \kappa^{m+1} , \tilde{\eta}^m \right)_{\Gamma^m} + \left( \hat{X}^{m+1} - \hat{X}^m , \tilde{\eta}^m \right)_{\Gamma^m} &= 0 \quad \forall \tilde{\eta} \in V^h, & (10c)
\end{align*}
\]

where \( \pi^h : C(I) \to W^h \) is the standard interpolation operator at the nodes \( \{q_j\}_{j=1}^N \). We note that the weak formulation of (1) and (3), on which (10) is based, can be derived from (1), (2) and (3a), respectively, by multiplying with a suitable test function and then performing integration by parts. Then (10a) is a standard finite element approximation of (3), while (10b), (10c) for the case \( \alpha_2 = 0 \) collapse to the scheme introduced in [4] for (1) with \( \alpha_2 = 0 \), i.e. for the geometric evolution law of surface diffusion.

Before we can proceed to prove existence and uniqueness of a solution to the system (10), we have to make the following very mild assumption, first introduced in [4].

**Proof.** We first notice that the equations for \( \phi^{m+1} \) and \((\hat{X}^{m+1}, \kappa^{m+1})\) decouple. The existence of a unique solution for (10a) is trivial. The existence of a solution \((\hat{X}^{m+1}, \kappa^{m+1})\) for (10b), (10c) follows from uniqueness. To prove the latter we need to show that the only solution to the homogeneous system is the zero solution, and this has been shown in [4, Theorem 2.1]. We do not repeat the simple proof here, but we observe that it relies on the assumption (A).

The stability result (12) can be obtained by choosing \( \chi = \kappa^{m+1} \) in (10b) and \( \tilde{\eta} = \hat{X}^{m+1} - \hat{X}^m \) in (10c), on noting that

\[
\left( \hat{X}_s^{m+1} , \hat{X}_s^{m+1} - \hat{X}_s^m \right)_{\Gamma^m} = |\Gamma^{m+1}| - |\Gamma^m|;
\]

see [4, Theorem 2.3] for details.

We note that the stability result (12) for \( \alpha_2 = 0 \) is the direct discrete analogue of (5).

### 3.1. Semidiscrete continuous-in-time approximation

It is worthwhile to consider a continuous-in-time semidiscrete version of our fully discrete scheme (10). To this end, we introduce the following definitions, where we assume that \( \Gamma^h(t) \) is a polygonal
approximation of $\Gamma(t)$. Let $\Omega^h_{\pm}(t)$ and $\Omega^h_{\pm}(t)$ be the interior and the exterior of $\Gamma^h(t)$, respectively. We can then define $T^h_+(t) := \{ o \in T^h: o \cap \Omega^h_{\pm}(t) \neq \emptyset \}$, and $\Omega^h_{\pm}(t) := \bigcup_{o \in T^h_+(t)} o$. In addition, we define

$$S^h_2(t) := \{ \chi \in C(\Omega^h_{\pm}(t)) : \chi |_o \text{ is linear } \forall o \in T^h_+(t), \chi |_{\partial^\pm \Omega} = g^\pm \} ,$$

$$S^h_0(t) := \{ \chi \in C(\Omega^h_{\pm}(t)) : \chi |_o \text{ is linear } \forall o \in T^h_+(t), \chi |_{\partial^\pm \Omega} = 0 \} ,$$

as well as the inner products $\langle \cdot, \cdot \rangle_{\Gamma^h_0(t)}$ and $\langle \cdot, \cdot \rangle_{\Gamma^h_1(t)}$ on $\Gamma^h(t)$; analogously to (7) and (8).

The semidiscrete variant of (10) can then be formulated as follows. Let $\Gamma^h(0)$ be given. Then for $t \in (0,T)$ find $\Gamma^h(t)$, with $\Gamma^h(t) = \bar{X}^h(I,t)$ for $\bar{X}^h(t) \in \mathbf{V}^h$, and $\phi^h(t) \in S^h_0(t)$, $\kappa^h(t) \in W^h$ such that for almost all times $t \in (0,T)$ it holds that

$$\int_{\Omega^h_{\pm}(t)} \nabla \phi^h \cdot \nabla \psi \, dx = 0 \quad \forall \psi \in S^h_0(t) , \quad (13a)$$

$$\langle \bar{X}_{\bar{t}}^h, \chi \bar{\nu}^h \rangle_{\Gamma^h_0(t)} - \alpha_1 \langle \kappa^h, \chi_t \rangle_{\Gamma^h_0(t)} = - \alpha_2 \langle (\pi^h \phi^h)_s, \chi_s \rangle_{\Gamma^h_0(t)} \quad \forall \chi \in W^h , \quad (13b)$$

$$\langle \kappa^h, \bar{\nu}^h, \bar{\eta}^h \rangle_{\Gamma^h_0(t)} + \langle \bar{X}_{\bar{t}}^h, \bar{\eta}^h \rangle_{\Gamma^h_0(t)} = 0 \quad \forall \bar{\eta} \in W^h , \quad (13c)$$

where $\bar{\nu}^h(t) = - \frac{(\bar{X}_{\bar{t}}^h)^+(t)}{|(\bar{X}_{\bar{t}}^h)^+(t)|}$ is the unit normal to $\Gamma^h(t)$.

Let us define $\bar{h}_j(t) = \bar{X}^h(q_j,t) - \bar{X}^h(q_{j-1},t)$ for $j = 1, \ldots, N$. We are now in a position to prove an exact area conservation property for (13), as well as an equidistribution property.

**Theorem 3.2.** Let $(\phi^h, \bar{X}^h, \kappa^h) \in S^h_0(t) \times \mathbf{V}^h \times W^h$ be a solution of (13). Then it holds that

$$\frac{d}{dt} |\Omega^h_+(t)| = 0 , \quad (14)$$

and, if $\alpha_2 = 0$, then we also have that

$$\frac{d}{dt} |\Gamma^h(t)| \leq 0 . \quad (15)$$

Moreover, it holds that

$$|\bar{h}_j(t)| = |\bar{h}_{j-1}(t)| \quad \text{if} \quad \bar{h}_j(t) \parallel \bar{h}_{j-1}(t) \quad j = 1, \ldots, N . \quad (16)$$

**Proof.** The exact conservation of the enclosed area can be shown by choosing $\chi = 1$ in (13b) and taking into account (8). Then it holds that

$$0 = \langle \bar{X}_{\bar{t}}^h, \bar{\nu}^h \rangle_{\Gamma^h_0(t)} = \int_{\Gamma^h_0(t)} \bar{X}_{\bar{t}}^h \cdot \bar{\nu}^h \, ds = \frac{d}{dt} |\Omega^h_+(t)| , \quad (17)$$

which is the desired result (14). Furthermore, choosing $\chi = \kappa^h$ in (13b) and $\bar{\eta} = \bar{X}_{\bar{t}}^h$ in (13c) yields that

$$\frac{d}{dt} |\Gamma^h(t)| = \langle \bar{X}_{\bar{t}}^h, (\bar{X}_{\bar{t}}^h)_s \rangle_{\Gamma^h_0(t)} = - \alpha_1 \langle \kappa^h, \kappa^h \rangle_{\Gamma^h_0(t)} \leq 0 , \quad (18)$$

and so the length of the curve $\Gamma^h(t)$ decreases over time, i.e. (15) holds. A proof of (16) can be found in [4, Remark 2.4]. We repeat a modified version here for the benefit of the reader. Choosing $\bar{\eta} = (\bar{h}_{j+1} + \bar{h}_j) \phi_j \in \mathbf{V}^h$ in (13c), where we recall that $\{ \phi_j \}_{j=1}^N$ denote the basis functions of $W^h$, and noting the analogues of (8) and (11) for $\Gamma^h(t)$, yields that

$$0 = \langle \bar{X}_{\bar{t}}^h, [(\bar{h}_{j+1} + \bar{h}_j) \phi_j]_s \rangle_{\Gamma^h_0(t)} = \left[ \frac{\bar{h}_{j+1}}{|\bar{h}_{j+1}|} - \frac{\bar{h}_j}{|\bar{h}_j|} \right] \cdot (\bar{h}_{j+1} + \bar{h}_j) . \quad (19)$$

It immediately follows from (19) that $(|\bar{h}_{j+1}| - |\bar{h}_j|)(|\bar{h}_{j+1}| |\bar{h}_j| - \bar{h}_{j+1} \cdot \bar{h}_j) = 0$, which means that the
desired result (16) follows directly from the Cauchy–Schwarz inequality.

Clearly, (14) is the natural discrete analogue to the continuous area preservation property (4), while (15) is the discrete analogue of (5). Finally, (16) proves that the vertices of $\Gamma^m(t)$ equidistribute except for regions where the elements of $\Gamma^h(t)$ are locally parallel. The proof of Theorem 3.2 shows that this property, which is also called weak equidistribution property, immediately follows from (13c), which is the novel approximation of (2) first introduced in [4]. While it does not seem possible to prove the weak equidistribution property for the fully discrete scheme (10), in practice we observe that the vertices on $\Gamma^m$ asymptotically equidistribute. In particular, the vertices always remain well distributed and no remeshings need to be performed.

In addition, we observe that the fully discrete scheme (10) approximately preserves the area of $\Omega^m$. In fact, when the maximal time step size $\tau$ converges to zero, we observe that the relative area loss for simulations with (10) tends to zero. In all of the numerical simulations presented in this paper, the observed relative area loss was always less than 0.01%.

4. Solution method

Due to the special structure of the system (10), the equations for $\phi^{m+1}$ and $(\hat{X}^{m+1}, \kappa^{m+1})$ decouple. In practice, we can find the unique solution to (10) as follows. First we find $\phi^{m+1} \in S^m$ such that

$$\Theta_m \phi^{m+1} = 0, \tag{20}$$

where $\Theta_m \in \mathbb{R}^{K \times K}$ is the standard stiffness matrix for the Laplacian on $\Omega^{m,h}$, i.e.

$$(\Theta_m)_{kl} := \int_{\Omega^{m,h}} \nabla \psi^m_k \cdot \nabla \psi^m_l \, dx,$$

where $\{\psi^m_k\}_{k=1}^K$ are the basis functions of the unconstrained finite element space $S^m$. In the above we have ignored the effect of the Dirichlet boundary conditions. Hence, in practice, $\Theta_m$ and the corresponding right-hand side in (20) need to be adjusted appropriately in order to include the Dirichlet boundary conditions. For the solution of (20) we use the sparse factorisation package UMFPACK (see [17]) in practice.

Having obtained $\phi^{m+1}$ from (20), we proceed with solving the equations (10b), (10c), which give rise to the following linear system of equations, where we define $\delta \hat{X}^{m+1} = \hat{X}^{m+1} - X^m$. Find $\delta \hat{X}^{m+1} \in \underline{1}^h$ and $\kappa^{m+1} \in W^h$ such that

$$\begin{pmatrix} \alpha_1 A_m & -\frac{1}{\tau_m} \hat{N}^T_m \\ \hat{N}^T_m & \hat{A}_m \end{pmatrix} \begin{pmatrix} \kappa^{m+1} \\ \delta \hat{X}^{m+1} \end{pmatrix} = \begin{pmatrix} \alpha_2 A_m \phi^{m+1} \\ -\hat{A}_m \hat{X}^m \end{pmatrix}, \tag{21}$$

where $\phi^{m+1} \in W^h$ denotes the trace on $\Gamma^m$ of $\phi^{m+1} \in S^m$, i.e.

$$\phi^{m+1}(q_j) = \phi^{m+1}(X^m(q_j)) \quad j = 1, \ldots, N.$$

In the above, we have introduced the matrices $\hat{N}_m \in (\mathbb{R}^2)^{N \times N}$, $A_m \in \mathbb{R}^{N \times N}$ and $\hat{A}_m \in (\mathbb{R}^{2 \times 2})^{N \times N}$, with entries

$$[\hat{N}^T_m]_{kl} := (\phi_k, \phi_l \hat{d}^m)^h_{\Gamma_m}, \quad [A_m]_{kl} := (\langle \phi_k \rangle_s, \langle \phi_l \rangle_s)_{\Gamma_m},$$

where we recall that $\{\phi_k\}_{k=1}^N$ are the basis functions of our finite element space of piecewise linear continuous functions $W^h$. In addition, $[\hat{A}_m]_{kl} := [A_m]_{kl} \hat{I}d$, where $\hat{I}d \in \mathbb{R}^{2 \times 2}$ is the identity matrix.

In order to solve (21) a Schur complement approach as introduced in [4] can be used. However, in our experience a Krylov subspace iterative solver, coupled with an efficient preconditioner, directly applied to (21) performs better in practice. Hence we solve (21) with a BiCGSTAB solver, see e.g. [9]. Since the matrix of the system is not very well conditioned, a good preconditioner is required. We make use of the
following operator as preconditioner, which has also been considered in [15]:

$$P_c = \left( \alpha_1 A_m - \frac{1}{\tau_m} \tilde{N}_m^T \right)^{-1} \left( \begin{array}{c} \tilde{N}_m \\ \text{diag} (\tilde{A}_m) \end{array} \right). \quad (22)$$

Here \(\text{diag} (\tilde{A}_m)\) denotes the diagonal part of the matrix \(\tilde{A}_m\). In order to apply the preconditioner \(P_c\), we need to solve systems of the form

$$\left( \begin{array}{cc} \alpha_1 A_m & -\frac{1}{\tau_m} \tilde{N}_m^T \\ \tilde{N}_m & \text{diag} (\tilde{A}_m) \end{array} \right) \left( \begin{array}{c} \kappa \\ \delta \tilde{X} \end{array} \right) = \left( \begin{array}{c} c \\ \tilde{g} \end{array} \right). \quad (23)$$

Now (23) can be solved with a Schur complement approach, leading to

$$\left( \alpha_1 A_m + \frac{1}{\tau_m} \tilde{N}_m^T (\text{diag}(\tilde{A}_m))^{-1} \tilde{N}_m \right) \kappa + \frac{1}{\tau_m} \tilde{N}_m^T (\text{diag}(\tilde{A}_m))^{-1} \tilde{g} = c \quad (24a)$$

and

$$\delta \tilde{X} = (\text{diag}(\tilde{A}_m))^{-1} (\tilde{g} - \tilde{N}_m \kappa). \quad (24b)$$

We note that (24a) is a symmetric, positive definite system, where we observe that the second matrix on the left hand side of (24a) is a positive diagonal matrix. In practice we first solve (24a) with the direct solver UMFPACK, and then substitute in (24b). Here we note that the system matrix of (24a) only needs to be factorised once before the BiCGSTAB iteration starts, which means that the application of the preconditioner (22) during the iteration is cheap. We also stress that the dimension of the matrix in (24a) is much smaller than the matrix for the block (21). In particular, in our experience solving the block (21) with a sparse factorisation package such as UMFPACK is less efficient than the preconditioned BiCGSTAB iteration proposed above.

### 4.1. Mesh adaptation

Our unfitted finite element approximation (10) is based on triangulations \(T_m\) of the whole domain \(\Omega\), which vary in time. Here the aim is to use an adaptive mesh for \(\Omega\), where we resolve the regions close to \(\Gamma^m\) much finer than far away from the interface. The exact refinement procedure is detailed in this subsection. The selection of the elements that belong to \(T^m\), recall (9), will be described in §4.2.

Given a polygonal approximation \(\Gamma^m, m \geq 0\), of the interface, we employ the following mesh adaptation strategy for the bulk mesh triangulation \(T^m\). The same strategy has been used in [7] for an unfitted finite element approximation of anisotropic solidification problems. It results in a fine mesh around \(\Gamma^m\) and a coarse mesh further away from it. In particular, given two integer parameters \(N_f > N_c\), we set:

$$h_f = \frac{2 L_2}{N_f} \quad \text{and} \quad h_c = \frac{2 L_2}{N_c} \quad (25a)$$

$$a_f = \frac{h_f^2}{2} \quad \text{and} \quad a_c = \frac{h_c^2}{2}, \quad (25b)$$

that is, \(a_f\) denotes the area of a right-angled and isosceles triangle with side length \(h_f\), and similarly for \(a_c\).

Now starting with the triangulation \(T^{m-1}\) from the previous time step, where here for convenience we define \(T^{-1}\) to be a uniform partitioning of mesh size \(h_c\), we obtain \(T^m\) as follows. First any element \(o^{m-1} \in T^{m-1}\) satisfying \(|o^{m-1}| \geq 2 a_f\) and \(o^{m-1} \cap \Gamma^m \neq \emptyset\) is marked for refinement. In addition, any element satisfying \(|o^{m-1}| \geq 2 a_f\) for which a direct neighbour intersects \(\Gamma^m\) is also marked for refinement. Similarly, an element that is not marked for refinement is marked for coarsening if it satisfies \(|o^{m-1}| \leq \frac{1}{2} a_c\) and \(o^{m-1} \cap \Gamma^m = \emptyset\). Now all the elements marked for refinement are halved into two smaller elements with the help of a simple bisectioning procedure, see [11, 10]. In order to avoid hanging nodes, this will in general lead to refinements of elements that were not originally marked for refinement. Similarly, an element that is marked for coarsening is coarsened only if all of its neighbouring elements are marked for coarsening as well. For more details on the refining and coarsening itself, we refer to [11, 10, 27].
This marking and refinement process is repeated until no more elements are required to be refined or coarsened. In practice, it can be observed that only at the first time step, \( m = 0 \), more than one of the described refinement cycles are needed.

In theory it is possible to use local mesh refinement also for the discrete interface \( \Gamma^m \), which is totally independent from \( T^m \). However, the weak equidistribution property (16) means that in practice no refinement of \( \Gamma^m \) is necessary. In fact, the vertices of \( \Gamma^m \) are in general very well distributed, so that mesh smoothing (redistribution) for the interface mesh is also not necessary in practice.

![Figure 3: Portion of the computational domain showing the bulk mesh close to the discrete interface.](image)

4.2. Definition of the bulk region

As already introduced in Section 3, a crucial aspect of our approach is the identification of a suitable region \( \Omega_{m,h}^+ \) where the approximation \( \phi^{m+1} \) to the electric potential is to be computed. Our method is based on an adapted triangulation \( T^m \) of the whole domain \( \Omega \). In order to define the submesh \( T^m_+ \), which defines the computational domain \( \Omega_{m,h}^+ \), we need to perform two steps. First we need to find all the elements that are cut by the discrete interface \( \Gamma^m \), and then we need to find all the elements of \( T_+^m \), recall (9). For the first step we need to be able to detect intersections between a segment \([\vec{X}_m(q_j), \vec{X}_m(q_{j-1})] =: [Q_1, Q_2] \) of \( \Gamma^m \), say, and a triangle \( \triangle(P_0, P_1, P_2) \) of \( T^m \). Such intersections can be detected with the help of the following algorithm.

Once all the “cut” elements have been correctly identified with the help of Algorithm 1, we use the following algorithm to find the elements of \( T^m_+ \). Here we adapt the strategy from [3], where an unfitted
Algorithm 1: Computing the intersection between the segment \([Q_1, Q_2]\) and the triangle \(\triangle(P_0, P_1, P_2)\).

- if \(Q_1 \in \triangle\) or \(Q_2 \in \triangle\), then the segment intersects the triangle;
- else if \([Q_1, Q_2] \cap [P_0, P_1] \neq \emptyset\), then the segment intersects the triangle;
- else if \([Q_1, Q_2] \cap [P_1, P_2] \neq \emptyset\), then the segment intersects the triangle;
- else if \([Q_1, Q_2] \cap [P_0, P_2] \neq \emptyset\), then the segment intersects the triangle;
- otherwise there is no intersection between the segment and the triangle.

finite element approximation for dendritic crystal growth with thermal convection was studied.

Algorithm 2: Finding the subset \(T^m_+\) of \(T^m\).

- Mark all the elements of \(T^m\) as “clear”.
- Assuming that \(\Gamma^m\) does not intersect the boundary \(\partial \Omega\) of the domain, proceed as follows:
  1. mark all the elements cut by the interface as “cut”;
  2. mark all boundary elements as “outside”;
  3. mark all clear neighbours of “outside” elements as “outside” until no more such neighbours can be found.
  4. mark all “cut” elements as “outside”.

The above algorithm produces a partition of the original bulk triangulation \(T^m\), where the “outside” triangles are the elements in \(T^m_+\). We note that \(T^m_+\) contains all the elements that are intersected by \(\Gamma^m\). This is motivated by the fact that we need to evaluate \(\varphi^{m+1}_s\) on \(\Gamma^m\) in (10b), and this is only guaranteed to be well-defined if \(\varphi^{m+1}\) is defined on all such intersected elements.

4.3. Topological changes

For ease of presentation, in Section 3 we have restricted ourselves to the case of \(\Gamma^m\) being a single closed curve, which can be parameterised over \(I\), the “periodic” interval \([0,1]\). It is straightforward to extend our approximation (10) to the case where \(\Gamma^m\) is given by a family of closed curves. Then each connected component of \(\Gamma^m\) is discretised individually, and its evolution is described by the analogues of (10b) and (10c).

In particular, the ability of our method to deal with a family of curves also allows us to perform topological changes, such as the merging of two curves into one, or the pinching-off of one curve from another. In practice we monitor the need for topological changes, and then implement the changes, with the help of the 2D variant of the package El-Topo, see [14]. Our usage of this library can be summarised as follows.

Let \(Q^m\) be the mesh configuration at time \(t = t_m\), consisting of (i) the current positions of the vertices of \(\Gamma^m\) and (ii) the connectivity of the grid in terms of pairs of vertex indices. As input parameters El-Topo expects the current mesh configuration \(Q^m\) as well as a velocity function, which in our case is given by \(\frac{1}{\tau_m} \delta X^{m+1}\), and the time step size \(\tau_m\). This allows El-Topo to define a predicted mesh configuration \(\hat{Q}^{m+1}\), where each vertex is transported with its own velocity, and where no topological changes are performed. If \(Q^{m+1}\) features self-intersections, then topological changes are performed to produce a final mesh configuration \(Q^{m+1}\) which is as close as possible to \(\hat{Q}^{m+1}\), but which is guaranteed to be intersection free. For more details on how El-Topo proceeds to determine the necessary topological changes, we refer to the description of the 3D counterpart in [14].
5. Numerical experiments

We implemented our finite element approximation (10) within the framework of the C++-based software DUNE, see [11, 10]. Throughout this section we use uniform time steps $\tau_m = \tau$, $m = 0, \ldots, M-1$. As we will often compare our numerical results to the phase field computations in [8], we also fix $\alpha_1 = \frac{1}{16} \pi^2$ throughout this section.

Our first experiment refers to (6a), where the true solution of a circular void, moving at constant speed through an infinite conductor, is known. We chose the following parameters: $L_1 = 1.5$, $L_2 = 0.5$, $\alpha_2 = 3\pi^2$. The initial geometry is a circle with radius $R = 0.25$ and centre $z = (-0.5, 0)$, while $T = 2 \times 10^{-3}$. Following [6], we define the error $\mathcal{E} = \| \vec{X} - \vec{x} \|_{L^\infty} := \max_{m=1 \to M} \| \vec{X}^m - \vec{x}(\cdot, t_m) \|_{L^\infty}$, where $\| \vec{X}^m - \vec{x}(t_m) \|_{L^\infty} := \max_{i=1 \to N} \{ \min_{\vec{y} \in \Gamma(t)} | \vec{X}^m(\vec{y}) - \vec{x}(\vec{y}, t_m) | \}$ between $\vec{X}$ and the true solution on the interval $[0, T]$. Since the exact solution is known, it is worth calculating an experimental order of convergence. To this end, we employ (25a) with

$$ N = N_f = 16 N_c = N_i := 2^{7+i}, \quad i = 0 \rightarrow 2. $$

The experimental order of convergence EOC is computed as $\log (\frac{\mathcal{E}_{i+1}}{\mathcal{E}_i}) / \log (\frac{N_i}{N_{i-1}})$. The corresponding errors are listed in Table 1, where it appears that we observe a convergence of at least $O(h)$ in the measured error.

<table>
<thead>
<tr>
<th>$i$</th>
<th>$\tau$</th>
<th>$N$</th>
<th>$N_f$</th>
<th>$h_f$</th>
<th>$N_c$</th>
<th>$h_c$</th>
<th>$| \vec{X} - \vec{x} |_{L^\infty}$</th>
<th>EOC</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$8 \times 10^{-6}$</td>
<td>128</td>
<td>128</td>
<td>$7.81 \times 10^{-3}$</td>
<td>8</td>
<td>$1.25 \times 10^{-1}$</td>
<td>16.459</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>$2 \times 10^{-6}$</td>
<td>256</td>
<td>256</td>
<td>$3.91 \times 10^{-3}$</td>
<td>16</td>
<td>$6.25 \times 10^{-2}$</td>
<td>7.556</td>
<td>1.1232</td>
</tr>
<tr>
<td>2</td>
<td>$5 \times 10^{-7}$</td>
<td>512</td>
<td>512</td>
<td>$1.95 \times 10^{-3}$</td>
<td>32</td>
<td>$3.13 \times 10^{-2}$</td>
<td>3.474</td>
<td>1.1212</td>
</tr>
</tbody>
</table>

Table 1: Results of the convergence test.

The next experiment corresponds to [8, Fig. 2], see also [13, Fig. 4]. We chose the radius of the initially circular void to be relatively large compared to the width of the conductor, $2L_2$. We used the following parameters: $L_1 = 1$, $L_2 = 0.5$, $\alpha_2 = \frac{512 \pi^2}{\pi}$, $\tau = 4.5 \times 10^{-7}$, $N = 1024$. As initial data we chose a circle with radius 0.375 and centre $(-0.5, 0)$; the refinement parameters were $N_f = 512$ and $N_c = 4$, respectively. In Figure 4 we plot the results of the simulation at times $t = 0.8 \times 10^{-5}$, and $T = 3.6 \times 10^{-4}$. We note the good agreement with both [13, Fig. 4] and [8, Fig. 2]. In the phase-field approximation discussed in the latter, the evolution appears to be slightly faster, which is likely to be due to the choice of Robin boundary conditions there, instead of the simpler Dirichlet boundary conditions prescribed in (3b).

The next experiment corresponds to [8, Fig. 6], see also [23, Fig. 9]. We used the following parameters: $L_1 = 0.5$, $L_2 = 0.5$, $\alpha_2 = 3\pi^2$, $\tau = 2 \times 10^{-7}$, $N = 2232$. As initial data we chose two ellipses, the left one with horizontal semiaxis 0.14, vertical semiaxis 0.2 and centre $(-0.15, 0)$, the right one with horizontal semiaxis 0.12, vertical semiaxis 0.24 and centre $(0.15, 0)$. The refinement parameters were $N_f = 512$ and $N_c = 4$, respectively. In Figure 5 we plot the results of the simulation at times $t = 3.04 \times 10^{-5}$, $3.8 \times 10^{-5}$, $4.56 \times 10^{-5}$ and $T = 1.5 \times 10^{-4}$. We observe that as the two elliptical voids try to attain a more circular shape they touch and merge into a single void. This represents a change of topology, which here is performed with the help of the library El-Topo, as discussed in §4.3. Here we note that the time at which the two ellipses merge is sensitive to the choice of the tolerance parameters employed in El-Topo. Due to the fast evolution immediately after the merging, we used much smaller time steps ($\approx 10^{-11}$) for some time afterwards (roughly, an interval of $10^{-6}$), as otherwise we observed a relatively large area loss. We note the good agreement with the results presented in [8, Fig. 6].

Our final experiment corresponds to [8, Fig. 7]. We used the following parameters: $L_1 = 1.5$, $L_2 = 0.5$, $\alpha_2 = 30 \pi^2$, $\tau = 3.32 \times 10^{-7}$, $N = 1024$. As initial data we chose an ellipse with horizontal semiaxis 0.4, vertical semiaxis 0.2 and centre $(-0.8, 0)$. The refinement parameters were $N_f = 512$ and $N_c = 4$, respectively. In Figure 6 we plot the results of the simulation at times $t = 0.875 \times 10^{-5}$, $1.75 \times 10^{-4}$, $2.625 \times 10^{-4}$ and $T = 3.32 \times 10^{-4}$. Here a different topological change can be observed during the evolution. As the void elongates in the direction of the applied electric field, the front of the moving void pinches off and
Figure 4: \((\alpha^2 = \frac{512}{9} \pi^2)\) Plots of the interface curve at times \(t = 0, 8 \times 10^{-5}, T = 3.6 \times 10^{-4}\), and adaptive bulk mesh at time \(t = T\).

Figure 5: \((\alpha^2 = 3\pi^2)\) Plots of the interface curve at times \(t = 0, 3.04 \times 10^{-5}, 3.8 \times 10^{-5}, 4.56 \times 10^{-5}, T = 1.5 \times 10^{-4}\), and adaptive bulk mesh at time \(t = T\).
then separates. Like in Figure 5, we used much smaller time steps after the pinch-off, to avoid a relatively large area loss. After the split the smaller void travels faster than the main part of the void. Here, once again, we note the good agreement with the numerical results for the phase-field approximation discussed in [8, Fig. 7].


