A mixed formulation of the Stefan problem with surface tension

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A dual formulation and finite element method is proposed and analyzed for simulating the Stefan problem with surface tension. The method uses a mixed form of the heat equation in the solid and liquid (bulk) domains, and imposes a weak formulation of the interface motion law (on the solid-liquid interface) as a constraint. The basic unknowns are the heat fluxes and temperatures in the bulk, and the velocity and temperature on the interface. The formulation, as well as its discretization, is viewed as a saddle point system. Well-posedness of the time semi-discrete and fully discrete formulations is proved in three dimensions, as well as an a priori (stability) bound and conservation law. Simulations of interface growth (in two dimensions) are presented to illustrate the method.

1. Introduction

1.1 *Background*

The Stefan problem describes the geometric evolution of a solidifying (or melting) interface. It is a classic problem in phase transitions. The model consists of time-dependent heat diffusion in the solid and liquid phases, with an interfacial condition on the solid-liquid interface known as the Gibbs-Thomson relation with kinetic undercooling [41, 42, 61]. A thermodynamic derivation of the model can be found in [29]. Applications range from modeling the freezing (or melting) of water to the solidification of crystals from a melt and dendritic growth [15, 30, 38, 51, 52, 59]. Mathematical theory for the Stefan problem with Gibbs-Thomson law is available for local and global in time solutions [13, 25, 36, 39, 45–48]. Well-posedness results are also available if the heat equation in the bulk phases is replaced by a quasi-static approximation (i.e. the Mullins–Sekerka problem) [18, 20, 24, 40, 49].

Efficient numerical schemes for simulating these models is necessary to allow for design, prediction, and optimization of these processes. Phase-field methods have been used for simulating solidification and dendrite growth [6, 35, 55]. Level set methods have also been used to handle the evolutions of the two phase interface [12, 23, 44, 54]. The method we present uses a front-tracking approach where the interface parametrization conforms to a surrounding bulk mesh. Other front-tracking methods for the Stefan problem have also been given [2, 4, 34, 35, 50–53].

Our paper presents a *completely* mixed formulation of the Stefan problem, including the bulk heat equations [8]. In other words, we formulate the problem in a saddle-point framework, where the heat equations are in mixed form, and the interface motion law appears as a constraint in the system of equations with a balancing Lagrange multiplier that represents the interface temperature. To the best of our knowledge, this is a new method for the Stefan problem with surface tension. Some highlights of our method are the following.

- We prove that *both* the time semi-discrete and fully discrete systems have a priori bounds (in time) that mimic the continuous model. This assumes the interface velocity is reasonably regular and that there are no topological changes. Moreover, we can prove that both the time semi-discrete and fully discrete systems maintain conservation of thermal energy. In [5], they only achieve this for their discrete in space, continuous in time, scheme.
- The interface is represented by a surface triangulation that conforms to the bulk mesh which deforms with the interface. Hence, occasional re-meshing is needed, which is done by the method in [63]. One advantage of this method is that all integrals in the finite element formulation can be computed exactly. In addition, we do not need to compute the intersection of meshes at adjacent time steps to transfer solution variables from one mesh to the next (e.g. for computing L^2 projections from one mesh to another).
- Our method can be modified to include anisotropic surface tension via [5], which is relevant to crystal growth. The well-posedness of the method remains unchanged, as well as the a priori bound and conservation law.
- Other variations of the Stefan problem (e.g. Mullins–Sekerka) can be formulated with our approach by straightforward modifications. One can even include moving contact line effects when the solid phase is attached to a rigid boundary [60, 64].

1.2   *Summary*

In Section 2, we describe the governing equations. Section 3 describes the fully continuous weak formulation and derives a formal a priori bound and conservation law. Section 4 explains the time-discretization and how the interface motion is handled. A variational formulation of the time semi-discrete problem is given, its well-posedness is shown, and an a priori bound and conservation law is proved. We then do the same for the fully-discrete formulation (Section 5). Section 6 concludes with numerical simulations to demonstrate the method.

2.   Model for the Stefan problem with surface tension

The particular mathematical model we consider can be found in [5, 29]. In this section, we present the strong form of the Stefan problem.

2.1   *Notation*

Let Ω be a fixed domain in $\mathbb{R}^d$ (for $d = 2, 3$), with outer boundary $\partial\Omega$, that contains two phases, liquid and solid, denoted respectively by the open sets Ω_l and Ω_s, i.e. $\Omega = \text{int}(\overline{\Omega_l} \cup \overline{\Omega_s})$ and $\Omega_l \cap \Omega_s = \emptyset$ (see Figure 1). Furthermore, $\partial\Omega$ partitions into two pieces: $\partial\Omega = \overline{\partial_D\Omega} \cup \overline{\partial_N\Omega}$ such that $\partial_D\Omega \cap \partial_N\Omega = \emptyset$ and $|\partial_D\Omega| > 0$ (set of positive measure).

The solid-liquid interface between the phases is $\Gamma = \overline{\Omega_l} \cap \overline{\Omega_s}$ (a closed surface). The domains Ω_l, Ω_s, and Γ are time-dependent, and we assume that $\Gamma(t) \subset \Omega$ for all t. Moreover, in order to

write the strong form of the Stefan problem (Section 2.2), we assume $\Gamma(t)$ is smooth and let $\mathbf{X}(t)$ denote a parametrization of $\Gamma(t)$:

$$\mathbf{X}(\cdot, t) : \mathfrak{M} \to \mathbb{R}^d, \quad \text{where } \mathfrak{M} \subset \mathbb{R}^d \text{ is a given reference manifold,} \tag{2.1}$$

i.e. $\Gamma(t) = \mathbf{X}(\mathfrak{M}, t)$. Furthermore, we introduce *fixed* reference domains $\widehat{\Omega}_1$, $\widehat{\Omega}_s$ for the liquid and solid domains such that $\Omega = \text{int}(\overline{\widehat{\Omega}_1} \cup \overline{\widehat{\Omega}_s})$ and $\mathfrak{M} = \overline{\widehat{\Omega}_1} \cap \overline{\widehat{\Omega}_s}$. We can extend $\mathbf{X}$ to be defined on all of Ω and such that $\Omega_1(t) = \mathbf{X}(\widehat{\Omega}_1, t)$ and $\Omega_s(t) = \mathbf{X}(\widehat{\Omega}_s, t)$ (slight abuse of notation here). This is needed later when specifying the function spaces.

The surface Γ has a unit normal vector ν that is assumed to point into Ω_1 (see Figure 1). For quantities q in Ω_1 (Ω_s), we append a subscript: q_1 (q_s). The symbol κ represents the *summed* curvature of the interface Γ (sum of the principle curvatures), and we assume the convention that κ is *positive* when Ω_s is convex (contrary to [5]).

Table 1 summarizes the notation we use for the physical domain and the physical variables (e.g. temperature, etc.). The physical coefficient symbols that appear in the model, as well as their values, are given in Table 2. The non-dimensional parameters are given in Table 3.
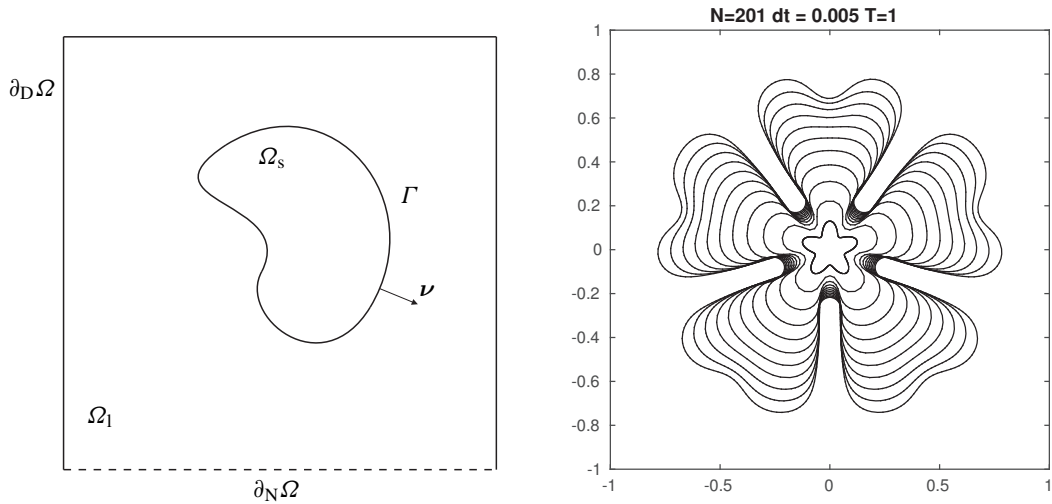

FIG. 1: Left: Domains in the Stefan problem. The entire "box" is $\Omega = \text{int}(\overline{\Omega_1} \cup \overline{\Omega_s})$ (containing two phases Ω_1, Ω_s) with Dirichlet boundary $\partial_D \Omega$ denoted by the dashed line. A Neumann condition is applied on the remaining sides $\partial_N \Omega$. The interface between the phases is $\Gamma = \overline{\Omega_1} \cap \overline{\Omega_s}$ with unit normal vector ν pointing into Ω_1. Right: Simulation using the method developed in this paper (isotropic surface tension). Several time-lapses are shown to illustrate the evolution with initial interface having a "star" shape. See Section 6 for more simulations.

TABLE 1: General notation and symbols

Symbol	Name	Units
Ω, Ω_l, Ω_s	Bulk Domains: Entire, Liquid, Solid	—
$\partial\Omega$	Boundary of Ω	—
$\partial_D\Omega$, $\partial_N\Omega$	Partition of $\partial\Omega = \overline{\partial_D\Omega} \cup \overline{\partial_N\Omega}$	—
Γ	Interface between Ω_l and Ω_s phases	—
$\mathbf{X}$, $\mathbf{V}$	Interface (Γ) Parametrization and Velocity	m, m s^{-1}
u_l, u_s	Temperature in Ω_l and Ω_s	K (deg. Kelvin)
f_l, f_s	Heat sources in Ω_l and Ω_s	J m^{-3} s^{-1}
∇_Γ, Δ_Γ	Surface Gradient and Laplace–Beltrami Operator	m^{-1}, m^{-2}
$\boldsymbol{\nu}$	Unit Normal Vector of Γ	—
$\nabla_\Gamma\mathbf{X} := \mathbf{I} - \boldsymbol{\nu} \otimes \boldsymbol{\nu}$	Projection onto Tangent Space of Γ	—
κ, $\kappa\boldsymbol{\nu} := -\Delta_\Gamma\mathbf{X}$	Summed Curvature and Curvature Vector of Γ	m^{-1}

TABLE 2: Physical parameters and values

Symbol	Name	Units
ϑ	Volumetric Heat Capacity	J m^{-3}K^{-1}
K_l, K_s	Thermal Conductivity in Ω_l and Ω_s	J s^{-1}m^{-1}K^{-1}
L	Latent Heat Coefficient	J m^{-3}
α	Surface Tension Coefficient of Γ	J m^{-2}
S	Volumetric Entropy Coefficient	J m^{-3}K^{-1}
ρ	Kinetic Coefficient	J s m^{-4}
β	Mobility Coefficient	—
D	Length Scale	m
$U_0 = T_M$	Temperature Scale	K
t_0	Time Scale	seconds (s)
$F_0 = \vartheta U_0/t_0$	Heat Source Scale	J m^{-3} s^{-1}

TABLE 3: Nondimensional parameters

Symbol	Name	Value
$\widehat{S} = S/\vartheta$	entropy coefficient	2
$\widehat{\beta}_0 = \vartheta U_0 t_0/(\rho D)$	mobility coefficient	0.01
$\widehat{\beta} = \widehat{\beta}_0\beta$	mobility function	-
$\widehat{K}_l = K_l t_0/(D^2\vartheta)$	liquid conductivity	1
$\widehat{K}_s = K_s t_0/(D^2\vartheta)$	solid conductivity	1
$\widehat{\alpha} = \alpha/(U_0 D\vartheta)$	surface tension coefficient	0.0005

2.2 *Strong formulation*

The Stefan problem is as follows. Find $u : \Omega \times [0, T] \rightarrow \mathbb{R}$ and interface $\Gamma(t) \subset \Omega$ for all $t \in (0, T]$, such that $u|_{\Omega_\mathrm{l}} = u_\mathrm{l}$, $u|_{\Omega_\mathrm{s}} = u_\mathrm{s}$, and the following bulk conditions hold:

$$
\begin{aligned}
\vartheta\, \partial_t u_\mathrm{l} - K_\mathrm{l} \Delta u_\mathrm{l} &= f_\mathrm{l}, \text{ in } \Omega_\mathrm{l}(t), \\
\vartheta\, \partial_t u_\mathrm{s} - K_\mathrm{s} \Delta u_\mathrm{s} &= f_\mathrm{s}, \text{ in } \Omega_\mathrm{s}(t), \\
\boldsymbol{\nu}_\Omega \cdot \nabla u &= 0, \text{ on } \partial_\mathrm{N}\Omega, \\
u &= u_\mathrm{D}, \text{ on } \partial_\mathrm{D}\Omega, \\
u(\cdot, 0) &= u_0, \text{ in } \Omega,
\end{aligned}
\tag{2.2}
$$

where u_0 is the initial temperature, and the following interface conditions hold:

$$
\begin{aligned}
u_\mathrm{l} - u_\mathrm{s} &= 0, \text{ on } \Gamma(t), \\
\boldsymbol{\nu} \cdot (K_\mathrm{l}\nabla u_\mathrm{l} - K_\mathrm{s}\nabla u_\mathrm{s}) + L\, \partial_t \mathbf{X} \cdot \boldsymbol{\nu} &= 0, \text{ on } \Gamma(t), \\
\frac{\rho}{\beta(\boldsymbol{\nu})} \partial_t \mathbf{X} \cdot \boldsymbol{\nu} + \alpha\kappa + Su &= 0, \text{ on } \Gamma(t), \\
\mathbf{X}(\cdot, 0) - \mathbf{X}_0(\cdot) &= \mathbf{0}, \text{ on } \mathfrak{M}, \\
\Gamma(0) &= \Gamma_0, \text{ in } \Omega,
\end{aligned}
\tag{2.3}
$$

where Γ_0 is the initial interface (parameterized by $\mathbf{X}_0$) and $\mathbf{X}(\cdot, t)$ parameterizes $\Gamma(t)$. Note that $u = T - T_\mathrm{M}$, where T is the temperature in degrees Kelvin and T_M is the melting temperature at the interface Γ, and that u is continuous across the interface. As noted in [5], we must have

$$
S = \frac{L}{T_\mathrm{M}}.
\tag{2.4}
$$

2.3 *Non-dimensionalization*

We non-dimensionalize the variables, but use the same variable symbols for convenience. This gives

$$
\begin{aligned}
\partial_t u_\mathrm{l} - \widehat{K}_\mathrm{l} \Delta u_\mathrm{l} &= f_\mathrm{l}, \text{ in } \Omega_\mathrm{l}(t), \\
\partial_t u_\mathrm{s} - \widehat{K}_\mathrm{s} \Delta u_\mathrm{s} &= f_\mathrm{s}, \text{ in } \Omega_\mathrm{s}(t), \\
\boldsymbol{\nu}_\Omega \cdot \nabla u &= 0, \text{ on } \partial_\mathrm{N}\Omega, \\
u &= u_\mathrm{D}, \text{ on } \partial_\mathrm{D}\Omega, \\
u(\cdot, 0) &= u_0, \text{ in } \Omega, \\
u_\mathrm{l} - u_\mathrm{s} &= 0, \text{ on } \Gamma(t), \\
\boldsymbol{\nu} \cdot (\widehat{K}_\mathrm{l}\nabla u_\mathrm{l} - \widehat{K}_\mathrm{s}\nabla u_\mathrm{s}) + \widehat{S}\, \partial_t \mathbf{X} \cdot \boldsymbol{\nu} &= 0, \text{ on } \Gamma(t), \\
\frac{1}{\widehat{\beta}(\boldsymbol{\nu})} \partial_t \mathbf{X} \cdot \boldsymbol{\nu} + \widehat{\alpha}\kappa + \widehat{S}\, u &= 0, \text{ on } \Gamma(t), \\
\mathbf{X}(\cdot, 0) - \mathbf{X}_0(\cdot) &= \mathbf{0}, \text{ on } \mathfrak{M}, \\
\Gamma(0) &= \Gamma_0, \text{ in } \Omega.
\end{aligned}
\tag{2.5, 2.6}
$$

Throughout the paper, we assume the non-dimensional coefficients satisfy

$$\infty > \widehat{K}_1, \widehat{K}_s, \widehat{\alpha}, \widehat{S} > 0, \quad \infty \geqslant \widehat{\beta}(\boldsymbol{\nu}) \geqslant \widehat{\beta}_- > 0, \quad \text{where } \widehat{\beta}_- \text{ is a constant.}$$

REMARK 2.1 The case of $\vartheta = 0$ (i.e. $\widehat{\alpha}, \widehat{S}, \widehat{K}_1, \widehat{K}_s = \infty$) corresponds to the steady-state heat equation in Ω_1 and Ω_s and if $\rho = 0$ (i.e. $\widehat{\beta}(\boldsymbol{\nu}) \equiv \infty$) then (2.5) and (2.6) becomes the Mullins–Sekerka problem with Gibbs-Thomson law [41]. Our formulation can easily be modified to implement this model. If $\widehat{S} \equiv \infty$ only, then $\partial_t \mathbf{X} \cdot \boldsymbol{\nu} \equiv 0$, so (2.5) and (2.6) reduce to the time-dependent heat equation on a stationary domain with $u_1 = u_s = 0$ on Γ.

3. Weak formulation

3.1 *Function spaces*

Since the domain and interface deform in time, we define the function spaces using a reference domain [5]. For simplicity, we shall assume that $\partial \Omega \cap \partial \Omega_1 = \partial \Omega$ (see Figure 1); thus, $\overline{\Omega_s} \subset \Omega$. We use standard notation for denoting Sobolev spaces [1, 57], e.g. $L^2(\Omega)$ is the space of square integrable functions on Ω. For any vector-valued function $\boldsymbol{\eta}$, if we write $\boldsymbol{\eta} \in L^2(\Omega)$, we mean each component of $\boldsymbol{\eta}$ is in $L^2(\Omega)$. Continuing, we have $H^1(\Omega) = \{u \in L^2(\Omega) : \nabla u \in L^2(\Omega)\}$ and $H(\text{div}, \Omega) = \{\boldsymbol{\eta} \in L^2(\Omega) : \nabla \cdot \boldsymbol{\eta} \in L^2(\Omega)\}$. The norms on these spaces are defined in the obvious way, i.e. $\|u\|^2_{L^2(\Omega)} = \int_\Omega |u|^2$, $\|u\|^2_{H^1(\Omega)} = \|u\|^2_{L^2(\Omega)} + \|\nabla u\|^2_{L^2(\Omega)}$, $\|\boldsymbol{\eta}\|^2_{H(\text{div}, \Omega)} = \|\boldsymbol{\eta}\|^2_{L^2(\Omega)} + \|\nabla \cdot \boldsymbol{\eta}\|^2_{L^2(\Omega)}$.

For a general function $f : \Omega \to \mathbb{R}$, we denote its *trace* (or restriction) to a sub-domain $\Sigma \subset \Omega$ (of co-dimension 1) by $f|_\Sigma$. The trace of a function in $H^1(\Omega)$ is well-defined; for a function in $L^2(\Omega)$, the trace is *not* well-defined. Moreover, the trace of all functions (on $\Sigma \subset \Omega$) in $H^1(\Omega)$ spans a Hilbert space, denoted $H^{1/2}(\Sigma)$, which is a proper dense subspace of $L^2(\Sigma)$. Referring to [7, pg. 48], the norm for $H^{1/2}(\partial \Omega)$ is defined by

$$\|v\|_{H^{1/2}(\partial \Omega)} := \inf_{\substack{w \in H^1(\Omega) \\ w|_{\partial \Omega} = v}} \|w\|_{H^1(\Omega)} = \|\bar{v}\|_{H^1(\Omega)}, \tag{3.1}$$

where $\bar{v}$ is the unique weak solution of $-\Delta \bar{v} + \bar{v} = 0$ in Ω, with $\bar{v} = v$ on $\partial \Omega$. We also have $H^{-1/2}(\partial \Omega)$, i.e. the dual space of $H^{1/2}(\partial \Omega)$ with the dual norm,

$$\|\varrho\|_{H^{-1/2}(\partial \Omega)} := \sup_{v \in H^{1/2}(\partial \Omega)} \frac{\langle \varrho, v \rangle_{\partial \Omega}}{\|v\|_{H^{1/2}(\partial \Omega)}}, \tag{3.2}$$

where $\langle \cdot, \cdot \rangle_{\partial \Omega}$ denotes the duality pairing between $H^{-1/2}(\partial \Omega)$ and $H^{1/2}(\partial \Omega)$.

It is well known [26, Theorem 1.7], [7, Lemma 2.1.1] that $\boldsymbol{\eta} \cdot \boldsymbol{\nu}|_{\partial \Omega}$ is in $H^{-1/2}(\partial \Omega)$ for all $\boldsymbol{\eta}$ in $H(\text{div}, \Omega)$ ($\boldsymbol{\nu}_\Omega$ is the unit normal vector on $\partial \Omega$). In fact, by [26, (1.44)], we have that

$$\|\boldsymbol{\eta} \cdot \boldsymbol{\nu}\|_{H^{-1/2}(\partial \Omega)} \lesssim \|\boldsymbol{\eta}\|_{H(\text{div}, \Omega)}, \text{ for all } \boldsymbol{\eta} \in H(\text{div}, \Omega). \tag{3.3}$$

With this, one can show that $\|v\|_{H^{1/2}(\partial \Omega)}$ has a dual norm realization.

PROPOSITION 3.1

$$\|v\|_{H^{1/2}(\partial \Omega)} = \sup_{\boldsymbol{\eta} \in H(\text{div}, \Omega)} \frac{\langle \boldsymbol{\eta} \cdot \boldsymbol{\nu}, v \rangle_{\partial \Omega}}{\|\boldsymbol{\eta}\|_{H(\text{div}, \Omega)}}.$$

Enforcing boundary conditions requires the trace. To this end, let $H^1_{0,D}(\Omega) = \{u \in H^1(\Omega) : u|_{\partial_D \Omega} = 0\}$. On the reference domains $\widehat{\Omega}_1$ and $\widehat{\Omega}_s$, we introduce:

$$
\begin{aligned}
\mathbb{V} &= H(\mathrm{div}, \Omega), & \mathbb{V}(g) &= \{\boldsymbol{\eta} \in \mathbb{V} : \langle \boldsymbol{\eta} \cdot \boldsymbol{\nu}_\Omega - g, q \rangle_{\partial \Omega} = 0, \ \forall q \in H^1_{0,D}(\Omega)\}, \\
\mathbb{V}_1 &= H(\mathrm{div}, \widehat{\Omega}_1), & \mathbb{V}_1(g) &= \{\boldsymbol{\eta} \in \mathbb{V}_1 : \langle \boldsymbol{\eta} \cdot \boldsymbol{\nu}_\Omega - g, q \rangle_{\partial \Omega} = 0, \ \forall q \in H^1_{0,D}(\Omega)\}, \\
\mathbb{V}_s &= H(\mathrm{div}, \widehat{\Omega}_s),
\end{aligned}
\tag{3.4}
$$

where g is in $H^{-1/2}(\partial \Omega)$ (see [7, Remark 2.1.3]). We also have the spaces

$$
\mathbb{Q} = L^2(\Omega), \quad \mathbb{Q}_1 = L^2(\widehat{\Omega}_1), \quad \mathbb{Q}_s = L^2(\widehat{\Omega}_s).
\tag{3.5}
$$

On the reference manifold $\mathfrak{M}$, we define [1]

$$
\mathbb{M} = H^{1/2}(\mathfrak{M}, \mathbb{R}), \qquad \mathbb{Y} = H^1(\mathfrak{M}, \mathbb{R}^d).
\tag{3.6}
$$

The norm for $\mathbb{Y}$ is $\|\mathbf{V}\|^2_{H^1(\Gamma)} = \int_\Gamma |\mathbf{V}|^2 + \int_\Gamma |\nabla_\Gamma \mathbf{V}|^2$ (see Section 3.2.1 for ∇_Γ).

We use the following abuse of notation, similar to [5]. We identify functions $\boldsymbol{\eta}_1$ in $\mathbb{V}_1$ with $\boldsymbol{\eta}_1 \circ \mathbf{X}^{-1}$ defined on $\Omega_1(t)$ (recall $\Omega_1(t) = \mathbf{X}(\widehat{\Omega}_1, t)$), and denote both functions simply as $\boldsymbol{\eta}_1$; similar considerations are made for functions $\boldsymbol{\eta}_s$ in $\mathbb{V}_s$. Likewise, we identify $\mathbf{V}$ in $\mathbb{Y}$ with $\mathbf{V} \circ \mathbf{X}^{-1}$ defined on $\Gamma(t)$, and denote both functions as $\mathbf{V}$; similar considerations are made for functions μ in $\mathbb{M}$. Along these lines, we have $\mathbb{V}_1 \simeq H(\mathrm{div}, \Omega_1)$, $\mathbb{V}_s \simeq H(\mathrm{div}, \Omega_s)$, $\mathbb{Q}_1 \simeq L^2(\Omega_1)$, $\mathbb{Q}_s \simeq L^2(\Omega_s)$, $\mathbb{M} \simeq H^{1/2}(\Gamma)$, $\mathbb{Y} \simeq H^1(\Gamma)$, provided the mapping $\mathbf{X}$ is not degenerate.

For technical reasons, we need two versions of the $H^{1/2}(\Gamma)$ norm related to Ω_1 and Ω_s. Define

$$
\|v\|_{H^{1/2}_1(\Gamma)} := \sup_{\boldsymbol{\eta}_1 \in \mathbb{V}_1(0)} \frac{\langle \boldsymbol{\eta}_1 \cdot \boldsymbol{\nu}, v \rangle_\Gamma}{\|\boldsymbol{\eta}_1\|_{H(\mathrm{div}, \Omega_1)}}, \quad \|v\|_{H^{1/2}_s(\Gamma)} := \sup_{\boldsymbol{\eta}_s \in \mathbb{V}_s} \frac{\langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}, v \rangle_\Gamma}{\|\boldsymbol{\eta}_s\|_{H(\mathrm{div}, \Omega_s)}}.
\tag{3.7}
$$

Basically, these norms are related to the "side" of Γ on which we take the trace. We also define the $H^{1/2}$ and $H^{-1/2}$ norm on Γ by

$$
\|v\|_{H^{1/2}(\Gamma)} := \frac{1}{2} \left(\|v\|_{H^{1/2}_1(\Gamma)} + \|v\|_{H^{1/2}_s(\Gamma)} \right), \qquad \|\varrho\|_{H^{-1/2}(\Gamma)} := \sup_{v \in H^{1/2}(\Gamma)} \frac{\langle \varrho, v \rangle_\Gamma}{\|v\|_{H^{1/2}(\Gamma)}}.
\tag{3.8}
$$

To conclude this section, we define the dual norm for $H^{-1}(\Gamma)$:

$$
\|\varrho\|_{H^{-1}(\Gamma)} := \sup_{v \in H^1(\Gamma)} \frac{\langle \varrho, v \rangle_\Gamma}{\|v\|_{H^1(\Gamma)}},
\tag{3.9}
$$

where $\langle \varrho, v \rangle_\Gamma$ is understood to be the duality pairing between $H^{-1}(\Gamma)$ and $H^1(\Gamma)$.

3.2 *Curvature*

3.2.1 *Differential geometry.*
First, we review some differential geometry [17, 37]. Let $\boldsymbol{\Psi} : U \to \Gamma$ be a local parameterization of $\Gamma \subset \mathbb{R}^3$ where $U \subset \mathbb{R}^2$ with local variables (s_1, s_2). The first

fundamental form $g : U \to \mathbb{R}^{2\times2}$ is given by $g_{ij} = \partial_{s_i}\boldsymbol{\Psi} \cdot \partial_{s_j}\boldsymbol{\Psi}$ for $1 \leqslant i, j \leqslant 2$. Then the tangential gradient (or surface gradient) of $\omega : \Gamma \to \mathbb{R}$ is defined as

$$(\nabla_\Gamma \omega) \circ \boldsymbol{\Psi} := \sum_{i,j=1}^{2} g^{ij} \partial_{s_i}(\omega \circ \boldsymbol{\Psi})\partial_{s_j}\boldsymbol{\Psi},$$

where $[g^{ij}]_{i,j=1}^{2} = g^{-1}$ (matrix inverse). Given $\mathbf{Y} : \Gamma \to \mathbb{R}^3$, we have $\nabla_\Gamma \mathbf{Y} = (\nabla_\Gamma Y_1, \nabla_\Gamma Y_2, \nabla_\Gamma Y_3)$ (a 3×3 matrix). Moreover, we have the tangential divergence $\nabla_\Gamma \cdot \mathbf{Y} :=$ trace$(\nabla_\Gamma \mathbf{Y})$.

The Laplace–Beltrami operator is defined by $\Delta_\Gamma \omega = \nabla_\Gamma \cdot \nabla_\Gamma \omega$ which expands out to

$$(\Delta_\Gamma \omega) \circ \boldsymbol{\Psi} := \sum_{i,j=1}^{2} g^{ij} \partial_{s_i} \left(\sum_{r,k=1}^{2} g^{rk} \partial_{s_r}(\omega \circ \boldsymbol{\Psi})\partial_{s_k}\boldsymbol{\Psi} \right) \cdot \partial_{s_j}\boldsymbol{\Psi}.$$

Note: When Γ is a one-dimensional curve with oriented unit tangent vector $\boldsymbol{\tau}$, we have $\nabla_\Gamma \equiv \boldsymbol{\tau}\partial_s$ and $\Delta_\Gamma \equiv \partial_s^2$, where ∂_s is the derivative with respect to arc-length.

Therefore, taking $\mathbf{X}(\cdot, t)$ to be a local parameterization of $\Gamma(t)$, the vector curvature $\kappa\boldsymbol{\nu}$ of $\Gamma(t)$ [17, 37] is given by $-\Delta_\Gamma \mathbf{X} = \kappa\boldsymbol{\nu}$, where κ is the sum of the principle curvatures.

3.2.2 *Weak form.* In the rest of the paper, we take advantage of a weak formulation of the vector curvature [3, 19]. If Γ is a closed C^2 manifold, then the following integration by parts relation is true:

$$\int_\Gamma \kappa\boldsymbol{\nu} \cdot \mathbf{Y} = \int_\Gamma \nabla_\Gamma \mathbf{X} : \nabla_\Gamma \mathbf{Y}, \quad \text{for all } \mathbf{Y} \text{ in } \mathbb{Y}, \tag{3.10}$$

where $\nabla_\Gamma \mathbf{X}$ is a symmetric matrix that represents the projection operator onto the tangent space of Γ, i.e. $\nabla_\Gamma \mathbf{X} = \mathbf{I} - \boldsymbol{\nu} \otimes \boldsymbol{\nu}$. We use (3.10) to derive the weak form (3.12).

3.3 *Fully continuous*

We present a mixed formulation of (2.5), (2.6) that is partly related to [8] for the heat equation. Define the flux variables $\boldsymbol{\sigma}_1 = -\widehat{K}_1 \nabla u_1$, $\boldsymbol{\sigma}_s = -\widehat{K}_s \nabla u_s$, and take $u_D(\cdot, t)$ in $H_{0,N}^1(\Omega) = \{u \in H^1(\Omega) : u|_{\partial_N\Omega} = 0\}$. Then, for given input data $f_1(\cdot, t)$, $f_s(\cdot, t)$ in $H^1(\Omega)$, and initial data $\mathbf{X}(\cdot, 0) = \mathbf{X}_0$, $u_s(\cdot, 0) = u_{s,0}$, $u_1(\cdot, 0) = u_{1,0}$, find time-dependent functions $\boldsymbol{\sigma}_1(\cdot, t)$ in $\mathbb{V}_1(0)$, $\boldsymbol{\sigma}_s(\cdot, t)$ in $\mathbb{V}_s$, $\mathbf{X}(\cdot, t)$ in $\mathbb{Y}$, $u_1(\cdot, t)$ in $\mathbb{Q}_1$, $u_s(\cdot, t)$ in $\mathbb{Q}_s$, $\lambda(\cdot, t)$ in $\mathbb{M}$ such that

$$\frac{1}{\widehat{K}_1} \int_{\Omega_1(t)} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\eta}_1 - \int_{\Omega_1(t)} u_1 \nabla \cdot \boldsymbol{\eta}_1 - \int_{\Gamma(t)} \lambda\boldsymbol{\eta}_1 \cdot \boldsymbol{\nu} = -\int_{\partial\Omega} u_D\boldsymbol{\eta}_1 \cdot \boldsymbol{\nu}_\Omega, \quad \text{for all } \boldsymbol{\eta}_1 \in \mathbb{V}_1(0),$$

$$-\int_{\Omega_1(t)} q_1 \nabla \cdot \boldsymbol{\sigma}_1 - \int_{\Omega_1(t)} q_1 \partial_t u_1 = -\int_{\Omega_1(t)} q_1 f_1, \quad \text{for all } q_1 \in \mathbb{Q}_1,$$

$$\frac{1}{\widehat{K}_s} \int_{\Omega_s(t)} \boldsymbol{\sigma}_s \cdot \boldsymbol{\eta}_s - \int_{\Omega_s(t)} u_s \nabla \cdot \boldsymbol{\eta}_s + \int_{\Gamma(t)} \lambda\boldsymbol{\eta}_s \cdot \boldsymbol{\nu} = 0, \quad \text{for all } \boldsymbol{\eta}_s \in \mathbb{V}_s,$$

$$-\int_{\Omega_s(t)} q_s \nabla \cdot \boldsymbol{\sigma}_s - \int_{\Omega_s(t)} q_s \partial_t u_s = -\int_{\Omega_s(t)} q_s f_s, \quad \text{for all } q_s \in \mathbb{Q}_s,$$

$$\tag{3.11}$$

$$\int_{\Gamma(t)} \frac{1}{\widehat{\beta}(\boldsymbol{\nu})} (\partial_t \mathbf{X} \cdot \boldsymbol{\nu})(\mathbf{Y} \cdot \boldsymbol{\nu}) + \widehat{\alpha} \int_{\Gamma(t)} \nabla_\Gamma \mathbf{X} : \nabla_\Gamma \mathbf{Y} + \widehat{S} \int_{\Gamma(t)} \lambda (\mathbf{Y} \cdot \boldsymbol{\nu}) = 0, \quad \text{for all } \mathbf{Y} \in \mathbb{Y},$$

$$\widehat{S} \int_{\Gamma(t)} \mu \, \partial_t \mathbf{X} \cdot \boldsymbol{\nu} - \int_{\Gamma(t)} \mu \boldsymbol{\sigma}_1 \cdot \boldsymbol{\nu} + \int_{\Gamma(t)} \mu \boldsymbol{\sigma}_s \cdot \boldsymbol{\nu} = 0, \quad \text{for all } \mu \in \mathbb{M},$$

(3.12)

where we have dropped the differential measure symbols $d\mathbf{x}$, $dS(\mathbf{x})$, etc., for brevity. Note: Integration by parts shows that $\lambda = u_1 = u_s$ on $\Gamma(t)$.

3.4 *Formal estimates*

Well-posedness of the fully continuous problem (3.11), (3.12) is challenging. One must handle the *parameterized deforming domain* appropriately and be able to obtain a priori estimates of the interface velocity, curvature, and improved regularity estimates of the variables [14, 31]. However, one may formally derive a priori bounds by assuming existence and uniqueness of a solution as well as sufficient regularity to allow for choosing test functions.

3.4.1 *A priori bound.*   For simplicity, take $u_D = 0$. In (3.11) and (3.12), choose $\boldsymbol{\eta}_1 = \boldsymbol{\sigma}_1$, $\boldsymbol{\eta}_s = \boldsymbol{\sigma}_s$, $\mathbf{Y} = \partial_t \mathbf{X}$, $q_1 = -u_1$, $q_s = -u_s$, $\mu = -\lambda$, and add the equations together to get:

$$\frac{1}{\widehat{K}_1} \int_{\Omega_1(t)} |\boldsymbol{\sigma}_1|^2 + \frac{1}{\widehat{K}_s} \int_{\Omega_s(t)} |\boldsymbol{\sigma}_s|^2 + \int_{\Gamma(t)} \frac{1}{\widehat{\beta}(\boldsymbol{\nu})} |\partial_t \mathbf{X} \cdot \boldsymbol{\nu}|^2 + \widehat{\alpha} \int_{\Gamma(t)} \nabla_\Gamma (\partial_t \mathbf{X}) : \nabla_\Gamma \mathbf{X}$$

$$+ \int_{\Omega_1(t)} u_1 \partial_t u_1 + \int_{\Omega_s(t)} u_s \partial_t u_s = \int_{\Omega_1(t)} u_1 f_1 + \int_{\Omega_s(t)} u_s f_s.$$

(3.13)

Next, we make some preliminary calculations for some of the terms in (3.13). By standard shape differentiation [16, 32, 56], we have

$$\frac{d}{dt} \left(\int_{\Omega_1(t)} u_1^2 \right) = \int_{\Omega_1(t)} \partial_t (u_1^2) - \int_{\Gamma(t)} u_1^2 (\partial_t \mathbf{X}) \cdot \boldsymbol{\nu},$$

$$\frac{d}{dt} \left(\int_{\Omega_s(t)} u_s^2 \right) = \int_{\Omega_s(t)} \partial_t (u_s^2) + \int_{\Gamma(t)} u_s^2 (\partial_t \mathbf{X}) \cdot \boldsymbol{\nu},$$

(3.14)

where we have accounted for the orientation of the normal vector $\boldsymbol{\nu}$ of $\Gamma(t)$. Thus,

$$\int_{\Omega_1(t)} u_1 \partial_t u_1 + \int_{\Omega_s(t)} u_s \partial_t u_s = \frac{1}{2} \left(\int_{\Omega_1(t)} \partial_t (u_1^2) + \int_{\Omega_s(t)} \partial_t (u_s^2) \right)$$

$$= \frac{1}{2} \frac{d}{dt} \left(\int_{\Omega_1(t)} u_1^2 + \int_{\Omega_s(t)} u_s^2 \right) + \frac{1}{2} \int_{\Gamma(t)} (u_1^2 - u_s^2) \partial_t \mathbf{X} \cdot \boldsymbol{\nu} \quad (3.15)$$

$$= \frac{1}{2} \frac{d}{dt} \left(\int_{\Omega_1(t)} u_1^2 + \int_{\Omega_s(t)} u_s^2 \right),$$

where the last term is dropped because (formally) $u_1 = u_s$ on $\Gamma(t)$.

Now note that shape differentiation also tells us that [16, 32, 56]

$$\int_{\Gamma(t)} \nabla_\Gamma (\partial_t \mathbf{X}) : \nabla_\Gamma \mathbf{X} = \frac{d}{dt} |\Gamma(t)|.$$

(3.16)

Therefore, we arrive at an identity

$$\int_{\Gamma(t)} \frac{1}{\widehat{\beta}(\nu)} [(\partial_t \mathbf{X}) \cdot \nu]^2 + \frac{1}{\widehat{K}_1} \|\sigma_1\|^2_{L^2(\Omega_1(t))} + \frac{1}{\widehat{K}_s} \|\sigma_s\|^2_{L^2(\Omega_s(t))} + \widehat{\alpha} \frac{d}{dt} |\Gamma(t)|$$
$$+ \frac{1}{2} \frac{d}{dt} \left(\int_{\Omega_1(t)} u_1^2 + \int_{\Omega_s(t)} u_s^2 \right) = \int_{\Omega_1(t)} u_1 f_1 + \int_{\Omega_s(t)} u_s f_s, \tag{3.17}$$

which is a variation of a result in [5, eqn. (2.13)].

To continue, we recall a variant of a Grönwall type inequality in [43, Lemma 3.1].

LEMMA 3.2 Let $g, h, r, w : [0, T] \rightarrow \mathbb{R}$ be measurable and positive functions such that

$$r^2(t) + g(t) + \int_0^t w(\tau) \, d\tau \leqslant r^2(0) + g(0) + \int_0^t r(\tau) h(\tau) \, d\tau, \quad \text{for all } t \in [0, T]. \tag{3.18}$$

Then,

$$r^2(t) + g(t) + \int_0^t w(\tau) \, d\tau \leqslant 2(r^2(0) + g(0)) + t \int_0^t h^2(\tau) \, d\tau, \quad \text{for all } t \in [0, T]. \tag{3.19}$$

Now make the following identifications with the functions in Lemma 3.2:

$$h(t) = \sqrt{2} \left(\|f_1(t)\|^2_{L^2(\Omega_1(t))} + \|f_s(t)\|^2_{L^2(\Omega_s(t))} \right)^{1/2},$$

$$r(t) = \frac{1}{\sqrt{2}} \left(\|u_1(t)\|^2_{L^2(\Omega_1(t))} + \|u_s(t)\|^2_{L^2(\Omega_s(t))} \right)^{1/2}, \qquad g(t) = \widehat{\alpha} |\Gamma(t)|,$$

$$w(t) = \|\widehat{\beta}^{-1/2}(\nu)(\partial_t \mathbf{X}) \cdot \nu\|^2_{L^2(\Gamma(t))} + \frac{1}{\widehat{K}_1} \|\sigma_1(t)\|^2_{L^2(\Omega_1(t))} + \frac{1}{\widehat{K}_s} \|\sigma_s(t)\|^2_{L^2(\Omega_s(t))}.$$

Using Cauchy–Schwarz twice on the right-hand-side of (3.17) and integrating, we get

$$\int_0^t w(\tau) \, d\tau + r^2(t) + g(t) \leqslant r^2(0) + g(0) + \int_0^t r(\tau) h(\tau) \, d\tau.$$

Applying Lemma 3.2 delivers the a priori estimate:

$$\frac{1}{2} \left(\|u_1(t)\|^2_{L^2(\Omega_1(t))} + \|u_s(t)\|^2_{L^2(\Omega_s(t))} \right) + \widehat{\alpha} |\Gamma(t)|$$
$$+ \int_0^t \left(\|\widehat{\beta}^{-1/2}(\nu)(\partial_t \mathbf{X}) \cdot \nu\|^2_{L^2(\Gamma(\tau))} + \frac{1}{\widehat{K}_1} \|\sigma_1(\tau)\|^2_{L^2(\Omega_1(\tau))} + \frac{1}{\widehat{K}_s} \|\sigma_s(\tau)\|^2_{L^2(\Omega_s(\tau))} \right) d\tau$$
$$\leqslant \left(\|u_1(0)\|^2_{L^2(\Omega_1(0))} + \|u_s(0)\|^2_{L^2(\Omega_s(0))} \right) + 2\widehat{\alpha} |\Gamma(0)|$$
$$+ 2t \int_0^t \left(\|f_1(\tau)\|^2_{L^2(\Omega_1(\tau))} + \|f_s(\tau)\|^2_{L^2(\Omega_s(\tau))} \right) d\tau, \quad \text{for all } t \in [0, T]. \tag{3.20}$$

See (4.27) for the semi-discrete version of (3.20).

3.4.2 *Conservation law.* We also have a conservation law for the system which is simply a thermal energy balance. Choosing $q_l = 1$, $q_s = 1$ in (3.11), and $\mu = 1$ in (3.12) gives

$$-\int_{\partial_D \Omega} \boldsymbol{\sigma}_l \cdot \boldsymbol{\nu}_\Omega + \int_{\Gamma(t)} \boldsymbol{\sigma}_l \cdot \boldsymbol{\nu} = \int_{\Omega_l(t)} \partial_t u_l - \int_{\Omega_l(t)} f_l,$$

$$-\int_{\Gamma(t)} \boldsymbol{\sigma}_s \cdot \boldsymbol{\nu} = \int_{\Omega_s(t)} \partial_t u_s - \int_{\Omega_s(t)} f_s,$$

$$\widehat{S} \int_{\Gamma(t)} (\partial_t \mathbf{X}) \cdot \boldsymbol{\nu} = \int_{\Gamma(t)} \boldsymbol{\sigma}_l \cdot \boldsymbol{\nu} - \int_{\Gamma(t)} \boldsymbol{\sigma}_s \cdot \boldsymbol{\nu}.$$

Adding them together gives the balance law:

$$\int_{\Omega_l(t)} f_l + \int_{\Omega_s(t)} f_s - \int_{\partial_D \Omega} \boldsymbol{\sigma}_l \cdot \boldsymbol{\nu}_\Omega = \int_{\Omega_l(t)} \partial_t u_l + \int_{\Omega_s(t)} \partial_t u_s - \widehat{S} \int_{\Gamma(t)} (\partial_t \mathbf{X}) \cdot \boldsymbol{\nu}, \qquad (3.21)$$

where the left side is the thermal (power) input and the right side is the rate of change in the stored thermal energy of the system. Note that energy is stored in the *phase change* associated with the velocity $\partial_t \mathbf{X}$ of $\Gamma(t)$. See (4.34) for the semi-discrete version of (3.21).

4. Time semi-discrete formulation

We now partition the time interval $(0, T)$ into subintervals of size Δt. We use a superscript i to denote a time dependent quantity at time t_i. Furthermore, let $(\cdot, \cdot)_\Sigma$ denote the L^2 inner product on the generic domain Σ. For a general domain Σ, let $\langle \cdot, \cdot \rangle_\Sigma$ denote the duality pairing on Σ between $H^{-1/2}(\Sigma)$ and $H^{1/2}(\Sigma)$ or between $H^{-1}(\Sigma)$ and $H^1(\Sigma)$ (the context will make it clear).

4.1 *Domain velocity*

4.1.1 *Map Γ^i to Γ^{i+1}.* We introduce the interface velocity $\mathbf{V} := \partial_t \mathbf{X}$ as a new variable. Thus, we approximate the interface position at time t_{i+1} by a backward Euler scheme:

$$\mathbf{X}^{i+1} = \mathbf{X}^i + \Delta t \, \mathbf{V}^{i+1}, \quad \text{where } \mathbf{V}^{i+1} : \Gamma^i \to \mathbb{R}^3. \qquad (4.1)$$

Thus, knowing $\mathbf{V}^{i+1}$ and $\mathbf{X}^i$ we can update the parametrization of the interface and obtain the interface Γ^{i+1} at t_{i+1}. Note that $\mathbf{X}^i(\cdot) \equiv \text{id}_{\Gamma^i}(\cdot)$ (the identity map) on Γ^i.

REMARK 4.1 We shall assume throughout this paper that $\mathbf{V}^{i+1}$ (for all i) is at least in $W^{1,\infty}(\Gamma^i)$ in order for the update (4.1) to make sense.

4.1.2 *Map Ω_l^i, Ω_s^i to Ω_l^{i+1}, Ω_s^{i+1}.* Clearly, the bulk domains Ω_l, Ω_s follow the interface Γ. Given $\mathbf{V}^{i+1}$ on Γ^i, it can be extended to the entire domain Ω by a harmonic extension [22, 65], i.e. if $\mathbf{V}_E^{i+1}$ denotes the extension, then

$$\mathbf{V}_E^{i+1} \in H^1(\Omega): \quad -\Delta \mathbf{V}_E^{i+1} = \mathbf{0}, \text{ in } \Omega_l^i \cup \Omega_s^i, \quad \mathbf{V}_E^{i+1} = \mathbf{V}^{i+1}, \text{ on } \Gamma^i, \quad \mathbf{V}_E^{i+1} = \mathbf{0}, \text{ on } \partial\Omega, \qquad (4.2)$$

In the following, we drop the E subscript and use $\mathbf{V}^{i+1}$ to denote the extension. This induces a map $\Phi_{i+1} : \Omega^i \to \Omega^{i+1}$ for "updating" the domain:

$$\Phi_{i+1}(\mathbf{x}) = \text{id}_{\Omega^i}(\mathbf{x}) + \Delta t \mathbf{V}^{i+1}(\mathbf{x}), \quad \text{for all } \mathbf{x} \in \Omega^i. \qquad (4.3)$$

See [27, 28] for similar constructions in an ALE (Arbitrary-Lagrangian-Eulerian) context.

Note that Φ_{i+1} is defined over both Ω_l^i and Ω_s^i, and $\Omega_l^{i+1} := \Phi_{i+1}(\Omega_l^i)$, $\Omega_s^{i+1} := \Phi_{i+1}(\Omega_s^i)$ conform to Γ^{i+1}. Similarly as for (4.1), we assume $\mathbf{V}^{i+1}$ (on Ω^i) is at least in $W^{1,\infty}(\Omega^i)$. Furthermore, we assume Φ_{i+1} is a bijective map and $\det([\nabla_{\mathbf{x}}\Phi_{i+1}(\mathbf{x})]) > 0$. We note the following properties satisfied by Φ_{i+1} [33, 58].

- If $\mathbf{y} = \Phi_{i+1}(\mathbf{x})$, then $(\nabla_{\mathbf{y}}\Phi_{i+1}^{-1} \circ \Phi_{i+1})(\mathbf{x}) = [\nabla_{\mathbf{x}}\Phi_{i+1}(\mathbf{x})]^{-1}$.
- If $f : \Omega^{i+1} \to \mathbb{R}$, then $\int_{\Omega^{i+1}} f(\mathbf{y})\, d\mathbf{y} = \int_{\Omega^i} f(\Phi_{i+1}(\mathbf{x})) \det([\nabla_{\mathbf{x}}\Phi_{i+1}(\mathbf{x})])\, d\mathbf{x}$.

We use the map Φ_{i+1} to transform the functions u_l^{i+1}, u_s^{i+1} on Ω^i to new functions on Ω^{i+1} in order to advance the solution to the next time step (see (4.7)).

REMARK 4.2 (Time Step Restriction) In order for (4.3) to remain bijective, Δt cannot be too large. In fact, it depends on $\|\nabla \mathbf{V}^{i+1}\|_{L^\infty(\Omega)}$ because $\det(\nabla \Phi_{i+1})$ depends on $\nabla \mathbf{V}^{i+1}$. There is also a similar restriction on the time step in Theorem 4.14 (a priori bound).

4.1.3 *Time derivative: Eulerian vs. Lagrangian.* Similar to (4.1), we use a backward Euler method to discretize the temperature time derivatives at each time step:

$$(\partial_t u_l)^{i+1} \approx \frac{u_l^{i+1} - u_l^i}{\Delta t}, \quad (\partial_t u_s)^{i+1} \approx \frac{u_s^{i+1} - u_s^i}{\Delta t}.$$

But, because the domain is changing, u_j^{i+1}, u_j^i ($j = 1, s$) are defined on different domains (Ω_j^i, Ω_j^{i-1}, respectively; see next section). This means u_j^i must be *transferred* to the new domain in order to compute the (discrete) Eulerian time derivative. The transference can be accomplished by an L^2 projection, for instance, but is not so convenient for a numerical method.

Therefore, we make use of the material derivative [58]. Using the standard formula $\dot{u}_j = \partial_t u_j + \mathbf{V} \cdot \nabla u_j$, and introducing the flux variables, we have $\dot{u}_j = \partial_t u_j - \widehat{K}_1^{-1} \mathbf{V} \cdot \boldsymbol{\sigma}_j$ for $j = 1, s$. Thus, we adopt the following discretization of $\partial_t u_l$ and $\partial_t u_s$:

$$(\partial_t u_j)^{i+1} \approx \frac{u_j^{i+1} - u_j^i \circ \Phi_i^{-1}}{\Delta t} + \frac{1}{\widehat{K}_j}\left(\boldsymbol{\sigma}_j^i \cdot \mathbf{V}^i\right) \circ \Phi_i^{-1}, \quad \text{for } j = 1, s. \tag{4.4}$$

Note that we have treated the convective term explicitly, and (formally) taking $\Delta t \to 0$ recovers the standard material derivative formula. The advantage here is that computing $u_j^i \circ \Phi_i^{-1}$ and $\left(\boldsymbol{\sigma}_j^i \cdot \mathbf{V}^i\right) \circ \Phi_i^{-1}$ ($j = 1, s$), in the fully discrete method, is straightforward (see (5.3) and Remark 5.8).

4.2 *Weak formulation*

We now present the semi-discrete formulation of equations (3.11) and (3.12). The main idea is to write all integrals over the current domain Ω^i, Γ^i but set all of the solution variables at the next time step t_{i+1} (i.e. a semi-implicit method). Moreover, we apply (4.1) and (4.4) and set $u_D^{i+1} = u_D(\cdot, t_{i+1})$, $f_l^{i+1} = f_l(\cdot, t_{i+1})$, and $f_s^{i+1} = f_s(\cdot, t_{i+1})$. Thus, we arrive at the following weak formulation. At time t_i, find $\boldsymbol{\sigma}_l^{i+1}$ in $\mathbb{V}_l^i(0)$, $\boldsymbol{\sigma}_s^{i+1}$ in $\mathbb{V}_s^i$, $\mathbf{V}^{i+1}$ in $\mathbb{Y}^i$, u_l^{i+1} in $\mathbb{Q}_l^i$, u_s^{i+1} in $\mathbb{Q}_s^i$, λ^{i+1}

in $\mathbb{M}^i$ such that

$$\frac{1}{\widehat{K}_1}(\boldsymbol{\sigma}_1^{i+1}, \boldsymbol{\eta}_1)_{\Omega_1^i} - (u_1^{i+1}, \nabla \cdot \boldsymbol{\eta}_1)_{\Omega_1^i} - \langle \boldsymbol{\eta}_1 \cdot \boldsymbol{\nu}^i, \lambda^{i+1} \rangle_{\Gamma^i} = -\langle \boldsymbol{\eta}_1 \cdot \boldsymbol{\nu}_\Omega, u_D^{i+1} \rangle_{\partial\Omega},$$
$$\text{for all } \boldsymbol{\eta}_1 \in \mathbb{V}_1^i(0),$$

$$-(\nabla \cdot \boldsymbol{\sigma}_1^{i+1}, q_1)_{\Omega_1^i} - \frac{1}{\Delta t}(u_1^{i+1}, q_1)_{\Omega_1^i} + \frac{1}{\Delta t}(\overline{u_1}^i, q_1)_{\Omega_1^i} = -(f_1^{i+1}, q_1)_{\Omega_1^i}, \text{ for all } q_1 \in \mathbb{Q}_1^i, \quad (4.5)$$

$$\frac{1}{\widehat{K}_s}(\boldsymbol{\sigma}_s^{i+1}, \boldsymbol{\eta}_s)_{\Omega_s^i} - (u_s^{i+1}, \nabla \cdot \boldsymbol{\eta}_s)_{\Omega_s^i} + \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}^i, \lambda^{i+1} \rangle_{\Gamma^i} = 0, \text{ for all } \boldsymbol{\eta}_s \in \mathbb{V}_s^i,$$

$$-(\nabla \cdot \boldsymbol{\sigma}_s^{i+1}, q_s)_{\Omega_s^i} - \frac{1}{\Delta t}(u_s^{i+1}, q_s)_{\Omega_s^i} + \frac{1}{\Delta t}(\overline{u_s}^i, q_s)_{\Omega_s^i} = -(f_s^{i+1}, q_s)_{\Omega_s^i}, \text{ for all } q_s \in \mathbb{Q}_s^i,$$

$$(\widehat{\beta}^{-1}(\boldsymbol{\nu}^i)\mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i, \mathbf{Y} \cdot \boldsymbol{\nu}^i)_{\Gamma^i} + \Delta t\widehat{\alpha}(\nabla_{\Gamma^i}\mathbf{V}^{i+1}, \nabla_{\Gamma^i}\mathbf{Y})_{\Gamma^i}$$
$$+\widehat{S}(\mathbf{Y} \cdot \boldsymbol{\nu}^i, \lambda^{i+1})_{\Gamma^i} = -\widehat{\alpha}(\nabla_{\Gamma^i}\mathbf{X}^i, \nabla_{\Gamma^i}\mathbf{Y})_{\Gamma^i}, \quad (4.6)$$
$$\text{for all } \mathbf{Y} \in \mathbb{Y}^i,$$

$$\widehat{S}(\mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i, \mu)_{\Gamma^i} - \langle \boldsymbol{\sigma}_1^{i+1} \cdot \boldsymbol{\nu}^i, \mu \rangle_{\Gamma^i} + \langle \boldsymbol{\sigma}_s^{i+1} \cdot \boldsymbol{\nu}^i, \mu \rangle_{\Gamma^i} = 0, \text{ for all } \mu \in \mathbb{M}^i,$$

where the function spaces are defined over the current (known) domain Ω^i, Γ^i. Then we use (4.1) to obtain the new interface position, which induces a map $\Phi_{i+1} : \Omega^i \to \Omega^{i+1}$. Because of (4.4), the temperature from the previous time index, $u_j^i : \Omega_j^{i-1} \to \mathbb{R}$, is mapped onto Ω_j^i by

$$\overline{u_j}^i := u_j^i \circ \Phi_i^{-1} - \Delta t \frac{1}{\widehat{K}_j} \left(\boldsymbol{\sigma}_j^i \cdot \mathbf{V}^i \right) \circ \Phi_i^{-1}, \text{ for } j = 1, s. \quad (4.7)$$

Iterating this procedure gives a time semi-discrete approximation of the fully continuous problem (3.11), (3.12).

REMARK 4.3 (How To Start The Method) From (4.7), it is clear we need $\mathbf{V}^0$ to compute $\overline{u_1}^0$, $\overline{u_s}^0$. However, we start solving (4.5), (4.6) at $i = 0$, which only gives $\mathbf{V}^1$. Hence, we must do one of the following. (i) specify $\mathbf{V}^0$, $\boldsymbol{\sigma}_1^0$, $\boldsymbol{\sigma}_s^0$; (ii) set $\mathbf{V}^0 = \boldsymbol{\sigma}_1^0 = \boldsymbol{\sigma}_s^0 = \mathbf{0}$ (i.e. choose $\overline{u_1}^0$, $\overline{u_s}^0$ directly); (iii) or apply (ii) with a small time step to obtain an approximation of $\mathbf{V}^0$, $\boldsymbol{\sigma}_1^0$, $\boldsymbol{\sigma}_s^0$. Either way, the error in approximating $\overline{u_1}^0$, $\overline{u_s}^0$ is only $O(\Delta t)$.

4.3 *Abstract formulation*

In order to simplify notation, we shall drop the time index notation and remember that we are solving for all variables on the current known domain $\Omega \equiv \Omega^i$, $\Gamma \equiv \Gamma^i$ with the current known normal vector $\boldsymbol{\nu} \equiv \boldsymbol{\nu}^i$. In particular, we take

$$\boldsymbol{\sigma}_1^{i+1} \equiv \boldsymbol{\sigma}_1, \ \boldsymbol{\sigma}_s^{i+1} \equiv \boldsymbol{\sigma}_s, \ \mathbf{V}^{i+1} \equiv \mathbf{V}, \ u_1^{i+1} \equiv u_1, \ u_s^{i+1} \equiv u_s, \ \lambda^{i+1} \equiv \lambda,$$
$$f_1^{i+1} \equiv f_1, \ f_s^{i+1} \equiv f_s, \ u_D^{i+1} \equiv u_D, \ \overline{u_1}^i \equiv \overline{u_1}, \ \overline{u_s}^i \equiv \overline{u_s}, \ \mathbf{X}^i \equiv \overline{\mathbf{X}}, \ \nabla_{\Gamma^i} \equiv \nabla_{\Gamma}.$$

4.3.1 *Bilinear and linear forms.* For notational convenience, we introduce the following bilinear forms. The primal form is

$$
a\big((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V})\big) = \frac{1}{\widehat{K}_l}(\boldsymbol{\eta}_l, \boldsymbol{\sigma}_l)_{\Omega_l} + \frac{1}{\widehat{K}_s}(\boldsymbol{\eta}_s, \boldsymbol{\sigma}_s)_{\Omega_s} \\
+ (\widehat{\beta}^{-1}(\boldsymbol{\nu})\mathbf{Y} \cdot \boldsymbol{\nu}, \mathbf{V} \cdot \boldsymbol{\nu})_\Gamma + \Delta t \widehat{\alpha}(\nabla_\Gamma \mathbf{Y}, \nabla_\Gamma \mathbf{V})_\Gamma,
$$

(4.8)

the constraint form is

$$
b\big((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (q_l, q_s, \mu)\big) = -(\nabla \cdot \boldsymbol{\eta}_l, q_l)_{\Omega_l} - (\nabla \cdot \boldsymbol{\eta}_s, q_s)_{\Omega_s} \\
- \langle \boldsymbol{\eta}_l \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma + \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma + \widehat{S}\,(\mathbf{Y} \cdot \boldsymbol{\nu}, \mu)_\Gamma,
$$

(4.9)

and the lower diagonal form is

$$
c\big((q_l, q_s, \mu), (u_l, u_s, \lambda)\big) = \frac{1}{\Delta t}(q_l, u_l)_{\Omega_l} + \frac{1}{\Delta t}(q_s, u_s)_{\Omega_s}.
$$

(4.10)

The linear forms are defined by

$$
\chi(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}) = -\big(\langle \boldsymbol{\eta}_l \cdot \boldsymbol{\nu}_\Omega, u_D \rangle_{\partial\Omega} + \widehat{\alpha}(\nabla_\Gamma \overline{\mathbf{X}}, \nabla_\Gamma \mathbf{Y})_\Gamma\big),
$$
$$
\psi(q_l, q_s, \mu) = -\Big((f_l, q_l)_{\Omega_l} + (f_s, q_s)_{\Omega_s} + \frac{1}{\Delta t}(\overline{u_l}, q_l)_{\Omega_l} + \frac{1}{\Delta t}(\overline{u_s}, q_s)_{\Omega_s}\Big).
$$

(4.11)

4.3.2 *Saddle-point formulation.* Define the primal space by

$$
\mathbb{Z} = \mathbb{V}_l(0) \times \mathbb{V}_s \times \mathbb{Y},
$$

(4.12)

and the multiplier space by

$$
\mathbb{T} = \mathbb{Q}_l \times \mathbb{Q}_s \times \mathbb{M}.
$$

(4.13)

With the above notation, the formulation (4.5), (4.6) can be written as a saddle-point problem.

VARIATIONAL FORMULATION 4.4 Find $(\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V})$ in $\mathbb{V}_l(0) \times \mathbb{V}_s \times \mathbb{Y}$ and (u_l, u_s, λ) in $\mathbb{Q}_l \times \mathbb{Q}_s \times \mathbb{M}$ such that

$$
a\big((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V})\big) + b\big((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (u_l, u_s, \lambda)\big) = \chi(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}),
$$
$$
b\big((\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V}), (q_l, q_s, \mu)\big) - c\big((q_l, q_s, \mu), (u_l, u_s, \lambda)\big) = \psi(q_l, q_s, \mu),
$$

(4.14)

for all $(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})$ in $\mathbb{V}_l(0) \times \mathbb{V}_s \times \mathbb{Y}$, and (q_l, q_s, μ) in $\mathbb{Q}_l \times \mathbb{Q}_s \times \mathbb{M}$. The temperatures u_l, u_s are Lagrange multipliers as well as the interface temperature λ.

4.4 Norms

4.4.1 *Non-degenerate interface.* The purpose of the following assumption is to avoid a case where Γ is closed and very flat (e.g. the surface of a pancake). It is necessary to ensure the equivalence of the norms in Proposition 4.6.

ASSUMPTION 4.5 Assume that Γ is a Lipschitz or polyhedral manifold. In addition, for any non-zero constant vector $\mathbf{a} \in \mathbb{R}^3$, assume there exists an open neighborhood $\mathfrak{N} \subset \Gamma$ such that $|\mathfrak{N}| \geq c_0 > 0$ and

$$
\mathbf{a} \cdot \boldsymbol{\nu}(\mathbf{x}) > 0, \quad \forall \mathbf{x} \in \mathfrak{N}, \quad \text{or} \quad \mathbf{a} \cdot \boldsymbol{\nu}(\mathbf{x}) < 0, \quad \forall \mathbf{x} \in \mathfrak{N}.
$$

4.4.2 *Primal norm.* Clearly, $\|(\boldsymbol{\eta}_\mathrm{l}, \boldsymbol{\eta}_\mathrm{s}, \mathbf{Y})\|^2_{\mathbb{Z}\diamond} := \|\boldsymbol{\eta}_\mathrm{l}\|^2_{H(\mathrm{div}, \Omega_\mathrm{l})} + \|\boldsymbol{\eta}_\mathrm{s}\|^2_{H(\mathrm{div}, \Omega_\mathrm{s})} + \|\mathbf{Y}\|^2_{H^1(\Gamma)}$ is a norm on $\mathbb{Z}$. But because of the form of the equations, we shall use a different norm. First, we note an equivalent norm to the standard H^1 norm on Γ (recall that $\|\mathbf{Y}\|^2_{H^1(\Gamma)} = \|\mathbf{Y}\|^2_{L^2(\Gamma)} + \|\nabla_\Gamma \mathbf{Y}\|^2_{L^2(\Gamma)}$).

PROPOSITION 4.6 Let Γ be a Lipschitz or polyhedral manifold. Define:

$$|||\mathbf{Y}|||^2 = \|\mathbf{Y} \cdot \boldsymbol{\nu}\|^2_{H^{-1/2}(\Gamma)} + \|\nabla_\Gamma \mathbf{Y}\|^2_{L^2(\Gamma)}.$$

Then, $|||\mathbf{Y}||| \approx \|\mathbf{Y}\|_{H^1(\Gamma)}$, with constants that only depend on the domain.

Proof. First, verify that $|||\mathbf{Y}|||$ is a norm on $H^1(\Gamma)$. We just need to check that $|||\mathbf{Y}||| = 0 \Leftrightarrow \mathbf{Y} = \mathbf{0}$ since the other norm properties are trivial to verify. If $|||\mathbf{Y}||| = 0$, then $\|\nabla_\Gamma \mathbf{Y}\|_{L^2(\Gamma)} = 0$, so $\mathbf{Y} = \mathbf{a} \in \mathbb{R}^3$ (constant vector). If $\mathbf{a} \neq \mathbf{0}$, then by Assumption 4.5, $\mathbf{a} \cdot \boldsymbol{\nu} > 0$ (or < 0) on a set of positive measure. Thus, $\|\mathbf{Y} \cdot \boldsymbol{\nu}\|^2_{H^{-1/2}(\Gamma)} \neq 0$, but this is a contradiction, so then $\mathbf{a} = \mathbf{0}$. Since $||| \cdot |||$ is a norm on $H^1(\Gamma)$, the equivalence with $\| \cdot \|_{H^1(\Gamma)}$ follows by a classical compactness argument [1, 21]. $\qquad\square$

In light of the above, we define the following primal norm:

$$\|(\boldsymbol{\eta}_\mathrm{l}, \boldsymbol{\eta}_\mathrm{s}, \mathbf{Y})\|^2_{\mathbb{Z}} = \frac{1}{\widehat{K}_\mathrm{l}} \|\boldsymbol{\eta}_\mathrm{l}\|^2_{H(\mathrm{div}, \Omega_\mathrm{l})} + \frac{1}{\widehat{K}_\mathrm{s}} \|\boldsymbol{\eta}_\mathrm{s}\|^2_{H(\mathrm{div}, \Omega_\mathrm{s})} + \|\widehat{\beta}^{-1/2} \mathbf{Y} \cdot \boldsymbol{\nu}\|^2_{L^2(\Gamma)}$$
$$+ \|\mathbf{Y} \cdot \boldsymbol{\nu}\|^2_{H^{-1/2}(\Gamma)} + \Delta t \widehat{\alpha} \|\nabla_\Gamma \mathbf{Y}\|^2_{L^2(\Gamma)}. \quad (4.15)$$

The choice of $H^{-1/2}(\Gamma)$ is the most convenient for our formulation.

4.4.3 *Multiplier norm.* The obvious multiplier norm is $\|(q_\mathrm{l}, q_\mathrm{s}, \mu)\|^2_{\mathbb{T}\diamond} := \|q_\mathrm{l}\|^2_{L^2(\Omega_\mathrm{l})} + \|q_\mathrm{s}\|^2_{L^2(\Omega_\mathrm{s})} + \|\mu\|^2_{H^{1/2}(\Gamma)}$. However, because of the form of the bilinear form b (4.9), it is more advantageous to use the following equivalent norm:

$$\|(q_\mathrm{l}, q_\mathrm{s}, \mu)\|^2_{\mathbb{T}} = \|\tilde{q}_\mathrm{l}\|^2_{L^2(\Omega_\mathrm{l})} + \|\tilde{q}_\mathrm{s}\|^2_{L^2(\Omega_\mathrm{s})} + \|\mu - \hat{q}_\mathrm{l}\|^2_{H^{1/2}_\mathrm{l}(\Gamma)}$$
$$+ \|\mu - \hat{q}_\mathrm{s}\|^2_{H^{1/2}_\mathrm{s}(\Gamma)} + \widehat{S} \|\mu \nu\|^2_{H^{-1}(\Gamma)}, \quad (4.16)$$

where we introduced the mean value: $\hat{q}_i := \frac{1}{|\Omega_i|} \int_{\Omega_i} q_i$, and $\tilde{q}_i := q_i - \hat{q}_i$ (for $i = 1, \mathrm{s}$). We also define the mean value on Γ: $\hat{\mu} := \frac{1}{|\Gamma|} \int_\Gamma \mu$, and $\tilde{\mu} := \mu - \hat{\mu}$.

PROPOSITION 4.7 (Equivalence of Multiplier Norms) Let Γ be a Lipschitz or polyhedral manifold. Then, $\|(q_\mathrm{l}, q_\mathrm{s}, \mu)\|_{\mathbb{T}\diamond} \approx \|(q_\mathrm{l}, q_\mathrm{s}, \mu)\|_{\mathbb{T}}$, with constants that only depend on the domain and $\widehat{S}$.

Proof. Again, use a compactness argument. $\qquad\square$

4.5 *Well-posedness*

This section verifies the conditions needed for well-posedness of (4.14) [9, 11].

4.5.1 *Main conditions.*

LEMMA 4.8 (Continuity of Forms) For all $(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V})$ in $\mathbb{Z}$ and $(q_l, q_s, \mu), (u_l, u_s, \lambda)$ in $\mathbb{T}$,

$$
\left| a\big((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V})\big) \right| \leqslant C_a \|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}} \|(\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V})\|_{\mathbb{Z}},
$$
$$
\left| b\big((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (q_l, q_s, \mu)\big) \right| \leqslant C_b \|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}} \|(q_l, q_s, \mu)\|_{\mathbb{T}},
$$
$$
\left| c\big((q_l, q_s, \mu), (u_l, u_s, \lambda)\big) \right| \leqslant \Delta t^{-1} \big(\|q_l\|_{L^2(\Omega_l)} \|u_l\|_{L^2(\Omega_l)} + \|q_s\|_{L^2(\Omega_s)} \|u_s\|_{L^2(\Omega_s)} \big),
$$
$$
\left| \chi(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}) \right| \leqslant C_\chi \|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}},
$$
$$
\left| \psi(q_l, q_s, \mu) \right| \leqslant C_\psi \|(q_l, q_s, \mu)\|_{\mathbb{T}},
$$

where $C_a, C_b, C_\chi, C_\psi > 0$ are constants that depend on physical parameters and domain geometry. In addition, C_χ depends on u_D, $\Delta t^{-1/2}$, and C_ψ depends on f_l, f_s, $\overline{u_l}, \overline{u_s}$ and Δt^{-1}.

Proof. The first result comes from two uses of the Schwarz inequality. The second estimate follows by noting

$$
-(\nabla \cdot \boldsymbol{\eta}_l, q_l)_{\Omega_l} - \langle \boldsymbol{\eta}_l \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma \leqslant \big(\|q_l\|_{L^2(\Omega_l)} + \|\mu\|_{H^{1/2}(\Gamma)} \big) \|\boldsymbol{\eta}_l\|_{H(\mathrm{div}, \Omega_l)},
$$
$$
-(\nabla \cdot \boldsymbol{\eta}_s, q_s)_{\Omega_s} + \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma \leqslant \big(\|q_s\|_{L^2(\Omega_s)} + \|\mu\|_{H^{1/2}_s(\Gamma)} \big) \|\boldsymbol{\eta}_s\|_{H(\mathrm{div}, \Omega_s)},
$$

where we used Cauchy–Schwarz and (3.7). In addition, by (3.8), we have

$$
\widehat{S} \int_\Gamma \mu(\mathbf{Y} \cdot \boldsymbol{\nu}) = \widehat{S} \langle \mathbf{Y} \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma \leqslant \widehat{S} \|\mathbf{Y} \cdot \boldsymbol{\nu}\|_{H^{-1/2}(\Gamma)} \|\mu\|_{H^{1/2}(\Gamma)}.
$$

The bound on b then follows by combining these results and using Proposition 4.7. The bound on c is obvious. Next, we have

$$
\chi(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}) \leqslant \|u_D\|_{H^{1/2}(\partial\Omega)} \|\boldsymbol{\eta}_l \cdot \boldsymbol{\nu}_\Omega\|_{H^{-1/2}(\partial\Omega)} + C_1 \widehat{\alpha} \|\nabla_\Gamma \mathbf{Y}\|_{L^2(\Gamma)} \leqslant C \|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}},
$$

where C depends on $\Delta t^{-1/2}$ and the data u_D. The last inequality follows from (4.11) where the constant depends on Δt^{-1} and the problem data. $\square$

LEMMA 4.9 (Coercivity) Let $(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}) \in \mathbb{Z}$ with $b((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (q_l, q_s, \mu)) = 0$ for all $(q_l, q_s, \mu) \in \mathbb{T}$. Then,

$$
\left| a((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})) \right| \geqslant C \|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}}^2,
$$

where $C > 0$ is a constant depending on $\widehat{S}$, $\widehat{K}_l$, $\widehat{K}_s$, and the domain. This is true even if $\widehat{\beta} \to \infty$.

Proof. From (4.8), we get

$$
\begin{aligned}
a\big((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\big) &\geqslant \frac{1}{\widehat{K}_l} \|\boldsymbol{\eta}_l\|_{L^2(\Omega_l)}^2 + \frac{1}{\widehat{K}_s} \|\boldsymbol{\eta}_s\|_{L^2(\Omega_s)}^2 + \|\widehat{\beta}^{-1/2} \mathbf{Y} \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)}^2 \\
&\qquad + \Delta t \widehat{\alpha} \|\nabla_\Gamma \mathbf{Y}\|_{L^2(\Gamma)}^2 \\
&= \frac{1}{\widehat{K}_l} \|\boldsymbol{\eta}_l\|_{H(\mathrm{div}, \Omega_l)}^2 + \frac{1}{\widehat{K}_s} \|\boldsymbol{\eta}_s\|_{H(\mathrm{div}, \Omega_s)}^2 \\
&\qquad + \|\widehat{\beta}^{-1/2} \mathbf{Y} \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)}^2 + \Delta t \widehat{\alpha} \|\nabla_\Gamma \mathbf{Y}\|_{L^2(\Gamma)}^2,
\end{aligned}
$$

where the last step follows from the hypothesis $\nabla \cdot \boldsymbol{\eta}_l = \nabla \cdot \boldsymbol{\eta}_s = 0$. Also by hypothesis, we have

$$\widehat{S}\,(\mathbf{Y} \cdot \boldsymbol{\nu}, \mu)_\Gamma = \langle \boldsymbol{\eta}_l \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma - \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma, \quad \text{for all } \mu \in H^{1/2}(\Gamma).$$

Hence, using (3.7) and (3.8), we have

$$\widehat{S}\,\|\mathbf{Y} \cdot \boldsymbol{\nu}\|_{H^{-1/2}(\Gamma)} = \sup_{\mu \in H^{1/2}(\Gamma)} \frac{\widehat{S}\,(\mathbf{Y} \cdot \boldsymbol{\nu}, \mu)_\Gamma}{\|\mu\|_{H^{1/2}(\Gamma)}} \leqslant 2\left(\|\boldsymbol{\eta}_l\|_{H(\mathrm{div},\Omega_l)} + \|\boldsymbol{\eta}_s\|_{H(\mathrm{div},\Omega_s)}\right).$$

Combining these inequalities yields the assertion. $\qquad\square$

LEMMA 4.10 (Inf-Sup) For all $(q_l, q_s, \mu) \in \mathbb{T}$, the following "inf-sup" condition holds

$$\sup_{(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}) \in \mathbb{Z}} \frac{b((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (q_l, q_s, \mu))}{\|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}^\diamond}} \geqslant C\,\|(q_l, q_s, \mu)\|_\mathbb{T},$$

where $C > 0$ depends on the domain and $\widehat{S}$. If $\|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}^\diamond}$ is replaced by $\|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_\mathbb{Z}$ in the denominator, then the inf-sup still holds, except C also depends on $\widehat{K}_l$, $\widehat{K}_s$, $\widehat{\alpha}$, and $\widehat{\beta}_-$. Furthermore, C does *not* depend on the time step Δt, as long as $\Delta t \leqslant 1$.

Proof. Setting $\boldsymbol{\eta}_l \cdot \boldsymbol{\nu}_\Omega = 0$ on $\partial\Omega$, and accounting for the orientation of the normal vector and using the divergence theorem, we have

$$
\begin{aligned}
b\big((\boldsymbol{\eta}_l, &\boldsymbol{\eta}_s, \mathbf{Y}), (q_l, q_s, \mu)\big) \\
&= -(\nabla \cdot \boldsymbol{\eta}_l, q_l)_{\Omega_l} - (\nabla \cdot \boldsymbol{\eta}_s, q_s)_{\Omega_s} - \langle \boldsymbol{\eta}_l \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma + \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma + \widehat{S}\,(\mathbf{Y} \cdot \boldsymbol{\nu}, \mu)_\Gamma \\
&= -(\nabla \cdot \boldsymbol{\eta}_l, \tilde{q}_l)_{\Omega_l} - (\nabla \cdot \boldsymbol{\eta}_s, \tilde{q}_s)_{\Omega_s} - \langle \boldsymbol{\eta}_l \cdot \boldsymbol{\nu}, \mu - \hat{q}_l \rangle_\Gamma + \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}, \mu - \hat{q}_s \rangle_\Gamma \\
&\qquad\qquad\qquad\qquad\qquad + \widehat{S}\,(\mathbf{Y} \cdot \boldsymbol{\nu}, \mu)_\Gamma.
\end{aligned}
$$

By definition of the $H_l^{1/2}(\Gamma)$ norm (3.7), there exists a $\boldsymbol{\xi} \in \mathbb{V}_l(0)$ such that $-\langle \boldsymbol{\xi} \cdot \boldsymbol{\nu}, \mu - \hat{q}_l \rangle_\Gamma = \|\mu - \hat{q}_l\|_{H_l^{1/2}(\Gamma)}$ and $\|\boldsymbol{\xi}\|_{H(\mathrm{div},\Omega_l)} = 1$. With this, we construct the vector field $\boldsymbol{\eta}_l \in H(\mathrm{div}, \Omega_l)$. Let ϕ_1, ϕ_2 in $H^1(\Omega_l)$ (with zero mean value) be weak solutions of the following elliptic problems,

$$-\Delta\phi_1 = \frac{\tilde{q}_l}{\|\tilde{q}_l\|_{L^2(\Omega_l)}}, \text{ in } \Omega_l, \quad \boldsymbol{\nu} \cdot \nabla\phi_1 = 0, \text{ on } \partial\Omega_l \equiv \Gamma \cup \partial\Omega,$$

$$-\Delta\phi_2 = \frac{1}{|\Omega_l|}\int_{\partial\Omega_l} \boldsymbol{\xi} \cdot \boldsymbol{\nu}, \text{ in } \Omega_l, \quad \boldsymbol{\nu} \cdot \nabla\phi_2 = \boldsymbol{\xi} \cdot \boldsymbol{\nu}, \text{ on } \partial\Omega_l,$$

and define $\boldsymbol{\eta}_l = \nabla\phi_1 + \nabla\phi_2$ (note that $\nabla\phi_1$ and $\nabla\phi_2$ are in $\mathbb{V}_l(0)$). This gives

$$
\begin{aligned}
-(\nabla \cdot \boldsymbol{\eta}_l, \tilde{q}_l)_{\Omega_l} - \langle \boldsymbol{\eta}_l \cdot \boldsymbol{\nu}, \mu - \hat{q}_l \rangle_\Gamma &= (-\Delta\phi_1, \tilde{q}_l)_{\Omega_l} + (-\Delta\phi_2, \tilde{q}_l)_{\Omega_l} - \langle \boldsymbol{\nu} \cdot \nabla\phi_2, \mu - \hat{q}_l \rangle_\Gamma \\
&= \|\tilde{q}_l\|_{L^2(\Omega_l)} + \|\mu - \hat{q}_l\|_{H_l^{1/2}(\Gamma)}.
\end{aligned}
$$

Now bound $\|\boldsymbol{\eta}_l\|_{H(\mathrm{div},\Omega_l)}$. Since (3.2) and (3.3) hold with Ω replaced by Ω_l, we get $\|\Delta\phi_2\|_{L^2(\Omega_l)} \leqslant C_0|\langle \boldsymbol{\xi} \cdot \boldsymbol{\nu}, 1 \rangle_{\partial\Omega_l}| \leqslant C_1\|\boldsymbol{\xi} \cdot \boldsymbol{\nu}\|_{H^{-1/2}(\partial\Omega_l)} \leqslant C_1\|\boldsymbol{\xi}\|_{H(\mathrm{div},\Omega_l)} = C_1$. Moreover, a standard a priori bound gives $\|\phi_2\|_{H^1(\Omega_l)} \leqslant C_2\left(\|\Delta\phi_2\|_{L^2(\Omega_l)} + \|\boldsymbol{\xi} \cdot \boldsymbol{\nu}\|_{H^{-1/2}(\partial\Omega_l)}\right) \leqslant C_2(C_1 + 1)$. Similarly, we deduce that $\|\Delta\phi_1\|_{L^2(\Omega_l)} = 1$ and $\|\phi_1\|_{H^1(\Omega_l)} \leqslant C_3$. Hence, we arrive at the following result

$$\|\boldsymbol{\eta}_l\|_{H(\mathrm{div},\Omega_l)} \leqslant \|\Delta\phi_1\|_{L^2(\Omega_l)} + \|\Delta\phi_2\|_{L^2(\Omega_l)} + \|\phi_1\|_{H^1(\Omega_l)} + \|\phi_2\|_{H^1(\Omega_l)} \leqslant C_4,$$

where $C_4 > 0$ depends on Ω_l and Γ. Analogous results show there exists an $\boldsymbol{\eta}_s$ in $\mathbb{V}_s$ such that

$$-(\nabla \cdot \boldsymbol{\eta}_s, \tilde{q}_s)_{\Omega_l} + \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}, \mu - \hat{q}_s \rangle_\Gamma = \|\tilde{q}_s\|_{L^2(\Omega_s)} + \|\mu - \hat{q}_s\|_{H_s^{1/2}(\Gamma)}, \quad \|\boldsymbol{\eta}_s\|_{H(\mathrm{div}, \Omega_s)} \leqslant C_5,$$

where $C_5 > 0$ depends on Ω_s and Γ.

By the definition of the $H^{-1}(\Gamma)$ norm (3.9), there exists a $\mathbf{Y}$ in $H^1(\Gamma)$ such that

$$(\mathbf{Y} \cdot \boldsymbol{\nu}, \mu)_\Gamma = \langle \mathbf{Y}, \mu\boldsymbol{\nu} \rangle_\Gamma = \|\mu\boldsymbol{\nu}\|_{H^{-1}(\Gamma)}, \quad \|\mathbf{Y}\|_{H^1(\Gamma)} = 1.$$

Taking all this together gives the result.   □

4.5.2 *Summary.*

For saddle-point problems, one usually needs to only check the continuity, coercivity, and inf-sup conditions to verify well-posedness. However, there is the third bilinear form $c(\cdot, \cdot)$, whose continuity constant depends on Δt^{-1} (see Lemma 4.8). As long as $\Delta t > 0$, the system (4.14) is well-posed with a bounded solution [9, 11]. But it is important to know how the time step affects the well-posedness, especially as $\Delta t \to 0$.

The following lemma is a modification of a result in [9, Lemma 4.14], applied to our formulation, which illustrates the effect of Δt.

LEMMA 4.11 Let $(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})$ in $\mathbb{Z}$ such that $b((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (0, 0, \mu)) = 0$ for all $\mu \in \mathbb{M}$. Then, the bilinear forms a and b in (4.8), (4.9) satisfy

$$\frac{a((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}))}{\|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}^*}} + \sup_{(q_l, q_s) \in \mathbb{Q}_l \times \mathbb{Q}_s} \frac{b((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (q_l, q_s, 0))}{\Delta t^{-1/2}(\|q_l\|^2_{L^2(\Omega_l)} + \|q_s\|^2_{L^2(\Omega_s)})^{1/2}}$$

$$\geqslant C \|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}^*},$$

where $C > 0$ depends on the physical parameters and the domain, with norm defined by

$$\|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|^2_{\mathbb{Z}^*} := \frac{1}{\widehat{K}_l} \left(\|\boldsymbol{\eta}_l\|^2_{L^2(\Omega_l)} + \Delta t \|\nabla \cdot \boldsymbol{\eta}_l\|^2_{L^2(\Omega_l)} \right)$$

$$+ \frac{1}{\widehat{K}_s} \left(\|\boldsymbol{\eta}_s\|^2_{L^2(\Omega_s)} + \Delta t \|\nabla \cdot \boldsymbol{\eta}_s\|^2_{L^2(\Omega_s)} \right)$$

$$+ \|\widehat{\beta}^{-1/2} \mathbf{Y} \cdot \boldsymbol{\nu}\|^2_{L^2(\Gamma)} + \Delta t \|\mathbf{Y} \cdot \boldsymbol{\nu}\|^2_{H^{-1/2}(\Gamma)} + \Delta t \widehat{\alpha} \|\nabla_\Gamma \mathbf{Y}\|^2_{L^2(\Gamma)}.$$

Lemma 4.11, and [9, Theorem 4.11, 4.13], yields the well-posedness of (4.14), but one can see more clearly how the norm is affected. An extra factor of Δt multiplies $\|\nabla \cdot \boldsymbol{\eta}_l\|^2_{L^2(\Omega_l)}$, $\|\nabla \cdot \boldsymbol{\eta}_s\|^2_{L^2(\Omega_s)}$, and $\|\mathbf{Y} \cdot \boldsymbol{\nu}\|^2_{H^{-1/2}(\Gamma)}$. This is reasonable given the parabolic nature of the problem. In particular, from (4.5), one can see that $\nabla \cdot \boldsymbol{\eta}_l$ and $\nabla \cdot \boldsymbol{\eta}_s$ depends on the discrete time derivative of u_l and u_s.

4.6 *Estimates*

The semi-discrete system (4.5), (4.6) satisfies both an a priori stability bound in time and a conservation law (see the following sections). First, we note some basic results we will need.

PROPOSITION 4.12 Let $\mathbf{A}$ be a constant 3×3 matrix and define $\mathbf{G}(\gamma) = \mathbf{I} + \gamma\mathbf{A}$ for all γ in $\mathbb{R}$. Then

$$\det \mathbf{G}(\gamma) = 1 + \gamma \operatorname{trace}(\mathbf{A}) + \frac{1}{2}\gamma^2 \underbrace{\left[(\operatorname{trace}(\mathbf{A}))^2 - \operatorname{trace}(\mathbf{A}^2)\right]}_{=:\Xi_1(\mathbf{A})} + \frac{1}{6}\gamma^3 \Xi_2(\mathbf{A}),$$

where $\Xi_1(\mathbf{A})$ and $\Xi_2(\mathbf{A})$ are functions of $\mathbf{A}$ that satisfy $|\Xi_1(\mathbf{A})| \leqslant C|\mathbf{A}|^2$, $|\Xi_2(\mathbf{A})| \leqslant C|\mathbf{A}|^3$, where $|\cdot|$ is any matrix norm and $C > 0$ is a constant that only depends on the norm.

LEMMA 4.13 (Discrete Grönwall Inequality) Let $c \geqslant 0$ and suppose $\{r_i\}_{i \geqslant 0}$ and $\{g_i\}_{i \geqslant 0}$ are non-negative sequences. Then the following is true:

$$r_n \leqslant c + \sum_{k=0}^{n-1} g_k r_k, \quad \text{for all } n \geqslant 0, \quad \Rightarrow \quad r_n \leqslant c \exp\left(\sum_{k=0}^{n-1} g_k\right), \quad \text{for all } n \geqslant 0,$$

where the sum is zero when $n = 0$.

4.6.1 *A priori bound.* We begin as we did in Section 3.4.1. Again, take $u_{\mathrm{D}}^{i+1} = 0$ for $i \geqslant 0$. In (4.5) and (4.6), choose $\boldsymbol{\eta}_{\mathrm{l}} = \boldsymbol{\sigma}_{\mathrm{l}}^{i+1}$, $\boldsymbol{\eta}_{\mathrm{s}} = \boldsymbol{\sigma}_{\mathrm{s}}^{i+1}$, $\mathbf{Y} = \mathbf{V}^{i+1}$, $q_{\mathrm{l}} = -u_{\mathrm{l}}^{i+1}$, $q_{\mathrm{s}} = -u_{\mathrm{s}}^{i+1}$, $\mu = -\lambda^{i+1}$, and add the equations together to get

$$\begin{aligned}
\frac{1}{\widehat{K}_{\mathrm{l}}}\|\boldsymbol{\sigma}_{\mathrm{l}}^{i+1}\|_{L^2(\Omega_{\mathrm{l}}^i)}^2 + \frac{1}{\widehat{K}_{\mathrm{s}}}\|\boldsymbol{\sigma}_{\mathrm{s}}^{i+1}\|_{L^2(\Omega_{\mathrm{s}}^i)}^2 &+ \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu}^i)\mathbf{V}^{i+1}\cdot\boldsymbol{\nu}^i\|_{L^2(\Gamma^i)}^2 \\
&+ \widehat{\alpha}\left[(\nabla_{\Gamma^i}(\Delta t\mathbf{V}^{i+1}), \nabla_{\Gamma^i}\mathbf{V}^{i+1})_{\Gamma^i} + (\nabla_{\Gamma^i}\mathbf{X}^i, \nabla_{\Gamma^i}\mathbf{V}^{i+1})_{\Gamma^i}\right] \\
&+ \frac{1}{\Delta t}(u_{\mathrm{l}}^{i+1}, (u_{\mathrm{l}}^{i+1} - \overline{u_{\mathrm{l}}}^i))_{\Omega_{\mathrm{l}}^i} + \frac{1}{\Delta t}(u_{\mathrm{s}}^{i+1}, (u_{\mathrm{s}}^{i+1} - \overline{u_{\mathrm{s}}}^i))_{\Omega_{\mathrm{s}}^i} \\
&= (u_{\mathrm{l}}^{i+1}, f_{\mathrm{l}}^{i+1})_{\Omega_{\mathrm{l}}^i} + (u_{\mathrm{s}}^{i+1}, f_{\mathrm{s}}^{i+1})_{\Omega_{\mathrm{s}}^i}.
\end{aligned} \tag{4.17}$$

Next, focus on the discrete time derivative terms. Using $2a(a-b) = a^2 - b^2 + (a-b)^2$, we obtain

$$(u_{\mathrm{l}}^{i+1}, (u_{\mathrm{l}}^{i+1} - \overline{u_{\mathrm{l}}}^i))_{\Omega_{\mathrm{l}}^i} = \frac{1}{2}\left(\int_{\Omega_{\mathrm{l}}^i}(u_{\mathrm{l}}^{i+1})^2 - \int_{\Omega_{\mathrm{l}}^i}(\overline{u_{\mathrm{l}}}^i)^2 + \int_{\Omega_{\mathrm{l}}^i}(u_{\mathrm{l}}^{i+1} - \overline{u_{\mathrm{l}}}^i)^2\right). \tag{4.18}$$

Now use (4.7) and a change of variables to show

$$\begin{aligned}
\int_{\Omega_{\mathrm{l}}^i}(\overline{u_{\mathrm{l}}}^i)^2 &= \int_{\Omega_{\mathrm{l}}^{i-1}}\left(\overline{u_{\mathrm{l}}}^i \circ \Phi_i(\mathbf{x})\right)^2 \det\left([\nabla_{\mathbf{x}}\Phi_i(\mathbf{x})]\right) d\mathbf{x} \\
&= \int_{\Omega_{\mathrm{l}}^{i-1}}\left(u_{\mathrm{l}}^i - \Delta t\,\widehat{K}_{\mathrm{l}}^{-1}\boldsymbol{\sigma}_{\mathrm{l}}^i\cdot\mathbf{V}^i\right)^2 \det\left([\nabla\Phi_i]\right).
\end{aligned} \tag{4.19}$$

Combining (4.3) and Proposition 4.12 with (4.19), and expanding, gives

$$
\int_{\Omega_1^i} (\overline{u_1^i})^2 \leqslant \int_{\Omega_1^{i-1}} \left((u_1^i)^2 + 2\Delta t\, \widehat{K}_1^{-1} |u_1^i||\sigma_1^i||\mathbf{V}^i| + \Delta t^2\, \widehat{K}_1^{-2} |\sigma_1^i|^2 |\mathbf{V}^i|^2 \right) \cdot
$$
$$
\cdot \left(1 + \Delta t |\nabla \cdot \mathbf{V}^i| + (\Delta t^2/2)|\Xi_1(\nabla \mathbf{V}^i)| + (\Delta t^3/6)|\Xi_2(\nabla \mathbf{V}^i)| \right) d\mathbf{x}
$$
$$
\leqslant \|u_1^i\|^2_{L^2(\Omega_1^{i-1})} + M_{1,i}\,\Delta t \left(\frac{2}{\widehat{K}_1} \|u_1^i\|_{L^2(\Omega_1^{i-1})} \|\sigma_1^i\|_{L^2(\Omega_1^{i-1})} + \|u_1^i\|^2_{L^2(\Omega_1^{i-1})} \right)
$$
$$
+ (M_{1,i}^2 \Delta t^2 + M_{1,i}^3 \Delta t^3)
$$
$$
\cdot \left(\frac{1}{\widehat{K}_1^2} \|\sigma_1^i\|^2_{L^2(\Omega_1^{i-1})} + \frac{2C}{\widehat{K}_1} \|u_1^i\|_{L^2(\Omega_1^{i-1})} \|\sigma_1^i\|_{L^2(\Omega_1^{i-1})} + C\|u_1^i\|^2_{L^2(\Omega_1^{i-1})} \right)
$$
$$
+ CM_{1,i}^4 \Delta t^4 \left(\frac{1}{\widehat{K}_1^2} \|\sigma_1^i\|^2_{L^2(\Omega_1^{i-1})} + \frac{2}{\widehat{K}_1} \|u_1^i\|_{L^2(\Omega_1^{i-1})} \|\sigma_1^i\|_{L^2(\Omega_1^{i-1})} \right)
$$
$$
+ CM_{1,i}^5 \Delta t^5 \frac{1}{\widehat{K}_1^2} \|\sigma_1^i\|^2_{L^2(\Omega_1^{i-1})}
$$
$$
\leqslant \|u_1^i\|^2_{L^2(\Omega_1^{i-1})}
$$
$$
+ 2\Delta t \frac{M_{1,i}}{\widehat{K}_1} \|u_1^i\|_{L^2(\Omega_1^{i-1})} \|\sigma_1^i\|_{L^2(\Omega_1^{i-1})} (1 + CM_{1,i}\Delta t + CM_{1,i}^2 \Delta t^2 + CM_{1,i}^3 \Delta t^3)
$$
$$
+ \Delta t M_{1,i} \|u_1^i\|^2_{L^2(\Omega_1^{i-1})} (1 + CM_{1,i}\Delta t + CM_{1,i}^2 \Delta t^2)
$$
$$
+ \Delta t^2 \frac{M_{1,i}^2}{\widehat{K}_1^2} \|\sigma_1^i\|^2_{L^2(\Omega_1^{i-1})} (1 + M_{1,i}\Delta t + CM_{1,i}^2 \Delta t^2 + CM_{1,i}^3 \Delta t^3),
$$

$$(4.20)$$

where $M_{1,i} = \|\mathbf{V}^i\|_{W^{1,\infty}(\Omega_1^{i-1})}$ and $C > 0$ is an independent constant. Next, choose Δt such that

$$
M_{1,i}\Delta t, \; CM_{1,i}\Delta t, \; CM_{1,i}^2 \Delta t^2, \; CM_{1,i}^3 \Delta t^3 \leqslant 1/3, \quad \Delta t M_{1,i}^2/\widehat{K}_1 \leqslant 1/4, \quad (4.21)
$$

and note the following weighted Young's inequality:

$$
\frac{\Delta t}{\widehat{K}_1} M_{1,i} 2\|u_1^i\|_{L^2(\Omega_1^{i-1})} \|\sigma_1^i\|_{L^2(\Omega_1^{i-1})} \leqslant \frac{\Delta t}{\widehat{K}_1} \left(4M_{1,i}^2 \|u_1^i\|^2_{L^2(\Omega_1^{i-1})} + \frac{1}{4}\|\sigma_1^i\|^2_{L^2(\Omega_1^{i-1})} \right).
$$

Hence, (4.20) implies

$$
\int_{\Omega_1^i} (\overline{u_1^i})^2 \leqslant \|u_1^i\|^2_{L^2(\Omega_1^{i-1})} + \Delta t \underbrace{\left(\frac{8M_{1,i}^2}{\widehat{K}_1} + 2M_{1,i} \right)}_{=: \widetilde{M_{1,i}}} \|u_1^i\|^2_{L^2(\Omega_1^{i-1})} + \frac{\Delta t}{\widehat{K}_1} \|\sigma_1^i\|^2_{L^2(\Omega_1^{i-1})},
$$

for all $i \geqslant 0$. (4.22)

A similar result holds for u_s^i, with constant $\widetilde{M_{s,i}} = (8M_{s,i}^2/\widehat{K}_s) + 2M_{s,i}$ where $M_{s,i} = \|\mathbf{V}^i\|_{W^{1,\infty}(\Omega_s^{i-1})}$.

Next, we note a result from [3, Lemma 1] which says that

$$\int_{\Gamma^i} \nabla_\Gamma \mathbf{X}^{i+1} \cdot \nabla_\Gamma (\mathbf{X}^{i+1} - \mathbf{X}^i) \geqslant |\mathbf{X}^{i+1}(\Gamma^i)| - |\Gamma^i| = |\Gamma^{i+1}| - |\Gamma^i|,$$

where $\Gamma^{i+1} := \mathbf{X}^{i+1}(\Gamma^i)$. Hence,

$$(\nabla_{\Gamma^i}(\Delta t \mathbf{V}^{i+1}), \nabla_{\Gamma^i} \mathbf{V}^{i+1})_{\Gamma^i} + (\nabla_{\Gamma^i} \mathbf{X}^i, \nabla_{\Gamma^i} \mathbf{V}^{i+1})_{\Gamma^i} = \Delta t^{-1}(\nabla_{\Gamma^i} \mathbf{X}^{i+1}, \nabla_{\Gamma^i}(\mathbf{X}^{i+1} - \mathbf{X}^i))_{\Gamma^i}$$

$$\geqslant \frac{|\Gamma^{i+1}| - |\Gamma^i|}{\Delta t}.$$
(4.23)

Now combine (4.22) with (4.18) and plug into (4.17) (and do the same for u_{s}^i). Using (4.23) then yields

$$\frac{1}{\widehat{K}_{\mathrm{l}}} \|\boldsymbol{\sigma}_{\mathrm{l}}^{i+1}\|_{L^2(\Omega_{\mathrm{l}}^i)}^2 - \frac{1}{2}\frac{1}{\widehat{K}_{\mathrm{l}}}\|\boldsymbol{\sigma}_{\mathrm{l}}^i\|_{L^2(\Omega_{\mathrm{l}}^{i-1})}^2 + \frac{1}{\widehat{K}_{\mathrm{s}}}\|\boldsymbol{\sigma}_{\mathrm{s}}^{i+1}\|_{L^2(\Omega_{\mathrm{s}}^i)}^2 - \frac{1}{2}\frac{1}{\widehat{K}_{\mathrm{s}}}\|\boldsymbol{\sigma}_{\mathrm{s}}^i\|_{L^2(\Omega_{\mathrm{s}}^{i-1})}^2$$

$$+ \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu}^i)\mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i\|_{L^2(\Gamma^i)}^2 + \widehat{\alpha}\frac{|\Gamma^{i+1}| - |\Gamma^i|}{\Delta t} + \frac{1}{\Delta t}\frac{1}{2}\left(\|u_{\mathrm{l}}^{i+1}\|_{L^2(\Omega_{\mathrm{l}}^i)}^2 - \|u_{\mathrm{l}}^i\|_{L^2(\Omega_{\mathrm{l}}^{i-1})}^2\right)$$

$$+ \frac{1}{\Delta t}\frac{1}{2}\left(\|u_{\mathrm{s}}^{i+1}\|_{L^2(\Omega_{\mathrm{s}}^i)}^2 - \|u_{\mathrm{s}}^i\|_{L^2(\Omega_{\mathrm{s}}^{i-1})}^2\right)$$

$$\leqslant (u_{\mathrm{l}}^{i+1}, f_{\mathrm{l}}^{i+1})_{\Omega_{\mathrm{l}}^i} + \frac{1}{2}\widetilde{M_{\mathrm{l},i}}\|u_{\mathrm{l}}^i\|_{L^2(\Omega_{\mathrm{l}}^{i-1})}^2 + (u_{\mathrm{s}}^{i+1}, f_{\mathrm{s}}^{i+1})_{\Omega_{\mathrm{s}}^i} + \frac{1}{2}\widetilde{M_{\mathrm{s},i}}\|u_{\mathrm{s}}^i\|_{L^2(\Omega_{\mathrm{s}}^{i-1})}^2. \quad (4.24)$$

Applying a weighted Young's inequality to the right-hand-side, multiplying by Δt, summing over i, and cancelling similar terms, we get

$$\frac{\Delta t}{2}\sum_{i=0}^{N-1}\left[\frac{1}{\widehat{K}_{\mathrm{l}}}\|\boldsymbol{\sigma}_{\mathrm{l}}^{i+1}\|_{L^2(\Omega_{\mathrm{l}}^i)}^2 + \frac{1}{\widehat{K}_{\mathrm{s}}}\|\boldsymbol{\sigma}_{\mathrm{s}}^{i+1}\|_{L^2(\Omega_{\mathrm{s}}^i)}^2\right] + \Delta t\sum_{i=0}^{N-1}\|\widehat{\beta}^{-1/2}(\boldsymbol{\nu}^i)\mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i\|_{L^2(\Gamma^i)}^2$$

$$+ \widehat{\alpha}|\Gamma^N| + \frac{1}{2}\|u_{\mathrm{l}}^N\|_{L^2(\Omega_{\mathrm{l}}^{N-1})}^2 + \frac{1}{2}\|u_{\mathrm{s}}^N\|_{L^2(\Omega_{\mathrm{s}}^{N-1})}^2$$

$$\leqslant \widehat{\alpha}|\Gamma^0| + \frac{1}{2}\left(\frac{\Delta t}{\widehat{K}_{\mathrm{l}}}\|\boldsymbol{\sigma}_{\mathrm{l}}^0\|_{L^2(\Omega_{\mathrm{l}}^{-1})}^2 + \frac{\Delta t}{\widehat{K}_{\mathrm{s}}}\|\boldsymbol{\sigma}_{\mathrm{s}}^0\|_{L^2(\Omega_{\mathrm{s}}^{-1})}^2 + \|u_{\mathrm{l}}^0\|_{L^2(\Omega_{\mathrm{l}}^{-1})}^2 + \|u_{\mathrm{s}}^0\|_{L^2(\Omega_{\mathrm{s}}^{-1})}^2\right)$$

$$+ \Delta t\sum_{i=0}^{N-1}\left[\|f_{\mathrm{l}}^{i+1}\|_{L^2(\Omega_{\mathrm{l}}^i)}^2 + \|f_{\mathrm{s}}^{i+1}\|_{L^2(\Omega_{\mathrm{s}}^i)}^2\right]$$

$$+ \frac{\Delta t}{2}\sum_{i=0}^{N-1}\left[\frac{1}{2}\|u_{\mathrm{l}}^{i+1}\|_{L^2(\Omega_{\mathrm{l}}^i)}^2 + \widetilde{M_{\mathrm{l},i}}\|u_{\mathrm{l}}^i\|_{L^2(\Omega_{\mathrm{l}}^{i-1})}^2 + \frac{1}{2}\|u_{\mathrm{s}}^{i+1}\|_{L^2(\Omega_{\mathrm{s}}^i)}^2 + \widetilde{M_{\mathrm{s},i}}\|u_{\mathrm{s}}^i\|_{L^2(\Omega_{\mathrm{s}}^{i-1})}^2\right],$$

where N is the last time index to compute. Making further simplifications, and assuming $\Delta t \leqslant 1$,

we arrive at

$$
\begin{aligned}
\frac{\Delta t}{2} \sum_{i=0}^{N-1} & \left[\frac{1}{\widehat{K}_{\mathrm{l}}} \| \sigma_{\mathrm{l}}^{i+1} \|_{L^2(\Omega_{\mathrm{l}}^i)}^2 + \frac{1}{\widehat{K}_{\mathrm{s}}} \| \sigma_{\mathrm{s}}^{i+1} \|_{L^2(\Omega_{\mathrm{s}}^i)}^2 \right] + \Delta t \sum_{i=0}^{N-1} \| \widehat{\beta}^{-1/2}(\boldsymbol{\nu}^i) \mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i \|_{L^2(\Gamma^i)}^2 \\
& + \widehat{\alpha} |\Gamma^N| + \frac{1}{4} \| u_{\mathrm{l}}^N \|_{L^2(\Omega_{\mathrm{l}}^{N-1})}^2 + \frac{1}{4} \| u_{\mathrm{s}}^N \|_{L^2(\Omega_{\mathrm{s}}^{N-1})}^2 \\
\leqslant \widehat{\alpha} |\Gamma^0| & + \frac{1}{2} \left(\frac{\Delta t}{\widehat{K}_{\mathrm{l}}} \| \sigma_{\mathrm{l}}^0 \|_{L^2(\Omega_{\mathrm{l}}^{-1})}^2 + \frac{\Delta t}{\widehat{K}_{\mathrm{s}}} \| \sigma_{\mathrm{s}}^0 \|_{L^2(\Omega_{\mathrm{s}}^{-1})}^2 + \| u_{\mathrm{l}}^0 \|_{L^2(\Omega_{\mathrm{l}}^{-1})}^2 + \| u_{\mathrm{s}}^0 \|_{L^2(\Omega_{\mathrm{s}}^{-1})}^2 \right) \\
& + \Delta t \sum_{i=0}^{N-1} \left[\| f_{\mathrm{l}}^{i+1} \|_{L^2(\Omega_{\mathrm{l}}^i)}^2 + \| f_{\mathrm{s}}^{i+1} \|_{L^2(\Omega_{\mathrm{s}}^i)}^2 \right] \\
& + \frac{\Delta t}{2} \sum_{i=0}^{N-1} \mathcal{V}_i \left[\| u_{\mathrm{l}}^i \|_{L^2(\Omega_{\mathrm{l}}^{i-1})}^2 + \| u_{\mathrm{s}}^i \|_{L^2(\Omega_{\mathrm{s}}^{i-1})}^2 \right],
\end{aligned}
\tag{4.25}
$$

where $\mathcal{V}_i > 0$ is a constant that depends on $\| \mathbf{V}^i \|_{W^{1,\infty}(\Omega)}$. Note that u_{l}^0 (u_{s}^0) is the initial temperature on the initial domain Ω_{l}^{-1} (Ω_{s}^{-1}); similar for the flux σ_{l}^0 (σ_{s}^0).

Applying Lemma 4.13 to (4.25) yields

$$
\frac{1}{4} \left[\| u_{\mathrm{l}}^k \|_{L^2(\Omega_{\mathrm{l}}^{k-1})}^2 + \| u_{\mathrm{s}}^k \|_{L^2(\Omega_{\mathrm{s}}^{k-1})}^2 \right] \leqslant A_0 \exp \left(2\Delta t \sum_{p=0}^{k-1} \mathcal{V}_p \right), \quad \text{for all } k \geqslant 0,
\tag{4.26}
$$

where A_0 is given in Theorem 4.14, which we have now proved.

THEOREM 4.14 Suppose (4.5), (4.6), (4.7) is solved on Ω^i at time index i, with $u_{\mathrm{D}}^{i+1} = 0$, and assume $\mathbf{V}^{i+1}$ is in $W^{1,\infty}(\Omega^i)$ and that Φ_{i+1} is a bijective map in $W^{1,\infty}(\Omega^i)$ with bounded inverse. Suppose this holds for $i = 0, ..., N-1$. If $\Delta t \leqslant 1$ also satisfies

$$
\Delta t \leqslant \frac{B_0}{\max_{0 \leqslant i \leqslant N} \| \mathbf{V}^i \|_{W^{1,\infty}(\Omega)}} \quad \text{and} \quad \Delta t \leqslant B_0 \frac{\max(\widehat{K}_{\mathrm{l}}, \widehat{K}_{\mathrm{s}})}{\max_{0 \leqslant i \leqslant N} \| \mathbf{V}^i \|_{W^{1,\infty}(\Omega)}^2},
$$

for some independent constant $B_0 > 0$, then

$$
\begin{aligned}
\frac{\Delta t}{2} \sum_{i=0}^{N-1} & \left[\frac{1}{\widehat{K}_{\mathrm{l}}} \| \sigma_{\mathrm{l}}^{i+1} \|_{L^2(\Omega_{\mathrm{l}}^i)}^2 + \frac{1}{\widehat{K}_{\mathrm{s}}} \| \sigma_{\mathrm{s}}^{i+1} \|_{L^2(\Omega_{\mathrm{s}}^i)}^2 \right] + \Delta t \sum_{i=0}^{N-1} \| \widehat{\beta}^{-1/2}(\boldsymbol{\nu}^i) \mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i \|_{L^2(\Gamma^i)}^2 \\
& + \widehat{\alpha} |\Gamma^N| + \frac{1}{4} \| u_{\mathrm{l}}^N \|_{L^2(\Omega_{\mathrm{l}}^{N-1})}^2 + \frac{1}{4} \| u_{\mathrm{s}}^N \|_{L^2(\Omega_{\mathrm{s}}^{N-1})}^2 \\
& \leqslant A_0 + A_0 2\Delta t \sum_{i=0}^{N-1} \mathcal{V}_i \exp \left(2\Delta t \sum_{p=0}^{i-1} \mathcal{V}_p \right), \quad (4.27)
\end{aligned}
$$

where

$$A_0 = \widehat{\alpha}|\Gamma^0| + \frac{1}{2}\left(\frac{\Delta t}{\widehat{K}_1}\|\boldsymbol{\sigma}_1^0\|_{L^2(\Omega_1^{-1})}^2 + \frac{\Delta t}{\widehat{K}_s}\|\boldsymbol{\sigma}_s^0\|_{L^2(\Omega_s^{-1})}^2 + \|u_1^0\|_{L^2(\Omega_1^{-1})}^2 + \|u_s^0\|_{L^2(\Omega_s^{-1})}^2\right)$$

$$+ \Delta t \sum_{i=0}^{N-1}\left[\|f_1^{i+1}\|_{L^2(\Omega_1^i)}^2 + \|f_s^{i+1}\|_{L^2(\Omega_s^i)}^2\right],$$

where $\mathcal{V}_i > 0$ is a constant that depends on $\|\mathbf{V}^i\|_{W^{1,\infty}(\Omega)}$. Note: the final time for the semi-discrete evolution is $T = \Delta t N$.

REMARK 4.15 Using an L^2 projection for the temperatures from one time step to the next would give a better estimate (i.e. more in-line with the fully continuous result (3.20)). The approach taken here is more complicated because we introduced the material derivative with an explicit treatment of the convective term (recall (4.4) and (4.7)); see Remark 5.8 for the reason. Theorem 4.14 can be easily modified to allow $u_D^{i+1} \neq 0$.

4.6.2 *Conservation law.* Analogous to Section 3.4.2, choose $q_1 = 1$, $q_s = 1$ in (4.5), and $\mu = 1$ in (4.6) to get

$$-\int_{\partial_D\Omega}\boldsymbol{\sigma}_1^{i+1}\cdot\boldsymbol{\nu}_\Omega + \int_{\Gamma^i}\boldsymbol{\sigma}_1^{i+1}\cdot\boldsymbol{\nu}^i = \frac{1}{\Delta t}\left(\int_{\Omega_1^i}u_1^{i+1} - \int_{\Omega_1^i}\overline{u_1}^i\right) - \int_{\Omega_1^i}f_1^{i+1},$$

$$-\int_{\Gamma^i}\boldsymbol{\sigma}_s^{i+1}\cdot\boldsymbol{\nu}^i = \frac{1}{\Delta t}\left(\int_{\Omega_s^i}u_s^{i+1} - \int_{\Omega_s^i}\overline{u_s}^i\right) - \int_{\Omega_s^i}f_s^{i+1}, \quad\quad (4.28)$$

$$\widehat{S}\int_{\Gamma^i}\mathbf{V}^{i+1}\cdot\boldsymbol{\nu}^i = \int_{\Gamma^i}\boldsymbol{\sigma}_1^{i+1}\cdot\boldsymbol{\nu}^i - \int_{\Gamma^i}\boldsymbol{\sigma}_s^{i+1}\cdot\boldsymbol{\nu}^i.$$

Just as in (4.19), we have

$$\int_{\Omega_1^i}\overline{u_1}^i = \int_{\Omega_1^{i-1}}\overline{u_1}^i\circ\Phi_i(\mathbf{x})\det([\nabla_{\mathbf{x}}\Phi_i(\mathbf{x})])\,d\mathbf{x} = \int_{\Omega_1^{i-1}}\left(u_1^i - \Delta t\,\widehat{K}_1^{-1}\boldsymbol{\sigma}_1^i\cdot\mathbf{V}^i\right)\det([\nabla\Phi_i]).$$

$$(4.29)$$

Combining (4.3) and Proposition 4.12 with (4.29), and expanding, gives

$$\int_{\Omega_1^i}\overline{u_1}^i = \int_{\Omega_1^{i-1}}\left(u_1^i - \Delta t\,\widehat{K}_1^{-1}\boldsymbol{\sigma}_1^i\cdot\mathbf{V}^i\right)$$

$$\cdot\left(1 + \Delta t\nabla\cdot\mathbf{V}^i + (\Delta t^2/2)\mathcal{E}_1(\nabla\mathbf{V}^i) + (\Delta t^3/6)\mathcal{E}_2(\nabla\mathbf{V}^i)\right) \quad (4.30)$$

$$= \int_{\Omega_1^{i-1}}u_1^i + \Delta t\int_{\Omega_1^{i-1}}\left(u_1^i\nabla\cdot\mathbf{V}^i - \widehat{K}_1^{-1}\boldsymbol{\sigma}_1^i\cdot\mathbf{V}^i\right) + \Delta t^2 I_1,$$

where I_1 contains the higher order terms (c.f. (4.20)):

$$I_1 = \int_{\Omega_1^{i-1}}\left\{(u_1^i/2)\mathcal{E}_1(\nabla\mathbf{V}^i) - \widehat{K}_1^{-1}\boldsymbol{\sigma}_1^i\cdot\mathbf{V}^i(\nabla\cdot\mathbf{V}^i)\right.$$

$$\left. + \Delta t\left[(u_1^i/6)\mathcal{E}_2(\nabla\mathbf{V}^i) - (1/2)\widehat{K}_1^{-1}\boldsymbol{\sigma}_1^i\cdot\mathbf{V}^i\mathcal{E}_1(\nabla\mathbf{V}^i)\right] - \Delta t^2(1/6)\widehat{K}_1^{-1}\boldsymbol{\sigma}_1^i\cdot\mathbf{V}^i\mathcal{E}_2(\nabla\mathbf{V}^i)\right\}.$$

Next, by making judicious use of the weak formulation (4.5), we can simplify the $O(\Delta t)$ term in (4.30). Choose $\boldsymbol{\eta}_l = \mathbf{V}^i|_{\Omega_l} \in \mathbb{V}_l^{i-1}(0)$ in (4.5) on Ω_l^{i-1} for any $i \geqslant 1$, and note (4.2):

$$\int_{\Omega_l^{i-1}} \widehat{K}_l^{-1} \boldsymbol{\sigma}_l^i \cdot \mathbf{V}^i - \int_{\Omega_l^{i-1}} u_l^i \nabla \cdot \mathbf{V}^i = \int_{\Gamma^{i-1}} \lambda^i \mathbf{V}^i \cdot \boldsymbol{\nu}^{i-1}. \tag{4.31}$$

Thus, we arrive at

$$\int_{\Omega_l^i} \overline{u_l}^i = \int_{\Omega_l^{i-1}} u_l^i - \Delta t \int_{\Gamma^{i-1}} \lambda^i \mathbf{V}^i \cdot \boldsymbol{\nu}^{i-1} + \Delta t^2 I_1, \quad \text{for all } i \geqslant 1,$$

$$|I_1| \leqslant C_0 M_{l,i}^2 \left[\|u_l^i\|_{L^1(\Omega_l^{i-1})}(1 + \Delta t M_{l,i}) + \widehat{K}_l^{-1} \|\boldsymbol{\sigma}_l^i\|_{L^1(\Omega_l^{i-1})}(1 + \Delta t M_{l,i} + \Delta t^2 M_{l,i}^2) \right], \tag{4.32}$$

where $M_{l,i} = \|\mathbf{V}^i\|_{W^{1,\infty}(\Omega_l^{i-1})}$ and $C_0 > 0$ is an independent constant. Note that setting the initial velocity $\mathbf{V}^0 = \mathbf{0}$ gives $\int_{\Omega_l^0} \overline{u_l}^0 \equiv \int_{\Omega_l^{-1}} u_l^0$. Similar results hold for u_s^i:

$$\int_{\Omega_s^i} \overline{u_s}^i = \int_{\Omega_s^{i-1}} u_s^i + \Delta t \int_{\Gamma^{i-1}} \lambda^i \mathbf{V}^i \cdot \boldsymbol{\nu}^{i-1} + \Delta t^2 I_s, \quad \text{for all } i \geqslant 1,$$

$$|I_s| \leqslant C_0 M_{s,i}^2 \left[\|u_s^i\|_{L^1(\Omega_s^{i-1})}(1 + \Delta t M_{s,i}) + \widehat{K}_s^{-1} \|\boldsymbol{\sigma}_s^i\|_{L^1(\Omega_s^{i-1})}(1 + \Delta t M_{s,i} + \Delta t^2 M_{s,i}^2) \right], \tag{4.33}$$

where $M_{s,i} = \|\mathbf{V}^i\|_{W^{1,\infty}(\Omega_s^{i-1})}$.

Therefore, adding the equations in (4.28), and using (4.32) and (4.33), gives a time-discrete thermal power balance for each $i = 0, \ldots, N - 1$:

$$\int_{\Omega_l^i} f_l^{i+1} + \int_{\Omega_s^i} f_s^{i+1} - \int_{\partial_D \Omega} \boldsymbol{\sigma}_l^{i+1} \cdot \boldsymbol{\nu}_\Omega = \frac{1}{\Delta t} \left(\int_{\Omega_l^i} u_l^{i+1} - \int_{\Omega_l^{i-1}} u_l^i \right)$$

$$+ \frac{1}{\Delta t} \left(\int_{\Omega_s^i} u_s^{i+1} - \int_{\Omega_s^{i-1}} u_s^i \right) - \widehat{S} \int_{\Gamma^i} \mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i - \Delta t (I_1 + I_s). \tag{4.34}$$

Finally, summing (4.34) over the time steps, and bounding I_1 and I_s, yields the following theorem.

THEOREM 4.16 Assume the hypothesis of Theorem 4.14 and suppose $\mathbf{V}^0 \equiv \mathbf{0}$ on Ω. Then,

$$\left| \Delta t \sum_{i=0}^{N-1} \left(\int_{\Omega_l^i} f_l^{i+1} + \int_{\Omega_s^i} f_s^{i+1} - \int_{\partial_D \Omega} \boldsymbol{\sigma}_l^{i+1} \cdot \boldsymbol{\nu}_\Omega \right) + \int_{\Omega_l^{-1}} u_l^0 + \int_{\Omega_s^{-1}} u_s^0 \right.$$

$$\left. - \int_{\Omega_l^{N-1}} u_l^N - \int_{\Omega_s^{N-1}} u_s^N + \Delta t \widehat{S} \sum_{i=0}^{N-1} \int_{\Gamma^i} \mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i \right| \leqslant \Delta t B_1, \tag{4.35}$$

where

$$B_1 = \Delta t \sum_{i=0}^{N-1} \mathcal{V}_i \left[\frac{1}{\widehat{K}_l} \|\boldsymbol{\sigma}_l^i\|_{L^1(\Omega_l^{i-1})} + \frac{1}{\widehat{K}_s} \|\boldsymbol{\sigma}_s^i\|_{L^1(\Omega_s^{i-1})} + \|u_l^i\|_{L^1(\Omega_l^{i-1})} + \|u_s^i\|_{L^1(\Omega_s^{i-1})} \right],$$

and $\mathcal{V}_i > 0$ is a constant that depends on $\|\mathbf{V}^i\|_{W^{1,\infty}(\Omega)}$. Note that B_1 is uniformly bounded (with respect to Δt) by Theorem 4.14.

REMARK 4.17 Theorem 4.16 is a discrete time integral version of (3.21), except with an $O(\Delta t)$ error. The conservation property in [5, Remark 3.5] is exact but only applies to a time-continuous version of their numerical scheme. We note that Theorem 4.16 can be modified to allow $u_{\mathrm{D}}^{i+1} \neq 0$ and $\mathbf{V}^0 \neq \mathbf{0}$.

5. Fully discrete formulation

5.1 *Discretization*

5.1.1 *Non-degenerate interface.* Let $\boldsymbol{\nu}_h$ denote the unit normal vector on Γ_h and $\partial\Omega_h$. The following assumption is the space discrete version of Assumption 4.5 in Section 4.4.1. It is necessary to ensure the equivalence of the norms in the space discrete version of Proposition 4.6 when $\|\cdot\|_{H^{-1/2}}$ is replaced by a *discrete* norm $\|\cdot\|_{H_h^{-1/2}}$.

ASSUMPTION 5.1 Assume that Γ_h is a polyhedral manifold (i.e. a surface triangulation). For any vertex v, let $\mathrm{Star}(v)$ be the set of triangle faces in Γ_h that contain v as a vertex. For any non-zero constant vector $\mathbf{a} \in \mathbb{R}^3$, assume there exists a vertex v in Γ_h such that $|\mathrm{Star}(v)| \geqslant c_0 > 0$ and

$$\mathbf{a} \cdot \boldsymbol{\nu}_h(\mathbf{x}) > 0, \quad \forall \mathbf{x} \in \mathrm{Star}(v), \quad \text{or} \quad \mathbf{a} \cdot \boldsymbol{\nu}_h(\mathbf{x}) < 0, \quad \forall \mathbf{x} \in \mathrm{Star}(v).$$

5.1.2 *Formulation.* We begin by approximating the domains Ω_1^i, Ω_s^i by three dimensional triangulations $\Omega_{1,h}^i$, $\Omega_{s,h}^i$ such that $\Gamma_h^i = \overline{\Omega_{1,h}^i} \cap \overline{\Omega_{s,h}^i}$ is an embedded polyhedral surface contained in the faces of the mesh. A standard Galerkin approximation of equations (4.5), (4.6) takes the form: find $\boldsymbol{\sigma}_{1,h}^{i+1}$ in $\mathbb{V}_{1,h}^i(0) \subset \mathbb{V}_1^i(0)$, $\boldsymbol{\sigma}_{s,h}^{i+1}$ in $\mathbb{V}_{s,h}^i \subset \mathbb{V}_s^i$, $\mathbf{V}_h^{i+1}$ in $\mathbb{Y}_h^i \subset \mathbb{Y}^i$, $u_{1,h}^{i+1}$ in $\mathbb{Q}_{1,h}^i \subset \mathbb{Q}_1^i$, $u_{s,h}^{i+1}$ in $\mathbb{Q}_{s,h}^i \subset \mathbb{Q}_s^i$, λ_h^{i+1} in $\mathbb{M}_h^i \subset \mathbb{M}^i$ such that for all $\boldsymbol{\eta}_1 \in \mathbb{V}_{1,h}^i(0)$, $\boldsymbol{\eta}_s \in \mathbb{V}_{s,h}^i$, $q_1 \in \mathbb{Q}_{1,h}^i$, $q_s \in \mathbb{Q}_{s,h}^i$, $\mathbf{Y} \in \mathbb{Y}_h^i$, $\mu \in \mathbb{M}_h^i$,

$$\frac{1}{\widehat{K}_1}(\boldsymbol{\sigma}_{1,h}^{i+1}, \boldsymbol{\eta}_1)_{\Omega_{1,h}^i} - (u_{1,h}^{i+1}, \nabla \cdot \boldsymbol{\eta}_1)_{\Omega_{1,h}^i} - \langle \boldsymbol{\eta}_1 \cdot \boldsymbol{\nu}_h^i, \lambda_h^{i+1} \rangle_{\Gamma_h^i} = -\langle \boldsymbol{\eta}_1 \cdot \boldsymbol{\nu}_h^i, u_{\mathrm{D}}^{i+1} \rangle_{\partial\Omega_h},$$

$$-(\nabla \cdot \boldsymbol{\sigma}_{1,h}^{i+1}, q_1)_{\Omega_{1,h}^i} - \frac{1}{\Delta t}(u_{1,h}^{i+1}, q_1)_{\Omega_{1,h}^i} + \frac{1}{\Delta t}(\overline{u_{1,h}}^i, q_1)_{\Omega_{1,h}^i} = -(f_1^{i+1}, q_1)_{\Omega_{1,h}^i},$$

$$\frac{1}{\widehat{K}_s}(\boldsymbol{\sigma}_{s,h}^{i+1}, \boldsymbol{\eta}_s)_{\Omega_{s,h}^i} - (u_{s,h}^{i+1}, \nabla \cdot \boldsymbol{\eta}_s)_{\Omega_{s,h}^i} + \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}_h^i, \lambda_h^{i+1} \rangle_{\Gamma_h^i} = 0, \tag{5.1}$$

$$-(\nabla \cdot \boldsymbol{\sigma}_{s,h}^{i+1}, q_s)_{\Omega_{s,h}^i} - \frac{1}{\Delta t}(u_{s,h}^{i+1}, q_s)_{\Omega_{s,h}^i} + \frac{1}{\Delta t}(\overline{u_{s,h}}^i, q_s)_{\Omega_{s,h}^i} = -(f_s^{i+1}, q_s)_{\Omega_{s,h}^i},$$

$$(\widehat{\beta}^{-1}(\boldsymbol{\nu}_h^i)\mathbf{V}_h^{i+1} \cdot \boldsymbol{\nu}_h^i, \mathbf{Y} \cdot \boldsymbol{\nu}_h^i)_{\Gamma_h^i} + \Delta t \widehat{\alpha}(\nabla_\Gamma \mathbf{V}_h^{i+1}, \nabla_\Gamma \mathbf{Y})_{\Gamma_h^i}$$
$$+ \widehat{S}(\mathbf{Y} \cdot \boldsymbol{\nu}_h^i, \lambda_h^{i+1})_{\Gamma_h^i} = -\widehat{\alpha}(\nabla_\Gamma \mathbf{X}^i, \nabla_\Gamma \mathbf{Y})_{\Gamma_h^i}, \tag{5.2}$$

$$\widehat{S}(\mathbf{V}_h^{i+1} \cdot \boldsymbol{\nu}_h^i, \mu)_{\Gamma_h^i} - \langle \boldsymbol{\sigma}_{1,h}^{i+1} \cdot \boldsymbol{\nu}_h^i, \mu \rangle_{\Gamma_h^i} + \langle \boldsymbol{\sigma}_{s,h}^{i+1} \cdot \boldsymbol{\nu}_h^i, \mu \rangle_{\Gamma_h^i} = 0,$$

where the discrete spaces are defined over the current (known) domain Ω_h^i, Γ_h^i. We then use the space discrete version of (4.1) to compute the new interface Γ_h^{i+1}, followed by the space discrete version of (4.2), (4.3) to compute the map $\Phi_{i+1,h} : \Omega_h^i \to \Omega_h^{i+1}$.

REMARK 5.2 (Finite Element Space For Domain Velocity) The extension (4.2) of $\mathbf{V}_h^{i+1}$ to all of Ω_h^i is computed by solving a discrete Laplace equation using a finite element space $\mathbb{L}_h^i$ on Ω_h^i whose restriction to Γ_h^i contains $\mathbb{Y}_h^i$. Because of (4.1), (4.3), the shape of the tetrahedral elements T in Ω_h^i must be representable by functions in $\mathbb{L}_h^i$, i.e. the parametrization of T must be expressed as a linear combination of basis functions in the local finite element space of $\mathbb{L}_h^i$. For example, this is achieved when $\mathbb{L}_h^i$ is piecewise linear and Ω_h^i consists of affine tetrahedra.

The space discrete version of the temperature update formula (4.7) is then given by

$$\overline{u_{j,h}}^i := \left[u_{j,h}^i - \Delta t \frac{1}{\widehat{K}_j} \Pi_{\mathbb{Q}_{j,h}^i} \left(\sigma_{j,h}^i \cdot \mathcal{Q}_{\mathring{\mathbb{V}}_h^i} \mathbf{V}_h^i \right) \right] \circ \Phi_{i,h}^{-1}, \text{ for } j = 1, \text{s}, \tag{5.3}$$

where $\Pi_{\mathbb{Q}_{j,h}^i} : L^2(\Omega_{j,h}^i) \to \mathbb{Q}_{j,h}^i$ is the standard L^2 projection onto $\mathbb{Q}_{j,h}^i$ and $\mathcal{Q}_{\mathring{\mathbb{V}}_h^i} : H_0^1(\Omega_h^i) \to \mathring{\mathbb{V}}_h^i$ is a suitable interpolant; see Section 5.2 for a description of these operators and Section 5.4 for the reasons we need them. Iterating this procedure gives the fully discrete approximation of (3.11), (3.12).

Just as in Section 4.3, *we drop the time index notation* when considering (5.1), (5.2) at a single time step. This leads to a fully discrete version of (4.14).

VARIATIONAL FORMULATION 5.3 Find $(\sigma_{1,h}, \sigma_{s,h}, \mathbf{V}_h)$ in $\mathbb{Z}_h$ and $(u_{1,h}, u_{s,h}, \lambda_h)$ in $\mathbb{T}_h$ such that

$$\begin{aligned}
a_h\big((\eta_1, \eta_s, \mathbf{Y}), (\sigma_{1,h}, \sigma_{s,h}, \mathbf{V}_h)\big) + b_h\big((\eta_1, \eta_s, \mathbf{Y}), (u_{1,h}, u_{s,h}, \lambda_h)\big) &= \chi_h(\eta_1, \eta_s, \mathbf{Y}), \\
+b_h\big((\sigma_{1,h}, \sigma_{s,h}, \mathbf{V}_h), (q_1, q_s, \mu)\big) - c_h\big((q_1, q_s, \mu), (u_{1,h}, u_{s,h}, \lambda_h)\big) &= \psi_h(q_1, q_s, \mu),
\end{aligned} \tag{5.4}$$

for all $(\eta_1, \eta_s, \mathbf{Y})$ in $\mathbb{Z}_h$, and (q_1, q_s, μ) in $\mathbb{T}_h$.

The discrete version of the forms in Section 4.3.1 are defined in the obvious way. The discrete product spaces are defined similar to (4.12), (4.13): $\mathbb{Z}_h = \mathbb{V}_{1,h}(0) \times \mathbb{V}_{s,h} \times \mathbb{Y}_h$, $\mathbb{T}_h = \mathbb{Q}_{1,h} \times \mathbb{Q}_{s,h} \times \mathbb{M}_h$.

5.1.3 *Discrete norms.* The discrete multiplier norm is slightly different. We first introduce a discrete version of the $H^{1/2}(\Gamma_h)$ norm. For any $\mu \in H^{1/2}(\Gamma_h)$, define the discrete version of (3.7):

$$\|\mu\|_{H_{1,h}^{1/2}(\Gamma_h)} := \sup_{\eta_1 \in \mathbb{V}_{1,h}(0)} \frac{\langle \eta_1 \cdot \nu_h, \mu \rangle_{\Gamma_h}}{\|\eta_1\|_{H(\mathrm{div}, \Omega_{1,h})}}, \quad \|\mu\|_{H_{s,h}^{1/2}(\Gamma_h)} := \sup_{\eta_s \in \mathbb{V}_{s,h}} \frac{\langle \eta_s \cdot \nu_h, \mu \rangle_{\Gamma_h}}{\|\eta_s\|_{H(\mathrm{div}, \Omega_{s,h})}}. \tag{5.5}$$

Clearly, for $j = 1, \text{s}$, $\|\mu\|_{H_{j,h}^{1/2}(\Gamma_h)} \lesssim \|\mu\|_{H_j^{1/2}(\Gamma_h)}$ and $\langle \eta \cdot \nu_h, \mu \rangle_{\Gamma_h} \lesssim \|\eta\|_{H(\mathrm{div}, \Omega_{j,h})} \|\mu\|_{H_{j,h}^{1/2}(\Gamma_h)}$ (discrete Schwarz inequality). We shall also use a discrete version of the $H^{-1}(\Gamma_h)$ norm to control the mean value of $\mu \in \mathbb{M}_h$. For all $\mathbf{v}$ in $H^{-1}(\Gamma_h)$, define

$$\|\mathbf{v}\|_{H_h^{-1}(\Gamma_h)} := \sup_{\mathbf{Y} \in \mathbb{Y}_h} \frac{\langle \mathbf{v}, \mathbf{Y} \rangle_{\Gamma_h}}{\|\mathbf{Y}\|_{H^1(\Gamma_h)}}, \tag{5.6}$$

which also satisfies $\|\mathbf{v}\|_{H_h^{-1}(\Gamma_h)} \lesssim \|\mathbf{v}\|_{H^{-1}(\Gamma_h)}$ and $\langle \mathbf{v}, \mathbf{Y} \rangle_{\Gamma_h} \lesssim \|\mathbf{v}\|_{H_h^{-1}(\Gamma_h)} \|\mathbf{Y}\|_{H^1(\Gamma_h)}$ (discrete Schwarz inequality). Then the discrete version of $\|(q_1, q_s, \mu)\|_{\mathbb{T}^\diamond}^2$ is $\|(q_1, q_s, \mu)\|_{\mathbb{T}_h^\diamond}^2 = \|q_1\|_{L^2(\Omega_{1,h})}^2 + \|q_s\|_{L^2(\Omega_{s,h})}^2 + \|\mu\|_{H_h^{1/2}(\Gamma_h)}^2$, where

$$\|\mu\|_{H_h^{1/2}(\Gamma_h)} := \frac{1}{2} \left(\|\mu\|_{H_{1,h}^{1/2}(\Gamma_h)} + \|\mu\|_{H_{s,h}^{1/2}(\Gamma_h)} \right). \tag{5.7}$$

and the discrete version of (4.16) is

$$
\begin{aligned}
\|(q_l, q_s, \mu)\|_{\mathbb{T}_h}^2 = \|\tilde{q}_l\|_{L^2(\Omega_{l,h})}^2 + \|\tilde{q}_s\|_{L^2(\Omega_{s,h})}^2 \\
+ \|\mu - \hat{q}_l\|_{H_{l,h}^{1/2}(\Gamma_h)}^2 + \|\mu - \hat{q}_s\|_{H_{s,h}^{1/2}(\Gamma_h)}^2 + \widehat{S}\|\mu \nu_h\|_{H_h^{-1}(\Gamma_h)}^2.
\end{aligned}
\tag{5.8}
$$

A discrete version of Proposition 4.7 also holds, i.e. $\|(q_l, q_s, \mu)\|_{\mathbb{T}_h^\diamond} \approx \|(q_l, q_s, \mu)\|_{\mathbb{T}_h}$.

The discrete version of the primal norm (4.15) is also slightly different. It requires a discrete version of the $H^{-1/2}(\Gamma_h)$ norm to control the mean value of $\mathbf{Y} \cdot \nu_h$ for $\mathbf{Y} \in \mathbb{Y}_h$. For any $\mathbf{Y} \cdot \nu_h \in H^{-1/2}(\Gamma_h)$, define

$$
\|\mathbf{Y} \cdot \nu_h\|_{H_h^{-1/2}(\Gamma_h)} := \sup_{\mu_h \in \mathbb{M}_h} \frac{\langle \mathbf{Y} \cdot \nu_h, \mu_h \rangle_{\Gamma_h}}{\|\mu_h\|_{H_h^{1/2}(\Gamma_h)}},
\tag{5.9}
$$

Clearly, $\langle \mathbf{Y} \cdot \nu_h, \mu_h \rangle_{\Gamma_h} \leqslant \|\mathbf{Y} \cdot \nu_h\|_{H_h^{-1/2}(\Gamma_h)} \|\mu_h\|_{H_h^{1/2}(\Gamma_h)}$ (discrete Schwarz inequality). Then the discrete version of $\|(\eta_l, \eta_s, \mathbf{Y})\|_{\mathbb{Z}}^2$ is obtained by replacing $\|\mathbf{Y} \cdot \nu\|_{H^{-1/2}(\Gamma)}$ with $\|\mathbf{Y} \cdot \nu_h\|_{H_h^{-1/2}(\Gamma_h)}$. A discrete version of Proposition 4.6 also holds.

5.2 *Space assumptions*

To prove well-posedness of the discrete system, we must prove the discrete version of Lemmas 4.8, 4.9, and 4.10. In addition, we want to obtain discrete versions of Theorems 4.14 and 4.16. To facilitate this, we make the following general assumptions on the choice of finite dimensional subspaces (see Section 5.5 for the specific spaces used).

Let $\mathbb{V}_h$ be a conforming finite dimensional subspace, i.e. $\mathbb{V}_h \subset \mathbb{V} \equiv H(\mathrm{div}, \Omega)$, and define

$$
\mathring{\mathbb{V}}_h := \{\eta \in \mathbb{V}_h : \eta \cdot \nu_h = 0, \text{ on } \partial\Omega_h\} \subset \{\eta \in \mathbb{V} : \langle \eta \cdot \nu_h, q \rangle_{\partial\Omega_h} = 0, \ \forall q \in H^1(\Omega_h)\}.
$$

Furthermore, assume that for any η in $\mathring{\mathbb{V}}_h$, we have $\eta|_{\Omega_{l,h}} \in \mathbb{V}_{l,h}(0)$ and $\eta|_{\Omega_{s,h}} \in \mathbb{V}_{s,h}$.

Next, take $\mathring{\mathbb{V}}_{l,h} = \{\eta_l \in \mathbb{V}_{l,h} : \eta_l \cdot \nu_h = 0, \text{ on } \partial\Omega_{l,h}\}$ and $\hat{\mathbb{Q}}_{l,h} = \{q \in \mathbb{Q}_{l,h} : \int_{\Omega_{l,h}} q \, dx = 0\}$, and assume that $\nabla \cdot \mathbb{V}_{l,h} = \mathbb{Q}_{l,h}$, $\nabla \cdot \mathring{\mathbb{V}}_{l,h} = \hat{\mathbb{Q}}_{l,h}$, and $\mathbb{V}_{l,h}$ contains continuous piecewise linear functions on Γ_h. Analogous definitions are made for $\mathbb{V}_{s,h}$ and $\mathbb{Q}_{s,h}$. Moreover, assume $(\mathbb{V}_{l,h}, \mathbb{Q}_{l,h})$ and $(\mathbb{V}_{s,h}, \mathbb{Q}_{s,h})$ satisfy

$$
\sup_{\eta_l \in \mathbb{V}_{l,h}} \frac{-(\nabla \cdot \eta_l, q_l)_{\Omega_{l,h}}}{\|\eta_l\|_{H(\mathrm{div},\Omega_{l,h}))}} \geqslant c\|q_l\|_{L^2(\Omega_{l,h})}, \qquad \sup_{\eta_s \in \mathbb{V}_{s,h}} \frac{-(\nabla \cdot \eta_s, q_s)_{\Omega_{s,h}}}{\|\eta_s\|_{H(\mathrm{div},\Omega_{s,h}))}} \geqslant c\|q_s\|_{L^2(\Omega_{s,h})}, \quad (5.10)
$$

for all $q_l \in \mathbb{Q}_{l,h}$, $q_s \in \mathbb{Q}_{s,h}$, with c independent of h and that an analogous condition is satisfied for $(\mathring{\mathbb{V}}_{l,h}, \hat{\mathbb{Q}}_{l,h})$ and $(\mathring{\mathbb{V}}_{s,h}, \hat{\mathbb{Q}}_{s,h})$. This implies that we can solve the discrete mixed form of Laplace's equation. As for $\mathbb{Y}_h$ and $\mathbb{M}_h$, assume they are spaces of continuous functions.

Regarding (5.3), we have a "Fortin interpolant" [9, 11] $\ell_{\mathring{\mathbb{V}}_h} : H_0^1(\Omega_h) \to \mathring{\mathbb{V}}_h$ that satisfies for any $\mathbf{V} \in H_0^1(\Omega_h)$:

$$
\|\ell_{\mathring{\mathbb{V}}_h} \mathbf{V}\|_{L^2(\Omega_h)} \lesssim C\|\mathbf{V}\|_{H^1(\Omega_h)}, \text{ and } (q, \nabla \cdot \mathbf{V} - \nabla \cdot \ell_{\mathring{\mathbb{V}}_h} \mathbf{V})_{\Omega_{j,h}} = 0, \ \forall \, q \in \mathbb{Q}_{j,h}, \text{ for } j = l, s.
\tag{5.11}
$$

And the L^2 projections $\Pi_{\mathbb{Q}_{j,h}} : L^2(\Omega_{j,h}) \to \mathbb{Q}_{j,h}$ (for $j = l, s$) satisfy for any $v \in L^2(\Omega_{j,h})$:

$$
\|\Pi_{\mathbb{Q}_{j,h}} v\|_{L^2(\Omega_{j,h})} \lesssim \|v\|_{L^2(\Omega_{j,h})}, \text{ and } (q, v - \Pi_{\mathbb{Q}_{j,h}} v)_{\Omega_{j,h}} = 0, \ \forall \, q \in \mathbb{Q}_{j,h}, \text{ for } j = l, s. \tag{5.12}
$$

5.3   *Well-posedness*

We follow a similar outline as Section 4.5.

5.3.1   *Main conditions.*

LEMMA 5.4 (Continuity of Forms)

$$|a_h((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V}))| \leqslant C_{a_h} \|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h} \|(\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V})\|_{\mathbb{Z}_h}, \ \forall (\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V}) \in \mathbb{Z}_h,$$

$$|b_h((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (q_l, q_s, \mu))| \leqslant C_{b_h} \|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h} \|(q_l, q_s, \mu)\|_{\mathbb{T}_h},$$
$$\forall (\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}) \in \mathbb{Z}_h, \ (q_l, q_s, \mu) \in \mathbb{T}_h,$$

$$|c_h((q_l, q_s, \mu), (u_l, u_s, \lambda))| \leqslant \Delta t^{-1} (\|q_l\|_{L^2(\Omega_{l,h})} \|u_l\|_{L^2(\Omega_{l,h})} + \|q_s\|_{L^2(\Omega_{s,h})} \|u_s\|_{L^2(\Omega_{s,h})}),$$
$$\forall (q_l, q_s, \mu), (u_l, u_s, \lambda) \in \mathbb{T}_h,$$

$$|\chi_h(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})| \leqslant C_{\chi_h} \|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h}, \ \forall (\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}) \in \mathbb{Z}_h,$$

$$|\psi_h(q_l, q_s, \mu)| \leqslant C_{\psi_h} \|(q_l, q_s, \mu)\|_{\mathbb{T}_h}, \ \forall (q_l, q_s, \mu) \in \mathbb{T}_h,$$

where $C_{a_h}, C_{b_h}, C_{\chi_h}, C_{\psi_h} > 0$ are constants that depend on physical parameters and domain geometry. In addition, C_{χ_h} depends on u_D, $\Delta t^{-1/2}$, and C_{ψ_h} depends on f_l, f_s, $\overline{u_l}, \overline{u_s}$ and Δt^{-1}.

Proof. The proof is analogous to the proof of Lemma 4.8. Minor modifications are: one must use the discrete Schwarz inequalities associated with the discrete $H_{l,h}^{1/2}$, $H_{s,h}^{1/2}$, and $H_h^{-1/2}$ norms, and use the discrete versions of Propositions 4.6 and 4.7. □

LEMMA 5.5 (Coercivity) Let $(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}) \in \mathbb{Z}_h$ with $b_h((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (q_l, q_s, \mu)) = 0$ for all $(q_l, q_s, \mu) \in \mathbb{T}_h$. Then,

$$\left| a_h\big((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\big) \right| \geqslant C \left\| (\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}) \right\|_{\mathbb{Z}_h}^2,$$

where $C > 0$ is a constant depending on $\widehat{S}$, $\widehat{K}_l$, $\widehat{K}_s$, and the domain. This is true even if $\widehat{\beta} \to \infty$.

Proof. Follows the same argument as in Lemma 4.9, except the discrete $H_h^{-1/2}$ norm (5.9) is used. □

LEMMA 5.6 (Inf-Sup) For all $(q_l, q_s, \mu) \in \mathbb{T}_h$, the following "inf-sup" condition holds

$$\sup_{(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}) \in \mathbb{Z}_h} \frac{b_h\big((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (q_l, q_s, \mu)\big)}{\|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h^\diamond}} \geqslant C \|(q_l, q_s, \mu)\|_{\mathbb{T}_h},$$

where $C > 0$ depends on the domain and $\widehat{S}$. If $\|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h^\diamond}$ is replaced by $\|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h}$ in the denominator, then the inf-sup still holds, except C also depends on $\widehat{K}_l$, $\widehat{K}_s$, $\widehat{\alpha}$, and $\widehat{\beta}_-$. Furthermore, C does *not* depend on the time step Δt, as long as $\Delta t \leqslant 1$.

Proof. Starting as we did in the proof of Lemma 4.10, we have

$$b_h\big((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (q_l, q_s, \mu)\big) = -(\nabla \cdot \boldsymbol{\eta}_l, \tilde{q}_l)_{\Omega_{l,h}} - (\nabla \cdot \boldsymbol{\eta}_s, \tilde{q}_s)_{\Omega_{s,h}} - \langle \boldsymbol{\eta}_l \cdot \boldsymbol{\nu}_h, \mu - \hat{q}_l \rangle_{\Gamma_h}$$
$$+ \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}_h, \mu - \hat{q}_s \rangle_{\Gamma_h} + \widehat{S} \langle \mathbf{Y} \cdot \boldsymbol{\nu}_h, \mu \rangle_{\Gamma_h}.$$

Next, let us focus on $-(\nabla \cdot \boldsymbol{\eta}_{\mathrm{s}}, \tilde{q}_{\mathrm{s}})_{\Omega_{\mathrm{s},h}} + \langle \boldsymbol{\eta}_{\mathrm{s}} \cdot \boldsymbol{\nu}_h, \mu - \hat{q}_{\mathrm{s}} \rangle_{\Gamma_h}$ only. By (5.10), there exists a unique $(\mathbf{w}, \omega)$ in $(\mathring{\mathbb{V}}_{\mathrm{s},h}, \hat{\mathbb{Q}}_{\mathrm{s},h})$ such that

$$
\begin{aligned}
(\mathbf{w}, \mathbf{v})_{\Omega_{\mathrm{s},h}} - (\omega, \nabla \cdot \mathbf{v})_{\Omega_{\mathrm{s},h}} &= 0, & \forall \mathbf{v} \in \mathring{\mathbb{V}}_{\mathrm{s},h}, \\
-(\nabla \cdot \mathbf{w}, r)_{\Omega_{\mathrm{s},h}} &= (\tilde{q}_{\mathrm{s}}, r)_{\Omega_{\mathrm{s},h}}, & \forall r \in \hat{\mathbb{Q}}_{\mathrm{s},h},
\end{aligned}
\tag{5.13}
$$

and $\|\mathbf{w}\|_{H(\mathrm{div}, \Omega_{\mathrm{s},h})} \leqslant C_0 \|\tilde{q}_{\mathrm{s}}\|_{L^2(\Omega_{\mathrm{s},h})}$. By (5.5), there exists $\boldsymbol{\xi} \in \mathbb{V}_{\mathrm{s},h}$ such that

$$
\langle \boldsymbol{\xi} \cdot \boldsymbol{\nu}_h, \mu - \hat{q}_{\mathrm{s}} \rangle_{\Gamma_h} = \|\mu - \hat{q}_{\mathrm{s}}\|_{H_{\mathrm{s},h}^{1/2}(\Gamma_h)}^2, \quad \|\boldsymbol{\xi}\|_{H(\mathrm{div}, \Omega_{\mathrm{s},h})} = \|\mu - \hat{q}_{\mathrm{s}}\|_{H_{\mathrm{s},h}^{1/2}(\Gamma_h)}.
$$

Similar to (5.13), there exists a $\mathbf{z}$ in $\mathring{\mathbb{V}}_{\mathrm{s},h}$ such that

$$
-\nabla \cdot \mathbf{z} = \nabla \cdot \boldsymbol{\xi} - \frac{1}{|\Omega_{\mathrm{s},h}|} \left(\int_{\Gamma_h} \boldsymbol{\xi} \cdot \boldsymbol{\nu}_h \right), \text{ on } \Omega_{\mathrm{s},h}, \quad \|\mathbf{z}\|_{H(\mathrm{div}, \Omega_{\mathrm{s},h})} \leqslant C_1 \|\boldsymbol{\xi}\|_{H(\mathrm{div}, \Omega_{\mathrm{s},h})}. \tag{5.14}
$$

Now let $\mathbf{d} = \mathbf{z} + \boldsymbol{\xi}$. Then,

$$
\nabla \cdot \mathbf{d} = \frac{1}{|\Omega_{\mathrm{s},h}|} \left(\int_{\Gamma_h} \boldsymbol{\xi} \cdot \boldsymbol{\nu}_h \right), \text{ on } \Omega_{\mathrm{s},h}, \quad \mathbf{d} \cdot \boldsymbol{\nu}_h = \boldsymbol{\xi} \cdot \boldsymbol{\nu}_h, \text{ on } \Gamma_h,
$$

where $\|\mathbf{d}\|_{H(\mathrm{div}, \Omega_{\mathrm{s},h})} \leqslant (1 + C_1) \|\boldsymbol{\xi}\|_{H(\mathrm{div}, \Omega_{\mathrm{s},h})} = (1 + C_1) \|\mu - \hat{q}_{\mathrm{s}}\|_{H_{\mathrm{s},h}^{1/2}(\Gamma_h)}$.

Next, define $\mathbf{y} := \mathbf{w} + \mathbf{d} \in \mathbb{V}_{\mathrm{s},h}$ and note $\|\mathbf{y}\|_{H(\mathrm{div}, \Omega_{\mathrm{s},h})} \leqslant C_0 \|\tilde{q}_{\mathrm{s}}\|_{L^2(\Omega_{\mathrm{s},h})} + (1 + C_1) \|\mu - \hat{q}_{\mathrm{s}}\|_{H_{\mathrm{s},h}^{1/2}(\Gamma_h)}$. Thus, setting $\boldsymbol{\eta}_{\mathrm{s}} := \mathbf{y} / \|\mathbf{y}\|_{H(\mathrm{div}, \Omega_{\mathrm{s},h})}$ gives

$$
\begin{aligned}
-(\nabla \cdot \boldsymbol{\eta}_{\mathrm{s}}, \tilde{q}_{\mathrm{s}})_{\Omega_{\mathrm{s},h}} + \langle \boldsymbol{\eta}_{\mathrm{s}} \cdot \boldsymbol{\nu}_h, \mu - \hat{q}_{\mathrm{s}} \rangle_{\Gamma_h} &= \frac{1}{\|\mathbf{y}\|_{H(\mathrm{div}, \Omega_{\mathrm{s},h})}} \left(\|\tilde{q}_{\mathrm{s}}\|_{L^2(\Omega_{\mathrm{s},h})}^2 + \langle \mathbf{d} \cdot \boldsymbol{\nu}_h, \mu - \hat{q}_{\mathrm{s}} \rangle_{\Gamma_h} \right) \\
&\geqslant C_2 \left(\|\tilde{q}_{\mathrm{s}}\|_{L^2(\Omega_{\mathrm{s},h})} + \|\mu - \hat{q}_{\mathrm{s}}\|_{H_{\mathrm{s},h}^{1/2}(\Gamma_h)} \right),
\end{aligned}
$$

with $\|\boldsymbol{\eta}_{\mathrm{s}}\|_{H(\mathrm{div}, \Omega_{\mathrm{s},h})} = 1$. Similarly, there exists $\boldsymbol{\eta}_{\mathrm{l}} \in \mathbb{V}_{\mathrm{l},h}(0)$ such that

$$
-(\nabla \cdot \boldsymbol{\eta}_{\mathrm{l}}, \tilde{q}_{\mathrm{l}})_{\Omega_{\mathrm{l},h}} - \langle \boldsymbol{\eta}_{\mathrm{l}} \cdot \boldsymbol{\nu}_h, \mu - \hat{q}_{\mathrm{l}} \rangle_{\Gamma_h} \geqslant C_3 \left(\|\tilde{q}_{\mathrm{l}}\|_{L^2(\Omega_{\mathrm{l},h})} + \|\mu - \hat{q}_{\mathrm{l}}\|_{H_{\mathrm{l},h}^{1/2}(\Gamma_h)} \right),
$$

with $\|\boldsymbol{\eta}_{\mathrm{l}}\|_{H(\mathrm{div}, \Omega_{\mathrm{l},h})} = 1$.

By the definition of the discrete $H^{-1}(\Gamma_h)$ norm (5.6), there exists a $\mathbf{Y}$ in $\mathbb{Y}_h$ such that

$$
(\mathbf{Y} \cdot \boldsymbol{\nu}_h, \mu)_{\Gamma_h} = \langle \mathbf{Y}, \mu \boldsymbol{\nu}_h \rangle_{\Gamma_h} = \|\mu \boldsymbol{\nu}_h\|_{H_{\bar{h}}^{-1}(\Gamma_h)}, \quad \|\mathbf{Y}\|_{H^1(\Gamma_h)} = 1.
$$

Combining the above results gives the assertion. □

5.3.2 *Summary.*   A discussion analogous to the one in Section 4.5.2 applies to the fully discrete problem also. Hence, the discrete problem is well-posed, but one must modify the norm $\| \cdot \|_{\mathbb{Z}_h}^2$ to include an extra factor of Δt multiplying $\|\nabla \cdot \boldsymbol{\eta}_{\mathrm{l}}\|_{L^2(\Omega_{\mathrm{l},h})}^2$, $\|\nabla \cdot \boldsymbol{\eta}_{\mathrm{s}}\|_{L^2(\Omega_{\mathrm{s},h})}^2$, and $\|\mathbf{Y} \cdot \boldsymbol{\nu}_h\|_{H_h^{-1/2}(\Gamma_h)}^2$.

5.4 *Discrete estimates*

Applying the same arguments in Section 4.6.1 to the fully discrete problem (5.1), (5.2), (5.3), and using the stability properties in (5.11), (5.12), we get the fully discrete version of Theorem 4.14.

For the conservation law, the argument in Section 4.6.2 changes slightly. Recalling (5.3), the discrete counterpart of (4.30) is

$$\int_{\Omega^i_{1,h}} \overline{u_{1,h}}^i = \int_{\Omega^{i-1}_{1,h}} u^i_{1,h} + \Delta t \underbrace{\int_{\Omega^{i-1}_{1,h}} \left(u^i_{1,h} \nabla \cdot \mathbf{V}^i_h - \widehat{K}_1^{-1} \Pi_{\mathbb{Q}^i_{1,h}} \left(\boldsymbol{\sigma}^i_{1,h} \cdot \ell_{\mathbb{V}^i_h} \mathbf{V}^i_h \right) \right)}_{=: R_1} + O(\Delta t^2). \tag{5.15}$$

Using the properties of $\ell_{\mathbb{V}^i_h}$ and $\Pi_{\mathbb{Q}^i_{1,h}}$ (5.11), (5.12), we see that

$$R_1 = \int_{\Omega^{i-1}_{1,h}} u^i_{1,h} \nabla \cdot \ell_{\mathbb{V}^i_h} \mathbf{V}^i_h - \int_{\Omega^{i-1}_{1,h}} \widehat{K}_1^{-1} \boldsymbol{\sigma}^i_{1,h} \cdot \ell_{\mathbb{V}^i_h} \mathbf{V}^i_h = -\int_{\Gamma^{i-1}_h} \lambda^i_h (\ell_{\mathbb{V}^i_h} \mathbf{V}^i_h) \cdot \boldsymbol{\nu}^{i-1}_h,$$

where the last equality follows by choosing $\eta_1 = \ell_{\mathbb{V}^i_h} \mathbf{V}^i_h|_{\Omega_{1,h}} \in \mathbb{V}^{i-1}_{1,h}(0)$ in (5.1) on $\Omega^{i-1}_{1,h}$ for any $i \geqslant 1$. Thus, we arrive at

$$\int_{\Omega^i_{1,h}} \overline{u_{1,h}}^i = \int_{\Omega^{i-1}_{1,h}} u^i_{1,h} - \Delta t \int_{\Gamma^{i-1}_h} \lambda^i_h (\ell_{\mathbb{V}^i_h} \mathbf{V}^i_h) \cdot \boldsymbol{\nu}^{i-1}_h + O(\Delta t^2), \quad \text{for all } i \geqslant 1.$$

A similar relation holds for $u^i_{s,h}$, except with $+\Delta t$. The rest of the derivation in Section 4.6.2 remains the same (note that $\ell_{\mathbb{V}^i_h} \mathbf{V}^i_h$ is continuous across Γ^{i-1}_h), which delivers the fully discrete version of Theorem 4.16.

We summarize these results in the following theorem.

THEOREM 5.7 (A Priori Bound and Conservation Law) Suppose (5.1), (5.2), (5.3) is solved on Ω^i_h at time index i, with $u^{i+1}_D = 0$, and that $\Phi_{i+1,h}$ is a bijective map with bounded inverse. Suppose this holds for $i = 0, ..., N - 1$. If $\Delta t \leqslant 1$ also satisfies

$$\Delta t \leqslant \frac{B_0}{\max_{0 \leqslant i \leqslant N} \|\mathbf{V}^i_h\|_{W^{1,\infty}(\Omega)}} \quad \text{and} \quad \Delta t \leqslant B_0 \frac{\max(\widehat{K}_1, \widehat{K}_s)}{\max_{0 \leqslant i \leqslant N} \|\mathbf{V}^i_h\|^2_{W^{1,\infty}(\Omega)}},$$

for some independent constant $B_0 > 0$, then the fully discrete version of the a priori bound (4.27) is true, i.e. replace all pertinent variables in (4.27) by their discrete counterparts. Moreover, if $\mathbf{V}^0_h \equiv \mathbf{0}$ on Ω_h, then the fully discrete version of the conservation law (4.35) is also true.

We emphasize that the time step Δt does *not* depend on the mesh size h to guarantee stability or the conservation law; it only depends on $\|\mathbf{V}^{i+1}_h\|_{W^{1,\infty}(\Omega)}$ (see Remark 4.2).

REMARK 5.8 (Reason For The Lagrangian Update) Using a Lagrangian approach to update the temperatures (5.3) *avoids* having to compute the intersection of the mesh from one time step to the next (i.e. the L^2 projections (5.12) are only computed on the previous domains $\Omega^{i-1}_{1,h}, \Omega^{i-1}_{s,h}$). The alternative would have been to compute the L^2 projection (for $j = 1, s$) of $u^i_{j,h}$ from $\Omega^{i-1}_{j,h}$ to $\Omega^i_{j,h}$, which would require computing the intersection of the meshes representing $\Omega^{i-1}_{j,h}$ and $\Omega^i_{j,h}$.

5.5 *Specific realization*

The particulars of our implementation are as follows. Let $\mathfrak{T}_h$ denote a quasi-uniform, shape regular triangulation of $\overline{\Omega_h} = \overline{\Omega_{l,h}} \cup \overline{\Omega_{s,h}}$ consisting of affine tetrahedra T of maximum size $h \equiv h_T$ [10]. We choose the finite element spaces in the bulk to be $\mathbb{V}_{l,h} = \text{BDM}_1 \subset H(\text{div}, \Omega_{l,h})$, $\mathbb{V}_{s,h} = \text{BDM}_1 \subset H(\text{div}, \Omega_{s,h})$, i.e. the lowest order Brezzi-Douglas-Marini space of piecewise linear vector functions [7, 26], and $\mathbb{Q}_{l,h}$, $\mathbb{Q}_{s,h}$ to be the set of piecewise constants.

Next, assume that Γ_h is represented by a conforming set of faces $\mathfrak{F}_h$ in the triangulation $\mathfrak{T}_h$, i.e. $\mathfrak{F}_h$ is the surface triangulation obtained by restricting $\mathfrak{T}_h$ to Γ_h. Then choose $\mathbb{M}_h$ to be the space of continuous piecewise linear functions over $\mathfrak{F}_h$ and each of the three components of the space $\mathbb{Y}_h$ to be continuous piecewise linear functions over $\mathfrak{F}_h$. Recalling Remark 5.2, we choose $\mathbb{L}_h$ to be the space of continuous piecewise linear functions over Ω_h.

REMARK 5.9 (Choice Of Finite Element Spaces) It is well-known that these spaces satisfy the assumptions in Section 5.2. Indeed, it is possible to enforce zero boundary values point-wise with BDM_1. If different spaces were chosen that did not allow this, then one needs a reasonable compatibility condition between $\mathring{\mathbb{V}}_{l,h}$, $\mathring{\mathbb{V}}_{s,h}$ and $\mathbb{M}_h$ in order to prove Lemma 5.6.

Moreover, we take $\ell_{\mathring{\mathbb{V}}_h}$ in (5.11) to be the classic BDM_1 interpolant [7, 11]; the L^2 projections $\Pi_{\mathbb{Q}_{l,h}}$, $\Pi_{\mathbb{Q}_{s,h}}$ are standard [10]. Note that this allows (5.3) to be computed *locally* (i.e. element-by-element).

6. Numerical results

We present two dimensional simulations to illustrate our method (2-D for simplicity). All simulations were implemented in the package FELICITY [62]. The linear systems are solved by MATLAB's "backslash" command. Alternatively, one can use an iterative procedure such as Uzawa's algorithm; see [22, Section 7] for an example in a related problem.

For all simulations, the Dirichlet boundary is the entire outer boundary, i.e. $\partial_D \Omega \equiv \partial \Omega$ with $u_D = -0.5$. The initial temperature is $u_s^0 := 0$ in Ω_s and u_l^0 is a smooth function between 0 and -0.5 in Ω_l. For updating the temperatures, we initialized $\mathbf{V}^0 = \mathbf{0}$. We verified the conservation law by computing the left-hand-side of (4.35). The error was less than 10^{-3}, which is consistent with the $O(\Delta t)$ error estimate in Theorem 4.16. During the course of a simulation, the mesh topology was regenerated between three and five times which did not impact the computational time.

Error estimates for the spatial discretization will be discussed in a future publication.

6.1 *Isotropic surface energy*

The model in Section 2 assumes the surface tension coefficient $\widehat{\alpha}$ is constant (isotropic). In Figure 2, we show a simulation of our method with a non-trivial initial shape. Also see Figure 1 for another example with a different initial shape.
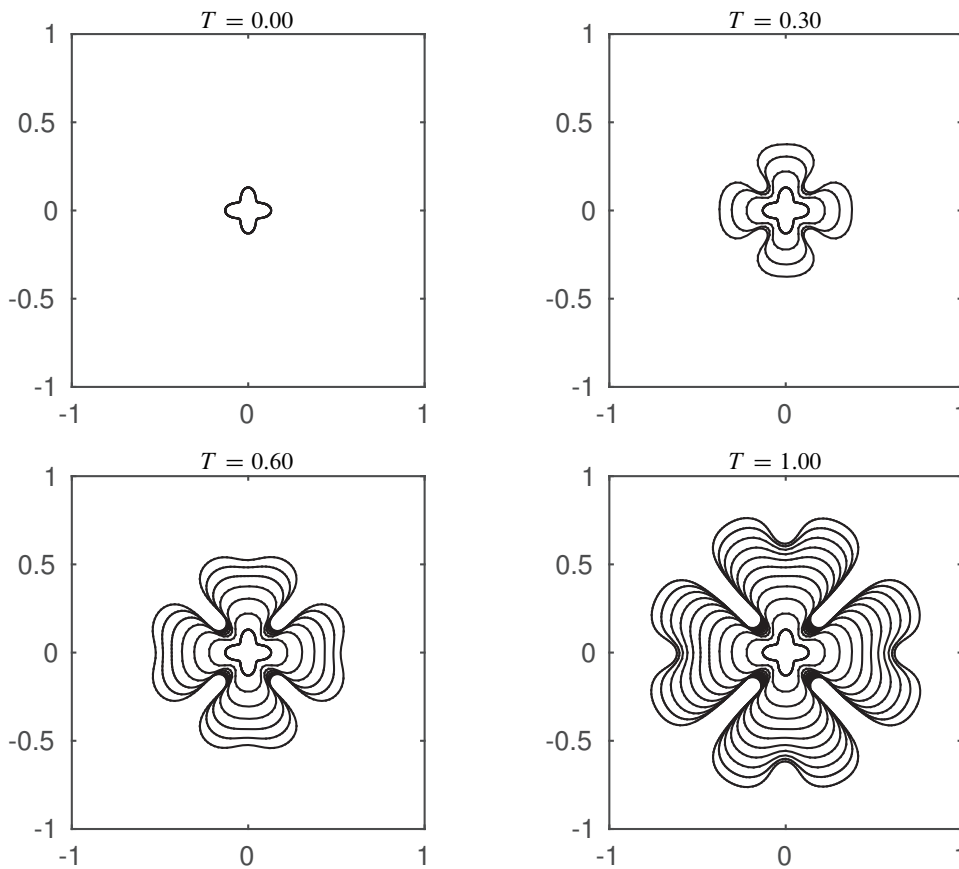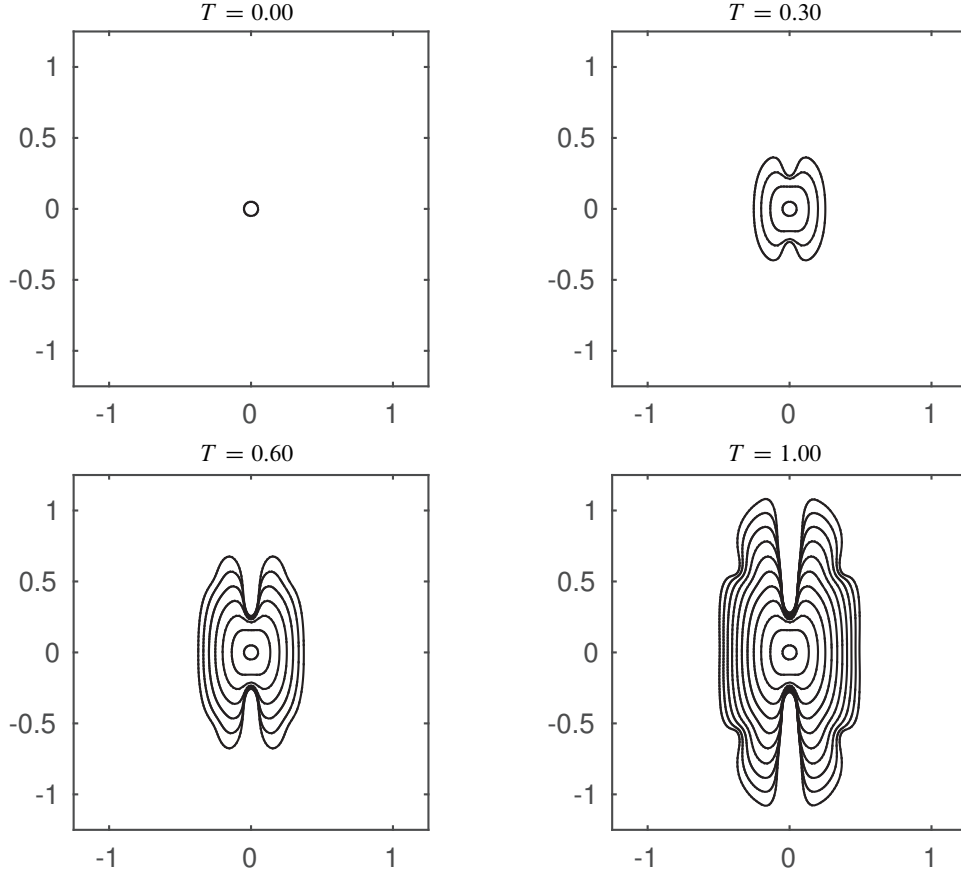
FIG. 2: Simulation with *isotropic* surface tension. Several time-lapses are shown to illustrate the evolution with initial interface having a "clover" shape.

6.2 *Anisotropic surface energy*

The model can be generalized to have an anisotropic surface tension coefficient, i.e. $\widehat{\alpha} \equiv \widehat{\alpha}(\nu)$. In particular, we consider anisotropies of the form:

$$\widehat{\alpha} = \widehat{\alpha}(\nu) := \widehat{\alpha}_0 \sum_{j=1}^{K} (\nu^T G_j \nu)^{1/2}, \tag{6.1}$$

where $\widehat{\alpha}_0 = 0.0005$ is a material constant, K is the number of anisotropies, and G_j is a symmetric positive definite matrix in $\mathbb{R}^{d \times d}$. We consider a class of matrices that have the structure $G_j = R_j^T D_j R_j$, where R_j is a rotation matrix that determines the "directions" of the anisotropy, and D_j is a diagonal matrix consisting of ones and small numbers, which controls the strength of the anisotropy. For our simulations, we set $\widehat{\beta} = \widehat{\beta}_0 \widehat{\alpha}(\nu)$, although this is not required. Note that isotropic surface tension is modeled by this as well with $K = 1$ and $G_1 = I_{2 \times 2}$ so that $\widehat{\alpha}(\nu) = \widehat{\alpha}_0$.
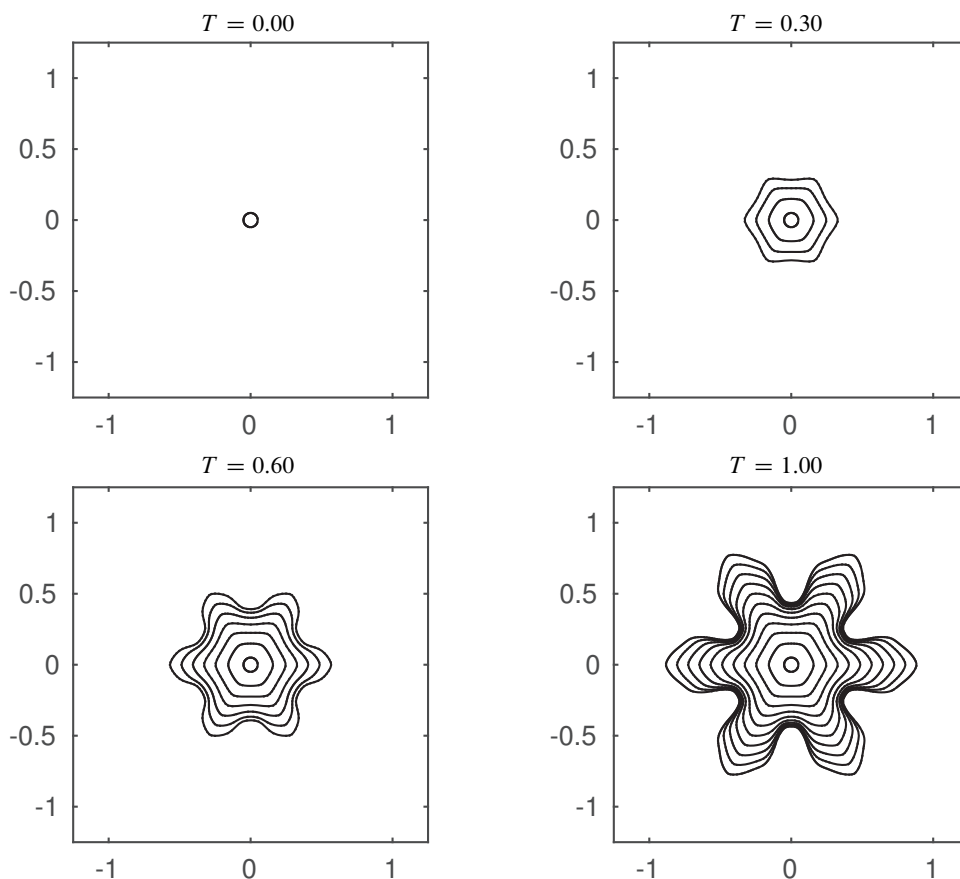
FIG. 3: Simulation with *anisotropic* surface tension. Several time-lapses are shown to illustrate the evolution with initial interface shape being a circle. A *one-fold* anisotropy is used which breaks the initial radial symmetry.

With the above, we can derive the modified form of (4.6) by standard shape differentiation [16, 32, 56]. Indeed,

$$\frac{d}{dt}\int_{\Gamma(t)}\widehat{\alpha}(\nu) = \int_{\Gamma(t)}\widehat{\alpha}(\nu)\nabla_\Gamma\mathbf{X} : \nabla_\Gamma\mathbf{V} - \int_{\Gamma(t)}\nu[\widehat{\alpha}'(\nu)]^T : \nabla_\Gamma\mathbf{V}, \tag{6.2}$$

where $\mathbf{V}$ is the velocity of Γ, and for $\mathbf{p} \in \mathbb{R}^d$, $\widehat{\alpha}'(\mathbf{p})$ is the gradient of $\widehat{\alpha}$ with respect to $\mathbf{p}$. We now obtain a semi-discrete formulation for the anisotropic case by combining (4.5), (4.6), and (6.2):

$$(\widehat{\beta}^{-1}(\nu^i)\mathbf{V}^{i+1}\cdot\nu^i, \mathbf{Y}\cdot\nu^i)_{\Gamma^i} + \Delta t(\widehat{\alpha}(\nu^i)\nabla_{\Gamma^i}\mathbf{V}^{i+1}, \nabla_{\Gamma^i}\mathbf{Y})_{\Gamma^i} + \widehat{S}(\mathbf{Y}\cdot\nu^i, \lambda^{i+1})_{\Gamma^i}$$
$$= -(\widehat{\alpha}(\nu^i)\nabla_{\Gamma^i}\mathbf{X}^i, \nabla_{\Gamma^i}\mathbf{Y})_{\Gamma^i} + (\nu^i[\widehat{\alpha}'(\nu^i)]^T, \nabla_{\Gamma^i}\mathbf{Y})_{\Gamma^i} \quad \text{for all } \mathbf{Y} \in \mathbb{Y}^i. \tag{6.3}$$

The fully discrete formulation follows straightforwardly. This type of anisotropy is studied in [5] where they handle the anisotropic surface energy by defining the local finite element basis functions to capture the anisotropic energy. Their approach allows for obtaining an energy law, which can also be combined with our method. But (6.3) is easier to implement. In fact, it allows us to consider more general coefficients $\widehat{\alpha}(\nu)$ other than (6.1). The main drawback of (6.3) is it makes the numerical scheme slightly explicit, which puts a constraint on the time step. From our experience, we need $\Delta t \leqslant Ch$ for some uniform constant C. Using the anisotropic approach in [5] would circumvent this.

In Figure 3, we present a simulation using (6.1) with $K = 1$ (i.e. a one-fold anisotropy). Figure 4 shows a simulation with $K = 3$ (i.e. a three-fold anisotropy).

FIG. 4: Simulation with *anisotropic* surface tension. Several time-lapses are shown to illustrate the evolution with initial interface shape being a circle. A *three-fold* anisotropy is used which breaks the initial radial symmetry.

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