

# A Saddle-Point Formulation And Finite Element Method For The Stefan Problem With Surface Tension

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## Abstract

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 bound and conservation law. In addition, error estimates are derived with reduced regularity assumptions on the solution. 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, 60] and a thermodynamic derivation of the model can be found in [28]. Applications range from modeling the freezing (or melting) of water to the solidification of crystals from a melt and dendritic growth [50, 51, 29, 36, 14, 58]. Mathematical theory for the Stefan problem with Gibbs-Thomson law is available for local and global in time solutions [12, 38, 24, 35, 44, 45, 47, 46]. 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) [17, 23, 19, 39, 48].

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 [34, 6, 54]. Level set methods have also been used to handle the evolutions of the two phase interface [22, 11, 43, 53]. 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, 49, 34, 33, 50, 51, 52, 4].

Our paper presents a *completely* mixed formulation of the Stefan problem, including the bulk heat equations [7]. 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, if a simple mapping procedure is used to update temperature fields on the deforming domain. This assumes the interface velocity is reasonably regular and that there are no topological changes. Moreover, if a different mapping procedure is used, then 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 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 [64]. One advantage of this method is that all integrals in the finite element formulation can be computed exactly.
- We obtain error estimates between the time semi-discrete and fully discrete solutions while making *low regularity* assumptions on the solution of the time semi-discrete system.
- 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. The error estimates must be modified slightly to account for the non-linearity induced by the anisotropic curvature term.
- 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 [59, 63].

## 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 and its well-posedness is shown. We then do the same for the fully-discrete formulation (Section 5). Error estimates and regularity assumptions are described in Section 6. Section 7 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 [28, 5]. In this section, we present the strong form of the Stefan problem.

### 2.1 Notation

Let  $\Omega$  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  $\Omega_l$  and  $\Omega_s$ , 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  $\Omega_l$ ,  $\Omega_s$ , and  $\Gamma$  are time-dependent, and we shall assume that  $\Gamma(t) \subset \Omega$  for all  $t$ . Moreover, we assume  $\Gamma(t)$  is smooth and let  $\mathbf{X}(t)$  denote a parametrization of  $\Gamma(t)$ :

$$\mathbf{X}(\cdot, t) : \mathcal{M} \rightarrow \mathbb{R}^d, \quad \text{where } \mathcal{M} \subset \mathbb{R}^d \text{ is a given reference manifold,} \quad (1)$$

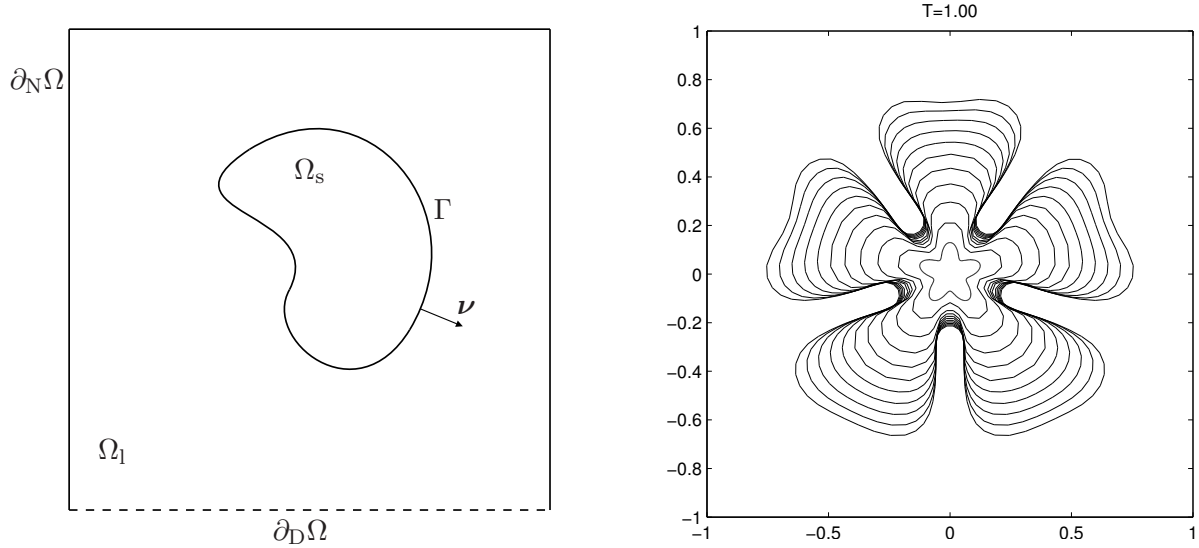


Figure 1: Left: Domains in the Stefan problem. The entire “box” is  $\Omega = \text{int}(\overline{\Omega_1} \cup \overline{\Omega_s})$  (containing two phases  $\Omega_1, \Omega_s$ ) with Dirichlet boundary  $\partial_D \Omega$  denoted by the dashed line. A Neumann condition is applied on the remaining sides  $\partial_N \Omega$ . The interface between the phases is  $\Gamma = \overline{\Omega_1} \cap \overline{\Omega_s}$  with unit normal vector  $\nu$  pointing into  $\Omega_1$ . 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 7 for more simulations.

i.e.  $\Gamma(t) = \mathbf{X}(\mathcal{M}, t)$ . 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  $\mathcal{M} = \overline{\widehat{\Omega}_1} \cap \overline{\widehat{\Omega}_s}$ . We can extend  $\mathbf{X}$  to be defined on all of  $\Omega$  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  $\Gamma$  has a unit normal vector  $\nu$  that is assumed to point into  $\Omega_1$  (see Figure 1). For quantities  $q$  in  $\Omega_1$  ( $\Omega_s$ ), we append a subscript:  $q_1$  ( $q_s$ ). The symbol  $\kappa$  represents the *total* curvature of the interface  $\Gamma$ , and we assume the convention that  $\kappa$  is *positive* when  $\Omega_s$  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.

## 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  $u|_{\Omega_1} = u_1$ ,  $u|_{\Omega_s} = u_s$ , and the following bulk conditions hold:

$$\begin{aligned}
 \vartheta \partial_t u_1 - K_1 \Delta u_1 &= f_1, \text{ in } \Omega_1(t), \\
 \vartheta \partial_t u_s - K_s \Delta u_s &= f_s, \text{ in } \Omega_s(t), \\
 \nu_\Omega \cdot \nabla u &= 0, \text{ on } \partial_N \Omega, \\
 u &= u_D, \text{ on } \partial_D \Omega, \\
 u(\cdot, 0) &= u_0, \text{ in } \Omega,
 \end{aligned} \tag{2}$$

Table 1: General notation and symbols.

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

Table 2: Physical parameters and values.

Symbol	Name	Units
$\vartheta$	Volumetric Heat Capacity	$\text{J m}^{-3} \text{K}^{-1}$
$K_l, K_s$	Thermal Conductivity in $\Omega_l$ and $\Omega_s$	$\text{J s}^{-1} \text{m}^{-1} \text{K}^{-1}$
$L$	Latent Heat Coefficient	$\text{J m}^{-3}$
$\alpha$	Surface Tension Coefficient of $\Gamma$	$\text{J m}^{-2}$
$S$	Volumetric Entropy Coefficient	$\text{J m}^{-3} \text{K}^{-1}$
$\rho$	Kinetic Coefficient	$\text{J s m}^{-4}$
$\beta$	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	$\text{J m}^{-3} \text{s}^{-1}$

Table 3: Nondimensional parameters.

Symbol	Name	Value
$\widehat{S} = S/\vartheta$	non-dim. entropy coefficient	2
$\widehat{\beta}_0 = \vartheta U_0 t_0 / (\rho D)$	non-dim. mobility coefficient	0.01
$\widehat{\beta} = \beta_0 \beta$	non-dim. mobility function	-
$\widehat{K}_l = K_l t_0 / (D^2 \vartheta)$	non-dim. liquid conductivity	1
$\widehat{K}_s = K_s t_0 / (D^2 \vartheta)$	non-dim. solid conductivity	1
$\widehat{C} = \alpha / (U_0 D \vartheta)$	non-dim. surface tension coefficient	0.0005

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

$$\begin{aligned}
u_1 - u_s &= 0, \text{ on } \Gamma(t), \\
\boldsymbol{\nu} \cdot (K_1 \nabla u_1 - K_s \nabla u_s) + L \partial_t \mathbf{X} \cdot \boldsymbol{\nu} &= 0, \text{ on } \Gamma(t), \\
\frac{\rho}{\beta(\boldsymbol{\nu})} \partial_t \mathbf{X} \cdot \boldsymbol{\nu} + \alpha \kappa + S u &= 0, \text{ on } \Gamma(t), \\
\mathbf{X}(\cdot, 0) - \mathbf{X}_0(\cdot) &= \mathbf{0}, \text{ on } \mathcal{M}, \\
\Gamma(0) &= \Gamma_0, \text{ in } \Omega,
\end{aligned} \tag{3}$$

where  $\Gamma_0$  is the initial interface (parameterized by  $\mathbf{X}_0$ ) and  $\mathbf{X}(\cdot, t)$  parameterizes  $\Gamma(t)$ . Note that  $u = T - T_M$ , where  $T$  is the temperature in degrees Kelvin and  $T_M$  is the melting temperature at the interface  $\Gamma$ , and that  $u$  is continuous across the interface. As noted in [5], we must have

$$S = \frac{L}{T_M}. \tag{4}$$

### 2.3 Non-Dimensionalization

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

$$\begin{aligned}
\partial_t u_1 - \widehat{K}_1 \Delta u_1 &= f_1, \text{ in } \Omega_1(t), \\
\partial_t u_s - \widehat{K}_s \Delta u_s &= f_s, \text{ in } \Omega_s(t), \\
\boldsymbol{\nu}_\Omega \cdot \nabla u &= 0, \text{ on } \partial_N \Omega, \\
u &= u_D, \text{ on } \partial_D \Omega, \\
u(\cdot, 0) &= u_0, \text{ in } \Omega,
\end{aligned} \tag{5}$$

$$\begin{aligned}
u_1 - u_s &= 0, \text{ on } \Gamma(t), \\
\boldsymbol{\nu} \cdot (\widehat{K}_1 \nabla u_1 - \widehat{K}_s \nabla u_s) + \widehat{S} \partial_t \mathbf{X} \cdot \boldsymbol{\nu} &= 0, \text{ on } \Gamma(t), \\
\frac{1}{\widehat{\beta}(\boldsymbol{\nu})} \partial_t \mathbf{X} \cdot \boldsymbol{\nu} + \widehat{\mathcal{C}} \kappa + \widehat{S} u &= 0, \text{ on } \Gamma(t), \\
\mathbf{X}(\cdot, 0) - \mathbf{X}_0(\cdot) &= \mathbf{0}, \text{ on } \mathcal{M}, \\
\Gamma(0) &= \Gamma_0, \text{ in } \Omega,
\end{aligned} \tag{6}$$

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

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

**Remark 1.** *The case of  $\vartheta = 0$  (i.e.  $\widehat{\mathcal{C}}, \widehat{S}, \widehat{K}_1, \widehat{K}_s = \infty$ ) corresponds to the steady-state heat equation in  $\Omega_1$  and  $\Omega_s$  and if  $\rho = 0$  (i.e.  $\widehat{\beta}(\boldsymbol{\nu}) \equiv \infty$ ) then (5) and (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 (5) and (6) reduce to the time-dependent heat equation on a stationary domain with  $u_1 = u_s = 0$  on  $\Gamma$ .*

## 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, e.g.  $L^2(\Omega)$  is the space of square integrable functions on  $\Omega$ ,  $H(\text{div}, \Omega)$  is the space of vector functions on  $\Omega$  that are square integrable and whose divergence is also square integrable, etc. On the reference domains  $\widehat{\Omega}_1$  and  $\widehat{\Omega}_s$ , we introduce:

$$\begin{aligned} \mathbb{V} &= H(\text{div}, \Omega), & \mathbb{V}(g) &= \{\boldsymbol{\eta} \in \mathbb{V} : \boldsymbol{\eta} \cdot \boldsymbol{\nu}_\Omega = g, \text{ on } \partial_N \Omega\}, \\ \mathbb{V}_1 &= H(\text{div}, \widehat{\Omega}_1), & \mathbb{V}_1(g) &= \{\boldsymbol{\eta} \in \mathbb{V}_1 : \boldsymbol{\eta} \cdot \boldsymbol{\nu}_\Omega = g, \text{ on } \partial_N \Omega\}, \\ \mathbb{V}_s &= H(\text{div}, \widehat{\Omega}_s), \end{aligned} \tag{7}$$

$$\mathbb{Q} = L^2(\Omega), \quad \mathbb{Q}_1 = L^2(\widehat{\Omega}_1), \quad \mathbb{Q}_s = L^2(\widehat{\Omega}_s). \tag{8}$$

On the reference manifold  $\mathcal{M}$ , we have

$$\mathbb{Y} = H^1(\mathcal{M}, \mathbb{R}^d), \tag{9}$$

$$\mathbb{M} = H^{1/2}(\mathcal{M}, \mathbb{R}). \tag{10}$$

We will use the following abuse of notation, similar to [5]. We identify functions  $\boldsymbol{\eta}$  in  $\mathbb{V}_1$  with  $\boldsymbol{\eta} \circ \mathbf{X}^{-1}$  defined on  $\Omega_1(t)$  (recall  $\Omega_1(t) = \mathbf{X}(\widehat{\Omega}_1, t)$ ), and denote both functions simply as  $\boldsymbol{\eta}$ ; similar considerations are made for functions  $\boldsymbol{\eta}$  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  $\mu$  in  $\mathbb{M}$ .

## 3.2 Curvature

### 3.2.1 Definition

Next, recall an equation relating  $\mathbf{X}(\cdot, t)$  to the vector curvature  $\kappa \boldsymbol{\nu}$  of  $\Gamma(t)$  [16]:

$$-\Delta_\Gamma \mathbf{X} = \kappa \boldsymbol{\nu},$$

where  $\Delta_\Gamma$  is the Laplace-Beltrami operator, which is defined by  $\Delta_\Gamma := \nabla_\Gamma \cdot \nabla_\Gamma$  where  $\nabla_\Gamma$  is the tangential gradient (or surface gradient) on the manifold  $\Gamma$ . Note:  $\nabla_\Gamma \equiv \boldsymbol{\tau} \partial_s$  and  $\Delta_\Gamma \equiv \partial_s^2$ , where  $\partial_s$  is the derivative with respect to arc-length, when  $\Gamma$  is a one-dimensional curve with oriented unit tangent vector  $\boldsymbol{\tau}$ .

### 3.2.2 Weak Form

In the rest of the paper, we take advantage of a weak formulation of the vector curvature [18, 3]. If  $\Gamma$  is a closed manifold, then the following integration by parts relation is true:

$$\int_\Gamma \kappa \boldsymbol{\nu} \cdot \mathbf{Y} = \int_\Gamma \nabla_\Gamma \mathbf{X} : \nabla_\Gamma \mathbf{Y}, \tag{11}$$

where  $\nabla_\Gamma \mathbf{X}$  is a symmetric matrix that represents the projection operator onto the tangent space of  $\Gamma$ , i.e.  $\nabla_\Gamma \mathbf{X} = \mathbf{I} - \boldsymbol{\nu} \otimes \boldsymbol{\nu}$ . We use (11) to derive the weak form (13).

## 3.3 Fully Continuous

We present a mixed formulation of (5), (6) that is partly related to [7] for the heat equation. Define the flux variables  $\boldsymbol{\sigma}_1 = -\widehat{K}_1 \nabla u_1$ ,  $\boldsymbol{\sigma}_s = -\widehat{K}_s \nabla u_s$ . Then, for given initial data  $\mathbf{X}(\cdot, 0) = \mathbf{X}_0$ ,

$u_s(\cdot, 0) = u_{s,0}$ ,  $u_1(\cdot, 0) = u_{1,0}$ , we want to 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

$$\begin{aligned} \frac{1}{\widehat{K}_1} \int_{\Omega_1(t)} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\eta} - \int_{\Omega_1(t)} u_1 \nabla \cdot \boldsymbol{\eta} - \int_{\Gamma(t)} \lambda \boldsymbol{\eta} \cdot \boldsymbol{\nu} &= - \int_{\partial_D \Omega} u_D \boldsymbol{\eta} \cdot \boldsymbol{\nu}_\Omega, \quad \text{for all } \boldsymbol{\eta} \in \mathbb{V}_1(0), \\ - \int_{\Omega_1(t)} q \nabla \cdot \boldsymbol{\sigma}_1 - \int_{\Omega_1(t)} q \partial_t u_1 &= - \int_{\Omega_1(t)} q f_1, \quad \text{for all } q \in \mathbb{Q}_1, \\ \frac{1}{\widehat{K}_s} \int_{\Omega_s(t)} \boldsymbol{\sigma}_s \cdot \boldsymbol{\eta} - \int_{\Omega_s(t)} u_s \nabla \cdot \boldsymbol{\eta} + \int_{\Gamma(t)} \lambda \boldsymbol{\eta} \cdot \boldsymbol{\nu} &= 0, \quad \text{for all } \boldsymbol{\eta} \in \mathbb{V}_s, \\ - \int_{\Omega_s(t)} q \nabla \cdot \boldsymbol{\sigma}_s - \int_{\Omega_s(t)} q \partial_t u_s &= - \int_{\Omega_s(t)} q f_s, \quad \text{for all } q \in \mathbb{Q}_s, \end{aligned} \tag{12}$$

$$\begin{aligned} \int_{\Gamma(t)} \frac{1}{\widehat{\beta}(\boldsymbol{\nu})} (\partial_t \mathbf{X} \cdot \boldsymbol{\nu})(\mathbf{Y} \cdot \boldsymbol{\nu}) + \widehat{\mathcal{C}} \int_{\Gamma(t)} \nabla_\Gamma \mathbf{X} : \nabla_\Gamma \mathbf{Y} + \widehat{S} \int_{\Gamma(t)} \lambda (\mathbf{Y} \cdot \boldsymbol{\nu}) &= 0, \quad \text{for all } \mathbf{Y} \in \mathbb{Y}, \\ \widehat{S} \int_{\Gamma(t)} \mu \partial_t \mathbf{X} \cdot \boldsymbol{\nu} - \int_{\Gamma(t)} \mu \boldsymbol{\sigma}_1 \cdot \boldsymbol{\nu} + \int_{\Gamma(t)} \mu \boldsymbol{\sigma}_s \cdot \boldsymbol{\nu} &= 0, \quad \text{for all } \mu \in \mathbb{M}, \end{aligned} \tag{13}$$

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 (12), (13) 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 [13, 30]. 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 (12) and (13), 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:

$$\begin{aligned} \frac{1}{\widehat{K}_1} \int_{\Omega_1(t)} |\boldsymbol{\sigma}_1|^2 + \frac{1}{\widehat{K}_s} \int_{\Omega_s(t)} |\boldsymbol{\sigma}_s|^2 + \int_{\Gamma(t)} \frac{1}{\widehat{\beta}(\boldsymbol{\nu})} |\partial_t \mathbf{X} \cdot \boldsymbol{\nu}|^2 + \widehat{\mathcal{C}} \int_{\Gamma(t)} \nabla_\Gamma(\partial_t \mathbf{X}) : \nabla_\Gamma \mathbf{X} \\ \int_{\Omega_1(t)} u_1 \partial_t u_1 + \int_{\Omega_s(t)} u_s \partial_t u_s = \int_{\Omega_1(t)} u_1 f_1 + \int_{\Omega_s(t)} u_s f_s. \end{aligned} \tag{14}$$

Next, we make some preliminary calculations for some of the terms in (14). By standard shape differentiation [55, 15, 31], we have

$$\begin{aligned} \frac{d}{dt} \left( \int_{\Omega_1(t)} u_1^2 \right) &= \int_{\Omega_1(t)} \partial_t (u_1^2) - \int_{\Gamma(t)} u_1^2 (\partial_t \mathbf{X}) \cdot \boldsymbol{\nu}, \\ \frac{d}{dt} \left( \int_{\Omega_s(t)} u_s^2 \right) &= \int_{\Omega_s(t)} \partial_t (u_s^2) + \int_{\Gamma(t)} u_s^2 (\partial_t \mathbf{X}) \cdot \boldsymbol{\nu}, \end{aligned} \tag{15}$$

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

$$\begin{aligned} \int_{\Omega_1(t)} u_1 \partial_t u_1 + \int_{\Omega_s(t)} u_s \partial_t u_s &= \frac{1}{2} \left( \int_{\Omega_1(t)} \partial_t (u_1^2) + \int_{\Omega_s(t)} \partial_t (u_s^2) \right) \\ &= \frac{1}{2} \frac{d}{dt} \left( \int_{\Omega_1(t)} u_1^2 + \int_{\Omega_s(t)} u_s^2 \right) + \frac{1}{2} \int_{\Gamma(t)} (u_1^2 - u_s^2) \partial_t \mathbf{X} \cdot \boldsymbol{\nu} \\ &= \frac{1}{2} \frac{d}{dt} \left( \int_{\Omega_1(t)} u_1^2 + \int_{\Omega_s(t)} u_s^2 \right), \end{aligned} \quad (16)$$

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

Now note that shape differentiation also tells us that

$$\int_{\Gamma(t)} \nabla_{\Gamma}(\partial_t \mathbf{X}) : \nabla_{\Gamma} \mathbf{X} = \frac{d}{dt} |\Gamma(t)|. \quad (17)$$

Therefore, we arrive at an identity

$$\begin{aligned} \int_{\Gamma(t)} \frac{1}{\widehat{\beta}(\boldsymbol{\nu})} [(\partial_t \mathbf{X}) \cdot \boldsymbol{\nu}]^2 + \frac{1}{\widehat{K}_1} \|\boldsymbol{\sigma}_1\|_{L^2(\Omega_1(t))}^2 + \frac{1}{\widehat{K}_s} \|\boldsymbol{\sigma}_s\|_{L^2(\Omega_s(t))}^2 + \widehat{C} \frac{d}{dt} |\Gamma(t)| \\ + \frac{1}{2} \frac{d}{dt} \left( \int_{\Omega_1(t)} u_1^2 + \int_{\Omega_s(t)} u_s^2 \right) = \int_{\Omega_1(t)} u_1 f_1 + \int_{\Omega_s(t)} u_s f_s, \end{aligned} \quad (18)$$

which is a variation of a result in [5]. Continuing, we assume there exists an ‘‘inf-sup’’ condition for the system (12), (13) (similar to Lemma 3), such that  $\|u_1\|_{L^2(\Omega_1)}^2 + \|u_s\|_{L^2(\Omega_s)}^2$  is bounded by a constant times the top line of (18). Hence, by using weighted Young’s inequalities on the right-hand-side of (18), we obtain the desired inequality

$$\begin{aligned} \int_{\Gamma(t)} \frac{1}{\widehat{\beta}(\boldsymbol{\nu})} [(\partial_t \mathbf{X}) \cdot \boldsymbol{\nu}]^2 + \|\boldsymbol{\sigma}_1\|_{L^2(\Omega_1(t))}^2 + \|\boldsymbol{\sigma}_s\|_{L^2(\Omega_s(t))}^2 + \frac{d}{dt} |\Gamma(t)| \\ + \frac{d}{dt} \left( \int_{\Omega_1(t)} u_1^2 + \int_{\Omega_s(t)} u_s^2 \right) \leq C \left( \|f_1\|_{L^2(\Omega_1)}^2 + \|f_s\|_{L^2(\Omega_s)}^2 \right), \end{aligned} \quad (19)$$

where  $C > 0$  only depends on the physical constants and domain geometry. See (41) for the semi-discrete version of (19).

### 3.4.2 Conservation Law

We also have a conservation law for the system which is simply a thermal energy balance. Choosing  $q_1 = 1$ ,  $q_s = 1$  in (12), and  $\mu = 1$  in (13) gives

$$\begin{aligned} - \int_{\partial_D \Omega} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\nu}_{\Omega} + \int_{\Gamma(t)} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\nu} &= \int_{\Omega_1(t)} \partial_t u_1 - \int_{\Omega_1(t)} f_1, \\ - \int_{\Gamma(t)} \boldsymbol{\sigma}_s \cdot \boldsymbol{\nu} &= \int_{\Omega_s(t)} \partial_t u_s - \int_{\Omega_s(t)} f_s, \\ \widehat{S} \int_{\Gamma(t)} (\partial_t \mathbf{X}) \cdot \boldsymbol{\nu} &= \int_{\Gamma(t)} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\nu} - \int_{\Gamma(t)} \boldsymbol{\sigma}_s \cdot \boldsymbol{\nu}. \end{aligned}$$



Adding them together gives the balance law:

$$\int_{\Omega_l(t)} f_l + \int_{\Omega_s(t)} f_s - \int_{\partial_D \Omega} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\nu}_\Omega = \int_{\Omega_l(t)} \partial_t u_l + \int_{\Omega_s(t)} \partial_t u_s - \widehat{S} \int_{\Gamma(t)} (\partial_t \mathbf{X}) \cdot \boldsymbol{\nu}, \quad (20)$$

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 (42) for the semi-discrete version of (20).

## 4 Time Semi-Discrete Formulation

We now partition the time interval  $(0, T)$  into subintervals of size  $\Delta t$ . 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  $\Sigma$ . In addition, let  $\langle \cdot, \cdot \rangle_\Sigma$  denote the duality pairing on  $\Sigma$  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 Interface Velocity

#### 4.1.1 Map $\Gamma^i$ to $\Gamma^{i+1}$

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:

$$\mathbf{X}^{i+1} = \mathbf{X}^i + \Delta t \mathbf{V}^{i+1}, \quad \text{where } \mathbf{V}^{i+1} : \Omega^i \rightarrow \mathbb{R}^3. \quad (21)$$

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

**Remark 2.** *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 (21) to make sense.*

#### 4.1.2 Map $\Omega_l^i, \Omega_s^i$ to $\Omega_l^{i+1}, \Omega_s^{i+1}$

Given  $\mathbf{V}^{i+1}$  on  $\Gamma^i$ , it can be extended to the entire domain  $\Omega$  by a harmonic extension [21, 65]. We use the same symbol  $\mathbf{V}^{i+1}$  to denote the extension. This induces a map  $\Phi_{i+1} : \Omega^i \rightarrow \Omega^{i+1}$  defined by

$$\Phi_{i+1}(\mathbf{x}) = \text{id}_{\Omega^i}(\mathbf{x}) + \Delta t \mathbf{V}^{i+1}(\mathbf{x}), \quad \text{for all } \mathbf{x} \in \Omega^i. \quad (22)$$

See [26, 27] for similar constructions in an ALE (Arbitrary-Lagrangian-Eulerian) context.

Note that  $\Phi_{i+1}$  is defined over both  $\Omega_l^i$  and  $\Omega_s^i$ . Similarly as for (21), we assume  $\mathbf{V}^{i+1}$  (on  $\Omega^i$ ) is at least in  $W^{1,\infty}(\Omega^i)$ . Moreover, we assume  $\Phi_{i+1}$  is a bijective map and  $\det([\nabla_{\mathbf{x}} \Phi_{i+1}(\mathbf{x})]) > 0$ . We note the following properties satisfied by  $\Phi_{i+1}$  [32, 57].

- 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  $f : \Omega^{i+1} \rightarrow \mathbb{R}$ , 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  $\Phi_{i+1}$  to transform the functions  $u_l^{i+1}, u_s^{i+1}$  on  $\Omega^i$  to new functions on  $\Omega^{i+1}$  in order to advance the solution to the next time step. See Section 4.6 for more details.

## 4.2 Weak Formulation

We now present the semi-discrete formulation of equations (12) and (13). The main idea is to write all integrals over the current domain  $\Omega^i, \Gamma^i$  but set all of the solution variables at the next time step  $t_{i+1}$  (i.e. a semi-implicit method). Moreover, we apply (21). Thus, we arrive at the following weak formulation. At time  $t_i$ , find  $\boldsymbol{\sigma}_1^{i+1}$  in  $\mathbb{V}_1^i(0)$ ,  $\boldsymbol{\sigma}_s^{i+1}$  in  $\mathbb{V}_s^i$ ,  $\mathbf{V}^{i+1}$  in  $\mathbb{Y}^i$ ,  $u_1^{i+1}$  in  $\mathbb{Q}_1^i$ ,  $u_s^{i+1}$  in  $\mathbb{Q}_s^i$ ,  $\lambda^{i+1}$  in  $\mathbb{M}^i$  such that

$$\begin{aligned} \frac{1}{\widehat{K}_1}(\boldsymbol{\sigma}_1^{i+1}, \boldsymbol{\eta})_{\Omega_1^i} - (u_1^{i+1}, \nabla \cdot \boldsymbol{\eta})_{\Omega_1^i} - \langle \boldsymbol{\eta} \cdot \boldsymbol{\nu}^i, \lambda^{i+1} \rangle_{\Gamma^i} &= -\langle \boldsymbol{\eta} \cdot \boldsymbol{\nu}_\Omega, u_D^{i+1} \rangle_{\partial_D \Omega}, \quad \text{for all } \boldsymbol{\eta} \in \mathbb{V}_1^i(0), \\ -(\nabla \cdot \boldsymbol{\sigma}_1^{i+1}, q)_{\Omega_1^i} - \frac{1}{\Delta t}(u_1^{i+1}, q)_{\Omega_1^i} + \frac{1}{\Delta t}(\overline{u}_1^i, q)_{\Omega_1^i} &= -(f_1^{i+1}, q)_{\Omega_1^i}, \quad \text{for all } q \in \mathbb{Q}_1^i, \\ \frac{1}{\widehat{K}_s}(\boldsymbol{\sigma}_s^{i+1}, \boldsymbol{\eta})_{\Omega_s^i} - (u_s^{i+1}, \nabla \cdot \boldsymbol{\eta})_{\Omega_s^i} + \langle \boldsymbol{\eta} \cdot \boldsymbol{\nu}^i, \lambda^{i+1} \rangle_{\Gamma^i} &= 0, \quad \text{for all } \boldsymbol{\eta} \in \mathbb{V}_s^i, \end{aligned} \quad (23)$$

$$\begin{aligned} -(\nabla \cdot \boldsymbol{\sigma}_s^{i+1}, q)_{\Omega_s^i} - \frac{1}{\Delta t}(u_s^{i+1}, q)_{\Omega_s^i} + \frac{1}{\Delta t}(\overline{u}_s^i, q)_{\Omega_s^i} &= -(f_s^{i+1}, q)_{\Omega_s^i}, \quad \text{for all } q \in \mathbb{Q}_s^i, \\ (\widehat{\beta}^{-1}(\boldsymbol{\nu}^i) \mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i, \mathbf{Y} \cdot \boldsymbol{\nu}^i)_{\Gamma^i} + \Delta t \widehat{\mathcal{C}}(\nabla_{\Gamma^i} \mathbf{V}^{i+1}, \nabla_{\Gamma^i} \mathbf{Y})_{\Gamma^i} \\ + \widehat{S}(\mathbf{Y} \cdot \boldsymbol{\nu}^i, \lambda^{i+1})_{\Gamma^i} &= -\widehat{\mathcal{C}}(\nabla_{\Gamma^i} \mathbf{X}^i, \nabla_{\Gamma^i} \mathbf{Y})_{\Gamma^i}, \quad \text{for all } \mathbf{Y} \in \mathbb{Y}^i, \end{aligned} \quad (24)$$

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

where the function spaces are defined over the current (known) domain  $\Omega^i, \Gamma^i$ . Then we use (21) to obtain the new interface position, which induces a map  $\Phi_{i+1} : \Omega^i \rightarrow \Omega^{i+1}$  that we use to update the temperatures  $u_1^{i+1}, u_s^{i+1}$  defined on  $\Omega^i$  to new functions  $\overline{u}_1^{i+1}, \overline{u}_s^{i+1}$  defined on  $\Omega^{i+1}$  (see Sections 4.1.2 and 4.6). Iterating this procedure gives a time semi-discrete approximation of the fully continuous problem (12), (13).

## 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

$$\begin{aligned} \boldsymbol{\sigma}_1^{i+1} &\equiv \boldsymbol{\sigma}_1, \quad \boldsymbol{\sigma}_s^{i+1} \equiv \boldsymbol{\sigma}_s, \quad \mathbf{V}^{i+1} \equiv \mathbf{V}, \quad u_1^{i+1} \equiv u_1, \quad u_s^{i+1} \equiv u_s, \quad \lambda^{i+1} \equiv \lambda, \\ f_1^{i+1} &\equiv \overline{f}_1, \quad f_s^{i+1} \equiv \overline{f}_s, \quad \overline{u}_1^i \equiv \overline{u}_1, \quad \overline{u}_s^i \equiv \overline{u}_s, \quad \mathbf{X}^i \equiv \overline{\mathbf{X}}, \quad \nabla_{\Gamma^i} \equiv \nabla_\Gamma. \end{aligned}$$

### 4.3.1 Bilinear and Linear Forms

For notational convenience, we introduce the following bilinear forms. The primal form is

$$\begin{aligned} a((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_s, \mathbf{V})) &= \frac{1}{\widehat{K}_1}(\boldsymbol{\eta}_1, \boldsymbol{\sigma}_1)_{\Omega_1} + \frac{1}{\widehat{K}_s}(\boldsymbol{\eta}_s, \boldsymbol{\sigma}_s)_{\Omega_s} \\ &+ (\widehat{\beta}^{-1}(\boldsymbol{\nu}) \mathbf{Y} \cdot \boldsymbol{\nu}, \mathbf{V} \cdot \boldsymbol{\nu})_\Gamma + \Delta t \widehat{\mathcal{C}}(\nabla_\Gamma \mathbf{Y}, \nabla_\Gamma \mathbf{V})_\Gamma, \end{aligned} \quad (25)$$

the constraint form is

$$\begin{aligned} b((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (q_1, q_s, \mu)) &= -(\nabla \cdot \boldsymbol{\eta}_1, q_1)_{\Omega_1} - (\nabla \cdot \boldsymbol{\eta}_s, q_s)_{\Omega_s} \\ &- \langle \boldsymbol{\eta}_1 \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma + \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma + \widehat{S}(\mathbf{Y} \cdot \boldsymbol{\nu}, \mu)_\Gamma, \end{aligned} \quad (26)$$

and the lower diagonal form is

$$c((q_1, q_s, \mu), (u_1, u_s, \lambda)) = \frac{1}{\Delta t}(q_1, u_1)_{\Omega_1} + \frac{1}{\Delta t}(q_s, u_s)_{\Omega_s}. \quad (27)$$

The linear forms are defined by

$$\begin{aligned}\chi(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}) &= - \left( \langle \boldsymbol{\eta}_l \cdot \boldsymbol{\nu}_\Omega, u_D \rangle_{\partial_D \Omega} + \widehat{\mathcal{C}}(\nabla_\Gamma \overline{\mathbf{X}}, \nabla_\Gamma \mathbf{Y})_\Gamma \right), \\ \psi(q_l, q_s, \mu) &= - \left( (\overline{f}_l, q_l)_{\Omega_l} + (\overline{f}_s, q_s)_{\Omega_s} + \frac{1}{\Delta t} (\overline{u}_l, q_l)_{\Omega_l} + \frac{1}{\Delta t} (\overline{u}_s, q_s)_{\Omega_s} \right).\end{aligned}\tag{28}$$

### 4.3.2 Saddle-Point Formulation

Define the primal space by

$$\mathbb{Z} = \mathbb{V}_l(0) \times \mathbb{V}_s \times \mathbb{Y},\tag{29}$$

and the multiplier space by

$$\mathbb{T} = \mathbb{Q}_l \times \mathbb{Q}_s \times \mathbb{M}.\tag{30}$$

With the above notation, the formulation (23), (24) can be written as a saddle-point problem.

**Variational Formulation 1.** Find  $(\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V})$  in  $\mathbb{V}_l(0) \times \mathbb{V}_s \times \mathbb{Y}$  and  $(u_l, u_s, \lambda)$  in  $\mathbb{Q}_l \times \mathbb{Q}_s \times \mathbb{M}$  such that

$$\begin{aligned}a((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V})) + b((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (u_l, u_s, \lambda)) &= \chi(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), \\ +b((\boldsymbol{\sigma}_l, \boldsymbol{\sigma}_s, \mathbf{V}), (q_l, q_s, \mu)) - c((q_l, q_s, \mu), (u_l, u_s, \lambda)) &= \psi(q_l, q_s, \mu),\end{aligned}\tag{31}$$

for all  $(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})$  in  $\mathbb{V}_l(0) \times \mathbb{V}_s \times \mathbb{Y}$ , and  $(q_l, q_s, \mu)$  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  $\lambda$ .

## 4.4 Norms

### 4.4.1 Non-degenerate Interface

The purpose of the following assumption is to avoid a case where  $\Gamma$  is closed and very flat (e.g. the surface of a pancake). It is necessary to ensure the equivalence of the norms in Proposition 1.

**Assumption 1.** Assume that  $\Gamma$  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  $\mathcal{N} \subset \Gamma$  such that  $|\mathcal{N}| \geq c_0 > 0$  and

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

### 4.4.2 Primal Norm

Clearly,  $\|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}^\circ}^2 := \|\boldsymbol{\eta}_l\|_{H(\text{div}, \Omega_l)}^2 + \|\boldsymbol{\eta}_s\|_{H(\text{div}, \Omega_s)}^2 + \|\mathbf{Y}\|_{H^1(\Gamma)}^2$  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  $\Gamma$  (i.e.  $\|\mathbf{Y}\|_{H^1(\Gamma)}^2 = \|\mathbf{Y}\|_{L^2(\Gamma)}^2 + \|\nabla_\Gamma \mathbf{Y}\|_{L^2(\Gamma)}^2$ ).

**Proposition 1.** Let  $\Gamma$  be a Lipschitz or polyhedral manifold. Define:

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

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 1,  $\mathbf{a} \cdot \boldsymbol{\nu} > 0$  (or  $< 0$ ) on a set of positive measure. Thus,  $\|\mathbf{Y} \cdot \boldsymbol{\nu}\|_{H^{-1/2}(\Gamma)}^2 \neq 0$ , 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, 20].  $\square$

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

$$\begin{aligned} \|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}}^2 &= \frac{1}{K_1} \|\boldsymbol{\eta}_1\|_{H(\operatorname{div}, \Omega_1)}^2 + \frac{1}{K_s} \|\boldsymbol{\eta}_s\|_{H(\operatorname{div}, \Omega_s)}^2 + \|\widehat{\beta}^{-1/2} \mathbf{Y} \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)}^2 \\ &\quad + \|\mathbf{Y} \cdot \boldsymbol{\nu}\|_{H^{-1/2}(\Gamma)}^2 + \Delta t \widehat{\mathcal{C}} \|\nabla_{\Gamma} \mathbf{Y}\|_{L^2(\Gamma)}^2. \end{aligned} \quad (32)$$

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

#### 4.4.3 Multiplier Norm

The obvious multiplier norm is  $\|(q_1, q_s, \mu)\|_{\mathbb{T}^\circ}^2 := \|q_1\|_{L^2(\Omega_1)}^2 + \|q_s\|_{L^2(\Omega_s)}^2 + \|\mu\|_{H^{1/2}(\Gamma)}^2$ . However, because of the form of the bilinear form  $b$  (26), it is more advantageous to use the following equivalent norm:

$$\|(q_1, q_s, \mu)\|_{\mathbb{T}}^2 = \|\tilde{q}_1\|_{L^2(\Omega_1)}^2 + \|\tilde{q}_s\|_{L^2(\Omega_s)}^2 + \|\mu - \hat{q}_1\|_{H^{1/2}(\Gamma)}^2 + \|\mu - \hat{q}_s\|_{H^{1/2}(\Gamma)}^2 + \widehat{S} \|\mu \boldsymbol{\nu}\|_{H^{-1}}^2, \quad (33)$$

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  $i = 1, s$ ). We also define the mean value on  $\Gamma$ :  $\hat{\mu} := \frac{1}{|\Gamma|} \int_{\Gamma} \mu$ , and  $\tilde{\mu} := \mu - \hat{\mu}$ .

**Proposition 2** (Equivalence of Multiplier Norms). *Let  $\Gamma$  be a Lipschitz or polyhedral manifold. Then,  $\|(q_1, q_s, \mu)\|_{\mathbb{T}^\circ} \approx \|(q_1, q_s, \mu)\|_{\mathbb{T}}$ , with constants that only depend on the domain and  $\widehat{S}$ .*

*Proof.* Again, use a compactness argument. □

### 4.5 Well-posedness

This section verifies the conditions needed for well-posedness of (31) [10, 8].

#### 4.5.1 Main Conditions

**Lemma 1** (Continuity of Forms).

$$\begin{aligned} |a((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_s, \mathbf{V}))| &\leq C_a \|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}} \|(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_s, \mathbf{V})\|_{\mathbb{Z}}, \quad \forall (\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_s, \mathbf{V}) \in \mathbb{Z}, \\ |b((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (q_1, q_s, \mu))| &\leq C_b \|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}} \|(q_1, q_s, \mu)\|_{\mathbb{T}}, \quad \forall (\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}) \in \mathbb{Z}, (q_1, q_s, \mu) \in \mathbb{T}, \\ |c((q_1, q_s, \mu), (u_1, u_s, \lambda))| &\leq \Delta t^{-1} (\|q_1\|_{L^2(\Omega_1)} \|u_1\|_{L^2(\Omega_1)} + \|q_s\|_{L^2(\Omega_s)} \|u_s\|_{L^2(\Omega_s)}), \quad \forall (q_1, q_s, \mu), (u_1, u_s, \lambda) \in \mathbb{T}, \\ |\chi((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}))| &\leq C_\chi \|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}}, \quad \forall (\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}) \in \mathbb{Z}, \\ |\psi(q_1, q_s, \mu)| &\leq C_\psi \|(q_1, q_s, \mu)\|_{\mathbb{T}}, \quad \forall (q_1, q_s, \mu) \in \mathbb{T}, \end{aligned}$$

where  $C_a, C_b, C_\chi, C_\psi > 0$  are constants that depend on physical parameters and domain geometry. In addition,  $C_\chi$  depends on  $u_D$ ,  $\Delta t^{-1/2}$ , and  $C_\psi$  depends on  $\overline{f}_1, \overline{f}_s, \overline{u}_1, \overline{u}_s$  and  $\Delta t^{-1}$ .

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

$$\begin{aligned} -(\nabla \cdot \boldsymbol{\eta}_1, q_1)_{\Omega_1} - \langle \boldsymbol{\eta}_1 \cdot \boldsymbol{\nu}, \mu \rangle_{\Gamma} &\leq C [\|q_1\|_{L^2(\Omega_1)} + \|\mu\|_{H^{1/2}(\Gamma)}] \|\boldsymbol{\eta}_1\|_{H(\operatorname{div}, \Omega_1)}, \\ -(\nabla \cdot \boldsymbol{\eta}_s, q_s)_{\Omega_s} + \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}, \mu \rangle_{\Gamma} &\leq C [\|q_s\|_{L^2(\Omega_s)} + \|\mu\|_{H^{1/2}(\Gamma)}] \|\boldsymbol{\eta}_s\|_{H(\operatorname{div}, \Omega_s)}, \end{aligned}$$

where we used an  $H^{-1/2}(\Gamma)$  trace estimate. In addition, we have

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

The bound on  $b$  then follows by combining these results and using Proposition 2. The bound on  $c$  is obvious. Next, we have

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

where  $C$  depends on  $\Delta t^{-1/2}$  and the data  $u_D$ . The last inequality follows from (28) where the constant depends on  $\Delta t^{-1}$  and the problem data.  $\square$

**Lemma 2** (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,*

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

where  $C > 0$  is a constant that depends on  $\widehat{S}$  and the domain. This is true even if  $\widehat{\beta} \rightarrow \infty$ .

*Proof.* From (25), we get

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

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, we have

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

Combining these inequalities yields the assertion.  $\square$

**Lemma 3** (Inf-Sup). *For all  $(q_l, q_s, \mu) \in \mathbb{T}$ , the following ‘‘inf-sup’’ condition holds*

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

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  $\widehat{K}_l$ ,  $\widehat{K}_s$ ,  $\widehat{\mathcal{C}}$ , and  $\widehat{\beta}_-$ . Furthermore,  $C$  does not depend on the time step  $\Delta t$ , as long as  $\Delta t \leq 1$ .

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

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

Next, by definition of the  $H^{1/2}(\Gamma)$  norm, there exists a  $\boldsymbol{\xi} \in H(\text{div}, \Omega_1)$  such that  $-\langle \boldsymbol{\xi} \cdot \boldsymbol{\nu}, \mu - \hat{q}_1 \rangle_\Gamma = \|\mu - \hat{q}_1\|_{H^{1/2}(\Gamma)}$  and  $\|\boldsymbol{\xi}\|_{H(\text{div}, \Omega_1)} = 1$ . With this, we construct the vector field  $\boldsymbol{\eta}_1 \in H(\text{div}, \Omega_1)$ . Let  $\phi_1, \phi_2$  in  $H^1(\Omega_1)$  satisfy

$$\begin{aligned} -\Delta\phi_1 &= \frac{\tilde{q}_1}{\|\tilde{q}_1\|_{L^2(\Omega_1)}}, \text{ in } \Omega_1, \quad \boldsymbol{\nu} \cdot \nabla\phi_1 = 0, \text{ on } \partial\Omega_1 \equiv \Gamma \cup \partial\Omega, \\ -\Delta\phi_2 &= \frac{1}{|\Omega_1|} \int_\Gamma \boldsymbol{\xi} \cdot \boldsymbol{\nu}, \text{ in } \Omega_1, \quad \boldsymbol{\nu} \cdot \nabla\phi_2 = \boldsymbol{\xi} \cdot \boldsymbol{\nu}, \text{ on } \Gamma, \quad \boldsymbol{\nu} \cdot \nabla\phi_2 = 0, \text{ on } \partial\Omega, \end{aligned}$$

and define  $\boldsymbol{\eta}_1 = \nabla\phi_1 + \nabla\phi_2$ . This gives

$$\begin{aligned} -(\nabla \cdot \boldsymbol{\eta}_1, \tilde{q}_1)_{\Omega_1} - \langle \boldsymbol{\eta}_1 \cdot \boldsymbol{\nu}, \mu - \hat{q}_1 \rangle_\Gamma &= (-\Delta\phi_1, \tilde{q}_1)_{\Omega_1} + (-\Delta\phi_2, \tilde{q}_1)_{\Omega_1} - \langle \boldsymbol{\nu} \cdot \nabla\phi_2, \mu - \hat{q}_1 \rangle_\Gamma \\ &= \|\tilde{q}_1\|_{L^2(\Omega_1)} + \|\mu - \hat{q}_1\|_{H^{1/2}(\Gamma)}. \end{aligned}$$

Furthermore, one can show

$$\|\boldsymbol{\eta}_1\|_{H(\text{div}, \Omega_1)} \leq C_1 \left( \frac{\|\tilde{q}_1\|_{L^2(\Omega_1)}}{\|\tilde{q}_1\|_{L^2(\Omega_1)}} + \|\boldsymbol{\xi} \cdot \boldsymbol{\nu}\|_{H^{-1/2}(\Gamma)} \right) \leq \frac{C_2}{2} (1 + \|\boldsymbol{\xi}\|_{H(\text{div}, \Omega_1)}) = C_2,$$

where  $C_2 > 0$  depends on  $\Omega_1$  and  $\Gamma$ . Similarly, there exists an  $\boldsymbol{\eta}_s$  in  $H(\text{div}, \Omega_s)$  such that

$$-(\nabla \cdot \boldsymbol{\eta}_s, \tilde{q}_s)_{\Omega_s} + \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}, \mu - \hat{q}_s \rangle_\Gamma = \|\tilde{q}_s\|_{L^2(\Omega_s)} + \|\mu - \hat{q}_s\|_{H^{1/2}(\Gamma)}, \quad \|\boldsymbol{\eta}_s\|_{H(\text{div}, \Omega_s)} \leq C_3,$$

where  $C_3 > 0$  depends on  $\Omega_s$  and  $\Gamma$ .

By the definition of the  $H^{-1}(\Gamma)$  norm, 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  $\Delta t^{-1}$  (see Lemma 1). As long as  $\Delta t > 0$ , the system (31) is well-posed with a bounded solution [10, 8]. But it is important to know how the time-step affects the solution, especially as  $\Delta t \rightarrow 0$ .

The following lemma is a modification of a result in [8, Lemma 4.14], applied to our formulation, which sheds some light on the effect of  $\Delta t$ .

**Lemma 4.** *Let  $(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})$  in  $\mathbb{Z}$  such that  $b((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (0, 0, \mu)) = 0$  for all  $\mu \in \mathbb{M}$ . Then, the bilinear forms  $a$  and  $b$  in (25), (26) satisfy*

$$\frac{a((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}))}{\|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}^*}} + \sup_{(q_1, q_s) \in \mathbb{Q}_1 \times \mathbb{Q}_s} \frac{b((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (q_1, q_s, 0))}{\Delta t^{-1/2} \left( \|q_1\|_{L^2(\Omega_1)}^2 + \|q_s\|_{L^2(\Omega_s)}^2 \right)^{1/2}} \geq C \|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}^*},$$

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

$$\begin{aligned} \|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}^*}^2 &:= \frac{1}{K_1} \left( \|\boldsymbol{\eta}_1\|_{L^2(\Omega_1)}^2 + \Delta t \|\nabla \cdot \boldsymbol{\eta}_1\|_{L^2(\Omega_1)}^2 \right) + \frac{1}{K_s} \left( \|\boldsymbol{\eta}_s\|_{L^2(\Omega_s)}^2 + \Delta t \|\nabla \cdot \boldsymbol{\eta}_s\|_{L^2(\Omega_s)}^2 \right) \\ &\quad + \|\hat{\beta}^{-1/2} \mathbf{Y} \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)}^2 + \Delta t \|\mathbf{Y} \cdot \boldsymbol{\nu}\|_{H^{-1/2}(\Gamma)}^2 + \Delta t \hat{C} \|\nabla_\Gamma \mathbf{Y}\|_{L^2(\Gamma)}^2. \end{aligned}$$

Lemma 4, and [8, Theorem 4.11, 4.13], yields the well-posedness of (31), but one can see more clearly how the norm is affected. An extra factor of  $\Delta t$  multiplies  $\|\nabla \cdot \boldsymbol{\eta}_1\|_{L^2(\Omega_1)}^2$ ,  $\|\nabla \cdot \boldsymbol{\eta}_s\|_{L^2(\Omega_s)}^2$ , and  $\|\mathbf{Y} \cdot \boldsymbol{\nu}\|_{H^{-1/2}(\Gamma)}^2$ . This is reasonable given the parabolic nature of the problem. In particular, from (23), one can see that  $\nabla \cdot \boldsymbol{\eta}_1$  and  $\nabla \cdot \boldsymbol{\eta}_s$  depends on the discrete time derivative of  $u_1$  and  $u_s$ .

## 4.6 Estimates

In order to derive a priori estimates for the semi-discrete scheme, we must specify how we map the temperatures  $u_1^{i+1}$ ,  $u_s^{i+1}$  from  $\Omega^i$  to  $\Omega^{i+1}$ . We propose two methods:

$$\text{(Method 1)} \quad \bar{u}_j^{i+1}(\mathbf{y}) = u_j^{i+1}(\mathbf{x}) \det([\nabla_{\mathbf{x}} \Phi_{i+1}(\mathbf{x})])^{-1/2}, \quad \forall \mathbf{x} \in \Omega^i, \quad j = 1, s, \quad (34)$$

and

$$\text{(Method 2)} \quad \bar{u}_j^{i+1}(\mathbf{y}) = u_j^{i+1}(\mathbf{x}) \det([\nabla_{\mathbf{x}} \Phi_{i+1}(\mathbf{x})])^{-1}, \quad \forall \mathbf{x} \in \Omega^i, \quad j = 1, s, \quad (35)$$

where  $\mathbf{y} = \Phi_{i+1}(\mathbf{x})$ . Method 1 allows us to obtain an a priori bound (Section 4.6.1). But Method 2 is more physically relevant because it yields a conservation law for the time semi-discrete system (Section 4.6.2).

### 4.6.1 A Priori Bound

We shall follow a similar derivation as in Section 3.4.1. Again, take  $u_D = 0$ . In (23) and (24), choose  $\boldsymbol{\eta}_1 = \boldsymbol{\sigma}_1^{i+1}$ ,  $\boldsymbol{\eta}_s = \boldsymbol{\sigma}_s^{i+1}$ ,  $\mathbf{Y} = \mathbf{V}^{i+1}$ ,  $q_1 = -u_1^{i+1}$ ,  $q_s = -u_s^{i+1}$ ,  $\mu = -\lambda^{i+1}$ , and add the equations together to get

$$\begin{aligned} & \frac{1}{\widehat{K}_1} \|\boldsymbol{\sigma}_1^{i+1}\|_{L^2(\Omega_1^i)}^2 + \frac{1}{\widehat{K}_s} \|\boldsymbol{\sigma}_s^{i+1}\|_{L^2(\Omega_s^i)}^2 + \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu}^i) \mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i\|_{L^2(\Gamma^i)}^2 \\ & + \widehat{\mathcal{C}} [(\nabla_{\Gamma^i}(\Delta t \mathbf{V}^{i+1}), \nabla_{\Gamma^i} \mathbf{V}^{i+1})_{\Gamma^i} + (\nabla_{\Gamma^i} \mathbf{X}^i, \nabla_{\Gamma^i} \mathbf{V}^{i+1})_{\Gamma^i}] \\ & + \frac{1}{\Delta t} (u_1^{i+1}, (u_1^{i+1} - \bar{u}_1^i))_{\Omega_1^i} + \frac{1}{\Delta t} (u_s^{i+1}, (u_s^{i+1} - \bar{u}_s^i))_{\Omega_s^i} \\ & = (u_1^{i+1}, f_1^{i+1})_{\Omega_1^i} + (u_s^{i+1}, f_s^{i+1})_{\Omega_s^i}. \end{aligned} \quad (36)$$

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

$$(u_1^{i+1}, (u_1^{i+1} - \bar{u}_1^i))_{\Omega_1^i} = \frac{1}{2} \left( \int_{\Omega_1^i} (u_1^{i+1})^2 - \int_{\Omega_1^i} (\bar{u}_1^i)^2 + \int_{\Omega_1^i} (u_1^{i+1} - \bar{u}_1^i)^2 \right). \quad (37)$$

Assuming we use (34) as the transformation rule for  $u_1$ , a change of variables gives

$$\int_{\Omega_1^i} (\bar{u}_1^i)^2 = \int_{\Omega_1^i} (\bar{u}_1^i(\mathbf{y}))^2 d\mathbf{y} = \int_{\Omega_1^{i-1}} (u_1^i(\mathbf{x}))^2 \det([\nabla_{\mathbf{x}} \Phi_i(\mathbf{x})])^{-1} \cdot \det([\nabla_{\mathbf{x}} \Phi_i(\mathbf{x})]) d\mathbf{x} = \int_{\Omega_1^{i-1}} (u_1^i)^2. \quad (38)$$

If  $N$  is the last time index to solve for, then (37) and (38) imply

$$\sum_{i=0}^{N-1} (u_1^{i+1}, (u_1^{i+1} - \bar{u}_1^i))_{\Omega_1^i} \geq \frac{1}{2} \sum_{i=0}^{N-1} \left( \|u_1^{i+1}\|_{L^2(\Omega_1^i)}^2 - \|u_1^i\|_{L^2(\Omega_1^{i-1})}^2 \right) = \frac{1}{2} \|u_1^N\|_{L^2(\Omega_1^{N-1})}^2 - \frac{1}{2} \|u_1^0\|_{L^2(\Omega_1^{-1})}^2,$$

where  $u_1^0$  is the initial temperature on the initial domain  $\Omega_1^{-1}$ . A similar result holds for  $\{u_s^i\}$ .

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

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

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

$$\begin{aligned} (\nabla_{\Gamma^i}(\Delta t \mathbf{V}^{i+1}), \nabla_{\Gamma^i} \mathbf{V}^{i+1})_{\Gamma^i} + (\nabla_{\Gamma^i} \mathbf{X}^i, \nabla_{\Gamma^i} \mathbf{V}^{i+1})_{\Gamma^i} &= \Delta t^{-1} (\nabla_{\Gamma^i} \mathbf{X}^{i+1}, \nabla_{\Gamma^i} (\mathbf{X}^{i+1} - \mathbf{X}^i))_{\Gamma^i} \\ &\geq \frac{|\Gamma^{i+1}| - |\Gamma^i|}{\Delta t}. \end{aligned} \quad (39)$$

Plugging (39) into (36) gives

$$\begin{aligned} \frac{1}{K_1} \|\sigma_1^{i+1}\|_{L^2(\Omega_1^i)}^2 + \frac{1}{K_s} \|\sigma_s^{i+1}\|_{L^2(\Omega_s^i)}^2 + \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu}^i) \mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i\|_{L^2(\Gamma^i)}^2 + \widehat{C} \frac{|\Gamma^{i+1}| - |\Gamma^i|}{\Delta t} \\ + \frac{1}{\Delta t} (u_1^{i+1}, (u_1^{i+1} - \bar{u}_1^i))_{\Omega_1^i} + \frac{1}{\Delta t} (u_s^{i+1}, (u_s^{i+1} - \bar{u}_s^i))_{\Omega_s^i} \leq (u_1^{i+1}, f_1^{i+1})_{\Omega_1^i} + (u_s^{i+1}, f_s^{i+1})_{\Omega_s^i}. \end{aligned} \quad (40)$$

Using Lemma 3 and (31) (with the test function  $\mathbf{Y} = \mathbf{0}$ ), we get that (with  $u_D = 0$ )

$$\|u_1^{i+1}\|_{\Omega_1^i} \leq C_1 \left( \|\sigma_1^{i+1}\|_{L^2(\Omega_1^i)} + \|\sigma_s^{i+1}\|_{L^2(\Omega_s^i)} \right),$$

where  $C_1$  only depends on the physical parameters and the domain. Ergo, by using weighted Young's inequalities on the right-hand-side of (40), and summing over  $i$ , we obtain the following result.

**Theorem 1.** *Suppose (31) is solved on  $\Omega^i$  at time index  $i$  and assume  $\mathbf{V}^{i+1}$  is in  $W^{1,\infty}(\Gamma^i)$  and that  $\Phi_{i+1}$  is a bijective map in  $W^{1,\infty}(\Omega^i)$  with bounded inverse. Moreover, assume (34) is used to update  $u_1^i, u_s^i$ . Suppose this holds for  $i = 0, \dots, N-1$ . Then,*

$$\begin{aligned} \Delta t \sum_{i=0}^{N-1} \left( \|\sigma_1^{i+1}\|_{L^2(\Omega_1^i)}^2 + \|\sigma_s^{i+1}\|_{L^2(\Omega_s^i)}^2 + \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu}^i) \mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i\|_{L^2(\Gamma^i)}^2 \right) \\ + |\Gamma^N| + \|u_1^N\|_{L^2(\Omega_1^{N-1})}^2 + \|u_s^N\|_{L^2(\Omega_s^{N-1})}^2 \leq \\ C \left[ \|u_1^0\|_{L^2(\Omega_1^{-1})}^2 + \|u_s^0\|_{L^2(\Omega_s^{-1})}^2 + |\Gamma^0| + \Delta t \sum_{i=0}^{N-1} \left( \|f_1^{i+1}\|_{L^2(\Omega_1^i)}^2 + \|f_s^{i+1}\|_{L^2(\Omega_s^i)}^2 \right) \right], \end{aligned} \quad (41)$$

where  $T = \Delta t N$  and  $C > 0$  only depends on the physical parameters and domain geometry.

#### 4.6.2 Conservation Law

Analogous to Section 3.4.2, choose  $q_1 = 1, q_s = 1$  in (23), and  $\mu = 1$  in (24) to get

$$\begin{aligned} - \int_{\partial_D \Omega} \sigma_1^{i+1} \cdot \boldsymbol{\nu}_\Omega + \int_{\Gamma^i} \sigma_1^{i+1} \cdot \boldsymbol{\nu}^i &= \frac{1}{\Delta t} \left( \int_{\Omega_1^i} u_1^{i+1} - \int_{\Omega_1^i} \bar{u}_1^i \right) - \int_{\Omega_1^i} f_1^{i+1}, \\ - \int_{\Gamma^i} \sigma_s^{i+1} \cdot \boldsymbol{\nu}^i &= \frac{1}{\Delta t} \left( \int_{\Omega_s^i} u_s^{i+1} - \int_{\Omega_s^i} \bar{u}_s^i \right) - \int_{\Omega_s^i} f_s^{i+1}, \\ \widehat{S} \int_{\Gamma^i} \mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i &= \int_{\Gamma^i} \sigma_1^{i+1} \cdot \boldsymbol{\nu}^i - \int_{\Gamma^i} \sigma_s^{i+1} \cdot \boldsymbol{\nu}^i. \end{aligned}$$



If (35) is used, then  $\int_{\Omega_1^i} \bar{u}_1^i = \int_{\Omega_1^{i-1}} u_1^i$  and  $\int_{\Omega_s^i} \bar{u}_s^i = \int_{\Omega_s^{i-1}} u_s^i$ . Thus, adding the above equations together gives a thermal power balance for each  $i = 0, \dots, N-1$ :

$$\begin{aligned} \int_{\Omega_1^i} f_1^{i+1} + \int_{\Omega_s^i} f_s^{i+1} - \int_{\partial_D \Omega} \boldsymbol{\sigma}_1^{i+1} \cdot \boldsymbol{\nu}_\Omega = \\ \frac{1}{\Delta t} \left( \int_{\Omega_1^i} u_1^{i+1} - \int_{\Omega_1^{i-1}} u_1^i \right) + \frac{1}{\Delta t} \left( \int_{\Omega_s^i} u_s^{i+1} - \int_{\Omega_s^{i-1}} u_s^i \right) - \widehat{S} \int_{\Gamma^i} \mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i. \end{aligned} \quad (42)$$

Summing (42) over the time steps yields the following theorem.

**Theorem 2.** *Assume the hypothesis of Theorem 1, except assume (35) is used to update  $u_1^i, u_s^i$ . Suppose this holds for  $i = 0, \dots, N-1$ . Then,*

$$\begin{aligned} \Delta t \sum_{i=0}^{N-1} \left( \int_{\Omega_1^i} f_1^{i+1} + \int_{\Omega_s^i} f_s^{i+1} - \int_{\partial_D \Omega} \boldsymbol{\sigma}_1^{i+1} \cdot \boldsymbol{\nu}_\Omega \right) + \int_{\Omega_1^{-1}} u_1^0 + \int_{\Omega_s^{-1}} u_s^0 = \\ \int_{\Omega_1^{N-1}} u_1^N + \int_{\Omega_s^{N-1}} u_s^N - \Delta t \widehat{S} \sum_{i=0}^{N-1} \int_{\Gamma^i} \mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i. \end{aligned} \quad (43)$$

## 5 Fully Discrete Formulation

### 5.1 Discretization

#### 5.1.1 Non-degenerate Interface

The following assumption is the space discrete version of Assumption 1 in Section 4.4.1. It is necessary to ensure the equivalence of the norms in the space discrete version of Proposition 1 when  $\|\cdot\|_{H^{-1/2}}$  is replaced by a *discrete* norm  $\|\cdot\|_{H_h^{-1/2}}$ .

**Assumption 2.** *Assume that  $\Gamma_h$  is a polyhedral manifold (i.e. surface triangulation). For any vertex  $v$ , let  $\text{Star}(v)$  be the set of triangle faces in  $\Gamma_h$  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  $\Gamma_h$  such that  $|\text{Star}(v)| \geq c_0 > 0$  and*

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

#### 5.1.2 Formulation

We begin by approximating the domains  $\Omega_1, \Omega_s$  by three dimensional triangulations  $\Omega_{1,h}, \Omega_{s,h}$  such that  $\Gamma_h = \overline{\Omega_{1,h}} \cap \overline{\Omega_{s,h}}$  is an embedded polyhedral surface contained in the faces of the mesh. A standard Galerkin approximation of equations (23), (24) takes the form: find  $\boldsymbol{\sigma}_{1,h}$  in  $\mathbb{V}_{1,h}(0) \subset \mathbb{V}_1(0)$ ,  $\boldsymbol{\sigma}_{s,h}$  in  $\mathbb{V}_{s,h} \subset \mathbb{V}_s$ ,  $\mathbf{V}_h$  in  $\mathbb{Y}_h \subset \mathbb{Y}$ ,  $u_{1,h}$  in  $\mathbb{Q}_{1,h} \subset \mathbb{Q}_1$ ,  $u_{s,h}$  in  $\mathbb{Q}_{s,h} \subset \mathbb{Q}_s$ ,  $\lambda_h$  in  $\mathbb{M}_h \subset \mathbb{M}$  such that

$$\begin{aligned} \frac{1}{\widehat{K}_1} (\boldsymbol{\sigma}_{1,h}, \boldsymbol{\eta})_{\Omega_{1,h}} - (u_{1,h}, \nabla \cdot \boldsymbol{\eta})_{\Omega_{1,h}} - \langle \boldsymbol{\eta} \cdot \boldsymbol{\nu}_h, \lambda_h \rangle_{\Gamma_h} &= -\langle \boldsymbol{\eta} \cdot \boldsymbol{\nu}_\Omega, u_D \rangle_{\partial_D \Omega}, \quad \text{for all } \boldsymbol{\eta} \in \mathbb{V}_{1,h}(0), \\ -(\nabla \cdot \boldsymbol{\sigma}_{1,h}, q)_{\Omega_{1,h}} - \frac{1}{\Delta t} (u_{1,h}, q)_{\Omega_{1,h}} + \frac{1}{\Delta t} (\overline{u_{1,h}}, q)_{\Omega_{1,h}} &= -(\overline{f_1}, q)_{\Omega_{1,h}}, \quad \text{for all } q \in \mathbb{Q}_{1,h}, \\ \frac{1}{\widehat{K}_s} (\boldsymbol{\sigma}_{s,h}, \boldsymbol{\eta})_{\Omega_{s,h}} - (u_{s,h}, \nabla \cdot \boldsymbol{\eta})_{\Omega_{s,h}} + \langle \boldsymbol{\eta} \cdot \boldsymbol{\nu}_h, \lambda_h \rangle_{\Gamma_h} &= 0, \quad \text{for all } \boldsymbol{\eta} \in \mathbb{V}_{s,h}, \\ -(\nabla \cdot \boldsymbol{\sigma}_{s,h}, q)_{\Omega_{s,h}} - \frac{1}{\Delta t} (u_{s,h}, q)_{\Omega_{s,h}} + \frac{1}{\Delta t} (\overline{u_{s,h}}, q)_{\Omega_{s,h}} &= -(\overline{f_s}, q)_{\Omega_{s,h}}, \quad \text{for all } q \in \mathbb{Q}_{s,h}, \end{aligned} \quad (44)$$

$$\begin{aligned} & (\widehat{\beta}^{-1}(\boldsymbol{\nu}_h) \mathbf{V}_h \cdot \boldsymbol{\nu}_h, \mathbf{Y} \cdot \boldsymbol{\nu}_h)_{\Gamma_h} + \Delta t \widehat{\mathcal{C}}(\nabla_{\Gamma} \mathbf{V}_h, \nabla_{\Gamma} \mathbf{Y})_{\Gamma_h} \\ & + \widehat{\mathcal{S}}(\mathbf{Y} \cdot \boldsymbol{\nu}_h, \lambda_h)_{\Gamma_h} = -\widehat{\mathcal{C}}(\nabla_{\Gamma} \overline{\mathbf{X}}, \nabla_{\Gamma} \mathbf{Y})_{\Gamma_h}, \quad \text{for all } \mathbf{Y} \in \mathbb{Y}_h, \end{aligned} \quad (45)$$

$$\widehat{\mathcal{S}}(\mathbf{V}_h \cdot \boldsymbol{\nu}_h, \mu)_{\Gamma_h} - \langle \boldsymbol{\sigma}_{1,h} \cdot \boldsymbol{\nu}_h, \mu \rangle_{\Gamma_h} + \langle \boldsymbol{\sigma}_{s,h} \cdot \boldsymbol{\nu}_h, \mu \rangle_{\Gamma_h} = 0, \quad \text{for all } \mu \in \mathbb{M}_h,$$

where we again used an ‘‘overline’’ to denote data or variables from the previous time-step. This leads to a fully discrete version of (31).

**Variational Formulation 2.** Find  $(\boldsymbol{\sigma}_{1,h}, \boldsymbol{\sigma}_{s,h}, \mathbf{V}_h)$  in  $\mathbb{Z}_h$  and  $(u_{1,h}, u_{s,h}, \lambda_h)$  in  $\mathbb{T}_h$  such that

$$\begin{aligned} & a_h((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_{1,h}, \boldsymbol{\sigma}_{s,h}, \mathbf{V}_h)) + b_h((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (u_{1,h}, u_{s,h}, \lambda_h)) = \chi_h(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), \\ & + b_h((\boldsymbol{\sigma}_{1,h}, \boldsymbol{\sigma}_{s,h}, \mathbf{V}_h), (q_1, q_s, \mu)) - c_h((q_1, q_s, \mu), (u_{1,h}, u_{s,h}, \lambda_h)) = \psi_h(q_1, q_s, \mu), \end{aligned} \quad (46)$$

for all  $(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})$  in  $\mathbb{Z}_h$ , and  $(q_1, q_s, \mu)$  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 (29), (30):  $\mathbb{Z} = \mathbb{V}_{1,h}(0) \times \mathbb{V}_{s,h} \times \mathbb{Y}_h$ ,  $\mathbb{T}_h = \mathbb{Q}_{1,h} \times \mathbb{Q}_{s,h} \times \mathbb{M}_h$ .

### 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

$$\|\mu\|_{H_{j,h}^{1/2}(\Gamma_h)} := \sup_{\boldsymbol{\eta} \in \mathbb{V}_{j,h}} \frac{\langle \boldsymbol{\eta} \cdot \boldsymbol{\nu}_h, \mu \rangle_{\Gamma_h}}{\|\boldsymbol{\eta}\|_{H(\text{div}, \Omega_{j,h})}}, \quad \text{for } j = 1, s. \quad (47)$$

Clearly,  $\|\mu\|_{H_{j,h}^{1/2}(\Gamma_h)} \leq \|\mu\|_{H^{1/2}(\Gamma_h)}$  and  $\langle \boldsymbol{\eta} \cdot \boldsymbol{\nu}_h, \mu \rangle_{\Gamma_h} \leq \|\boldsymbol{\eta}\|_{H(\text{div}, \Omega_{j,h})} \|\mu\|_{H_{j,h}^{1/2}(\Gamma_h)}$  (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

$$\|\mathbf{v}\|_{H_h^{-1}(\Gamma_h)} := \sup_{\mathbf{Y} \in \mathbb{Y}_h} \frac{\langle \mathbf{v}, \mathbf{Y} \rangle_{\Gamma_h}}{\|\mathbf{Y}\|_{H^1(\Gamma_h)}}, \quad (48)$$

which also satisfies  $\|\mathbf{v}\|_{H_h^{-1}(\Gamma_h)} \leq \|\mathbf{v}\|_{H^{-1}(\Gamma_h)}$  and  $\langle \mathbf{v}, \mathbf{Y} \rangle_{\Gamma_h} \leq \|\mathbf{v}\|_{H_h^{-1}(\Gamma_h)} \|\mathbf{Y}\|_{H^1(\Gamma_h)}$  (discrete Schwarz inequality). Then the discrete version of  $\|(q_1, q_s, \mu)\|_{\mathbb{T}_h^\diamond}^2$  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

$$\|\mu\|_{H_h^{1/2}(\Gamma_h)} := \frac{1}{2} \left( \|\mu\|_{H_{1,h}^{1/2}(\Gamma_h)} + \|\mu\|_{H_{s,h}^{1/2}(\Gamma_h)} \right). \quad (49)$$

and the discrete version of (33) is

$$\begin{aligned} \|(q_1, q_s, \mu)\|_{\mathbb{T}_h^\diamond}^2 &= \|\tilde{q}_1\|_{L^2(\Omega_{1,h})}^2 + \|\tilde{q}_s\|_{L^2(\Omega_{s,h})}^2 \\ &+ \|\mu - \hat{q}_1\|_{H_{1,h}^{1/2}(\Gamma_h)}^2 + \|\mu - \hat{q}_s\|_{H_{s,h}^{1/2}(\Gamma_h)}^2 + \widehat{\mathcal{S}}\|\mu \boldsymbol{\nu}_h\|_{H_h^{-1}(\Gamma_h)}^2. \end{aligned} \quad (50)$$

A discrete version of Proposition 2 also holds, i.e.  $\|(q_1, q_s, \mu)\|_{\mathbb{T}_h^\diamond} \approx \|(q_1, q_s, \mu)\|_{\mathbb{T}_h}$ .

The discrete version of the primal norm (32) is also slightly different. It requires a discrete version of the  $H^{-1/2}(\Gamma_h)$  norm to control the mean value of  $\mathbf{Y} \cdot \boldsymbol{\nu}_h$  for  $\mathbf{Y} \in \mathbb{Y}_h$ . For any  $\mathbf{Y} \cdot \boldsymbol{\nu}_h \in H^{-1/2}(\Gamma_h)$ , define

$$\|\mathbf{Y} \cdot \boldsymbol{\nu}_h\|_{H_h^{-1/2}(\Gamma_h)} := \sup_{\mu_h \in \mathbb{M}_h} \frac{\langle \mathbf{Y} \cdot \boldsymbol{\nu}_h, \mu_h \rangle_{\Gamma_h}}{\|\mu_h\|_{H_h^{1/2}(\Gamma_h)}}, \quad (51)$$

Clearly,  $\langle \mathbf{Y} \cdot \boldsymbol{\nu}_h, \mu_h \rangle_{\Gamma_h} \leq \|\mathbf{Y} \cdot \boldsymbol{\nu}_h\|_{H_h^{-1/2}(\Gamma_h)} \|\mu_h\|_{H_h^{1/2}(\Gamma_h)}$  (discrete Schwarz inequality). Then the discrete version of  $\|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}}^2$  is obtained by replacing  $\|\mathbf{Y} \cdot \boldsymbol{\nu}\|_{H^{-1/2}(\Gamma)}$  with  $\|\mathbf{Y} \cdot \boldsymbol{\nu}_h\|_{H_h^{-1/2}(\Gamma_h)}$ . A discrete version of Proposition 1 also holds.

## 5.2 Space Assumptions

To prove well-posedness, we must prove the discrete version of the conditions of Lemmas 1, 2, and 3. To facilitate this, we make the following general assumptions on the choice of finite dimensional subspaces (see Section 6 for the specific spaces used).

Let  $\mathring{\mathbb{V}}_{1,h} = \{\boldsymbol{\eta}_1 \in \mathbb{V}_{1,h} : \boldsymbol{\eta}_1 \cdot \boldsymbol{\nu}_h = 0 \text{ on } \partial\Omega_{1,h}\}$  and  $\hat{\mathbb{Q}}_{1,h} = \{q \in \mathbb{Q}_{1,h} : \int_{\Omega_{1,h}} q \, dx = 0\}$ , and assume that  $\nabla \cdot \mathbb{V}_{1,h} = \mathbb{Q}_{1,h}$ ,  $\nabla \cdot \mathring{\mathbb{V}}_{1,h} = \hat{\mathbb{Q}}_{1,h}$ , and  $\mathbb{V}_{1,h}$  contains continuous piecewise linear functions on  $\Gamma_h$ . Analogous definitions are made for  $\mathbb{V}_{s,h}$  and  $\mathbb{Q}_{s,h}$ . Moreover, assume  $(\mathbb{V}_{1,h}, \mathbb{Q}_{1,h})$  and  $(\mathbb{V}_{s,h}, \mathbb{Q}_{s,h})$  satisfy

$$\sup_{\boldsymbol{\eta}_1 \in \mathring{\mathbb{V}}_{1,h}} \frac{-(\nabla \cdot \boldsymbol{\eta}_1, q_1)_{\Omega_{1,h}}}{\|\boldsymbol{\eta}_1\|_{H(\text{div}, \Omega_{1,h})}} \geq c \|q_1\|_{L^2(\Omega_{1,h})}, \quad \sup_{\boldsymbol{\eta}_s \in \mathring{\mathbb{V}}_{s,h}} \frac{-(\nabla \cdot \boldsymbol{\eta}_s, q_s)_{\Omega_{s,h}}}{\|\boldsymbol{\eta}_s\|_{H(\text{div}, \Omega_{s,h})}} \geq c \|q_s\|_{L^2(\Omega_{s,h})}, \quad (52)$$

for all  $q_1 \in \mathbb{Q}_{1,h}$ ,  $q_s \in \mathbb{Q}_{s,h}$ , with  $c$  independent of  $h$  and that an analogous condition is satisfied for  $(\mathring{\mathbb{V}}_{1,h}, \hat{\mathbb{Q}}_{1,h})$  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.

## 5.3 Well-posedness

We follow a similar outline as Section 4.5.

### 5.3.1 Main Conditions

**Lemma 5** (Continuity of Forms).

$$\begin{aligned} |a_h((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_s, \mathbf{V}))| &\leq C_{a_h} \|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h} \|(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_s, \mathbf{V})\|_{\mathbb{Z}_h}, \quad \forall (\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_s, \mathbf{V}) \in \mathbb{Z}_h, \\ |b_h((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (q_1, q_s, \mu))| &\leq C_{b_h} \|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h} \|(q_1, q_s, \mu)\|_{\mathbb{T}_h}, \quad \forall (\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}) \in \mathbb{Z}_h, (q_1, q_s, \mu) \in \mathbb{T}_h, \\ |c_h((q_1, q_s, \mu), (u_1, u_s, \lambda))| &\leq \Delta t^{-1} (\|q_1\|_{L^2(\Omega_{1,h})} \|u_1\|_{L^2(\Omega_{1,h})} + \|q_s\|_{L^2(\Omega_{s,h})} \|u_s\|_{L^2(\Omega_{s,h})}), \\ &\quad \forall (q_1, q_s, \mu), (u_1, u_s, \lambda) \in \mathbb{T}_h, \\ |\chi_h(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})| &\leq C_{\chi_h} \|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h}, \quad \forall (\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}) \in \mathbb{Z}_h, \\ |\psi_h(q_1, q_s, \mu)| &\leq C_{\psi_h} \|(q_1, q_s, \mu)\|_{\mathbb{T}_h}, \quad \forall (q_1, q_s, \mu) \in \mathbb{T}_h, \end{aligned}$$

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,  $C_{\chi_h}$  depends on  $u_D$ ,  $\Delta t^{-1/2}$ , and  $C_{\psi_h}$  depends on  $\bar{f}_1, \bar{f}_s, \bar{u}_1, \bar{u}_s$  and  $\Delta t^{-1}$ .

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

**Lemma 6** (Coercivity). *Let  $(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}) \in \mathbb{Z}_h$  with  $b_h((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (q_1, q_s, \mu)) = 0$  for all  $(q_1, q_s, \mu) \in \mathbb{T}_h$ . Then,*

$$|a_h((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}))| \geq C \|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h}^2,$$

where  $C > 0$  is a constant that depends on  $\hat{S}$  and the domain. This is true even if  $\hat{\beta} \rightarrow \infty$ .

*Proof.* Follows the same argument as in Lemma 2, except the discrete  $H^{-1/2}$  norm is used.  $\square$

**Lemma 7** (Inf-Sup). *For all  $(q_1, q_s, \mu) \in \mathbb{T}_h$ , the following "inf-sup" condition holds*

$$\sup_{(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}) \in \mathbb{Z}_h} \frac{b_h((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (q_1, q_s, \mu))}{\|(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h^\diamond}} \geq C \|(q_1, q_s, \mu)\|_{\mathbb{T}_h},$$

where  $C > 0$  depends on the domain and  $\widehat{S}$ . If  $\|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h^s}$  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  $\widehat{K}_1, \widehat{K}_s, \widehat{C},$  and  $\widehat{\beta}_-$ . Furthermore,  $C$  does not depend on the time step  $\Delta t$ , as long as  $\Delta t \leq 1$ .

*Proof.* Starting as we did in the proof of Lemma 3, we have

$$b_h((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (q_l, q_s, \mu)) = -(\nabla \cdot \boldsymbol{\eta}_l, \tilde{q}_l)_{\Omega_{1,h}} - (\nabla \cdot \boldsymbol{\eta}_s, \tilde{q}_s)_{\Omega_{s,h}} - \langle \boldsymbol{\eta}_l \cdot \boldsymbol{\nu}_h, \mu - \hat{q}_l \rangle_{\Gamma_h} + \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}_h, \mu - \hat{q}_s \rangle_{\Gamma_h} + \widehat{S}(\mathbf{Y} \cdot \boldsymbol{\nu}_h, \mu)_{\Gamma_h}.$$

Next, let us focus on  $-(\nabla \cdot \boldsymbol{\eta}_s, \tilde{q}_s)_{\Omega_{s,h}} + \langle \boldsymbol{\eta}_s \cdot \boldsymbol{\nu}_h, \mu - \hat{q}_s \rangle_{\Gamma_h}$  only. By (52), there exists a unique  $(\mathbf{w}, \omega)$  in  $(\mathring{\mathbb{V}}_{s,h}, \hat{\mathbb{Q}}_{s,h})$  such that

$$\begin{aligned} (\mathbf{w}, \mathbf{v})_{\Omega_{s,h}} - (\omega, \nabla \cdot \mathbf{v})_{\Omega_{s,h}} &= 0, & \forall \mathbf{v} \in \mathring{\mathbb{V}}_{s,h}, \\ -(\nabla \cdot \mathbf{w}, r)_{\Omega_{s,h}} &= (\tilde{q}_s, r)_{\Omega_{s,h}}, & \forall r \in \hat{\mathbb{Q}}_{s,h}, \end{aligned} \quad (53)$$

and  $\|\mathbf{w}\|_{H(\text{div}, \Omega_{s,h})} \leq C_0 \|\tilde{q}_s\|_{L^2(\Omega_{s,h})}$ . By (47), there exists  $\boldsymbol{\xi} \in \mathbb{V}_{s,h}$  such that

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

Similar to (53), there exists a  $\mathbf{z}$  in  $\mathring{\mathbb{V}}_{s,h}$  such that

$$-\nabla \cdot \mathbf{z} = \nabla \cdot \boldsymbol{\xi} - \frac{1}{|\Omega_{s,h}|} \left( \int_{\Gamma_h} \boldsymbol{\xi} \cdot \boldsymbol{\nu}_h \right), \quad \text{on } \Omega_{s,h}, \quad \|\mathbf{z}\|_{H(\text{div}, \Omega_{s,h})} \leq C_1 \|\boldsymbol{\xi}\|_{H(\text{div}, \Omega_{s,h})}. \quad (54)$$

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

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

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

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

Thus, setting  $\boldsymbol{\eta}_s := \mathbf{y} / \|\mathbf{y}\|_{H(\text{div}, \Omega_{s,h})}$  gives

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

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

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

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

By the definition of the discrete  $H^{-1}(\Gamma_h)$  norm (48), there exists a  $\mathbf{Y}$  in  $\mathbb{Y}_h$  such that

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

Combining the above results gives the assertion.  $\square$

### 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  $\Delta t$  multiplying  $\|\nabla \cdot \boldsymbol{\eta}_l\|_{L^2(\Omega_{l,h})}^2$ ,  $\|\nabla \cdot \boldsymbol{\eta}_s\|_{L^2(\Omega_{s,h})}^2$ , and  $\|\mathbf{Y} \cdot \boldsymbol{\nu}_h\|_{H_h^{-1/2}(\Gamma_h)}^2$ .

## 5.4 Discrete Estimates

All the results in Section 4.6 follow through for the fully discrete scheme. But the update rules (34), (35) are affected by the finite element spaces used. So some additional assumptions are needed for the fully discrete scheme.

- The extension of  $\mathbf{V}$  to all of  $\Omega_h$  is obtained by solving a discrete Laplace equation using a finite element space  $\mathbb{L}_h$  on  $\Omega_h$  whose restriction to  $\Gamma_h$  contains  $\mathbb{Y}_h$ .
- Because of the update rules (21), (22), the shape of the tetrahedral elements  $T$  in  $\Omega_h$  must be representable by functions in  $\mathbb{L}_h$ , i.e. the parametrization of  $T$  must be expressed as a linear combination of basis functions in the local finite element space of  $\mathbb{Y}_h$ .
- The spaces  $\mathbb{Q}_{l,h}$ ,  $\mathbb{Q}_{s,h}$  should be discontinuous across elements to allow for the update rules to be computed locally.

The most straightforward implementation is to use affine tetrahedral elements. This implies that  $\mathbb{Y}_h$  and  $\mathbb{L}_h$  are continuous piecewise linear spaces over  $\Gamma_h$  and  $\Omega_h$  (see Section 6). In this case,  $\Phi_{i+1}$  is continuous piecewise linear, so the Jacobian is *constant* over each element. Thus, the update rules (34), (35) can be implemented element-by-element. In fact, one can simply compute the ratio of individual element volumes from  $\Omega^i$  to  $\Omega^{i+1}$  to determine  $\det([\nabla_{\mathbf{x}} \Phi_{i+1}(\mathbf{x})])^{-1}$  locally.

Unfortunately, if the mesh elements are not affine, then it is not completely obvious how to update  $u_l^{i+1}$ ,  $u_s^{i+1}$  to the new domain  $\Omega^{i+1}$  and still obtain the a priori bound (41), or the conservation law (43). An alternative ALE scheme may be necessary [26, 27].

## 6 Error Estimates

In this section, we estimate the error over one time step, assuming that the “true” domain  $\Omega = \Omega_h$  is a polyhedral domain and that the solution from the previous time step is exact:  $\overline{u_{l,h}} = u_l$ ,  $\overline{u_{s,h}} = u_s$ . So we do not account for any variational crime due to approximation of the domain, and we do not consider the accumulated error over all time steps.

**Remark 3.** *Accounting for the accumulated error over all time steps can be done. However, the main issue is the fact that the domain changes with time. An important issue to overcome is whether the interface velocity  $\mathbf{V}$  is regular enough to make sense of updating the domain. This is connected to the regularity of the interface  $\Gamma$ , which is crucial for understanding the well-posedness of the fully time-continuous problem. Many of the constants in some of the estimates depend on the geometry of  $\Gamma$ . Therefore, proving a priori bounds on the domain geometry would be very useful, but challenging [13]. Moreover, there is also the issue of topological changes, where long time existence of a solution is not possible for general interface evolutions. Therefore, a full time-dependent error analysis is not warranted until these other issues are addressed.*

*But we do feel that an analysis of the error over one time step, with reasonable regularity assumptions, is useful for showing how well the method works. Besides, a formal time-dependent error analysis is a fairly minor modification of what we present below.*

*As for the variational crime, it is standard now [9, 37]. So we give no details on that here.*

Let  $\mathcal{T}_h$  denote a quasi-uniform, shape regular triangulation of  $\Omega$  consisting of tetrahedra  $T$  of maximum size  $h \equiv h_T$  [9]. The error estimates derived here are for the following choices of finite element spaces. Let  $\mathbb{V}_{1,h} = \text{BDM}_1 \subset H(\text{div}, \Omega_{1,h})$ ,  $\mathbb{V}_{s,h} = \text{BDM}_1 \subset H(\text{div}, \Omega_{s,h})$ , i.e. the lowest order Brezzi-Douglas-Marini space of piecewise linear vector functions, and  $\mathbb{Q}_{1,h}, \mathbb{Q}_{s,h}$  be the set of piecewise constants. It is well-known that these spaces satisfy the hypothesis (52).

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

## 6.1 Preliminaries

### 6.1.1 Domain Regularity

The ‘‘smoothness’’ of  $\Gamma$  affects the error analysis because the normal vector  $\boldsymbol{\nu}$  appears in the weak formulation. We use the following definition in Theorem 3 and Lemmas 11 and 12.

**Definition 1** ( $\gamma$  regularity). *Let  $\Gamma \subset \mathbb{R}^3$  be a polyhedral manifold with oriented unit normal vector  $\boldsymbol{\nu}$ . We say  $\Gamma$  is  $\gamma$  regular if there exists a unit vector field  $\boldsymbol{\nu}_\gamma : \Gamma \rightarrow \mathbb{R}^3$ , and corresponding function  $\gamma : \Gamma \rightarrow [0, 2]$ , with the following properties.*

- $\boldsymbol{\nu} \cdot \boldsymbol{\nu}_\gamma = 1 - \gamma$  on  $\Gamma$ .
- $\|\boldsymbol{\nu}_\gamma\|_{W^{1,\infty}(\Gamma)} \leq C_\gamma < \infty$ , for some positive constant  $C_\gamma$  depending on  $\Gamma$  and  $\gamma$ .

Furthermore, let  $\gamma_0 := \sup_{\mathbf{x} \in \Gamma} \gamma$ . We call  $\gamma_0$  the regularity coefficient and  $C_\gamma$  the  $W^{1,\infty}(\Gamma)$  stability constant.

The smaller both  $\gamma_0$  and  $C_\gamma$  are, the more regular  $\Gamma$  is. One way to construct  $\boldsymbol{\nu}_\gamma$  is by defining it to be a continuous piecewise linear function over  $\Gamma$  (linear on each face). Then set the value at each node  $v$ , with vertex coordinates  $\mathbf{x}$ , to be

$$\boldsymbol{\nu}_\gamma(\mathbf{x}) := \sum_{F \in \text{Star}(\mathbf{x})} \frac{\boldsymbol{\nu}_F}{|F|}, \quad \text{where } \boldsymbol{\nu}_F \text{ is the unit normal on } F.$$

If each star of faces is sufficiently flat, then  $\gamma_0 \leq \frac{1}{2}$ . Another example is if  $\Gamma$  is the piecewise linear interpolant of a  $C^2$  manifold  $\tilde{\Gamma}$ . Then, assuming  $\Gamma$  has sufficiently small faces, one can map  $\boldsymbol{\nu}_{\tilde{\Gamma}}$  from  $\tilde{\Gamma}$  to  $\Gamma$  and set  $\boldsymbol{\nu}_\gamma := \boldsymbol{\nu}_{\tilde{\Gamma}}$  with  $\gamma_0 \leq \frac{1}{2}$ . In this case,  $C_\gamma$  depends only on the curvature (and measure) of  $\tilde{\Gamma}$ . Note that, for polyhedral surfaces, it is not possible to construct  $\boldsymbol{\nu}_\gamma$  such that  $\|\boldsymbol{\nu}_\gamma\|_{W^{1,\infty}(\Gamma)} < \infty$  and  $\gamma_0 = 0$ . The following result gives additional properties of  $\boldsymbol{\nu}_\gamma$ .

**Lemma 8.** *Let  $\boldsymbol{\nu}_\gamma$  be given by Definition 1. Then,*

$$|\boldsymbol{\nu} - \boldsymbol{\nu}_\gamma| = \sqrt{2\gamma}, \quad \text{almost everywhere on } \Gamma. \quad (55)$$

*If  $\Gamma$  is a polyhedral surface that interpolates a  $C^2$  surface  $\tilde{\Gamma}$ , and there exists a smooth bijective map  $\Phi : \Gamma \rightarrow \tilde{\Gamma}$ , then  $\boldsymbol{\nu}_\gamma := \tilde{\boldsymbol{\nu}} \circ \Phi$ , where  $\tilde{\boldsymbol{\nu}}$  is the unit normal of  $\tilde{\Gamma}$ . In this case, on each face  $F$  (triangle) of  $\Gamma$ , we have*

$$\gamma \leq C (\text{diam}(F)K_0)^2, \quad \text{everywhere on } \Gamma, \quad (56)$$

*where  $C > 0$  is an independent constant,  $K_0 = \max_{\mathbf{x} \in \Gamma} \tilde{\kappa} \circ \Phi(\mathbf{x})$ , and  $\tilde{\kappa}$  is the curvature of  $\tilde{\Gamma}$ .*

*Proof.* The first result follows easily by

$$|\boldsymbol{\nu} - \boldsymbol{\nu}_\gamma|^2 = \boldsymbol{\nu} \cdot \boldsymbol{\nu} - 2\boldsymbol{\nu} \cdot \boldsymbol{\nu}_\gamma + \boldsymbol{\nu}_\gamma \cdot \boldsymbol{\nu}_\gamma = 2(1 - \boldsymbol{\nu} \cdot \boldsymbol{\nu}_\gamma) = 2\gamma.$$

For the second result, we have  $\gamma = 1 - \boldsymbol{\nu} \cdot \boldsymbol{\nu}_\gamma = 1 - \cos \varphi \leq \frac{1}{2}\varphi^2$ , where  $\varphi$  is the angle between  $\boldsymbol{\nu}$  and  $\boldsymbol{\nu}_\gamma$ . Because each facet is a linear approximation of the smooth surface  $\tilde{\Gamma}$ , a Taylor expansion argument shows that  $\varphi \leq C_0 \text{diam}(F) \max_{\mathbf{x} \in F} \tilde{\kappa} \circ \Phi(\mathbf{x})$ ; see [62] and [21, Lemma 6.1] for an example of this.  $\square$

**Remark 4.** *By using Definition 1, we can avoid making too strong of an assumption on the polyhedral interface  $\Gamma$ . For instance, if  $\Gamma$  interpolates a piecewise smooth manifold with a finite number of corners and edges, then it is still possible to construct  $\boldsymbol{\nu}_\gamma$  with  $\gamma_0 \leq \frac{1}{2}$  as long as  $h$  is sufficiently small.*

### 6.1.2 Projection Operators

We introduce standard projection operators for the spaces  $\mathbb{V}_{1,h}$ ,  $\mathbb{V}_{s,h}$  and  $\mathbb{Q}_{1,h}$ ,  $\mathbb{Q}_{s,h}$  that are useful for the error analysis. Let  $\boldsymbol{\sigma}_{1,I}$  ( $\boldsymbol{\sigma}_{s,I}$ ) be the canonical projection of  $\boldsymbol{\sigma}_1$  ( $\boldsymbol{\sigma}_s$ ) into  $\text{BDM}_1$ ,  $u_{1,I}$  ( $u_{s,I}$ ) the  $L^2$  projection of  $u_1$  ( $u_s$ ) into  $\mathbb{Q}_{1,h}$  ( $\mathbb{Q}_{s,h}$ ),  $\lambda_I$  the  $L^2$  projection of  $\lambda$  into  $\mathbb{M}_h$ , and  $\mathbf{V}_I$  the  $L^2$  projection of  $\mathbf{V}$  into  $\mathbb{Y}_h$ . Note that  $\boldsymbol{\sigma}_{1,I}$ ,  $\boldsymbol{\sigma}_{s,I}$  and  $u_{1,I}$ ,  $u_{s,I}$  satisfy

$$\int_F [\boldsymbol{\sigma}_j - \boldsymbol{\sigma}_{j,I}] \cdot \boldsymbol{\nu} z dS = 0, \quad z \in \mathcal{P}_1(F), \quad \int_T [u_j - u_{j,I}] d\mathbf{x} = 0, \quad j = 1, s, \quad (57)$$

for each face  $F$  of  $\mathcal{F}_h$  and tetrahedron  $T$  of  $\mathcal{T}_h$ . For  $\boldsymbol{\sigma}_j$  in  $H^1(\Omega_j)$ , we have the usual estimate

$$\|\boldsymbol{\sigma}_j - \boldsymbol{\sigma}_{j,I}\|_{L^2(\Omega_j)} \leq Ch \|\boldsymbol{\sigma}_j\|_{H^1(\Omega_j)}, \quad j = 1, s. \quad (58)$$

The above projections and interpolants satisfy the following results.

**Proposition 3.** *For  $j = 1, s$ , we have that*

$$(q, \nabla \cdot (\boldsymbol{\sigma}_j - \boldsymbol{\sigma}_{j,I}))_{\Omega_j} = 0, \quad \forall q \in \mathbb{Q}_{j,h}, \quad (u_j - u_{j,I}, \nabla \cdot \boldsymbol{\eta}_h)_{\Omega_j} = 0, \quad \forall \boldsymbol{\eta}_h \in \mathbb{V}_{j,h}, \\ \langle (\boldsymbol{\sigma}_j - \boldsymbol{\sigma}_{j,I}) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma = 0, \quad \forall \mu \in \mathbb{M}_h.$$

**Proposition 4.** *Let  $(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_s, \mathbf{V})$  in  $\mathbb{V}_1(0) \times \mathbb{V}_s \times \mathbb{Y}$  and  $(u_1, u_s, \lambda)$  in  $\mathbb{Q}_1 \times \mathbb{Q}_s \times \mathbb{M}$  be the solution of (31), and  $(\boldsymbol{\sigma}_{1,h}, \boldsymbol{\sigma}_{s,h}, \mathbf{V}_h)$  in  $\mathbb{Z}_h$  and  $(u_{1,h}, u_{s,h}, \lambda_h)$  in  $\mathbb{T}_h$  be the solution of (46). Then, we have*

$$-\nabla \cdot (\boldsymbol{\sigma}_{j,h} - \boldsymbol{\sigma}_{j,I}) = \Delta t^{-1}(u_{j,h} - u_{j,I}), \quad \text{for } j = 1, s.$$

*Proof.* Note the projection properties (57). From (23), (44), and Proposition 3, one can show

$$(q, -\nabla \cdot (\boldsymbol{\sigma}_{j,h} - \boldsymbol{\sigma}_{j,I}))_{\Omega_j} = \Delta t^{-1}(q, u_{j,h} - u_{j,I})_{\Omega_j}, \quad \forall q \in \mathbb{Q}_{j,h}, \quad \text{for } j = 1, s.$$

Since  $-\nabla \cdot (\boldsymbol{\sigma}_{j,h} - \boldsymbol{\sigma}_{j,I})$  and  $u_{j,h} - u_{j,I}$  are in  $\mathbb{Q}_{j,h}$ , we get the assertion.  $\square$

### 6.1.3 Properties Of The Piola Transform

Each tetrahedron  $T$  in  $\Omega$  is obtained by applying a linear bijective map  $F_T : T^* \rightarrow T$  to the reference simplex  $T^*$ , i.e.  $T = F_T(T^*)$ . The Jacobian matrix of the transformation is denoted by  $\nabla F_T$ . Scalar valued functions are mapped between  $T^*$  and  $T$  by composition with  $F_T$ , i.e.  $q = q^* \circ F_T^{-1}$ , where  $q$  is defined on  $T$  and  $q^*$  is defined on  $T^*$ .

Vector valued functions are mapped via the Piola transformation:

$$\boldsymbol{\sigma} = \left( \frac{1}{\det(\nabla F_T)} [\nabla F_T] \boldsymbol{\sigma}^* \right) \circ F_T^{-1},$$

where  $\boldsymbol{\sigma}$  is defined on  $T$  and  $\boldsymbol{\sigma}^*$  is defined on  $T^*$ . In particular, the local BDM<sub>1</sub> basis functions on  $T$  are obtained from applying the Piola transformation to the BDM<sub>1</sub> basis functions on  $T^*$ . The Piola transform satisfies the following properties [10]:

$$\int_T q \nabla \cdot \boldsymbol{\sigma} \, d\mathbf{x} = \int_{T^*} q^* \nabla \cdot \boldsymbol{\sigma}^* \, d\mathbf{x}^*, \quad \int_F q \boldsymbol{\sigma} \cdot \boldsymbol{\nu} \, dS(\mathbf{x}) = \int_{F^*} q^* \boldsymbol{\sigma}^* \cdot \boldsymbol{\nu}^* \, dS(\mathbf{x}^*), \quad (59)$$

where  $F$  ( $F^*$ ) is a face of  $\partial T$  ( $\partial T^*$ ).

#### 6.1.4 Non-standard Estimate

To the best of our knowledge, regularity estimates are not available for the formulation (31). Thus, we make a reduced regularity assumption in the error analysis. The following results are useful in this regard.

**Proposition 5.** *For all sufficiently regular functions, and  $r \geq 0$ , we have*

$$|\boldsymbol{\sigma}^*|_{H^r(T^*)} \leq C h_T^{r-1+d/2} |\boldsymbol{\sigma}|_{H^r(T)}, \quad |q^*|_{H^r(F^*)} \leq C h_T^{r+1/2-d/2} |q|_{H^r(F)}, \quad (60)$$

where  $d$  is the dimension of  $T$  and  $h_T$  is the diameter of  $T$ .

*Proof.* Follows by standard scaling arguments [9, 10].  $\square$

**Lemma 9.** *Fix  $r$  such that  $0 < r \leq \frac{1}{2}$ . Suppose  $\boldsymbol{\sigma}_j \in H^{r+1/2}(\Omega_j)$  and  $\boldsymbol{\sigma}_{j,I}$  is the BDM<sub>1</sub> interpolant of  $\boldsymbol{\sigma}_j$  for  $j = 1, s$ . Then,*

$$\|\boldsymbol{\sigma}_{j,I}\|_{L^2(\Omega_j)} \leq C \left( \|\boldsymbol{\sigma}_j\|_{L^2(\Omega_j)} + h^{r+1/2} |\boldsymbol{\sigma}_j|_{H^{r+1/2}(\Omega_j)} \right), \quad j = 1, s. \quad (61)$$

*Proof.* We show this for  $\boldsymbol{\sigma}_1$  only. Given any tetrahedron  $T$  in  $\Omega_1$ , we can write  $\boldsymbol{\sigma}_{1,I}$  in terms of a local basis  $\{\mathbf{v}_i\}_{i=1}^{12}$  on  $T$  such that  $\boldsymbol{\sigma}_{1,I}(\mathbf{x}) = \sum_{i=1}^{12} \alpha_i \mathbf{v}_i(\mathbf{x})$ . By the definition of the BDM<sub>1</sub> interpolant, the basis can be chosen such that

$$\alpha_i = \frac{1}{|F_i|} \int_{F_i} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\nu}) \phi_i,$$

where  $F_i$  is one of the (four) faces of  $T$  and  $\phi_i$  is one of the (three) standard ‘‘hat’’ basis functions on the face  $F_i$ .

Next, note the following standard trace inequality [1, 56]:

$$\|\boldsymbol{\sigma}_1^* \cdot \boldsymbol{\nu}^*\|_{H^r(F_i^*)} = \|\boldsymbol{\sigma}_1^*\|_{H^r(F_i^*)} \leq \|\boldsymbol{\sigma}_1^*\|_{H^r(\partial T^*)} \leq C \|\boldsymbol{\sigma}_1^*\|_{H^{r+1/2}(T^*)}.$$

Thus, by (59) and (60), we have

$$\begin{aligned} \int_{F_i} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\nu}) \phi_i &= \int_{F_i^*} (\boldsymbol{\sigma}_1^* \cdot \boldsymbol{\nu}^*) \phi_i^* \leq \|\boldsymbol{\sigma}_1^* \cdot \boldsymbol{\nu}^*\|_{H^r(F_i^*)} \|\phi_i^*\|_{(H^r(F_i^*))^*} \\ &\leq C_0 \left( \|\boldsymbol{\sigma}_1^*\|_{L^2(T^*)} + |\boldsymbol{\sigma}_1^*|_{H^{r+1/2}(T^*)} \right) \\ &\leq C_1 h_T^{1/2} \left( \|\boldsymbol{\sigma}_1\|_{L^2(T)} + h_T^{r+1/2} |\boldsymbol{\sigma}_1|_{H^{r+1/2}(T)} \right), \end{aligned}$$



where  $\|\phi_i^*\|_{(H^r(F_i^*))^*}$  is bounded by an independent constant because  $\phi_i^*$  is a fixed polynomial on  $F_i^*$ .

Next, for any  $T \subset \Omega_1$  we have  $\|\sigma_{1,I}\|_{L^2(T)}^2 \leq C_2|T|\sum_j \alpha_j^2$ . So, by shape regularity of the triangulation and the above results, we get

$$\begin{aligned} \|\sigma_{1,I}\|_{L^2(\Omega_1)}^2 &\leq C_2 \sum_{T \subset \Omega_1} |T| \sum_i \left( |F_i|^{-1} \int_{F_i} (\sigma_1 \cdot \nu) \phi_i \right)^2 \leq C_3 \sum_{T \subset \Omega_1} h_T^3 (h_T^2)^{-2} \sum_i \left( \int_{F_i} (\sigma_1 \cdot \nu) \phi_i \right)^2 \\ &\leq C_4 \sum_{T \subset \Omega_1} h_T^{-1} \left( C_1 h_T^{1/2} \left( \|\sigma_1\|_{L^2(T)} + h_T^{r+1/2} |\sigma_1|_{H^{r+1/2}(T)} \right) \right)^2 \\ &\leq C_5 \sum_{T \subset \Omega_1} \left( \|\sigma_1\|_{L^2(T)}^2 + h_T^{2r+1} |\sigma_1|_{H^{r+1/2}(T)}^2 \right) = C_5 \left( \|\sigma_1\|_{L^2(\Omega_1)}^2 + h^{2r+1} |\sigma_1|_{H^{r+1/2}(\Omega_1)}^2 \right), \end{aligned}$$

which is the assertion.  $\square$

The following lemma is analogous to a result in [21, Lemma 6.3]. However, the result in [21] only holds for two dimensional domains, where as Lemma 10 is true for three dimensional domains.

**Lemma 10.** *Assume the hypothesis of Lemma 9 and let  $s$  satisfy  $r + \frac{1}{2} \leq s \leq 1$ . Then,*

$$\|\sigma_j - \sigma_{j,I}\|_{L^2(\Omega_j)} \leq Ch^\theta \|\sigma_j\|_{H^s(\Omega_j)}, \quad \theta = \frac{s - (r + 1/2)}{1 - (r + 1/2)}, \quad \text{for } j = 1, s. \quad (62)$$

*Proof.* From (61), note that

$$\|\sigma_j - \sigma_{j,I}\|_{L^2(\Omega_j)} \leq C \|\sigma_j\|_{H^{r+1/2}(\Omega_j)}.$$

Next, we interpolate between  $H^{r+1/2}$  and  $H^1$  so that we can ‘‘tune’’ our regularity assumption on  $\sigma_j$ . From [56, Ch. 34], we have

$$W^{s,p}(\Omega_j) = (W^{m_1,p}(\Omega_j), W^{m_2,p}(\Omega_j))_{\theta,p}, \quad s = (1 - \theta)m_1 + \theta m_2,$$

In our case,  $p = 2$ ,  $m_1 = r + 1/2$ ,  $m_2 = 1$ , which implies  $H^s(\Omega_j) = (H^{r+1/2}(\Omega_j), H^1(\Omega_j))_{\theta,2}$ , with  $\theta = \frac{s - (r+1/2)}{1 - (r+1/2)}$ . Then, we can combine (61) and (58) to get the error estimate (62) (see [56, Lemma 22.3]). Note: if  $s = 1$ , then  $\theta = 1$ , and if  $s = r + 1/2$ , then  $\theta = 0$ .  $\square$

## 6.2 Primal Error Estimate

### 6.2.1 Main Estimate

We start with an initial estimate.

**Theorem 3.** *Assume  $\Gamma$  is  $\gamma$  regular with  $\gamma_0 \leq \frac{1}{2\sqrt{6}}$ . Let  $(\sigma_1, \sigma_s, \mathbf{V})$  in  $\mathbb{V}_1(0) \times \mathbb{V}_s \times \mathbb{Y}$  and  $(u_1, u_s, \lambda)$  in  $\mathbb{Q}_1 \times \mathbb{Q}_s \times \mathbb{M}$  be the solution of (31), and  $(\sigma_{1,h}, \sigma_{s,h}, \mathbf{V}_h)$  in  $\mathbb{Z}_h$  and  $(u_{1,h}, u_{s,h}, \lambda_h)$  in  $\mathbb{T}_h$  be the solution of (46). Then,*

$$\begin{aligned} &\|\sigma_{1,h} - \sigma_{1,I}\|_{H(\text{div}, \Omega_1)}^2 + \|\sigma_{s,h} - \sigma_{s,I}\|_{H(\text{div}, \Omega_s)}^2 + \|\widehat{\beta}^{-1/2}(\nu)(\mathbf{V}_h - \mathbf{V}_I) \cdot \nu\|_{L^2(\Gamma)}^2 \\ &+ \Delta t \|\nabla_\Gamma(\mathbf{V}_h - \mathbf{V}_I)\|_{L^2(\Gamma)}^2 + \Delta t^{-2} \|u_h - u_I\|_{L^2(\Omega)}^2 \\ &\leq C \left\{ \|\sigma_1 - \sigma_{1,I}\|_{L^2(\Omega_1)}^2 + \|\sigma_s - \sigma_{s,I}\|_{L^2(\Omega_s)}^2 + \|\widehat{\beta}^{-1/2}(\nu)(\mathbf{V} - \mathbf{V}_I) \cdot \nu\|_{L^2(\Gamma)}^2 \right. \\ &\quad + \Delta t \|\nabla_\Gamma(\mathbf{V} - \mathbf{V}_I)\|_{L^2(\Gamma)}^2 + \left( 1 + \frac{\Delta t}{h^2} \right) \|(\mathbf{V} - \mathbf{V}_I) \cdot \nu\|_{L^2(\Gamma)}^2 \\ &\quad \left. + \left( 1 + \varpi \frac{\gamma_0}{\Delta t} \right) \|\lambda - \lambda_I\|_{L^2(\Gamma)}^2 + \|\lambda - \lambda_I\|_{H^{1/2}(\Gamma)}^2 \right\}, \end{aligned} \quad (63)$$

where the constant  $C > 0$  only depends on the physical constants and the domain geometry. If  $\widehat{\beta}$  is unbounded, then  $\varpi = 1$  and  $C$  is independent of  $\widehat{\beta}$ ; otherwise,  $\varpi = 0$ .

*Proof.* For simplicity, we write  $c((q_1, q_s, \mu), (u_1, u_s, \lambda)) = \Delta t^{-1}(q, u)_\Omega$ , where  $u|_{\Omega_j} = u_j$  and  $q|_{\Omega_j} = q_j$  for  $j = 1, s$ . Then, by combining the continuous and discrete equations, we obtain the error equations

$$\begin{aligned} & a((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}, \boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}, \mathbf{V}_h - \mathbf{V}_I)) + b((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (u_{1,h} - u_{1,I}, u_{s,h} - u_{s,I}, \lambda_h - \lambda_I)) = \\ & a((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_{1,I}, \boldsymbol{\sigma}_s - \boldsymbol{\sigma}_{s,I}, \mathbf{V} - \mathbf{V}_I)) + b((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (u_1 - u_{1,I}, u_s - u_{s,I}, \lambda - \lambda_I)), \\ & b((\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}, \boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}, \mathbf{V}_h - \mathbf{V}_I), (q_1, q_s, \mu)) - \Delta t^{-1}(q, u_h - u_I)_\Omega = \\ & b((\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_{1,I}, \boldsymbol{\sigma}_s - \boldsymbol{\sigma}_{s,I}, \mathbf{V} - \mathbf{V}_I), (q_1, q_s, \mu)) - \Delta t^{-1}(q, u - u_I)_\Omega, \end{aligned}$$

for all  $(\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y})$  in  $\mathbb{Z}_h$  and all  $(q_1, q_s, \mu)$  in  $\mathbb{T}_h$ . Next, set the test functions:  $\boldsymbol{\eta}_1 = \boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}$ ,  $\boldsymbol{\eta}_s = \boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}$ ,  $\mathbf{Y} = \mathbf{V}_h - \mathbf{V}_I$ ,  $q_1 = \Delta t^{-1}(u_{1,h} - u_{1,I})$ ,  $q_s = \Delta t^{-1}(u_{s,h} - u_{s,I})$ , and  $\mu = \lambda_h - \lambda_I$ . Combining the error equations then yields

$$\begin{aligned} & a((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}, \boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}, \mathbf{V}_h - \mathbf{V}_I)) + \Delta t^{-1}(q, u_h - u_I)_\Omega = \Delta t^{-1}(q, u - u_I)_\Omega \\ & + a((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_{1,I}, \boldsymbol{\sigma}_s - \boldsymbol{\sigma}_{s,I}, \mathbf{V} - \mathbf{V}_I)) + b((\boldsymbol{\eta}_1, \boldsymbol{\eta}_s, \mathbf{Y}), (u_1 - u_{1,I}, u_s - u_{s,I}, \lambda - \lambda_I)) \\ & - b((\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_{1,I}, \boldsymbol{\sigma}_s - \boldsymbol{\sigma}_{s,I}, \mathbf{V} - \mathbf{V}_I), (q_1, q_s, \mu)), \end{aligned}$$

which, after using Young's inequality and moving terms to the left-hand-side, becomes

$$\begin{aligned} & \frac{1}{2} \left[ \widehat{K}_1^{-1} \|\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}\|_{L^2(\Omega_1)}^2 + \widehat{K}_s^{-1} \|\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}\|_{L^2(\Omega_s)}^2 + \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu})(\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)}^2 \right. \\ & \left. + \Delta t \widehat{\mathcal{C}} \|\nabla_\Gamma(\mathbf{V}_h - \mathbf{V}_I)\|_{L^2(\Gamma)}^2 \right] + \Delta t^{-2} \|u_h - u_I\|_{L^2(\Omega)}^2 \leq \\ & \frac{1}{2} \left[ \widehat{K}_1^{-1} \|\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_{1,I}\|_{L^2(\Omega_1)}^2 + \widehat{K}_s^{-1} \|\boldsymbol{\sigma}_s - \boldsymbol{\sigma}_{s,I}\|_{L^2(\Omega_s)}^2 + \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu})(\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)}^2 \right. \\ & \left. + \Delta t \widehat{\mathcal{C}} \|\nabla_\Gamma(\mathbf{V} - \mathbf{V}_I)\|_{L^2(\Gamma)}^2 \right] + \Delta t^{-1}(q, u - u_I)_\Omega \\ & - (\nabla \cdot (\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}), u_1 - u_{1,I})_{\Omega_1} - (\nabla \cdot (\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}), u_s - u_{s,I})_{\Omega_s} \\ & - \langle (\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}) \cdot \boldsymbol{\nu}, \lambda - \lambda_I \rangle_\Gamma + \langle (\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}) \cdot \boldsymbol{\nu}, \lambda - \lambda_I \rangle_\Gamma + \widehat{S}((\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \lambda - \lambda_I)_\Gamma \\ & + \Delta t^{-1}(\nabla \cdot (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_{1,I}), u_{1,h} - u_{1,I})_{\Omega_1} + \Delta t^{-1}(\nabla \cdot (\boldsymbol{\sigma}_s - \boldsymbol{\sigma}_{s,I}), u_{s,h} - u_{s,I})_{\Omega_s} \\ & + \langle (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_{1,I}) \cdot \boldsymbol{\nu}, \lambda_h - \lambda_I \rangle_\Gamma - \langle (\boldsymbol{\sigma}_s - \boldsymbol{\sigma}_{s,I}) \cdot \boldsymbol{\nu}, \lambda_h - \lambda_I \rangle_\Gamma - \widehat{S}((\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \lambda_h - \lambda_I)_\Gamma. \end{aligned}$$

Using (57) and Proposition 3, we can eliminate several terms to get

$$\begin{aligned} & \frac{1}{2} \left[ \widehat{K}_1^{-1} \|\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}\|_{L^2(\Omega_1)}^2 + \widehat{K}_s^{-1} \|\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}\|_{L^2(\Omega_s)}^2 + \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu})(\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)}^2 \right. \\ & \left. + \Delta t \widehat{\mathcal{C}} \|\nabla_\Gamma(\mathbf{V}_h - \mathbf{V}_I)\|_{L^2(\Gamma)}^2 \right] + \Delta t^{-2} \|u_h - u_I\|_{L^2(\Omega)}^2 \leq \\ & \frac{1}{2} \left[ \widehat{K}_1^{-1} \|\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_{1,I}\|_{L^2(\Omega_1)}^2 + \widehat{K}_s^{-1} \|\boldsymbol{\sigma}_s - \boldsymbol{\sigma}_{s,I}\|_{L^2(\Omega_s)}^2 + \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu})(\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)}^2 \right. \\ & \left. + \Delta t \widehat{\mathcal{C}} \|\nabla_\Gamma(\mathbf{V} - \mathbf{V}_I)\|_{L^2(\Gamma)}^2 \right] - \underbrace{\langle (\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}) \cdot \boldsymbol{\nu}, \lambda - \lambda_I \rangle_\Gamma}_{=:T_1} + \underbrace{\langle (\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}) \cdot \boldsymbol{\nu}, \lambda - \lambda_I \rangle_\Gamma}_{=:T_2} \\ & + \underbrace{\widehat{S}((\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \lambda - \lambda_I)_\Gamma}_{=:T_1} - \underbrace{\widehat{S}((\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \lambda_h - \lambda_I)_\Gamma}_{=:T_2}. \end{aligned} \tag{64}$$

Next, by a standard trace estimate and Proposition 4, we have

$$\begin{aligned} & -\langle (\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}) \cdot \boldsymbol{\nu}, \lambda - \lambda_I \rangle_\Gamma + \langle (\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}) \cdot \boldsymbol{\nu}, \lambda - \lambda_I \rangle_\Gamma \\ & \leq \sqrt{2} \left( \|\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}\|_{H^{-1/2}(\Gamma)}^2 + \|\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}\|_{H^{-1/2}(\Gamma)}^2 \right)^{1/2} \|\lambda - \lambda_I\|_{H^{1/2}(\Gamma)} \\ & \leq C \left( \|\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}\|_{L^2(\Omega_1)} + \|\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}\|_{L^2(\Omega_s)} + \Delta t^{-1} \|u_h - u_I\|_{L^2(\Omega)} \right) \|\lambda - \lambda_I\|_{H^{1/2}(\Gamma)}, \end{aligned}$$

which is then further bounded by weighted Young's inequalities and moving terms to the left-hand-side of (64). For  $T_1$ , if  $\widehat{\beta}$  is uniformly bounded with  $\widehat{\beta}_+ := \max_{\nu} \widehat{\beta}(\nu)$ , we can use the simple estimate

$$\widehat{S}((\mathbf{V}_h - \mathbf{V}_I) \cdot \nu, \lambda - \lambda_I)_\Gamma \leq \frac{1}{4} \|\widehat{\beta}^{-1/2}(\nu)(\mathbf{V}_h - \mathbf{V}_I) \cdot \nu\|_{L^2(\Gamma)}^2 + \widehat{\beta}_+ \widehat{S}^2 \|\lambda - \lambda_I\|_{L^2(\Gamma)}^2,$$

because the first term on the right can be absorbed into the left-hand-side of (64). If  $\widehat{\beta}_+ = \infty$ , then we must use Lemma 11. In this case, we get

$$\widehat{S}((\mathbf{V}_h - \mathbf{V}_I) \cdot \nu, \lambda - \lambda_I)_\Gamma \leq \frac{1}{8} \Delta t \widehat{C} \|\nabla_\Gamma(\mathbf{V}_h - \mathbf{V}_I)\|_{L^2(\Gamma)}^2 + C \frac{\gamma_0}{\Delta t} \|\lambda - \lambda_I\|_{L^2(\Gamma)}^2 + \dots,$$

where again the first term can be absorbed into the left-hand-side of (64), but the second term has the constant  $\frac{\gamma_0}{\Delta t}$ ; the remaining terms can be dealt with similarly by weighted Young's inequalities.

To bound  $T_2$ , we use Lemma 12 and more weighted Young's inequalities to obtain

$$\begin{aligned} \widehat{S}((\mathbf{V} - \mathbf{V}_I) \cdot \nu, \lambda_h - \lambda_I)_\Gamma &\leq C \left( \frac{\Delta t}{h^2} \|(\mathbf{V} - \mathbf{V}_I) \cdot \nu\|_{L^2(\Gamma)}^2 + \Delta t \|\nabla_\Gamma(\mathbf{V}_I - \mathbf{V})\|_{L^2(\Gamma)}^2 \right) \\ &\quad + \frac{1}{8} \Delta t \widehat{C} \|\nabla_\Gamma(\mathbf{V}_h - \mathbf{V}_I)\|_{L^2(\Gamma)}^2 + \dots \end{aligned}$$

The rest then follows by moving terms to the left-hand-side. Note: by Proposition 4, we can replace  $\|\sigma_{j,h} - \sigma_{j,I}\|_{L^2(\Omega_j)}$  on the left-hand-side of (64) by the full  $H(\text{div}, \Omega_j)$  norm.  $\square$

**Corollary 1.** *Assume the hypothesis of Theorem 3. Fix  $r$  such that  $0 < r \leq \frac{1}{2}$ , and assume  $\sigma_1 \in H^s(\Omega_1)$ ,  $\sigma_s \in H^s(\Omega_s)$  for some  $r + \frac{1}{2} \leq s \leq 1$  and define  $\theta = \frac{s - (r + 1/2)}{1 - (r + 1/2)}$ . Moreover, assume  $\mathbf{V} \in H^{1+\theta}(\Gamma)$  and  $u_1 \in H^\theta(\Omega_1)$ ,  $u_s \in H^\theta(\Omega_s)$ , and  $\lambda \in H^{1/2+\theta}(\Gamma)$ . Then,*

$$\begin{aligned} \|\sigma_1 - \sigma_{1,h}\|_{L^2(\Omega_1)} + \|\sigma_s - \sigma_{s,h}\|_{L^2(\Omega_s)} + \|\widehat{\beta}^{-1/2}(\nu)(\mathbf{V} - \mathbf{V}_h) \cdot \nu\|_{L^2(\Gamma)} \\ + \Delta t^{1/2} \|\nabla_\Gamma(\mathbf{V} - \mathbf{V}_h)\|_{L^2(\Gamma)} \leq Ch^\theta \left\{ \|\sigma_1\|_{H^s(\Omega_1)} + \|\sigma_s\|_{H^s(\Omega_s)} + \left[ h + \Delta t^{1/2} \right] \|\mathbf{V}\|_{H^{1+\theta}(\Gamma)} \right. \\ \left. + \left[ 1 + \varpi \left( \gamma_0 \frac{h}{\Delta t} \right)^{1/2} \right] \|\lambda\|_{H^{1/2+\theta}(\Gamma)} \right\}, \end{aligned} \quad (65)$$

where the constant  $C > 0$  only depends on the physical constants and the domain geometry. If  $\widehat{\beta}$  is unbounded (i.e.  $\widehat{\beta}_-^{-1/2} = 0$ ), then  $\varpi = 1$  and  $C$  is independent of  $\widehat{\beta}$ ; otherwise,  $\varpi = 0$ .

*Proof.* Use Proposition 4, Lemma 10, the triangle inequality, and standard interpolation estimates [9].  $\square$

**Corollary 2.** *Assume the hypothesis of Corollary 1. Then,*

$$\|u - u_h\|_{L^2(\Omega)} \leq Ch^\theta \|u\|_{H^\theta(\Omega)} + \Delta t \cdot (\text{right-hand-side of (65)}), \quad (66)$$

where the constant  $C > 0$  only depends on the physical constants and the domain geometry. If  $\widehat{\beta}$  is unbounded (i.e.  $\widehat{\beta}_-^{-1/2} = 0$ ), then  $\varpi = 1$  and  $C$  is independent of  $\widehat{\beta}$ ; otherwise,  $\varpi = 0$ .

*Proof.* Similar as before, except most terms on the left-hand-side of (63) are dropped.  $\square$

**Remark 5.** *The above error estimates suggest that the method converges (for a single time step), without requiring the true interface to be smooth, i.e. the true interface may contain corners or edges (see also Remark 4). This is important if we include anisotropic surface tension.*

*If  $\hat{\beta}$  is unbounded, then there is a restriction on the time step (for accuracy purposes only) that appears in (65):  $\Delta t \geq \gamma_0 h$ . By (56), if  $\Gamma$  interpolates a smooth surface  $\tilde{\Gamma}$ , then  $\Delta t \geq Ch^3$ , where  $C$  is proportional to the maximum curvature of  $\tilde{\Gamma}$ ; a rather mild restriction. If  $\hat{\beta}$  is uniformly bounded, then there is no time step restriction.*

## 6.2.2 Supporting Estimates

**Lemma 11.** *Assume the hypothesis of Theorem 3. Then,*

$$\begin{aligned} ((\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \lambda - \lambda_I)_\Gamma &\leq C\sqrt{\gamma_0} \|\lambda - \lambda_I\|_{L^2(\Gamma)} \left[ \|\nabla_\Gamma(\mathbf{V}_h - \mathbf{V}_I)\|_{L^2(\Gamma)} + \|(\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)} \right. \\ &\quad \left. + \|\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}\|_{L^2(\Omega_1)} + \|\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}\|_{L^2(\Omega_s)} + \Delta t^{-1} \|u_h - u_I\|_{L^2(\Omega)} \right]. \end{aligned}$$

*Proof.* Using the  $L^2$  projection property of  $\lambda_I$ , we have

$$((\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \lambda - \lambda_I)_\Gamma = ((\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu} - \mu, \lambda - \lambda_I)_\Gamma \leq \|\lambda - \lambda_I\|_{L^2(\Gamma)} \|(\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu} - \mu\|_{L^2(\Gamma)},$$

for all  $\mu \in \mathbb{M}_h$ . Next, choose

$$\mu(\mathbf{x}) := \sum_i (\mathbf{V}_h - \mathbf{V}_I)(\mathbf{x}_i) \cdot \boldsymbol{\nu}_\gamma(\mathbf{x}_i) \phi_i(\mathbf{x}),$$

where  $\boldsymbol{\nu}_\gamma$  is taken from Definition 1,  $\{\mathbf{x}_i\}$  are the vertices of  $\Gamma$ , and  $\{\phi_i\}$  are the piecewise linear basis functions of  $\mathbb{M}_h$ . Hence, on a particular face  $F$  of  $\Gamma$ , we have by (55)

$$(\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu} - \mu = \sum_{i=1}^3 (\boldsymbol{\nu}|_F - \boldsymbol{\nu}_\gamma(\mathbf{x}_i)) \cdot (\mathbf{V}_h - \mathbf{V}_I)(\mathbf{x}_i) \phi_i \leq \sqrt{2\gamma_0} \sum_{i=1}^3 |\mathbf{V}_h - \mathbf{V}_I|(\mathbf{x}_i) \phi_i,$$

which implies that  $\|(\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu} - \mu\|_{L^2(\Gamma)} \leq C_0 \sqrt{\gamma_0} \|\mathbf{V}_h - \mathbf{V}_I\|_{L^2(\Gamma)}$ .

Next, we bound  $\|\mathbf{V}_h - \mathbf{V}_I\|_{L^2(\Gamma)}$  by something more convenient because a similar term does not appear on the left-hand-side of (63) when  $\hat{\beta} \rightarrow \infty$ . By the discrete version of Proposition 1,

$$\|\mathbf{V}_h - \mathbf{V}_I\|_{L^2(\Gamma)}^2 \leq C_1 \left( \|\nabla_\Gamma(\mathbf{V}_h - \mathbf{V}_I)\|_{L^2(\Gamma)}^2 + \|(\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{H_h^{-1/2}(\Gamma)}^2 \right),$$

so we must bound  $|\langle (\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma|$ . Taking the difference of (24) and (45) gives for all  $\mu \in \mathbb{M}_h$

$$\begin{aligned} \widehat{S} \langle (\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma &= \widehat{S} \langle (\mathbf{V}_h - \mathbf{V}) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma + \widehat{S} \langle (\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma \\ &= \langle (\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_1) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma - \langle (\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_s) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma + \widehat{S} \langle (\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma \\ &= \langle (\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma - \langle (\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma + \widehat{S} \langle (\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma, \end{aligned}$$

where we used (57). Focusing on  $\langle (\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma$  and using discrete Schwarz yields

$$\begin{aligned} \langle (\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma &\leq \|(\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I})\|_{H(\text{div}, \Omega_s)} \|\mu\|_{H_{s,h}^{1/2}(\Gamma)} \\ &\leq (\|\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}\|_{L^2(\Omega_s)} + \Delta t^{-1} \|u_{s,h} - u_{s,I}\|_{L^2(\Omega_s)}) \|\mu\|_{H_{s,h}^{1/2}(\Gamma)}, \end{aligned}$$

where we used Proposition 4. A similar result holds for  $\langle (\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma$ .

For  $\langle (\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma$ , we need to use the fact that  $\|\mu\|_{L^2(\Gamma)} \leq C_2 \|\mu\|_{H_h^{1/2}(\Gamma)}$  for a constant  $C_2 > 0$  independent of  $h$ . This follows by [25, 40], where they show the existence of stable liftings of the normal trace for discrete  $H(\text{div})$  spaces such as Raviart-Thomas and Brezzi-Douglas-Marini; proofs are given in two dimensions, but the results also hold in three dimensions. So, combining this with (47) and (49) gives the bound. Therefore,

$$\langle (\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \mu \rangle_\Gamma \leq \|(\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)} \|\mu\|_{L^2(\Gamma)} \leq C_2 \|(\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)} \|\mu\|_{H_h^{1/2}(\Gamma)}, \quad \forall \mu \in \mathbb{M}_h.$$

Bringing everything together, we have

$$\begin{aligned} \|(\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{H_h^{-1/2}(\Gamma)} &= \sup_{\mu_h \in \mathbb{M}_h} \frac{\langle (\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \mu_h \rangle_{\Gamma_h}}{\|\mu_h\|_{H_h^{1/2}(\Gamma_h)}} \\ &\leq C_3 \left( \|\boldsymbol{\sigma}_{1,h} - \boldsymbol{\sigma}_{1,I}\|_{L^2(\Omega_1)}^2 + \|\boldsymbol{\sigma}_{s,h} - \boldsymbol{\sigma}_{s,I}\|_{L^2(\Omega_s)}^2 \right. \\ &\quad \left. + \Delta t^{-2} \|u_h - u_I\|_{L^2(\Omega)}^2 + \|(\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)}^2 \right)^{1/2}, \end{aligned}$$

which eventually gives the assertion.  $\square$

**Lemma 12.** *Assume the hypothesis of Theorem 3. Then,*

$$\begin{aligned} &\widehat{S}(\langle (\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \lambda_h - \lambda_I \rangle_\Gamma) \\ &\leq C \|(\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)} \left[ \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu})(\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)} + \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu})(\mathbf{V}_I - \mathbf{V}) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)} \right. \\ &\quad \left. + \Delta t \widehat{\mathcal{C}} h^{-1} \{ \|\nabla_\Gamma(\mathbf{V}_h - \mathbf{V}_I)\|_{L^2(\Gamma)} + \|\nabla_\Gamma(\mathbf{V}_I - \mathbf{V})\|_{L^2(\Gamma)} \} + \widehat{S} \|\lambda_I - \lambda\|_{L^2(\Gamma)} \right]. \end{aligned}$$

*Proof.* We start with  $\langle (\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \lambda_h - \lambda_I \rangle_\Gamma \leq \|(\mathbf{V} - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)} \|\lambda_h - \lambda_I\|_{L^2(\Gamma)}$ , and seek a bound for  $\|\lambda_h - \lambda_I\|_{L^2(\Gamma)}$ . From the error equations, we get

$$\begin{aligned} &(\widehat{\beta}^{-1}(\boldsymbol{\nu})(\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}, \mathbf{Y} \cdot \boldsymbol{\nu})_\Gamma + \Delta t \widehat{\mathcal{C}} (\nabla_\Gamma(\mathbf{V}_h - \mathbf{V}_I), \nabla_\Gamma \mathbf{Y})_\Gamma \\ &+ (\widehat{\beta}^{-1}(\boldsymbol{\nu})(\mathbf{V}_I - \mathbf{V}) \cdot \boldsymbol{\nu}, \mathbf{Y} \cdot \boldsymbol{\nu})_\Gamma + \Delta t \widehat{\mathcal{C}} (\nabla_\Gamma(\mathbf{V}_I - \mathbf{V}), \nabla_\Gamma \mathbf{Y})_\Gamma \\ &+ \widehat{S}(\mathbf{Y} \cdot \boldsymbol{\nu}, \lambda_I - \lambda)_\Gamma = \widehat{S}(\mathbf{Y} \cdot \boldsymbol{\nu}, \lambda_I - \lambda_h)_\Gamma, \quad \text{for all } \mathbf{Y} \in \mathbb{Y}_h. \end{aligned} \tag{67}$$

Next, set  $\mu_h := \lambda_I - \lambda_h$  and use  $\boldsymbol{\nu}_\gamma$  from Definition 1 to choose  $\mathbf{Y}$ :

$$\mathbf{Y}(\mathbf{x}) := \sum_i \mu_h(\mathbf{x}_i) \boldsymbol{\nu}_\gamma(\mathbf{x}_i) \phi_i(\mathbf{x}), \quad \text{where } \phi_i \text{ are piecewise linear basis functions of } \mathbb{Y}_h.$$

Then, since  $\boldsymbol{\nu}_\gamma(\mathbf{x}_i) \cdot \boldsymbol{\nu} = 1 - \gamma$ , over a single face  $F$  of  $\Gamma$  we have

$$\begin{aligned} \int_F \mu_h \mathbf{Y} \cdot \boldsymbol{\nu} &= \int_F \mu_h \sum_{i=1}^3 \mu_h(\mathbf{x}_i) \boldsymbol{\nu}_\gamma(\mathbf{x}_i) \cdot \boldsymbol{\nu} \phi_i(\mathbf{x}) = \|\mu_h\|_{L^2(F)}^2 - \int_F \mu_h \sum_{i=1}^3 \mu_h(\mathbf{x}_i) \gamma(\mathbf{x}_i) \phi_i(\mathbf{x}) \\ &\geq \|\mu_h\|_{L^2(F)}^2 - \|\mu_h\|_{L^2(F)} \|I_h(\mu_h \gamma)\|_{L^2(F)}, \end{aligned}$$

where  $I_h : C^0 \rightarrow \mathbb{Y}_h$  is the nodal interpolant on  $F$ . For piecewise linear basis functions, we have

$$\|I_h(\mu_h \gamma)\|_{L^2(F)}^2 \leq \frac{|F|}{4} \sum_{i=1}^3 (\mu_h(\mathbf{x}_i) \gamma(\mathbf{x}_i))^2 \leq \gamma_0^2 \frac{|F|}{4} \sum_{i=1}^3 (\mu_h(\mathbf{x}_i))^2 \leq \gamma_0^2 6 \|\mu_h\|_{L^2(F)}^2.$$

So combining with the previous inequality gives  $\int_F \mu_h \mathbf{Y} \cdot \boldsymbol{\nu} \geq (1 - \gamma_0 \sqrt{6}) \|\mu_h\|_{L^2(F)}^2 \geq \frac{1}{2} \|\mu_h\|_{L^2(F)}^2$ , which implies  $(\mathbf{Y} \cdot \boldsymbol{\nu}, \lambda_I - \lambda_h)_\Gamma \geq \frac{1}{2} \|\lambda_I - \lambda_h\|_{L^2(\Gamma)}^2$ . Moreover, we obtain by an inverse estimate

$$\|\mathbf{Y}\|_{L^2(\Gamma)} \leq C_1 \|\lambda_I - \lambda_h\|_{L^2(\Gamma)}, \quad \|\nabla_\Gamma \mathbf{Y}\|_{L^2(\Gamma)} \leq C_1 h^{-1} \|\lambda_I - \lambda_h\|_{L^2(\Gamma)}.$$

Taking all this together, from (67), we get

$$\begin{aligned} \widehat{S} \|\lambda_I - \lambda_h\|_{L^2(\Gamma)} &\leq C_2 \left[ \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu})(\mathbf{V}_h - \mathbf{V}_I) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)} + \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu})(\mathbf{V}_I - \mathbf{V}) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)} \right. \\ &\quad \left. + \Delta t \widehat{C} h^{-1} \left\{ \|\nabla_\Gamma(\mathbf{V}_h - \mathbf{V}_I)\|_{L^2(\Gamma)} + \|\nabla_\Gamma(\mathbf{V}_I - \mathbf{V})\|_{L^2(\Gamma)} \right\} \right. \\ &\quad \left. + \widehat{S} \|\lambda_I - \lambda\|_{L^2(\Gamma)} \right], \end{aligned}$$

which proves the inequality.  $\square$

### 6.3 Multiplier Error Estimate

We have an error estimate for  $\lambda - \lambda_h$  in the discrete  $H^{1/2}(\Gamma)$  norm by the next theorem and corollary.

**Theorem 4.** *Assume the hypothesis of Theorem 3. Then,*

$$\begin{aligned} \|\lambda_I - \lambda_h\|_{H_h^{1/2}(\Gamma)} &\leq C \left[ \|\lambda - \lambda_I\|_{H^{1/2}(\Gamma)} + \|u - u_h\|_{L^2(\Omega)} + \|\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_{1,h}\|_{L^2(\Omega_1)} + \|\boldsymbol{\sigma}_s - \boldsymbol{\sigma}_{s,h}\|_{L^2(\Omega_s)} \right. \\ &\quad \left. + \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu})(\mathbf{V} - \mathbf{V}_h) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)} + \Delta t^{1/2} \|\nabla_\Gamma(\mathbf{V} - \mathbf{V}_h)\|_{L^2(\Gamma)} \right]. \end{aligned} \quad (68)$$

where the constant  $C > 0$  only depends on the physical constants and the domain geometry.

*Proof.* Beginning as we did in the proof of Theorem 3, we have for all  $(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})$  in  $\mathbb{Z}_h$ :

$$\begin{aligned} &b((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (0, 0, \lambda_I - \lambda_h)) \\ &= b((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (u_{1,h} - u_1, u_{s,h} - u_s, \lambda_I - \lambda)) + b((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (u_1 - u_{1,h}, u_s - u_{s,h}, \lambda - \lambda_h)) \\ &= b((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (u_{1,h} - u_1, u_{s,h} - u_s, \lambda_I - \lambda)) - a((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_{1,h}, \boldsymbol{\sigma}_s - \boldsymbol{\sigma}_{s,h}, \mathbf{V} - \mathbf{V}_h)), \end{aligned}$$

which then yields

$$\begin{aligned} b((\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y}), (0, 0, \lambda_I - \lambda_h)) &\leq C \|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h} \left[ \|u - u_h\|_{L^2(\Omega)} + \|\lambda - \lambda_I\|_{H_h^{1/2}(\Gamma)} \right. \\ &\quad \left. + \|\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_{1,h}\|_{L^2(\Omega_1)} + \|\boldsymbol{\sigma}_s - \boldsymbol{\sigma}_{s,h}\|_{L^2(\Omega_s)} \right. \\ &\quad \left. + \|\widehat{\beta}^{-1/2}(\boldsymbol{\nu})(\mathbf{V} - \mathbf{V}_h) \cdot \boldsymbol{\nu}\|_{L^2(\Gamma)} + \Delta t^{1/2} \|\nabla_\Gamma(\mathbf{V} - \mathbf{V}_h)\|_{L^2(\Gamma)} \right]. \end{aligned}$$

Finally, use  $\|\lambda - \lambda_I\|_{H_h^{1/2}(\Gamma)} \leq \|\lambda - \lambda_I\|_{H^{1/2}(\Gamma)}$ , divide through by  $\|(\boldsymbol{\eta}_l, \boldsymbol{\eta}_s, \mathbf{Y})\|_{\mathbb{Z}_h}$ , take the supremum, and use Lemma 7.  $\square$

**Corollary 3.** *Assume the hypothesis of Theorem 3 and Corollary 1. Then,*

$$\begin{aligned} \|\lambda - \lambda_h\|_{H_h^{1/2}(\Gamma)} &\leq C h^\theta \|u\|_{H^\theta(\Omega)} \\ &\quad + C(1 + \Delta t) h^\theta \left\{ \|\boldsymbol{\sigma}_1\|_{H^s(\Omega_1)} + \|\boldsymbol{\sigma}_s\|_{H^s(\Omega_s)} + \left[ h + \Delta t^{1/2} \right] \|\mathbf{V}\|_{H^{1+\theta}(\Gamma)} \right. \\ &\quad \left. + \left[ 1 + \varpi \left( \gamma_0 \frac{h}{\Delta t} \right)^{1/2} \right] \|\lambda\|_{H^{1/2+\theta}(\Gamma)} \right\}, \end{aligned} \quad (69)$$

with the same conditions on  $C > 0$  and  $\varpi$  as in Theorem 3.

*Proof.* Combine Theorem 4 with Corollary 1, Corollary 2, the triangle inequality, and standard interpolation estimates.  $\square$

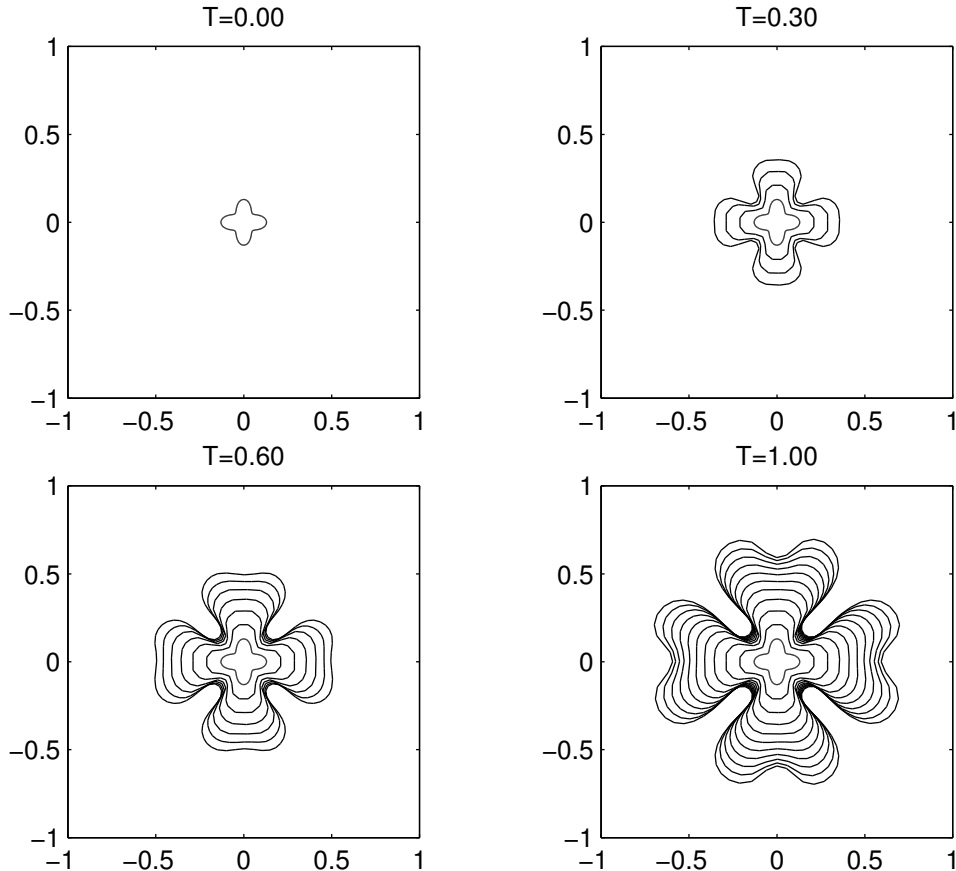


Figure 2: Simulation with **isotropic** surface tension. Several time-lapses are shown to illustrate the evolution with initial interface having a “clover” shape.

## 7 Numerical Results

We present two dimensional simulations to illustrate our method (2-D for simplicity). All simulations were implemented in the package FELICITY [61]. The linear systems are solved by MATLAB’s “backslash” command. Alternatively, one can use an iterative procedure such as Uzawa’s algorithm; see [21, Section 7] for a description.

For all simulations, the Dirichlet boundary is the entire outer boundary, i.e.  $\partial_{\text{D}}\Omega \equiv \partial\Omega$  with  $u_{\text{D}} = -0.5$ . The initial temperature is  $u_{\text{s}}^0 := 0$  in  $\Omega_{\text{s}}$  and  $u_{\text{l}}^0$  is a smooth function between 0 and  $-0.5$  in  $\Omega_{\text{l}}$ . For updating the temperatures, we used (35). We verified the conservation law by computing the difference of the left and right hand sides of (43). If the mesh was never regenerated, the difference was machine precision  $\approx 10^{-16}$ . If a re-mesh did occur, this induced a relative error of  $\approx 10^{-5}$ .

### 7.1 Isotropic Surface Energy

The model in Section 2 assumes the surface tension coefficient  $\widehat{\mathcal{C}}$  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.

## 7.2 Anisotropic Surface Energy

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

$$\widehat{\mathcal{C}} = \widehat{\mathcal{C}}(\boldsymbol{\nu}) := \widehat{\mathcal{C}}_0 \sum_{j=1}^K (\boldsymbol{\nu}^T G_j \boldsymbol{\nu})^{1/2}, \quad (70)$$

where  $\widehat{\mathcal{C}}_0 = 0.0005$  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  $\widehat{\beta} = \widehat{\beta}_0 \widehat{\mathcal{C}}(\boldsymbol{\nu})$ , 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  $\widehat{\mathcal{C}}(\boldsymbol{\nu}) = \widehat{\mathcal{C}}_0$ .

With the above, we can derive the modified form of (24) by standard shape differentiation [15, 55, 31]. Indeed,

$$\frac{d}{dt} \int_{\Gamma(t)} \widehat{\mathcal{C}}(\boldsymbol{\nu}) = \int_{\Gamma(t)} \widehat{\mathcal{C}}(\boldsymbol{\nu}) \nabla_{\Gamma} \mathbf{X} : \nabla_{\Gamma} \mathbf{V} - \int_{\Gamma(t)} \boldsymbol{\nu} [\widehat{\mathcal{C}}'(\boldsymbol{\nu})]^T : \nabla_{\Gamma} \mathbf{V}, \quad (71)$$

where  $\mathbf{V}$  is the velocity of  $\Gamma$ , and for  $\mathbf{p} \in \mathbb{R}^d$ ,  $\widehat{\mathcal{C}}'(\mathbf{p})$  is the gradient of  $\widehat{\mathcal{C}}$  with respect to  $\mathbf{p}$ . We now obtain a semi-discrete formulation for the anisotropic case by combining (23), (24), and (71):

$$\begin{aligned} & (\widehat{\beta}^{-1}(\boldsymbol{\nu}^i) \mathbf{V}^{i+1} \cdot \boldsymbol{\nu}^i, \mathbf{Y} \cdot \boldsymbol{\nu}^i)_{\Gamma^i} + \Delta t (\widehat{\mathcal{C}}(\boldsymbol{\nu}^i) \nabla_{\Gamma^i} \mathbf{V}^{i+1}, \nabla_{\Gamma^i} \mathbf{Y})_{\Gamma^i} + \widehat{S}(\mathbf{Y} \cdot \boldsymbol{\nu}^i, \lambda^{i+1})_{\Gamma^i} \\ & = -(\widehat{\mathcal{C}}(\boldsymbol{\nu}^i) \nabla_{\Gamma^i} \mathbf{X}^i, \nabla_{\Gamma^i} \mathbf{Y})_{\Gamma^i} + (\boldsymbol{\nu}^i [\widehat{\mathcal{C}}'(\boldsymbol{\nu}^i)]^T, \nabla_{\Gamma^i} \mathbf{Y})_{\Gamma^i} \quad \text{for all } \mathbf{Y} \in \mathbb{Y}^i. \end{aligned} \quad (72)$$

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 (72) is easier to implement. The main drawback of (72) is it makes the numerical scheme slightly explicit, which could put a constraint on the time step.

In Figure 3, we present a simulation using (70) with  $K = 1$  (i.e. a one-fold anisotropy). Figure 4 shows a simulation with  $K = 3$  (i.e. a three-fold anisotropy).

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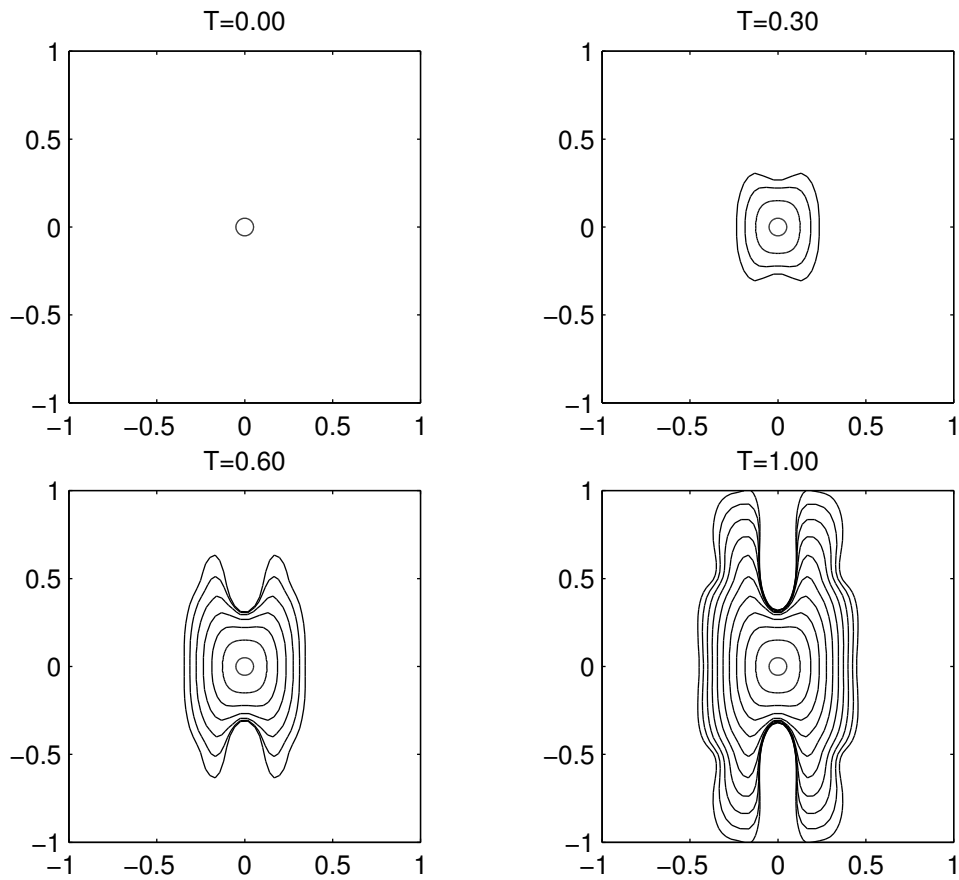


Figure 3: Simulation with **anisotropic** surface tension. Several time-lapses are shown to illustrate the evolution with initial interface shape being a circle. A *one-fold* anisotropy is used which breaks the initial radial symmetry.

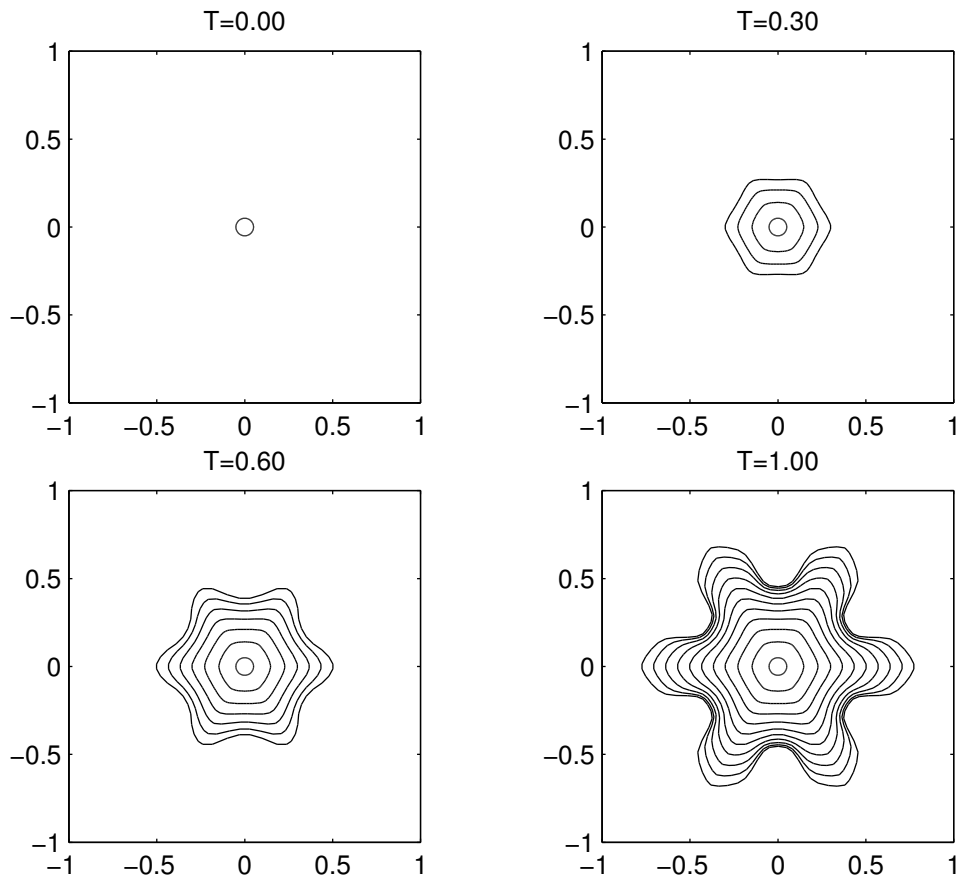


Figure 4: Simulation with **anisotropic** surface tension. Several time-lapses are shown to illustrate the evolution with initial interface shape being a circle. A *three-fold* anisotropy is used which breaks the initial radial symmetry.

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