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On the Cahn-Hilliard-Oono equation with dynamic boundary conditions

Relatore: Prof. Maurizio Grasselli

Tesi di Laurea di:
Antonello Gerbi
Matr. 765382

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Abstract

In the present work we describe and analyze the Cahn-Hilliard-Oono (CHO) equation (also known in literature as Ohta-Kawasaki) coupled with the so-called *dynamic boundary condition*.

CHO is a variant of the famous Cahn-Hilliard (CH) equation with the addition of a reaction term:

$$\begin{cases} \partial_t u + \sigma u = \Delta w & \text{in } \Omega,\ t > 0 \\ w = F'(u) - \varepsilon \Delta u & \text{in } \Omega,\ t > 0. \end{cases}$$

This fourth order, nonlinear PDE models the evolution in time of a binary mixture composed, for instance, of reacting components or diblock copolymers. Here u represents the order parameter, which is defined as the difference between the relative concentration of the two substances, w is the chemical potential, and F a double-well potential.

The above system can be coupled with different boundary conditions , the homogeneous Neumann being the most common choice for both u and w. However, it has not yet been studied with the dynamic boundary condition

$$\frac{1}{\omega}\partial_t u = \varepsilon_\Gamma \Delta_\Gamma u + \sigma_\Gamma u - \varepsilon \partial_n u - F'_\Gamma(u) \quad \text{on } \Gamma,\ t > 0$$

where $\Gamma = \partial\Omega$. The word *dynamic* refers to the fact that the time derivative of u appears explicitly in its formulation, thus making it a nonlinear parabolic PDE on the boundary. This choice is justified by physical and mathematical motivations explained in the text.
CHO with the above boundary condition is the system which is studied in this thesis.

The mathematical model thus obtained is particularly difficult to manage since, unlike the standard CH, the conservation of u is lost; moreover, the PDE on the boundary brings a large number of terms which have to be treated in an appropriate way. However, under a relatively small number of hypothesis, the following results are proven:

- Existence and uniqueness of a weak solution
- Continuous dependence of the solution on the initial data
- Existence of a connected global attractor

In addition to these theoretical aspects, a numerical analysis is made; assuming some stronger conditions (which are acceptable in the numerical setting) some error estimates for a $\mathbb{P}^1$ finite elements discretization are proven.
Finally, using the numerical results, various finite element simulations are conducted, with an implicit Euler time discretization; as the resulting system is nonlinear, a Newton method is implemented to solve the problem at each time step.

Sommario

In questa tesi viene descritta ed analizzata l'equazione di Cahn-Hilliard-Oono (CHO) (conosciuta in letteratura anche con il nome di Ohta-Kawasaki) con la cosiddetta *condizione al bordo dinamica.*

CHO è una variante della nota equazione di Cahn-Hilliard (CH) con l'aggiunta di un termine di reazione:

$$\begin{cases} \partial_t u + \sigma u = \Delta w & \text{in } \Omega,\ t > 0 \\ w = F'(u) - \varepsilon \Delta u & \text{in } \Omega,\ t > 0. \end{cases}$$

Questa EDP non lineare del quart'ordine modellizza l'evoluzione nel tempo di una miscela binaria composta, ad esempio, da elementi soggetti a reazione chimica o da diblocchi di copolimeri. u rappresenta il cosiddetto parametro d'ordine, ovvero la differenza tra le concentrazioni relative delle due sostanze, w è il potenziale chimico, e F un potenziale a doppio pozzo.

Il sistema sopra riportato può essere abbinato a diversi tipi di condizioni al bordo, ed una scelta di tipo Neumann omogeneo per u e w è la più comune. Tuttavia, non è stato ancora studiato con la condizione al bordo dinamica

$$\frac{1}{\omega}\partial_t u = \varepsilon_\Gamma \Delta_\Gamma u + \sigma_\Gamma u - \varepsilon \partial_n u - F'_\Gamma(u) \quad \text{on } \Gamma,\ t > 0$$

dove $\Gamma = \partial\Omega$. Il termine *dinamica* si riferisce al fatto che la derivata temporale di u appare esplicitamente nella sua formulazione, rendendola a tutti gli effetti una EDP parabolica, non lineare, sul bordo. Questo tipo di scelta è giustificato da motivazioni fisiche e matematiche discusse nel testo.
CHO con tale condizione al bordo rappresenta il sistema che viene analizzato in questa tesi.

Il modello matematico così ottenuto è particolarmente difficile da trattare poiché in questo caso, a differenza di CH standard, la quantità u non è conservata; inoltre, l'EDP sul bordo presenta un grande numero di termini che devono essere trattati in modo adeguato. Tuttavia, assumendo un numero relativamente limitato di ipotesi, i seguenti risultati sono dimostrati:

- Esistenza ed unicità di una soluzione debole
- Dipendenza continua della soluzione dai dati iniziali
- Esistenza di un attrattore globale connesso

Oltre a questi aspetti teorici, viene condotta un'analisi numerica; sotto alcune ipotesi più forti (che sono comunque accettabili nell'ambito numerico) alcune stime dell'errore per una discretizzazione ad elementi finiti di tipo $\mathbb{P}^1$ sono dimostrate.
Infine, sfruttando i risultati numerici, varie simulazioni ad elementi finiti sono effettuate, con una discretizzazione in tempo di tipo Eulero implicito; poiché il sistema così ottenuto è non lineare, un metodo di Newton è stato implementato per risolvere il problema ad ogni passo temporale.

Ringraziamenti

È estremamente difficile, se non impossibile, condensare in poche righe i ringraziamenti nei confronti di tutte le persone che hanno contribuito, direttamente e non, al mio percorso universitario ed alla stesura di questa tesi: farò quindi un tentativo che è ben lungi dall'essere completo.

Sicuramente il primo pensiero va alla mia famiglia, la quale in questi anni mi ha sostenuto e sopportato (anche e soprattutto in momenti in cui farlo deve essere stato piuttosto difficile).

Non potrei poi assolutamente dimenticare il professor Grasselli: innanzitutto come docente, ed in seguito nelle vesti di relatore. In entrambi i casi, posso dire di aver assorbito tanto l'amore per la materia, quanto il rigore necessario per poterla trattare: come se non bastasse, durante la stesura di questo lavoro, ha sempre mostrato una disponibilità ai limiti del sovrannaturale.

Gli anni trascorsi al Politecnico sarebbero stati senza dubbio ben più ardui da affrontare senza tutti gli amici, vecchi e nuovi, che hanno contribuito a superare i momenti di difficoltà e a rendere il percorso decisamente più piacevole; penso, in particolare, a tutti i compagni di corso con i quali ho condiviso gran parte della mia storia universitaria.
Tra tutti gli amici, Paolo Velati si è meritato una menzione speciale: senza i suoi potenti strumenti informatici, probabilmente starei ancora aspettando il risultato delle simulazioni numeriche.

Da ultimo, ma sicuramente non per importanza, devo ringraziare HSLT e tutto il mondo che vi ruota attorno. Nonostante in diversi momenti abbia assorbito il mio tempo anche più del Politecnico, è riuscita, tra le altre cose, nel difficile compito di sviluppare gli aspetti più sociali del mio carattere, contribuendo in modo fondamentale alla formazione della mia personalità.

Contents

List of Figures

Chapter 1

Introduction

The study of the evolution in time of incompatible binary mixtures is important in many fields of science and industrial processes; one can observe such phenomena in both nature and human driven experiments, and understanding its features is advantageous in different situations. The mathematical models which try to explain and predict the behavior of such systems are mainly based on the concept of an initially homogeneous alloy, which evolves into an unstable state when some parameter (usually temperature) is changed. The two components of the mixture are called phases, and this process is in turn known as *phase separation*. Often, this instability eventually leads to the formation of patterns - structures periodically repeated in space - which on the other hand strongly influence the macroscopical properties of the resulting material. The analysis of these models presents various intrinsic difficulties, and thus make it intriguing from a mathematical viewpoint too.

In this chapter we first present a more detailed phenomenological description of the problem, and then introduce the Cahn-Hilliard (CH) equation, which is probably the most known mathematical model, with its many variants, for phase separation. Next, we discuss the formulation of the Cahn-Hilliard-Oono (CHO) equation, which can be considered as a perturbation of CH, particularly suited to describe the phenomenon when the alloy is composed of diblock copolimers or reacting substances. Finally, to complete the description of the problem that we analyze in the subsequent chapters, we discuss how these equations can be coupled with boundary conditions, which take differently into account the interaction of the mixtures with the wall.

1.1 Phase separation in binary alloys

Consider a mixture of two incompatible substances A and B, which is homogeneously distributed and isothermal. Under certain circumstances, namely if the temperature is above a critical threshold T_c, this configuration is stable; however, if suddenly cooled down and kept at $\overline{T} < T_c$, the initially (macroscopically) homogeneous alloy evolves in a way such that A-rich and B-rich regions appear and grow. We can better describe what happens with the aid of the phase diagram in Figure 1.1, which is in good agreement with experimental evidence (see [5], [6]).

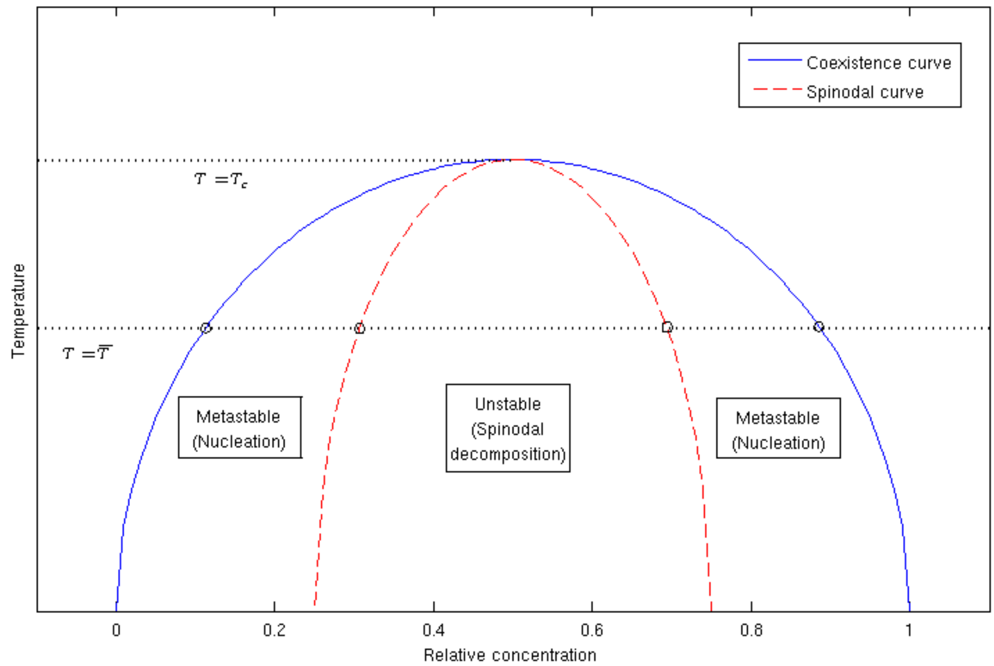

Figure 1.1: Phase diagram with coexistence and spinodal curves

On the x-axis the relative concentration of one of the two substances is represented, while temperature is on the y-axis where the critical threshold T_c is also highlighted. The state of the mixture is then described by the different locations on the graph relatively to the two curves.

The coexistence curve separates the diagram in regions where a homogeneous distribution is the only stable configuration (above) and where heterogeneous mixtures are allowed (under); on the points along the curve the mixed and unmixed states are in equilibrium with each other.
On the other hand, the spinodal curve divides the area under the coexistence curve in regions where the mixed configuration is metastable (that is, stable with respect to small perturbations) and unstable. The distinction in these two cases is due to a difference in the free energy of the configuration: the central region is characterized by the *spinodal decomposition* phenomenon, which is spontaneous since it is an unstable process; on the contrary *nucleation* happens in the metastable regions, but only if an external source is provided which make it possible to get over a local maximum in the free energy (see [7], where a description of the multicomponent case can be found too).

The evolution in the spinodal decomposition region is that of wave-like concentration fluctuations which ultimately form zones of the two phases, with a subsequent coarsening; the process comes to an end when the concentration lays on the intersection of the spinodal curve with the line $T = \overline{T}$.

As of nucleation, homogeneous A-rich and B-rich zones slowly aggregate in bubble-like structures and grow (Figure 1.2 shows the difference between the two phenomena). Here the (eventually asymptotic) final configuration is that of two approximately homogeneous single phase regions, and the concentration is given by the intersection of the coexistence curve with the line $T = \overline{T}$.

For more information about the whole process see e.g., amongst a vast literature, [8] and [9].

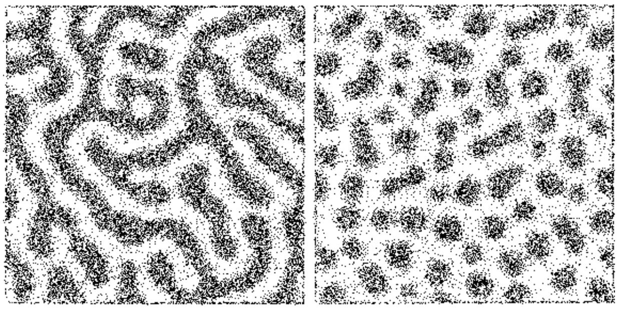

Figure 1.2: A numerical simulation taken from [1] shows the difference between spinodal decomposition (left) and nucleation (right)

1.2 The Cahn-Hilliard equation

The theory of patterns as emerging from bifurcations of an homogeneous state goes back to the work of Alan Turing in 1952 [10], but it was only six years later that Cahn and Hilliard proposed an energy approach in [11], later extended by Fisk and Widom in [12], with the aim of studying the spinodal decomposition process as that of an interfacial problem; we will now briefly describe their work.

If we consider a bounded domain $\Omega \subset \mathbb{R}^d$ filled with components A and B presenting different properties, we can define their relative mass fraction for every $\mathbf{x} \in \Omega$ as $u_A(\mathbf{x})$ and $u_B(\mathbf{x})$, assuming that they are non-uniform, were clearly $u_i : \Omega \to [0, 1]$ and $u_A(\mathbf{x}) + u_B(\mathbf{x}) = 1$. Choosing one of the two functions and relabeling it as $u(\mathbf{x})$, Cahn and Hilliard, under the additional hypothesis that the mixture is isothermal and that the molar volume is uniform and independent on pressure, proposed that the system goes towards the minimization of the following energy functional

$$E(u) = \int_\Omega \left(\frac{\varepsilon^2}{2} |\nabla u|^2 + F(u) \right), \tag{1.1}$$

$F(u)$ being the Helmholtz free energy density (of a single component)

$$F(u) = 2k_B T_c u(1-u) + k_B T(u \ln(u) + (1-u)\ln(1-u)).$$

Here k_B is the Boltzmann constant, T and T_c the temperature and its aforementioned critical threshold. With this description in mind, it is not surprising that T_c plays a crucial role in the process: if $T \geq T_c$, the behavior is trivial since $F(u)$ presents a single global minimum in $u = \frac{1}{2}$, and therefore the minimization of (1.1) is obtained with a homogeneous distribution $u(\mathbf{x}) = \frac{1}{2}\ \forall \mathbf{x} \in \Omega$. On the other hand, if $T < T_c$, a physically relevant double-well appears in the function's graph.

The first term in (1.1) takes into account the interfacial nature of the phenomenon: it clearly increases the energy in those regions of the space where both A and B are present (and thus u possess a high gradient). However, even if the substances separation looks sharp from a macroscopical point of view, there is experimental evidence of an intermediate, diffusive, stripe; the term ε^2 is then such that ε is proportional to the stripe's thickness.

In the mathematical treatment of the problem, one usually uses as a variable the so-called *order parameter* $u(\mathbf{x}) = u_A(\mathbf{x}) - u_B(\mathbf{x})$, such that $u : \Omega \to [-1, 1]$. The name is justified by the fact that it somehow measures the configuration's regularity, its extreme values representing the situation with a highest degree of order.
It can be easily shown that with this substitution, up to a multiplicative constant which therefore changes nothing in the description of the problem, (1.1) holds unmodified, while $F(u)$ becomes

$$F(u) = -c_0 u^2 + c_1((1+u)\ln(1+u) + (1-u)\ln(1-u)) \quad c_0 > c_1 > 0, \tag{1.2}$$

as we fixed $T < T_c$. Recalling now the hypothesis that the process minimizes (1.1) over time, we get a differential description of the phenomenon as

$$\partial_t u + \nabla \cdot \mathbf{J} = 0 \quad \text{in } \Omega.$$

where the flux $\mathbf{J}$ is defined by

$$\mathbf{J} = -M(u)\nabla\left(\frac{\delta E(u)}{\delta u}\right) = -M(u)\nabla\left(F'(u) - \varepsilon^2 \Delta u\right),$$

The function $M(u)$ is the mobility of the substances (which measures how much the molecules are free to move) and is of the form (see [13])

$$M(u) = (1-u^2)^k \overline{M}(u) \quad k \geq 1,\ \overline{M} \in C^1([-1,1], \mathbb{R}_0^+). \tag{1.3}$$

The equation is then usually decoupled, and finally written as

$$\begin{cases} \partial_t u = \nabla \cdot (M(u)\nabla w) \quad \text{in } \Omega & (1.4) \\ w = F'(u) - \varepsilon^2 \Delta u \quad \text{in } \Omega, & (1.5) \end{cases}$$

where w represents the chemical potential, a form of potential energy which, at every time t, depends on the mixture's configuration. System (1.4)-(1.5) represents the generic formulation of CH: clearly, as it is an evolution (with respect to u) PDE, an initial datum u_0 is needed, that is, the distribution of the substances at $t = 0$. Regarding the boundary conditions, we need two of them since the system is of the fourth order: a first, natural, choice is

$$\mathbf{n} \cdot M(u)\nabla w = 0 \quad \text{on } \Gamma, \tag{1.6}$$

where $\Gamma = \partial\Omega$ and $\mathbf{n}$ is the outer normal vector; in fact, integrating (1.4) over Ω and applying the divergence theorem we obtain

$$\frac{\mathrm{d}}{\mathrm{dt}} \int_\Omega u = 0,$$

that is, the conservation of u holds. As of a boundary condition for u, a Neumann homogeneous choice

$$\partial_n u = 0 \quad \text{on } \Gamma,$$

is the most common; however, we will discuss later the alternative proposed in this text.

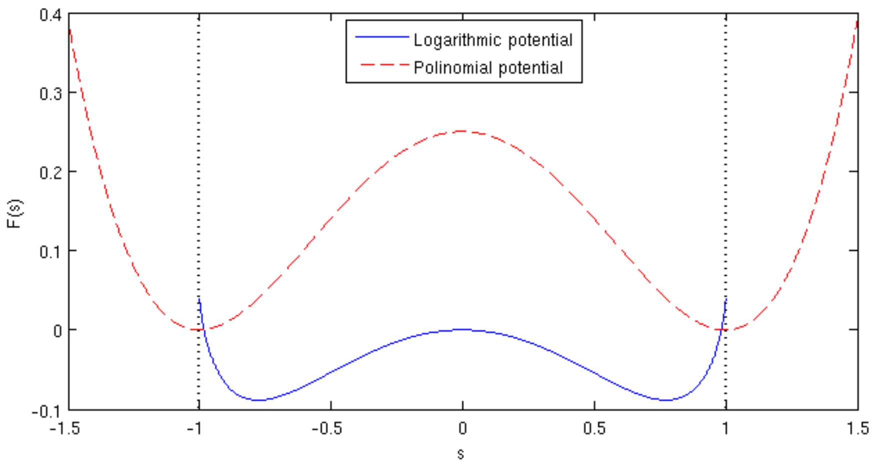

Figure 1.3: A comparison of the logarithmic potential (1.2) with $c_0 = 1$, $c_1 = \frac{1}{8}$ with the polynomial potential $F(s) = \frac{1}{4}(s-1)^2$

It is worth notice that system (1.4)-(1.5), although showing a deep phenomenological explanation, is very hard to treat mathematically because of the terms $F(u)$ and $M(u)$. One typically has to choose amongst the following alternatives concerning these nonlinearities:

- The potential $F(s)$ is called *singular* when defined as in (1.2), and *regular* when it is substituted with a proper approximation, which avoids the fact that $\lim_{|s|\to 1} F(s) = +\infty$. In order for the approximation to be significant, many

authors usually require that it still shows a double-well; moreover, the local minima should coincide with the pure phases (see [14] and references therein). A common choice is an even-degree polynomial with a positive leading coefficient, the case $F(s) = \frac{1}{4}(s^2 - 1)^2$ being by far the most present in literature. A comparison is shown in Figure 1.3.
We shall remark that in such case the solution of the problem (when it exists) is no longer guaranteed to assume values in $(-1, 1)$, as no maximum principle holds.

- A similar difficulty regards the mobility $M(u)$: it is indeed called *degenerate* if in the form (1.3). Here the problem is that $M(-1) = M(1) = 0$, thus the pure phases should be characterized by zero mobility. However, to simplify the treatment, it is often assumed - as we will do from now on - that $M(u) = constant$. See [13], [15] for an analysis of the CH equation with degenerate mobility.

The literature on the argument is extremely vast, as different combinations in the choice of $F(u)$, $M(u)$ and boundary conditions, in addition to the many variants of (1.4)-(1.5), lead to a deeply different treatment of the problem. With the above boundary conditions for u and w, we cite as references the articles [16], [17], [18], [19], [20], [21].

We stated by the beginning of the chapter that phase separation effects are present in different scopes. We will later discuss some industrial applications but, for the time being, we cite two examples of natural phenomena of this kind which can be modeled with the aforementioned equations.

Regarding the first one, in [22], Tremaine suggests that the irregular structure of Saturn's rings could be explained using a non-Newtonian fluid model coupled with the CH equation. On the other hand, in a recent article [2], the authors found that the spatial patterns in the distribution of mussels can be described with a CH model (see Figure 1.4).

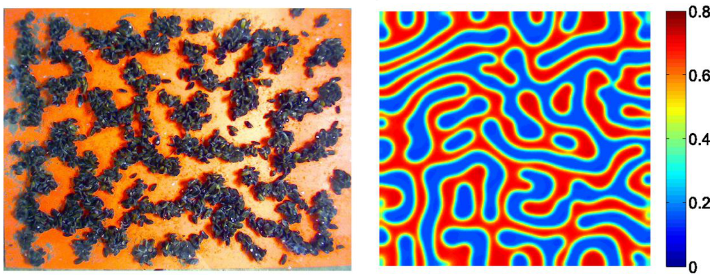

Figure 1.4: Spatial distribution of mussels in an experimental setting, compared with a numerical simulation of the model presented in [2]

1.3 The Cahn-Hilliard-Oono equation

We now focus on a particular case of phase separation, that occurs when the mixture is composed of diblock copolymers; these are organic binary chains, composed of two homogeneous linear subchains covalently joined with each other, e.g. polyisoprene and polystyrene. Here, the thermodynamical incompatibility between the two elements composing the subchains leads to phase separation, which is however inhibited at big scales because of the covalent bond. As a result, we observe a multitude of nanostructures which rise from this competing short and long range interactions (see Figure 1.5).

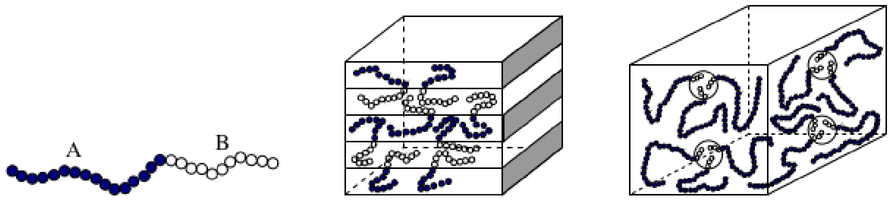

Figure 1.5: Diblock chains made of type A and B polymers and their distribution in the domain (image taken from [3])

Trying to model this phenomenon as a minimization problem over all the possible configurations is an incredibly hard task: using the statistical physics properties of polymer chains, one has to solve a highly nonlinear and nonlocal optimization problem. A different approach is given by the so-called *self-consistent field theory* (SCFT) [23], [24]; the models belonging to the SCFT, instead of considering all the interactions between the particles in a system, assume that the global effect can be though as that of a single, averaged, force field, and this is why SCFT is also called *mean field theory.* The power of these theory is clearly that of reducing a many-body problem to a one-body-problem: it has been however reported that this approximation could be inadequate in some cases, such as that of neutral polymers or polyelectrolyte solutions in dilute and semidilute concentration regimes [25].

A much simpler model was introduced by Ohta and Kawasaki in [26]; the authors proposed a Landau-type expansion in terms of monomer densities, and thus derived a free energy functional which is nothing but a perturbation of (1.1) with the addition of a non-local Coulombic type term, as showed in [27]. Moreover, Choksi and Ren proved in [28] that it can be obtained from SCFT by linearization about the disordered state. The functional reads

$$H(u) = \int_\Omega \left(\frac{\varepsilon^2}{2} |\nabla u|^2 + F(u) \right) + \frac{\sigma}{2} \int_\Omega \int_\Omega G(\mathbf{x}, \mathbf{y})(u(\mathbf{x}) - \overline{m})(u(\mathbf{y}) - \overline{m}), \qquad (1.7)$$

where $\overline{m} \in \mathbb{R}$. $G(\mathbf{x}, \mathbf{y})$ is the Green's function for $-\Delta$ in Ω with periodic or homogeneous Neumann conditions, i.e. the solution of

$$-\Delta G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}) \quad \text{in } \Omega.$$

In order to explain the meaning of the number $\overline{m}$, we proceed as in the previous section and get the differential equation

$$\begin{cases} \partial_t u + \sigma(u - \overline{m}) = \Delta w \quad \text{in } \Omega & (1.8) \\ w = F'(u) - \varepsilon^2 \Delta u \quad \text{in } \Omega. & (1.9) \end{cases}$$

We see that the perturbation led to an additional reaction term; moreover, if we consider again the boundary condition (1.6), what we get now is

$$\frac{\mathrm{d}}{\mathrm{dt}} \int_\Omega u = -\sigma \int_\Omega (u - \overline{m}),$$

so that the solution of this ODE is

$$\langle u \rangle = \overline{m} + \langle u_0 - \overline{m} \rangle e^{-\sigma t},$$

where $\langle u \rangle$ is the spatial average of u in Ω. As we are considering $\sigma > 0$ (the case $\sigma = 0$ being the standard CH equation), we clearly see that if $\langle u_0 \rangle \neq \overline{m}$, the mean value of u goes exponentially fast to this value.

In the case of diblock copolymers, $\overline{m} = \langle u_0 \rangle$ by definition. There is no global effect on the quantity of the two molecules, as no chemical reaction occurs between them; therefore the effect of σ is that of contrasting the formation of big structures (see Figure 1.6).
For more information on this model and how it is derived, see e.g. [28], [29], [3], [30]; some mathematical works of interest on the CHO equation are [31], [32].

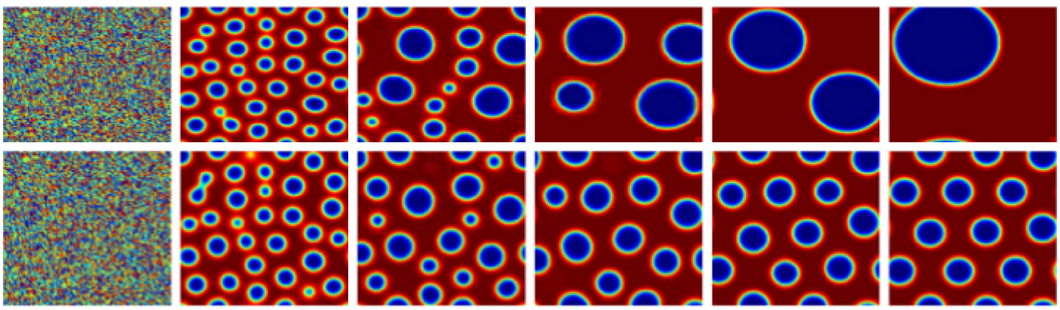

Figure 1.6: A numerical simulation which compares the pattern evolution over time using CHO with $\sigma = 0$ (first row) and $\sigma > 0$ (second row). The average of the solution is fixed, and the formation of big structures is clearly inhibited in the second case (image taken from [3])

CHO can also be applied to phase separation phenomena not related to diblock copolymers; this is the case of binary alloys in which a chemical reaction between the two elements actually happens, together with the spinodal decomposition. In this setting, $\overline{m}$ represents the global equilibrium for the reaction and (unless u_0 is chosen such that $\langle u_0 \rangle = \overline{m}$) the mean value decays in time towards this value, i.e. $\langle u(t) \rangle \to \overline{m}$ as $t \to \infty$. We will discuss this very important application in the following section.

We already pointed out the ubiquity of CH models, as they are used in a great variety of different fields. CHO-based equations are not an exception: some very interesting results have been obtained by Bertozzi et al. (see [33], [34]), which exploited a modified version of such equations in order to develop a filter for the inpainting (i.e., the filling of missing fragments) of binary images. Their algorithm proved to be good enough to be patented in the US in 2010.

1.4 An application of CHO: control of chemical reaction in phase separating alloys

Consider a mixture of substances A and B, as we did in the previous sections; moreover, now the two molecules undergo the following chemical reaction

$$\mathrm{A} \underset{\Gamma_2}{\overset{\Gamma_1}{\rightleftharpoons}} \mathrm{B}, \tag{1.10}$$

where Γ_1 and Γ_2 represent the rate at which such reaction occurs, respectively forward and backward: the presence of this effect, in addition to the phase separation, clearly alters the way in which A and B are spatially distributed. Actually, the reaction plays the role of a competing effect in contrast with spinodal decomposition and coarsening, and it has been observed in numerical experiments that the process may converge towards a steady state (see [4], [35]).
Glotzer et al. showed in [36] that in this case the following equation can be used to describe the phenomenon

$$\partial_t u_A = \Lambda \Delta \left(\frac{\delta E(u_A)}{\delta u_A} \right) - \Gamma_1 u_A + \Gamma_2 (1 - u_A),$$

which can be rewritten, as before, relatively to the concentration difference; this exactly leads to the CHO system

$$\begin{cases} \partial_t u = \Delta w - (\Gamma_1 + \Gamma_2) \left(u - \dfrac{\Gamma_1 - \Gamma_2}{\Gamma_1 + \Gamma_2} \right) & \text{in } \Omega \\ w = F'(u) - \varepsilon^2 \Delta u \quad \text{in } \Omega. \end{cases}$$

While linear analysis of (1.4)-(1.5) predicts an exponential growth of concentration fluctuations, it has also been shown that the concurrent presence of (1.10) induces a cutoff of the growth rate. Nonetheless numerical simulations show that this effect is present even in the long times, when the nonlinear results are important. Indeed, in the case $\Gamma_1 = \Gamma_2 = \Gamma_r$, the steady state structure size R_{eq} was found in [4] to be asymptotically proportional to a power of Γ_r, that is

$$R_{eq} \propto \left(\frac{1}{\Gamma_r} \right)^{1/3}.$$

This phenomenon can also be simulated (see Figure 1.7) by a Monte Carlo approach; in this case, the emerging pattern can be interpreted as the result of the competition between p_{exch} and p_r, where

$$p_{exch} = \frac{e^{-\Delta E/k_B T}}{1 + e^{-\Delta E/k_B T}},$$

is the acceptance probability for the exchange of two nearest-neighbors molecules, and $\Delta E = E_{final} - E_{initial}$ is the difference in the system's energy before and after the exchange. On the other hand, p_r represents the probability that a reaction between two nearest-neighbors molecules of type A and B eventually happens, and should be a value proportional to Γ_r.

It is evident from Figure 1.7 that using this method leads to the same conclusions as in the case of diblock copolymers; the size of the structures emerging from phase separation is clearly strongly influenced even by a small concurrent reaction.

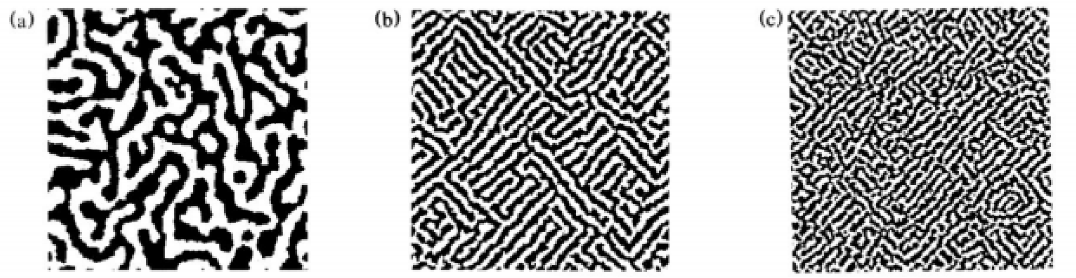

Figure 1.7: Monte Carlo simulation of pattern formation in a lattice following a quench to $T < T_c$, for a reaction probability of: (a) $p_r = 0$, (b) $p_r = 10^{-4}$, (c) $p_r = 5 \times 10^{-4}$. In all three cases, $t = 3 \times 10^5$ (image from [4])

The chance of acting on the chemical reaction rate is a very powerful tool; the tunability of the patterns gives a great way to control the final morphology of phase separated materials, which in turn gives raise to different properties of the derived alloy. Some applications in material sciences, with industrial consequences, are the production of polymer mixtures with induced isomerization, and the production of type-I superconductors with the aid of an external electric field. This kind of setting is of great interest in the scientific community, and has been studied, for instance, in [37], [38], [39].

The above arguments can also be applied to other pattern formation type phenomena: for instance, in [40], numerous experiments involving metal-ion catalyzed oxidation of organic compounds by bromate ions are discussed; here the result is an oscillatory reaction which goes under the name of Belousov-Zhabotinsky. More information about the pattern formation with concurrent reaction (and many other settings) can be found in [40], [41] and references therein.

1.5 Boundary conditions for phase separation models

We intentionally avoided a deep discussion about boundary conditions on u for problems (1.4)-(1.5) and (1.8)-(1.9). We showed that a Neumann homogeneous condition on w is more than acceptable from a physical viewpoint, as it leads to mass conservation if no reaction is present; however, a similar condition on u should not be taken lightly.

Taking the assumption that $\partial_n u = 0$ on Γ, as most works do, means that the gradient of u must be parallel with respect to the border. In other words, the interface must be orthogonal to Γ, and this may happen to be a strong hypothesis.
Instead, we now present (and give a brief justification of) a different condition which goes under the name of *dynamic boundary condition*, the word dynamic referring to the fact that the time derivative $\partial_t u|_\Gamma$ appears explicitly on the border. We use the same arguments showed in [42].

Given a regular enough function v on Ω, (consider for instance Sobolev spaces of increasing index), we know that its trace on the border is smooth too. Thus, one may denote the total mass not just by $\langle v \rangle$, but considering to this aim also the contribution on Γ (if $v|_\Gamma$ is at least in $L^1(\Gamma)$); in other words one may define it as

$$\int_{\overline{\Omega}} v \,\mathrm{dm} := \int_\Omega v \,\mathrm{d}\Omega + \int_\Gamma v \,\widetilde{w}\,\mathrm{d}\Gamma,$$

where $\widetilde{w}$ is some regular weight function which balances the contribute from Γ. It can be easily shown that dm is equivalent to the standard Lebesgue measure $\mathrm{d}\Omega \times \mathrm{d}\Gamma$. As we are admitting that some part of the mass is present on the border, it makes sense to take into account a contribution from Γ on the free energy defined in the previous sections. In the CH case, the new total free energy reads

$$E_{\mathrm{tot}}(u) = E(u) + E_\Gamma(u) = \int_\Omega \left(\frac{\varepsilon^2}{2} |\nabla u|^2 + F(u) \right) + \int_\Gamma \left(\frac{\varepsilon_\Gamma^2}{2} |\nabla_\Gamma u|^2 + F_\Gamma(u) \right),$$

where ∇_Γ is the surface gradient and F_Γ a potential, which may be defined as F. If we now evaluate the first variation of the total energy with respect to u and test it against a test function z, we get (formally operating in a suitable function space)

$$\left\langle \frac{\delta E_{\mathrm{tot}}(u)}{\delta u}, z \right\rangle = \int_\Omega \left(-\varepsilon \Delta u + F'(u) \right) z + \int_\Gamma \left(-\varepsilon_\Gamma \Delta_\Gamma u + \varepsilon \partial_n u + F_\Gamma'(u) \right) z,$$

Δ_Γ being the Laplace-Beltrami operator. We now assume that on Γ the density relaxes at a rate which is proportional to the part of the flux belonging to the border (as we did when we assumed the mobility to be constant). The resulting PDE is the boundary condition we were looking for

$$\frac{1}{\omega} \partial_t u = \varepsilon_\Gamma \Delta_\Gamma u - \varepsilon \partial_n u - F_\Gamma'(u) \quad \text{on } \Gamma,\ \omega > 0. \tag{1.11}$$

The formulation of (1.11) is relatively recent [43], but it has already been widely studied as a way to take into account non-permeable walls, especially with the CH equation (see [44], [45], [46], [47]). Moreover, it has also been coupled with the Caginalp system [48] in [49], and the Allen-Cahn equation [50] in [51], two phase separation models closely related to CH.
However, to the author's knowledge, the problem of using such a boundary condition with the CHO variant has not been studied yet; in such a case, as the reaction phenomenon should be present on Γ too, we propose the following modification of (1.11)

$$\frac{1}{\omega}\partial_t u = \varepsilon_\Gamma \Delta_\Gamma u + \sigma_\Gamma u - \varepsilon \partial_n u - F'_\Gamma(u) \quad \text{on } \Gamma,\ \omega > 0. \tag{1.12}$$

From a practical point of view this condition is not a new one, as it is the same as in, e.g., [45]; however, when present, the term $\sigma_\Gamma u$ is considered to come from the nonlinearity f_Γ, and made explicit for technical reasons. The main difference with the case we are considering is that this constant should be of the same order of magnitude of σ: we however allow it to be different to account the chance that the boundary boosts or inhibits the reaction.

1.6 CHO with dynamic boundary conditions

We now have all the elements to state the problem which is under analysis in this paper. We thus use (1.8)-(1.9) together with the boundary conditions (1.6), (1.12) and write

$$\begin{cases} \partial_t u + \sigma u - \Delta w = 0 & \text{in } \Omega,\ t > 0 \\ w = -\Delta u + F'(u) - g & \text{in } \Omega,\ t > 0 \\ \partial_n w = 0 & \text{on } \Gamma,\ t > 0 \\ \partial_t u + \partial_n u - \Delta_\Gamma u + F'_\Gamma(u) + \sigma_\Gamma u = g_\Gamma & \text{on } \Gamma,\ t > 0 \\ u|_{t=0} = u_0 & \text{on } \overline{\Omega} = \Omega \cup \Gamma \end{cases}$$

We also added the source terms g and g_Γ in order to consider a more generic formulation; we moreover set the parameters other than the reaction ones as $\overline{m} = 0$, $\varepsilon = \varepsilon_\Gamma = \omega = 1$ without loss of generality.

The plan of the thesis is the following:

- Chapter 2 is devoted to the proof of well-posedness of the above system; under some assumptions on the data the existence, uniqueness and continuous dependence on the initial datum are proven.
- In Chapter 3 we present a short introduction to the analysis of long time behavior for dissipative dynamical systems, and some theoretical results are then applied to our problem.

- In Chapter 4 a Galerkin $\mathbb{P}^1$ finite elements discretization is formulated, and some error estimates are proven; furthermore numerical simulations are executed with the aid of the FreeFem++ software, with various choices for the problem's parameters. These simulations are then discussed and compared with results found in literature.
- Conclusions and future work contains a brief summary of the results obtained, and some aspects of interest not covered in this work that might be explored.
- Appendix A contains the main results used throughout the paper, regarding both functional and numerical analysis; Appendix B contains the FreeFem++ code used for the simulations.

Chapter 2

Well-posedness

In this chapter, we show that the CHO equation, coupled with the dynamic boundary condition (1.12), is well posed. This means proving that for each initial datum u_0 there corresponds a unique solution to the problem, and that this solution is stable, in a suitable space, under small perturbations of u_0. These results are essential for both the study of the asymptotic behavior and the numerical analysis.

For the proof of existence we will use a Faedo-Galerkin method, following the same arguments used in [44]; we will then prove the continuous dependence on the initial datum, and the uniqueness as an immediate consequence.

2.1 Classical formulation and hypothesis

We recall the classical formulation of the problem we want to analyze

$$
\text{(CHO-D)}\begin{cases}
\partial_t u + \sigma u - \Delta w = 0 & \text{in } \Omega,\ t>0 \quad (2.1)\\
w = -\Delta u + f(u) - g & \text{in } \Omega,\ t>0 \quad (2.2)\\
\partial_n w = 0 & \text{on } \Gamma,\ t>0 \quad (2.3)\\
\partial_t u + \partial_n u - \Delta_\Gamma u + f_\Gamma(u) + \sigma_\Gamma u = g_\Gamma & \text{on } \Gamma,\ t>0 \quad (2.4)\\
u|_{t=0} = u_0 & \text{in } \overline{\Omega} \quad (2.5)
\end{cases}
$$

where $\Omega \subset \mathbb{R}^d$, $(d = 2, 3)$ is a smooth (at least of class C^2) and bounded domain, and Γ is its boundary; $T \in (0, +\infty)$ will represent, from now on, the final time. We also set $f = F'$ and $f_\Gamma = F'_\Gamma$.

We will use a regular potential as an approximation of the logarithmic one; f will therefore be, as explained in the introduction, an odd-degree polynomial with positive leading coefficient

$$
f(s) = \sum_{j=1}^{2p-1} a_j s^j, \qquad p \in \mathbb{N} \cap [2, +\infty),\ a_{2p-1} > 0, \tag{2.6}
$$

where the classical regular approximation is obtained with $p = 2$ and coefficients

$a_3 = 1$, $a_2 = 0$ and $a_1 = -1$ (see, e.g., [31], [52] and [53]). We remark that this definition, in particular, implies that f is dissipative

$$\liminf_{|s|\to\infty} f'(s) > 0,$$

and as a consequence, due to the regularity of the potential, there must exist a constant $c_0 \geq 0$ such that

$$f'(s) \geq -c_0, \qquad \forall s \in \mathbb{R}. \tag{2.7}$$

We observe that F is thus given by

$$F(s) = \int_0^s f(r)\mathrm{dr} = \sum_{j=2}^{2p} b_j s^j + C_F, \qquad C_F \in \mathbb{R},$$

where clearly $a_{j-1} = jb_j$, and the constant C_F is given.

It is not clear yet if $(\mathrm{CHO}-\mathrm{D})$ possesses a solution, without growth restrictions on f. So we will ask that, additionally, one of the following alternatives holds

$$\begin{gathered} p = 2, \qquad \text{if } d = 3, \\ \text{or} \\ p \in \mathbb{N} \cap [2, +\infty), \qquad \text{if } d = 2. \end{gathered} \tag{2.8}$$

We remark that these requirements are in agreement with the growth condition on f presented in many works dealing with a regular potential, such as [42], [44], [54].

Concerning the nonlinearity f_Γ, we will assume that it is of the form

$$f_\Gamma(s) = \sum_{j=1}^{2q-1} a_{\Gamma,j} s^j, \qquad q \in \mathbb{N} \cap [2, +\infty),\ a_{\Gamma,2q-1} > 0, \tag{2.9}$$

from which follows, in particular, that f_Γ too is dissipative; it hence holds

$$f'_\Gamma(s) \geq -c_{0,\Gamma}, \qquad \forall s \in \mathbb{R}, \tag{2.10}$$

for some nonnegative $c_{0,\Gamma}$. Finally, we ask for the following minimal requirements on data

$$\sigma > 0, \quad \sigma_\Gamma > 0, \tag{2.11}$$

$$g \in H^1(0, T; L^2(\Omega)), \quad g_\Gamma \in H^1(0, T; L^2(\Gamma)), \tag{2.12}$$

$$u_0 \in H^1(\Omega), \quad u_0|_\Gamma \in H^1(\Gamma). \tag{2.13}$$

Conditions (2.11) do not represent a real limitation, due to the symmetry of the order parameter u (see the Introduction); we however exclude the case $\sigma = 0$, since

it has already been widely studied in literature. On the other hand, the case with $\sigma_\Gamma = 0$ could be treated obtaining a term of the form $\lambda_\Gamma u$, $\lambda_\Gamma > 0$, simply modifying the nonlinearity f_Γ (such a procedure does not alter its definition).
Assumptions (2.12) are essential for the well-posedness to be established (as will be clear from the proof of existence of a discretized solution); we finally remark that (2.13) are necessary for the formulation of the problem to make sense at $t = 0$.

Arguing now similarly as we did when we presented the CHO equation in the Introduction, we multiply (2.1) by $\frac{1}{|\Omega|}$ and integrate over Ω; we then immediately see (due to (2.3)) that

$$\frac{\mathrm{d}}{\mathrm{dt}}\langle u\rangle + \sigma\langle u\rangle = 0, \tag{2.14}$$

where

$$\langle\phi\rangle = \frac{1}{|\Omega|}\int_\Omega \phi \qquad \forall\phi \in L^1(\Omega),$$

represents the mean value of function ϕ in Ω. The solution of ODE (2.14) is

$$\langle u\rangle = \langle u_0\rangle e^{-\sigma t}, \tag{2.15}$$

that is, the spatial average of the solution decays to 0 exponentially fast.
As already pointed out, if $\sigma = 0$, $(\mathrm{CHO}-\mathrm{D})$ becomes the well known CH equation endowed with dynamic boundary conditions; in this case, (2.15) simply tells us that the mean value of function u is fixed over time (that is, the mass is conserved).

Dealing with a function whose average is not fixed presents some intrinsic difficulties; it will be clear from the estimates that we will later develop that we need to work with a null mean function, defined as

$$\overline{u}(t) := u(t) - \langle u(t)\rangle = u(t) - \langle u_0\rangle e^{-\sigma t} \quad \forall t \geq 0. \tag{2.16}$$

This operation will prove to be essential, since it allows us to use many of the results collected in Appendix A; as an example, the well-known Poincaré inequality with its consequences. So, we use (2.16) to write $(\mathrm{CHO}-\mathrm{D})$ in the equivalent form

$$\begin{cases}
\partial_t\overline{u} + \sigma\overline{u} - \Delta w = 0 & \text{in } \Omega,\ t > 0 \quad (2.17)\\
w = -\Delta\overline{u} + f(u) - g & \text{in } \Omega,\ t > 0 \quad (2.18)\\
\partial_n w = 0 & \text{on } \Gamma,\ t > 0 \quad (2.19)\\
\partial_t\overline{u} + \partial_n\overline{u} - \Delta_\Gamma\overline{u} + f_\Gamma(u) + \sigma_\Gamma\overline{u} = g_\Gamma + (\sigma - \sigma_\Gamma)\langle u_0\rangle e^{-\sigma t} & \text{on } \Gamma,\ t > 0 \quad (2.20)\\
\overline{u}|_{t=0} = u_0 - \langle u_0\rangle & \text{in } \overline{\Omega} \quad (2.21)
\end{cases}$$

Remark 2.1 The last term in (2.20) is justified by the fact that (2.16) implies

$$\partial_t u = \partial_t \overline{u} - \sigma \langle u_0 \rangle e^{-\sigma t}$$

and

$$\sigma_\Gamma u = \sigma_\Gamma \overline{u} + \sigma_\Gamma \langle u_0 \rangle e^{-\sigma t}$$

while the other terms hold unchanged with respect to (CHO − D) for obvious reasons. We thus made explicit how the difference between the reaction parameters in Ω and Γ influences the problem, as it results in what can be seen as an additional source term on Γ, which vanishes exponentially fast as time goes to infinity.

Remark 2.2 By definition we have

$$\partial_t \overline{u} + \sigma \overline{u} = \partial_t u + \sigma u, \tag{2.22}$$

so, as a trivial consequence which will be useful in obtaining some of the a priori estimate, it holds

$$\partial_t \overline{u} = \partial_t u + \sigma (u - \overline{u}). \tag{2.23}$$

Remark 2.3 We point out a few rules that we will be following:

- As already did in the formulation of (2.17)-(2.21), we take for granted that $u = \overline{u} + \langle u_0 \rangle e^{-\sigma t}$; all of the theorems and formulations will refer to $\overline{u}$ throughout this chapter, the only exception being that of the continuous dependence on initial data. It is however trivial to show that, by a simple translation, every result is inherited by u.

- We will make use (especially in the a priori estimates) of various constants; when the dependence on the problem's parameters can be ignored, we will use the generic letters c, C, possibly numbered. Otherwise, we will add the parameter as a subscript when we want to emphasize this dependence, such as in C_R.

- We will write $|\cdot|_0$, $|\cdot|_1$ instead of $||\cdot||_{L^2(\Omega)}$, $||\nabla \cdot||_{L^2(\Omega)}$ (and equivalently for the norms on Γ) in order not to make the text too heavy.

- Finally, again for the sake of readability, we will use the same symbol for a function on Ω and its trace on Γ, as long as the difference is clear. We will however add the restriction operator $\cdot|_\Gamma$ when more care is needed.

2.2 Weak formulation and main results

We relabel for convenience the following function spaces

$$
\begin{gathered}
V = H^1(\Omega) \quad H = L^2(\Omega), \\
V_\Gamma = H^1(\Gamma) \quad H_\Gamma = L^2(\Gamma), \\
W = \{u \in V \mid u|_\Gamma \in V_\Gamma\} \\
V_0 = \{v \in V \mid \langle v \rangle = 0\} \quad V_0^* = \{v^* \in V^* \mid \langle v^* \rangle = 0\},
\end{gathered}
$$

for which it is well-known that the following embeddings hold

$$
\begin{gathered}
V \subset\subset H = H^* \subset V^*, \\
V_\Gamma \subset\subset H_\Gamma = (H_\Gamma)^* \subset (V_\Gamma)^*.
\end{gathered}
$$

Furthermore, we recall that W equipped with the graph norm

$$
||u||_W := \left(||u||_V^2 + ||u|_\Gamma||_{V_\Gamma}^2 \right)^{1/2} \quad \forall u \in W,
$$

is a Hilbert space with the induced inner product.

Our goal in this section is to write the weak formulation of (2.17)-(2.21), whose solution has to be looked for in some combination of these spaces.
To this aim, we multiply (2.17) and (2.18) by a test function and integrate over Ω, thus obtaining the weak formulation:

we look for a couple $(\overline{u}, w)$ such that

$$
\overline{u} \in L^2(0,T;V) \cap H^1(0,T;V^*), \tag{2.24}
$$

$$
\overline{u}|_\Gamma \in L^2(0,T;V_\Gamma) \cap H^1(0,T;H_\Gamma), \tag{2.25}
$$

$$
w \in L^2(0,T;V), \tag{2.26}
$$

$$
f(u) \in L^2(0,T;H), \quad f_\Gamma(u) \in L^2(0,T;H_\Gamma), \tag{2.27}
$$

$$
\overline{u}|_{t=0} = u_0 - \langle u_0 \rangle, \tag{2.28}
$$

and satisfying for a.a. $t \in (0,T)$

$$
\begin{cases}
\langle \partial_t \overline{u}, y \rangle_{V^*} + \sigma \int_\Omega \overline{u} y + \int_\Omega \nabla w \cdot \nabla y = 0 \qquad \forall y \in V, & (2.29) \\
\int_\Omega w y = \int_\Omega \nabla \overline{u} \cdot \nabla y + \int_\Omega (f(u) - g) y \\
\qquad + \int_\Gamma \partial_t \overline{u} y + \int_\Gamma \nabla_\Gamma \overline{u} \cdot \nabla_\Gamma y + \sigma_\Gamma \int_\Gamma \overline{u} y \\
\qquad + \int_\Gamma (f_\Gamma(u) - g_\Gamma) y - (\sigma - \sigma_\Gamma) \langle u_0 \rangle \int_\Gamma e^{-\sigma t} y \qquad \forall y \in W. & (2.30)
\end{cases}
$$

We can now state the main results of this chapter, that will be proved in the next two sections.

Theorem 2.4 *Assume* (2.6), (2.9) *and* (2.11)-(2.13). *If* (2.8) *holds, then there exists a unique couple* $(\overline{u}, w)$ *solving problem* (2.29)-(2.30) *and satisfying* (2.24)-(2.28).

Corollary 2.5 *Let the assumptions of Theorem 2.4 be satisfied. Then, if* $\overline{u}_1$ *and* $\overline{u}_2$ *are two solutions of* (2.29)-(2.30) *corresponding to initial data* $u_{0,1}$*,* $u_{0,2}$ *such that* $\max_{i=1,2} ||u_{0,i}||_W \leq R$*, it holds:*

$$||u_1 - u_2||_{C^0([0,T];V^*)} + ||u_1 - u_2||_{C^0([0,T];H_\Gamma)} \leq C_{R,T}||u_{0,1} - u_{0,2}||_W. \tag{2.31}$$

That is, the weak solution is continuously dependent on the initial datum with respect to the weaker metric

$$d_w(x, y) = ||x - y||_{V^*} + ||x - y||_{H_\Gamma}.$$

2.3 Proof of Theorem 2.4 and Corollary 2.5

As already pointed out, we will prove Theorem 2.4 using a Faedo-Galerkin procedure. So, as a first step, we write the problem in a finite-dimensional subspace V_n and show that it possess a unique (local in time) solution. Then, we develop some a priori estimates which allow us to extend the local solution to the whole $(0, T)$, and take the limit as $n \to \infty$, thus proving the existence of a solution for problem (2.29)-(2.30).

2.3.1 Discretized problem

Let $(e_k)_{k\in\mathbb{N}}$ be the set of eigenfunctions of the Laplace operator with homogeneous Neumann condition, which we normalize so that it forms an orthonormal base for $L^2(\Omega)$; we then denote by $(\mu_k)_{k\in\mathbb{N}}$ the corresponding eigenvalues, and we consider an ordering of these two sets such that

$$0 = \mu_1 < \mu_2 \leq \mu_3 \leq \dots$$

This is always possible, as well known from spectral theory.

If we define $V_n = \text{span}\{e_1, \dots, e_n\}$ as the finite dimensional discretization subspace, we can project our problem on it. Moreover, we define the approximation of the initial datum u_0^n as the $L^2(\Omega)$-projection of u_0 on V_n

$$u_0^n = \sum_{k=1}^{n} \left(\int_\Omega u_0 e_k \right) e_k.$$

The finite dimensional version of the problem then reads:

we look for a couple $(\overline{u}^n, w^n)$ such that

$$\overline{u}^n \in H^1(0,T;V_n), \quad w^n \in L^2(0,T;V_n), \tag{2.32}$$
$$\overline{u}^n(0) = u_0^n - \langle u_0 \rangle, \tag{2.33}$$

and satisfying for a.a. $t \in (0,T)$

$$\begin{cases} \int_\Omega \partial_t \overline{u}^n y + \sigma \int_\Omega \overline{u}^n y + \int_\Omega \nabla w^n \cdot \nabla y = 0 \qquad \forall y \in V_n, & (2.34) \\ \int_\Omega w^n y = \int_\Omega \nabla \overline{u}^n \cdot \nabla y + \int_\Omega (f(u^n) - g) y \\ \qquad + \int_\Gamma \partial_t \overline{u}^n y + \int_\Gamma \nabla_\Gamma \overline{u}^n \cdot \nabla_\Gamma y + \sigma_\Gamma \int_\Gamma \overline{u}^n y \\ \qquad + \int_\Gamma (f_\Gamma(u^n) - g_\Gamma) y - (\sigma - \sigma_\Gamma) \langle u_0 \rangle \int_\Gamma e^{-\sigma t} y \qquad \forall y \in V_n. & (2.35) \end{cases}$$

Remark 2.6 Since the domain is regular, exploiting a classical elliptic regularity result, the eigenfunctions are such that $e_k \in H^2(\Omega) \subset W \subset V$ for every k, and this justifies the choice of a test function in V_n for both (2.34) and (2.35).

Remark 2.7 It is clear that, as we chose $\{e_k\}_{k=1}^\infty$ such that this set forms an orthonormal base for $L^2(\Omega)$, we have in particular $e_1 = |\Omega|^{-1/2}$ and $\langle e_k \rangle = 0 \ \forall k > 1$ (as it is well known). Therefore it must also hold

$$\langle u_0^n \rangle = \left\langle \sum_{k=1}^n \left(\int_\Omega u_0 e_k \right) e_k \right\rangle = e_1^2 \int_\Omega u_0 = \langle u_0 \rangle,$$

and this is the reason why we wrote $\langle u_0 \rangle$ instead of $\langle u_0^n \rangle$ in both (2.33) and (2.35).

From this also follows the unsurprising fact

$$\langle \overline{u}^n(t) \rangle = 0 \quad \forall t \geq 0.$$

We can now prove the following

Proposition 2.8 *The discretized problem* (2.34)-(2.35) *possesses a unique local in time solution.*

Proof First we set

$$\overline{u}^n(t) := \sum_{j=1}^n \varphi_j(t) e_j, \quad w^n(t) := \sum_{j=1}^n w_j(t) e_j,$$
$$y = e_i \quad i = 1, \dots, n,$$

and define

$$a_{ij} := \int_\Omega e_j e_i = \delta_{ij}, \quad b_{ij} := \int_\Omega \nabla e_j \cdot \nabla e_i = \mu_i \delta_{ij},$$
$$a^\Gamma_{ij} := \int_\Gamma e_j e_i, \quad b^\Gamma_{ij} := \int_\Gamma \nabla_\Gamma e_j \cdot \nabla_\Gamma e_i,$$

which will denote the coefficients of matrices A, B, A_Γ and B_Γ, respectively. Then we notice that

$$\overline{u}^n(0) = u_0^n - \langle u_0 \rangle \quad \Rightarrow \quad \sum_{j=1}^n \varphi_j(0) e_j = \sum_{j=1}^n \left(\int_\Omega u_0 e_j \right) e_j - \langle u_0 \rangle.$$

Hence, if we take the mean value on both sides of the last equality, we can use the same argument of Remark 2.7 to show that

$$\varphi_1(0) = 0. \tag{2.36}$$

Now problem (2.34)-(2.35) can be rewritten in the equivalent form of a system of ODEs

$$\begin{cases} \dot{\boldsymbol{\varphi}}(t) + \sigma \boldsymbol{\varphi}(t) + B\mathbf{w}(t) = 0 & (2.37) \\ \mathbf{w}(t) = B\boldsymbol{\varphi}(t) + \mathbf{F}(\boldsymbol{\varphi}(t), t) - \mathbf{G}(t) + A_\Gamma \dot{\boldsymbol{\varphi}}(t) + B_\Gamma \boldsymbol{\varphi}(t) & \\ \qquad + \sigma_\Gamma A_\Gamma \boldsymbol{\varphi}(t) + \mathbf{F}_\Gamma(\boldsymbol{\varphi}(t), t) - \mathbf{G}_\Gamma(t) & (2.38) \\ \varphi_1(0) = 0 & \\ \varphi_j(0) = \int_\Omega u_0 e_j \quad j = 2, \dots, n, & \end{cases}$$

where we set $\boldsymbol{\varphi}(t) = (\varphi_j(t))_{j=1}^n$, $\mathbf{w}(t) = (w_j(t))_{j=1}^n$ and

$$F_j(\boldsymbol{\varphi}(t), t) := \int_\Omega f \left(\langle u_0 \rangle e^{-\sigma t} + \sum_{k=2}^n \varphi_k(t) e_k \right) e_j,$$
$$F_{\Gamma,j}(\boldsymbol{\varphi}(t), t) := \int_\Gamma f_\Gamma \left(\langle u_0 \rangle e^{-\sigma t} + \sum_{k=2}^n \varphi_k(t) e_k \right) e_j,$$
$$G_j(t) := \int_\Omega g(t) e_j, \qquad G_{\Gamma,j}(t) := \int_\Gamma \left(g_\Gamma(t) + (\sigma - \sigma_\Gamma) \langle u_0 \rangle e^{-\sigma t} \right) e_j.$$

Making explicit the term $\dot{\boldsymbol{\varphi}}(t)$ in (2.37) we get

$$\dot{\boldsymbol{\varphi}}(t) = -B\mathbf{w}(t) - \sigma \boldsymbol{\varphi}(t),$$

and substituting (2.38) in this equation leads to, after reordering

$$
\begin{aligned}
(I + BA_\Gamma)\dot{\boldsymbol{\varphi}}(t) = &- \Big(\sigma I + \sigma_\Gamma BA_\Gamma + BB + BB_\Gamma\Big)\boldsymbol{\varphi}(t) \\
&- B\Big(\mathbf{F}(\boldsymbol{\varphi}(t),t) + \mathbf{F}_\Gamma(\boldsymbol{\varphi}(t),t)\Big) + B\Big(\mathbf{G}(t) + \mathbf{G}_\Gamma(t)\Big).
\end{aligned} \tag{2.39}
$$

The first line of system (2.39), owing to the definition of B and to (2.36), is simply

$$
\frac{\mathrm{d}}{\mathrm{dt}}\varphi_1(t) = -\sigma\varphi_1(t) = 0, \quad \text{a.a. } t \geq 0,
$$

and this fact, together with (2.36), suggests us to eliminate the first row and column of (2.39), thus getting the reduced system

$$
\begin{cases}
(I_{n-1} + CD)\dot{\mathbf{x}}(t) = \boldsymbol{\Lambda}(t) - \boldsymbol{\Pi}(\mathbf{x}(t),t) \\
x_j(0) = \displaystyle\int_\Omega u_0 e_{j+1} \quad j = 1,\dots,n-1,
\end{cases} \tag{2.40}
$$

where we set for readability $\mathbf{x}(t) = (\varphi_2(t),\dots,\varphi_n(t))^T \in \mathbb{R}^{n-1}$, $C = B_{n-1}$, $D = A_{\Gamma,n-1}$, $E = B_{\Gamma,n-1}$ and

$$
\begin{aligned}
\boldsymbol{\Lambda}(t) &= C\left(\mathbf{G}_{n-1}(t) + \mathbf{G}_{\Gamma,n-1}(t)\right), \\
\boldsymbol{\Pi}(\mathbf{x}(t),t) &= (\sigma I_{n-1} + \sigma_\Gamma CD + CC + CE)\mathbf{x}(t) \\
&\quad + C(\mathbf{F}_{n-1}(\mathbf{x}(t),t) + \mathbf{F}_{\Gamma,n-1}(\mathbf{x}(t),t)).
\end{aligned}
$$

The $n-1$ subscript has the clear meaning of restriction by elimination of the first row and column.

We now show that the matrix on the left hand side of (2.40) is invertible.
Indeed C is diagonal and positive definite (since $\mu_k > 0\ \forall k > 1$), so C is invertible and C^{-1} is diagonal and positive definite. Moreover D is at least positive semidefinite, since this property holds for A_Γ

$$
\mathbf{z}^T A_\Gamma \mathbf{z} = \Big(\sum_{j=1}^n z_j \int_\Gamma \Big(\sum_{i=1}^n z_i e_i\Big) e_j\Big) = \int_\Gamma \Big(\sum_{j=1}^n z_j e_j\Big)^2 \geq 0 \quad \forall \mathbf{z} \in \mathbb{R}^n.
$$

Hence $(I_{n-1} + CD)$ is positive definite and we are allowed to write

$$
\begin{cases}
\dot{\mathbf{x}}(t) = (I_{n-1} + CD)^{-1}(\boldsymbol{\Lambda}(t) - \boldsymbol{\Pi}(\mathbf{x}(t),t)) \\
x_j(0) = \displaystyle\int_\Omega u_0 e_{j+1} \quad j = 1,\dots,n-1.
\end{cases}
$$

Since $g \in H^1(0,T;H)$ and $g_\Gamma \in H^1(0,T;H_\Gamma)$, we have $\boldsymbol{\Lambda}(t) \in H^1(0,T;\mathbb{R}^{n-1})$ and consequently $\boldsymbol{\Lambda}(t) \in C^0([0,T];\mathbb{R}^{n-1})$; moreover, $\boldsymbol{\Pi}(\mathbf{x}(t),t)$ is continuous in both t and $\mathbf{x}$, due to the continuity of f and f_Γ.
Then, it is trivial to check that $\boldsymbol{\Pi}(\mathbf{x}(t),t)$ is also (at least locally) Lipschitz in $\mathbf{x}$, uniformly with respect to t (since $\langle u_0\rangle e^{-\sigma t}$ is bounded), and so is the whole right hand side of the equation.

Hence, it finally suffices to invoke the well known Picard-Lindelöf theorem, obtaining the existence and uniqueness of a local solution in some interval $[0, T_n]$, where $T_n \in (0, T)$, for problem (2.34)-(2.35).

□

2.3.2 A priori estimates

We now prove some a priori estimates, independent on the discretization parameter n. Here the main difficulty is represented by the fact that we have to deal with both u^n and $\overline{u}^n$, as it is clear that we cannot exploit an expression like $f(\overline{u}^n)$ because of the nonlinearity of f. On the other hand, we will need to choose $\overline{u}^n$, $\partial_t \overline{u}^n$ as test functions in (2.35); therefore, the first estimate we prove is an upper bound for the quantities $f(u^n)\overline{u}^n$ and $f_\Gamma(u^n)\overline{u}^n$.

We will be extensively using the operator

$$\mathcal{N} : V_0^* \to V_0,$$

which is defined as the solution map for the Poisson problem with homogeneous Neumann condition

$$\int_\Omega \nabla v \cdot \nabla z = \langle g, z \rangle_{V^*} \qquad g \in V_0^*, \;\; \forall\, z \in V_0,$$

that is, $\mathcal{N}(g) = v$. This operator's properties are grouped in Appendix A.2.

A priori estimate for $f(u^n)\overline{u}^n$ and $f_\Gamma(u^n)\overline{u}^n$

We choose $y = \mathcal{N}(\overline{u}^n)$ as test function in (2.34), and $y = \overline{u}^n$ in (2.35). We are allowed to do so, as (2.36) gives us $\langle \overline{u}^n \rangle = 0$; it is moreover clear from the above definition of $\mathcal{N}$ that it must be $\mathcal{N}(\overline{u}^n) \in V_n$.

Thus, using $\mathcal{N}$ properties (A.8) and (A.9), we obtain

$$\begin{cases} \dfrac{1}{2}\dfrac{\mathrm{d}}{\mathrm{dt}}||\overline{u}^n||_*^2 + \sigma||\overline{u}^n||_*^2 + \displaystyle\int_\Omega \nabla w^n \cdot \nabla \mathcal{N}(\overline{u}^n) = 0 & (2.41) \\ \displaystyle\int_\Omega w^n \overline{u}^n = |\overline{u}^n|_1^2 + \int_\Omega f(u^n)\overline{u}^n - \int_\Omega g\overline{u}^n & \\ \qquad + \dfrac{1}{2}\dfrac{\mathrm{d}}{\mathrm{dt}}|\overline{u}^n|_{0,\Gamma}^2 + |\overline{u}^n|_{1,\Gamma}^2 + \sigma_\Gamma |\overline{u}^n|_{0,\Gamma}^2 & \\ \qquad + \displaystyle\int_\Gamma f_\Gamma(u^n)\overline{u}^n - \int_\Gamma g_\Gamma\, \overline{u}^n - (\sigma - \sigma_\Gamma)\langle u_0 \rangle \int_\Gamma e^{-\sigma t}\overline{u}^n. & (2.42) \end{cases}$$

The last term of the first equation and the first one of the second are equivalent due to the definition of $\mathcal{N}$, therefore we can substitute (2.42) in (2.41). After reordering and integrating the resulting equation in $(0,t)$, where $t \in [0,T_n]$, we get

$$
\begin{aligned}
&\frac{1}{2}||\overline{u}^n||_*^2 + \sigma\int_0^t ||\overline{u}^n||_*^2 + \int_0^t |\overline{u}^n|_1^2 + \frac{1}{2}|\overline{u}^n|_{0,\Gamma}^2 + \int_0^t |\overline{u}^n|_{1,\Gamma}^2 \\
&\quad + \sigma_\Gamma \int_0^t |\overline{u}^n|_{0,\Gamma}^2 + \int_0^t\int_\Omega f(u^n)\overline{u}^n + \int_0^t\int_\Gamma f_\Gamma(u^n)\overline{u}^n \\
&= \frac{1}{2}||\overline{u}^n(0)||_*^2 + \frac{1}{2}|\overline{u}^n(0)|_{0,\Gamma}^2 + \int_0^t\int_\Omega g\overline{u}^n + \int_0^t\int_\Gamma \left(g_\Gamma + (\sigma-\sigma_\Gamma)\langle u_0\rangle e^{-\sigma s}\right)\overline{u}^n.
\end{aligned}
$$

In order to find an upper bound, it suffices to use the Cauchy-Schwarz, Poincaré and Young inequalities, in addition to the L^p embedding results for bounded domains, according to the terms on the left; the right hand side can hence be maximized with

$$
\begin{aligned}
&\frac{1}{2}||u_0^n - \langle u_0\rangle||_*^2 + \frac{1}{2}|u_0^n - \langle u_0\rangle|_{0,\Gamma}^2 + C\int_0^t |g|_0|\overline{u}^n|_1 + \int_0^t |g_\Gamma|_{0,\Gamma}|\overline{u}^n|_{0,\Gamma} \\
&\quad + |\sigma-\sigma_\Gamma||\langle u_0\rangle||\Gamma|^{1/2}\int_0^t e^{-\sigma s}|\overline{u}^n|_{0,\Gamma} \\
&\le C\left(||u_0^n - \langle u_0\rangle||_W^2 + \int_0^t |g|_0^2 + \int_0^t |g_\Gamma|_{0,\Gamma}^2 + 1\right) + \frac{1}{2}\int_0^t |\overline{u}^n|_1^2 + \frac{\sigma_\Gamma}{2}\int_0^t |\overline{u}^n|_{0,\Gamma}^2
\end{aligned}
$$

so we get, simplifying and neglecting the remaining positive terms on the left hand side

$$
\int_0^t\int_\Omega f(u^n)\overline{u}^n + \int_0^t\int_\Gamma f_\Gamma(u^n)\overline{u}^n \le C\left(1 + ||u_0^n||_W^2 + \int_0^t |g|_0^2 + \int_0^t |g_\Gamma|_{0,\Gamma}^2\right) \tag{2.43}
$$

for every $t \in [0,T_n]$, where the constant C depends on $\langle u_0\rangle, \sigma, \sigma_\Gamma$, $|\Gamma|$ and Ω. We also remark that since

$$
\begin{aligned}
\int_0^t e^{-\sigma s}|\overline{u}^n|_{0,\Gamma} &\le C_\varepsilon \int_0^t e^{-2\sigma s} + \varepsilon\int_0^t |\overline{u}^n|_{0,\Gamma}^2 \\
&< \frac{C_\varepsilon}{2\sigma} + \varepsilon\int_0^t |\overline{u}^n|_{0,\Gamma}^2, \quad \forall\,\varepsilon > 0,\ \ \forall\, t\in[0,T_n],
\end{aligned} \tag{2.44}
$$

C, in particular, does not depend on T_n.

A priori estimate for $\overline{u}^n$ and $\partial_t\overline{u}^n$

We set $y = \mathcal{N}(\partial_t\overline{u}^n)$ in (2.34), $y = \partial_t\overline{u}^n$ in (2.35); such choices are once again admittable, as the arguments explained in the previous estimate hold almost unchanged.

Thus, proceeding in a similar fashion as in the previous paragraph, we get

$$
\begin{aligned}
&\int_0^t ||\partial_t \overline{u}^n||_*^2 + \frac{\sigma}{2}||\overline{u}^n||_*^2 + \frac{1}{2}|\overline{u}^n|_1^2 + \int_0^t |\partial_t \overline{u}^n|_{0,\Gamma}^2 + \frac{1}{2}|\overline{u}^n|_{1,\Gamma}^2 + \frac{\sigma_\Gamma}{2}|\overline{u}^n|_{0,\Gamma}^2 \\
&\quad + \int_0^t \int_\Omega f(u^n)\partial_t \overline{u}^n + \int_0^t \int_\Gamma f_\Gamma(u^n)\partial_t \overline{u}^n \\
&= \frac{\sigma}{2}||\overline{u}^n(0)||_*^2 + \frac{1}{2}|\overline{u}^n(0)|_1^2 + \frac{1}{2}|\overline{u}^n(0)|_{1,\Gamma}^2 + \frac{\sigma_\Gamma}{2}|\overline{u}^n(0)|_{0,\Gamma}^2 + \int_0^t \int_\Omega g\partial_t \overline{u}^n \\
&\quad + \int_0^t \int_\Gamma \left(g_\Gamma + (\sigma - \sigma_\Gamma)\langle u_0\rangle e^{-\sigma s}\right)\partial_t \overline{u}^n.
\end{aligned}
\tag{2.45}
$$

We now notice that, according to (2.23), the second to last term on the left hand side can be rewritten in the following way

$$
\begin{aligned}
\int_0^t \int_\Omega f(u^n)\partial_t \overline{u}^n &= \int_0^t \int_\Omega f(u^n)\partial_t u^n + \sigma \int_0^t \int_\Omega f(u^n)(u^n - \overline{u}^n) \\
&= \int_0^t \int_\Omega \frac{\mathrm{d}}{\mathrm{dt}} F(u^n) + \sigma \int_0^t \int_\Omega f(u^n)(u^n - \overline{u}^n) \\
&= \int_\Omega F(u^n) - \int_\Omega F(u^n(0)) + \sigma \int_0^t \int_\Omega f(u^n)u^n - \sigma \int_0^t \int_\Omega f(u^n)\overline{u}^n.
\end{aligned}
$$

Then, due to the definition of F, it is trivial to show that it holds (since $b_{2p} > 0$)

$$
-C_1 \leq F(s) \leq C_2|s|^{2p} + C_3 \quad \forall\, s \in \mathbb{R}.
$$

with C_i suitable positive constants. Moreover, because of (2.7) and the fact that $f(0) = 0$, we have

$$
f(s)s \geq -c_0|s|^2 \quad \forall\, s \in \mathbb{R}.
$$

Hence, collecting the above results, we get

$$
\begin{aligned}
\int_0^t \int_\Omega f(u^n)\partial_t \overline{u}^n \geq &- C\left(||u_0^n||_{L^{2p}(\Omega)}^{2p} + 1\right) - \sigma c_0 \int_0^t |u^n|_0^2 \\
&- \sigma \int_0^t \int_\Omega f(u^n)\overline{u}^n,
\end{aligned}
\tag{2.46}
$$

and move these terms to the right hand side of (2.45); we then remark that, because of (2.9)-(2.10), the same argument applies to f_Γ, and we will write

$$
\begin{aligned}
\int_0^t \int_\Gamma f_\Gamma(u^n)\partial_t \overline{u}^n \geq &- C\left(||u_0^n||_{L^{2q}(\Gamma)}^{2q} + 1\right) - \sigma c_{0,\Gamma} \int_0^t |u^n|_{0,\Gamma}^2 \\
&- \sigma \int_0^t \int_\Gamma f_\Gamma(u^n)\overline{u}^n.
\end{aligned}
\tag{2.47}
$$

We hence use (2.46) and (2.47) in (2.45), thus getting

$$\begin{aligned}
&\int_0^t ||\partial_t\overline{u}^n||_*^2 + \frac{\sigma}{2}||\overline{u}^n||_*^2 + \frac{1}{2}|\overline{u}^n|_1^2 + \int_0^t |\partial_t\overline{u}^n|_{0,\Gamma}^2 + \frac{1}{2}|\overline{u}^n|_{1,\Gamma}^2 + \frac{\sigma_\Gamma}{2}|\overline{u}^n|_{0,\Gamma}^2 \\
&\leq C\left(1 + ||u_0^n||_{L^{2p}(\Omega)}^{2p} + ||u_0^n||_{L^{2q}(\Gamma)}^{2q} + ||u_0^n||_W^2\right) + \int_0^t\int_\Omega g\partial_t\overline{u}^n \\
&\quad + \int_0^t\int_\Gamma \left(g_\Gamma + (\sigma-\sigma_\Gamma)\langle u_0\rangle e^{-\sigma s}\right)\partial_t\overline{u}^n + \sigma\left(\int_0^t\int_\Omega f(u^n)\overline{u}^n + \int_0^t\int_\Gamma f_\Gamma(u^n)\overline{u}^n\right) \\
&\quad + \sigma\left(c_0\int_0^t |u^n|_0^2 + c_{0,\Gamma}\int_0^t |u^n|_{0,\Gamma}^2\right),
\end{aligned} \tag{2.48}$$

where we also maximized the terms containing $\overline{u}^n(0)$. The terms in the second pair of brackets are exactly the ones we estimated in (2.43); on the other hand, the other integrals can be maximized as follows

$$\begin{aligned}
\int_0^t\int_\Omega g\partial_t\overline{u}^n &= \int_\Omega g\overline{u}^n - \int_\Omega g(0)\overline{u}^n(0) - \int_0^t\int_\Omega \partial_t g\overline{u}^n \\
&\leq \frac{1}{4}|g|_0^2 + |\overline{u}^n|_0^2 + \frac{1}{2}|g(0)|_0^2 + \frac{1}{2}|\overline{u}^n(0)|_0^2 + C\int_0^t |\partial_t g|_0^2 + \int_0^t |\overline{u}^n|_1^2 \\
&\leq C\left(1 + ||u_0^n||_W^2 + |g|_0^2 + |g(0)|_0^2 + \int_0^t |\partial_t g|_0^2\right) + |\overline{u}^n|_0^2 + \int_0^t |\overline{u}^n|_1^2.
\end{aligned} \tag{2.49}$$

Here we integrated by parts and applied the Poincaré, Cauchy-Schwarz and Young inequalities. We proceed in a similar fashion with the other terms and get

$$\begin{aligned}
\int_0^t\int_\Gamma \left(g_\Gamma + (\sigma-\sigma_\Gamma)\langle u_0\rangle e^{-\sigma s}\right)\partial_t\overline{u}^n &\leq \int_0^t (|g_\Gamma|_{0,\Gamma} + |\sigma-\sigma_\Gamma||\langle u_0\rangle||\Gamma|^{1/2}e^{-\sigma s})|\partial_t\overline{u}^n|_{0,\Gamma} \\
&\leq C\left(1 + \int_0^t |g_\Gamma|_{0,\Gamma}^2\right) + \frac{1}{2}\int_0^t |\partial_t\overline{u}^n|_{0,\Gamma}^2.
\end{aligned} \tag{2.50}$$

$$\sigma\left(c_0\int_0^t |u^n|_0^2 + c_{0,\Gamma}\int_0^t |u^n|_{0,\Gamma}^2\right) \leq C\left(1 + \int_0^t |\overline{u}^n|_1^2 + \int_0^t |\overline{u}^n|_{0,\Gamma}^2\right). \tag{2.51}$$

All of the constants labeled as C in the above inequalities are once again independent on T_n, as the same argument used for (2.44) holds.

Using now (2.43), (2.49)-(2.51), simplifying and reordering, (2.48) becomes

$$
\begin{aligned}
&\int_0^t ||\partial_t \overline{u}^n||_*^2 + \frac{\sigma}{2}||\overline{u}^n||_*^2 + \frac{1}{2}|\overline{u}^n|_1^2 + \frac{1}{2}\int_0^t |\partial_t \overline{u}^n|_{0,\Gamma}^2 + \frac{1}{2}|\overline{u}^n|_{1,\Gamma}^2 + \frac{\sigma_\Gamma}{2}|\overline{u}^n|_{0,\Gamma}^2 \\
&\leq C_1 \left(1 + ||u_0^n||_{L^{2p}(\Omega)}^{2p} + ||u_0^n||_{L^{2q}(\Gamma)}^{2q} + ||u_0^n||_W^2 + |g|_0^2 + |g(0)|_0^2 + \int_0^t |g|_0^2 \right. \\
&\quad \left. + \int_0^t |\partial_t g|_0^2 + \int_0^t |g_\Gamma|_{0,\Gamma}^2 \right) + C_2 \left(\int_0^t |\overline{u}^n|_{0,\Gamma}^2 + \int_0^t |\overline{u}^n|_1^2 \right) + |\overline{u}^n|_0^2, \quad \forall\, t \in [0, T_n].
\end{aligned} \tag{2.52}
$$

We then recall that, due to the well-known Sobolev embedding theorem, it holds

$$
\begin{aligned}
V &\hookrightarrow L^{p^*}(\Omega) \quad \forall\, p^* \in [2, \infty), \qquad \text{if } d = 2, \\
V &\hookrightarrow L^{p^*}(\Omega) \quad \forall\, p^* \in [2, 6], \qquad \text{if } d = 3.
\end{aligned}
$$

Therefore, for both alternatives in (2.8), we have

$$
||u_0^n||_{L^{2p}(\Omega)}^{2p} \leq c||u_0^n||_W^{2p} \leq C \left(||u_0^n - u_0||_W^{2p} + ||u_0||_W^{2p} \right) \leq C \left(1 + ||u_0||_W^{2p} \right),
$$

where we have exploited the fact that a converging sequence (see (A.2)) is bounded. Treating the term $||u_0^n||_{L^{2q}(\Gamma)}^{2q}$ in the same way, it suffices to use (A.11) on the last term of (2.52) and eliminate some positive quantities on the left in order to get

$$
||\overline{u}^n||_V^2 + |\overline{u}^n|_{0,\Gamma}^2 \leq \widetilde{C}_1 + \widetilde{C}_2 \int_0^t \left(||\overline{u}^n||_V^2 + |\overline{u}^n|_{0,\Gamma}^2 \right) \quad \forall\, t \in [0, T_n]. \tag{2.53}
$$

As already pointed out, $\widetilde{C}_2$ does not depend on T_n; moreover, $\widetilde{C}_1$ is an upper bound for the terms in the first pair of brackets of (2.52), which holds up to $t = T$ due to the sources' regularity (we remark that $|g|_0^2$ and $|g(0)|_0^2$ are bounded too, by $||g||_{H^1(0,T;H)}^2$, since $H^1(0, T; H) \hookrightarrow C^0([0, T]; H)$).
Because of these arguments, (2.53) is actually valid in the whole interval $[0, T]$.

Gronwall's Lemma can now be applied: we conclude that

$$
||\overline{u}^n(t)||_V^2 + |\overline{u}^n(t)|_{0,\Gamma}^2 \leq C \quad \forall\, t \in [0, T]. \tag{2.54}
$$

To be more precise, we point out that the constant C in (2.54) depends on $||u_0||_W$, σ, σ_Γ, Ω and $|\Gamma|$, as well as on f and f_Γ coefficients and the norms $||g||_{H^1(0,T;H)}$, $||g_\Gamma||_{L^2(0,T;H)}$; but it does not depend on n.

Using the last estimate in (2.52), we get the more general result

$$
||\overline{u}^n||_{L^\infty(0,T;V) \cap H^1(0,T;V^*)} + ||\overline{u}^n||_{L^\infty(0,T;V_\Gamma) \cap H^1(0,T;H_\Gamma)} \leq C. \tag{2.55}
$$

Remark 2.9 Estimate (2.55) tells us in particular that the unique, local solution of the discretized problem can be extended up to the final time T.

Remark 2.10 We make explicit an obvious, nonetheless useful, consequence of (2.55); if the initial data is chosen from a bounded subset of W

$$||u_0||_W \leq R, \tag{2.56}$$

while the other parameters are fixed, then it must hold

$$||u^n||_{L^\infty(0,T;V)} + ||u^n||_{L^\infty(0,T;V_\Gamma)} \leq C_R,$$

for every solution correspondent to an initial datum such that (2.56) is satisfied. Once the existence of the solution is proved, the same estimate will be valid for u: we will be using it in the proof of continuous dependence on the initial data.

A priori estimate for $f(u)$ and $f_\Gamma(u)$

We use once more the Sobolev embedding theorem cited in the previous paragraph. It is indeed straightforward to check that

$$||u^n||^{p^*}_{L^{p^*}(0,T;L^{p^*}(\Omega))} \leq C_1 + C_2||\overline{u}^n||^{p^*}_{L^\infty(0,T;V)} \leq C,$$

for every $p^* \geq 2$ if $d = 2$, and for $p^* \in [2, 6]$ if $d = 3$.

Therefore, for both options in (2.8), it holds

$$\begin{aligned} ||f(u^n)||^2_{L^2(0,T;H)} &= \int_0^T \int_\Omega \left| \sum_{j=1}^{2p-1} a_j \, [u^n]^j \right|^2 \leq C \int_0^T \int_\Omega \sum_{j=1}^{2p-1} |u^n|^{2j} \\ &\leq C \sum_{p^*=2}^{4p-2} ||u^n||^{p^*}_{L^{p^*}(0,T;L^{p^*}(\Omega))} \leq C, \end{aligned} \tag{2.57}$$

since $4p - 2 = 6$ when $d = 3$ (and hence $p = 2$).

Regarding f_Γ, we can clearly apply the same argument and get

$$||f_\Gamma(u^n)||^2_{L^2(0,T;H_\Gamma)} \leq C.$$

We remark that all these constants, as we exploited the previous estimates, depend on the same parameters as the bounds for $\overline{u}^n$ norms.

A priori estimate for w^n

If we test (2.34) by $y = w^n - \langle w^n \rangle$ and integrate over $(0,T)$, we obtain

$$\int_0^T \int_\Omega \partial_t \overline{u}^n (w^n - \langle w^n \rangle) + \sigma \int_0^T \int_\Omega \overline{u}^n (w^n - \langle w^n \rangle) + \int_0^T |w^n|_1^2 = 0.$$

The first integral can be seen as the duality pairing

$$\int_0^T \langle \partial_t \overline{u}^n, (w^n - \langle w^n \rangle) \rangle_{V^*},$$

with $\partial_t \overline{u}^n \in V^*$; so, applying once more the Cauchy-Schwarz and Young inequalities we get

$$\begin{aligned} \int_0^T |w^n|_1^2 &\leq \int_0^T ||\partial_t \overline{u}^n||_{V^*} ||w^n - \langle w^n \rangle||_V + \sigma \int_0^T |\overline{u}^n|_0 |w^n - \langle w^n \rangle|_0 \\ &\leq C + \frac{1}{2} \int_0^T |w^n|_1^2, \end{aligned} \tag{2.58}$$

where we also used the Poincaré inequality and the boundedness of $\overline{u}^n$ in $H^1(0,T;V^*)$ and $L^2(0,T;H)$.

Now that we have a bound for the norm of ∇w^n, we need one for its mean value in order to use (A.10). We get it by choosing $y = \frac{1}{|\Omega|}$ in (2.35), squaring and integrating over $(0,T)$

$$\begin{aligned} \int_0^T |\langle w^n \rangle|^2 \leq C \Bigg(&\int_0^T |f(u^n)|_0^2 + \int_0^T |g|_0^2 + \int_0^T |\partial_t \overline{u}^n|_{0,\Gamma}^2 + \int_0^T |\overline{u}^n|_{0,\Gamma}^2 \\ &+ \int_0^T |f_\Gamma(u^n)|_{0,\Gamma}^2 + \int_0^T |g_\Gamma|_{0,\Gamma}^2 + 1 \Bigg) \leq C, \end{aligned} \tag{2.59}$$

owing to the previous estimates.

Finally, we simply sum up (2.58) and (2.59), thus getting

$$\int_0^T ||w^n||_V^2 \leq C \int_0^T \left(|w^n|_1^2 + |\langle w^n \rangle|^2 \right) \leq C,$$

and concluding

$$||w^n(t)||_{L^2(0,T;V)}^2 \leq C.$$

2.3.3 Existence of a solution

We now take advantage of these estimates in order to get some convergence results that will be essential to prove Theorem 2.4, as we take the limit $n \to \infty$. In the previous subsection we found out that

$$\begin{aligned} \overline{u}^n \text{ is bounded in } L^\infty(0,T;V), \qquad & \overline{u}^n|_\Gamma \text{ is bounded in } L^\infty(0,T;V_\Gamma), \\ \partial_t \overline{u}^n \text{ is bounded in } L^2(0,T;V^*), \quad & \partial_t \overline{u}^n|_\Gamma \text{ is bounded in } L^2(0,T;H_\Gamma). \end{aligned}$$

We hence recall a result from [55] that we will be using to exploit these estimates

Theorem 2.11 *Let X, B and Y be Banach spaces such that*

$$X \subset\subset B \subset Y,$$

and F be a bounded set in $L^\infty(0,T;X)$ such that $\partial_t F = \{\partial_t f \mid f \in F\}$ is bounded in $L^p(0,T;Y)$, with $p > 1$. Then, F is relatively compact in $C([0,T],B)$.

The hypothesis fit our case with

$$X = V, \ B = H, \ Y = V^*, \quad F = (\overline{u}^n)_{n \in \mathbb{N}},$$

in Ω, and

$$X = V_\Gamma, \ B = Y = H_\Gamma, \quad F = (\overline{u}^n|_\Gamma)_{n \in \mathbb{N}},$$

on Γ. Theorem 2.11 then gives

$$\begin{gathered} \overline{u}^n \text{ is relatively compact in } C([0,T];H), \\ \overline{u}^n|_\Gamma \text{ is relatively compact in } C([0,T];H_\Gamma), \end{gathered}$$

thus obtaining

$$\begin{gathered} \overline{u}^n \to \overline{u} \text{ strongly in } C([0,T];H), \\ \overline{u}^n|_\Gamma \to \overline{u}|_\Gamma \text{ strongly in } C([0,T];H_\Gamma), \end{gathered} \tag{2.60}$$

at least for a subsequence.

Then, we notice that $L^\infty(0,T;V)) = (L^1(0,T;V^*))^*$ where $L^1(0,T;V^*)$ is separable; moreover $H^1(0,T;V^*)$ is reflexive. So, due to the Banach-Alaoglu theorem, we get the convergences

$$\overline{u}^n \overset{*}{\rightharpoonup} \overline{u} \text{ in } L^\infty(0,T;V), \quad \overline{u}^n \rightharpoonup \overline{u} \text{ in } H^1(0,T;V^*),$$

and similarly on Γ

$$\overline{u}^n|_\Gamma \overset{*}{\rightharpoonup} \overline{u}|_\Gamma \text{ in } L^\infty(0,T;V_\Gamma), \quad \overline{u}^n|_\Gamma \rightharpoonup \overline{u}|_\Gamma \text{ in } H^1(0,T;H_\Gamma).$$

Next, since $L^2(0,T;V)$, $L^2(0,T;H)$ and $L^2(0,T;H_\Gamma)$ are all reflexive spaces, it is once again easy to see that

$$w^n \rightharpoonup w \quad \text{in } L^2(0,T;V),$$

and

$$f(u^n) \rightharpoonup \phi \quad \text{in } L^2(0,T;H), \quad f_\Gamma(u^n) \rightharpoonup \phi_\Gamma \quad \text{in } L^2(0,T;H_\Gamma).$$

We remark that all of the above convergences are to be intended for at least a subsequence.

If we now set $Q = \Omega \times (0,T)$ and $\Sigma = \Gamma \times (0,T)$, owing to (2.60), we get

$$u^n \to u \quad \text{a.e. } (\mathbf{x},t) \in Q \quad \Rightarrow \quad f(u^n) \to f(u) \quad \text{a.e. } (\mathbf{x},t) \in Q,$$

and analogously

$$f_\Gamma(u^n) \to f_\Gamma(u) \quad \text{a.e. } (\mathbf{x},t) \in \Sigma.$$

This means that $f(u) = \phi$ almost everywhere in Q and $f_\Gamma(u) = \phi_\Gamma$ almost everywhere in Σ, so we conclude that

$$f(u^n) \rightharpoonup f(u) \quad \text{in } L^2(0,T;H), \qquad f_\Gamma(u^n) \rightharpoonup f_\Gamma(u) \quad \text{in } L^2(0,T;H_\Gamma).$$

We can finally take advantage of all these results. If $m \in \mathbb{N}$ is a fixed integer, we can write problem (2.34)-(2.35) in the following, equivalent, way

$$\begin{cases} \displaystyle\int_0^T \langle \partial_t \overline{u}^n, y \rangle_{V^*} + \sigma \int_Q \overline{u}^n y + \int_Q \nabla w^n y = 0 \quad \forall y \in L^2(0,T;V_m) \\ \displaystyle\int_Q w^n y = \int_Q \nabla \overline{u}^n \cdot \nabla y + \int_Q (f(u^n) - g) y \\ \displaystyle\qquad\qquad + \int_\Sigma \partial_t \overline{u}^n y + \int_\Sigma \nabla_\Gamma \overline{u}^n \cdot \nabla_\Gamma y + \sigma_\Gamma \int_\Gamma \overline{u}^n y \\ \displaystyle\qquad\qquad + \int_\Sigma (f_\Gamma(u^n) - g_\Gamma) y - (\sigma - \sigma_\Gamma) \langle u_0 \rangle \int_\Sigma e^{-\sigma t} y \quad \forall y \in L^2(0,T;V_m), \end{cases}$$

which holds for every $n \geq m$. If we now let $n \to \infty$, it is clear from the above arguments that every term converges so, roughly speaking, we can drop the n.
Since m was chosen arbitrarily, the same holds for every $y \in L^2(0,T;V_\infty)$; hence for every $y \in L^2(0,T;V)$ in the first equation, and $y \in L^2(0,T;W)$ in the second because of density arguments (which are proved in Lemma A.3).

To conclude the proof of existence, we just recall that Lemma A.1 guarantees the convergence of the initial datum too.

Remark 2.12 The solution is more regular with respect to the original requests (2.24)-(2.25), which were necessary for the weak formulation to be well defined. Indeed we additionally have

$$\overline{u} \in L^\infty(0,T;V) \cap C^0([0,T],H),$$
$$\overline{u}|_\Gamma \in L^\infty(0,T;V_\Gamma) \cap C^0([0,T],H_\Gamma).$$

2.3.4 Continuous dependence on initial data

We conclude the proof of Theorem 2.4 by proving first Corollary 2.5, the uniqueness of the solution being an immediate consequence.

To this aim, let $(\overline{u}_1, w_1)$, $(\overline{u}_2, w_2)$ be two solutions corresponding to initial data $u_{0,1}$ and $u_{0,2}$; we then set

$$u_0^\delta = u_{0,1} - u_{0,2}, \quad u^\delta = u_1 - u_2, \quad w^\delta = w_1 - w_2,$$

and consequently

$$\overline{u}^\delta = \overline{u}_1 - \overline{u}_2 = u^\delta - \langle u_{0,1} - u_{0,2} \rangle e^{-\sigma t} = u^\delta - \langle u^\delta \rangle.$$

By definition, for $i = 1, 2$, it must hold

$$\begin{cases} \langle \partial_t \overline{u}_i, y \rangle_{V^*} + \sigma \int_\Omega \overline{u}_i y + \int_\Omega \nabla w_i \cdot \nabla y = 0 \qquad \forall y \in V, \\ \int_\Omega w_i y = \int_\Omega \nabla \overline{u}_i \cdot \nabla y + \int_\Omega (f(u_i) - g) y \\ \qquad + \int_\Gamma \partial_t \overline{u}_i y + \int_\Gamma \nabla_\Gamma \overline{u}_i \cdot \nabla_\Gamma y + \sigma_\Gamma \int_\Gamma \overline{u}_i y \\ \qquad + \int_\Gamma (f_\Gamma(u_i) - g_\Gamma) y - (\sigma - \sigma_\Gamma) \langle u_{0,i} \rangle \int_\Gamma e^{-\sigma t} y \qquad \forall y \in W, \end{cases}$$

for a.a. $t \in [0,T]$. We now subtract the corresponding equations and test them by $y = \mathcal{N}(\overline{u}^\delta)$ and $y = \overline{u}^\delta$, respectively; exploiting the usual results, we obtain

$$\begin{aligned} &\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}} ||\overline{u}^\delta||_*^2 + \sigma ||\overline{u}^\delta||_*^2 + |\overline{u}^\delta|_1^2 + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}} |\overline{u}^\delta|_{0,\Gamma}^2 + |\overline{u}^\delta|_{1,\Gamma}^2 + \sigma_\Gamma |\overline{u}^\delta|_{0,\Gamma}^2 \\ &= - \int_\Gamma (f_\Gamma(u_1) - f_\Gamma(u_2)) \overline{u}^\delta + (\sigma - \sigma_\Gamma) \langle u_0^\delta \rangle \int_\Gamma e^{-\sigma t} \overline{u}^\delta \\ &\quad - \int_\Omega (f(u_1) - f(u_2)) \overline{u}^\delta. \end{aligned} \tag{2.61}$$

We start treating the last term. Using (2.7), we show that it satisfies

$$\begin{aligned}\int_\Omega (f(u_1)-f(u_2))\overline{u}^\delta &= \int_\Omega (f(u_1)-f(u_2))(u^\delta - \langle u^\delta\rangle)\\ &\geq -c_0|u^\delta|_0^2 - \langle u^\delta\rangle \int_\Omega (f(u_1)-f(u_2)).\end{aligned} \tag{2.62}$$

Furthermore, it holds

$$f(u_1)-f(u_2) = \sum_{j=1}^{2p-1} a_j(u_1^j - u_2^j) = (u_1-u_2)\sum_{j=1}^{2p-1} a_j \left[\sum_{k=0}^{j-1} u_1^{j-1-k}\, u_2^k\right].$$

It is now just a simple algebra exercise, using the Young inequality, to verify that

$$|f(u_1)-f(u_2)| \leq C|u^\delta|(1+|u_1|^{2(2p-3)}+|u_2|^{2(2p-3)}),$$

so, using this result, we estimate the last term in (2.62) with

$$\begin{aligned}\left|\langle u^\delta\rangle \int_\Omega (f(u_1)-f(u_2))\right| &\leq C|\langle u^\delta\rangle| \int_\Omega |u^\delta|\left(1+|u_1|^{2(2p-3)}+|u_2|^{2(2p-3)}\right)\\ &\leq C\left(|u^\delta|_0^2 + |\langle u^\delta\rangle|^2\left(1+||u_1||_{L^{p^*}(\Omega)}^{p^*}+||u_2||_{L^{p^*}(\Omega)}^{p^*}\right)\right),\end{aligned} \tag{2.63}$$

where we set $p^* = 4(2p-3)$ (note that, in particular, if $d=3$ and hence $p=2$, we have $p^*=4$).

We now use (A.14) on u^δ

$$|u^\delta|_0^2 \leq \epsilon|\overline{u}^\delta|_1^2 + C_\epsilon(||\overline{u}^\delta||_*^2 + |\langle u^\delta\rangle|^2) \qquad \forall \epsilon > 0, \tag{2.64}$$

so that we can finally collect these inequalities and estimate the last term of (2.61) with

$$\begin{aligned}&-\int_\Omega (f(u_1)-f(u_2))\overline{u}^\delta \leq c_0|u^\delta|_0^2 + \langle u^\delta\rangle \int_\Omega (f(u_1)-f(u_2))\\ &\leq \frac{1}{2}|\overline{u}^\delta|_1^2 + C\left(||\overline{u}^\delta||_*^2 + |\langle u^\delta\rangle|^2\right)\left(1+||u_1||_{L^{p^*}(\Omega)}^{p^*}+||u_2||_{L^{p^*}(\Omega)}^{p^*}\right).\end{aligned} \tag{2.65}$$

It is then straightforward to check that a similar bound holds for the integral with f_Γ, that is

$$\begin{aligned}&-\int_\Gamma (f_\Gamma(u_1)-f_\Gamma(u_2))\overline{u}^\delta\\ &\leq C\left(|\overline{u}^\delta|_{0,\Gamma}^2 + |\langle u^\delta\rangle|^2\right)\left(1+||u_1||_{L^{q^*}(\Gamma)}^{q^*}+||u_2||_{L^{q^*}(\Gamma)}^{q^*}\right),\end{aligned} \tag{2.66}$$

where $q^* = 4(2q-3)$. Hence, we use (2.65) and (2.66) back into (2.61) and write

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}||\overline{u}^\delta||_*^2+\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}|\overline{u}^\delta|_{0,\Gamma}^2+\sigma||\overline{u}^\delta||_*^2+\frac{1}{2}|\overline{u}^\delta|_1^2+|\overline{u}^\delta|_{1,\Gamma}^2+\sigma_\Gamma|\overline{u}^\delta|_{0,\Gamma}^2$$
$$\leq C\left(||\overline{u}^\delta||_*^2+|u^\delta|_{0,\Gamma}^2+|\langle u^\delta\rangle|^2\right)\left(1+\sum_{i=1,2}\left(||u_i||_{L^{p^*}(\Omega)}^{p^*}+||u_i||_{L^{q^*}(\Gamma)}^{q^*}\right)\right)$$
$$+|\sigma-\sigma_\Gamma||\langle u_0^\delta\rangle||\Gamma|^{1/2}|\overline{u}^\delta|_{0,\Gamma},$$

where we also exploited the usual inequalities to estimate the last term. We moreover apply the Young inequality on the latter and obtain

$$|\sigma-\sigma_\Gamma||\langle u_0^\delta\rangle||\Gamma|^{1/2}|\overline{u}^\delta|_{0,\Gamma}\leq C\left(|\langle u_0^\delta\rangle|^2+|\overline{u}^\delta|_{0,\Gamma}^2\right),$$

thus getting

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}||\overline{u}^\delta||_*^2+\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}|\overline{u}^\delta|_{0,\Gamma}^2+\sigma||\overline{u}^\delta||_*^2+\frac{1}{2}|\overline{u}^\delta|_1^2+|\overline{u}^\delta|_{1,\Gamma}^2+\sigma_\Gamma|\overline{u}^\delta|_{0,\Gamma}^2$$
$$\leq C_1|\langle u_0^\delta\rangle|^2+C_2\left(||\overline{u}^\delta||_*^2+|\langle u^\delta\rangle|^2+|\overline{u}^\delta|_{0,\Gamma}^2\right)\left(1+\sum_{i=1,2}\left(||u_i||_{L^{p^*}(\Omega)}^{p^*}+||u_i||_{L^{q^*}(\Gamma)}^{q^*}\right)\right).$$

Finally, noting that the squared absolute mean value of u^δ is clearly non-increasing

$$\frac{\mathrm{d}}{\mathrm{dt}}|\langle u^\delta\rangle|^2\leq 0,$$

we can add this quantity to the left. Simplifying the positive terms on the left, we conclude

$$\frac{\mathrm{d}}{\mathrm{dt}}\left(||\overline{u}^\delta||_*^2+|\overline{u}^\delta|_{0,\Gamma}^2+|\langle u^\delta\rangle|^2\right)$$
$$\leq C_1|\langle u_0^\delta\rangle|^2+C_2\left(||\overline{u}^\delta||_*^2+|\langle u^\delta\rangle|^2+|\overline{u}^\delta|_{0,\Gamma}^2\right)\left(1+\sum_{i=1,2}\left(||u_i||_{L^{p^*}(\Omega)}^{p^*}+||u_i||_{L^{q^*}(\Gamma)}^{q^*}\right)\right),$$

for a.a. $t\in[0,T]$; integrating this inequality in $(0,t)$ with $t\in[0,T]$, it follows from Gronwall's lemma that

$$||\overline{u}^\delta||_*^2+|\overline{u}^\delta|_{0,\Gamma}^2+|\langle u^\delta\rangle|^2\leq C\left(||\overline{u}^\delta(0)||_*^2+(1+t)|\langle u_0^\delta\rangle|^2+|\overline{u}^\delta(0)|_{0,\Gamma}^2\right)e^{\gamma(t)},\quad (2.67)$$

for every $t\in[0,T]$, and where

$$\gamma(t)=\int_0^t\left(1+\sum_{i=1,2}\left(||u_i||_{L^{p^*}(\Omega)}^{p^*}+||u_i||_{L^{q^*}(\Gamma)}^{q^*}\right)\right).$$

We now recall Remark 2.10: if we choose the initial data from a bounded set, i.e. there exists $R>0$ such that

$$||u_{0,i}||_W\leq R,$$

it is clear that it holds

$$\gamma(t) \le \gamma(T) \le C_R, \qquad \forall t \in [0,T],$$

since the only parameter that we are varying is the initial datum.

Therefore (2.67) becomes

$$||\overline{u}^\delta||_*^2 + |\overline{u}^\delta|_{0,\Gamma}^2 + |\langle u^\delta\rangle|^2 \le C_{R,T}\left(||\overline{u}^\delta(0)||_*^2 + |\langle u_0^\delta\rangle|^2 + |\overline{u}^\delta(0)|_{0,\Gamma}^2\right) \quad \forall t \in (0,T). \tag{2.68}$$

Then, we notice that

$$||u^\delta||_*^2 + |u^\delta|_{0,\Gamma}^2 \le C\left(||\overline{u}^\delta||_*^2 + |\overline{u}^\delta|_{0,\Gamma}^2 + |\langle u^\delta\rangle|^2\right),$$

and

$$\begin{aligned} ||\overline{u}^\delta||_*^2 + |\overline{u}^\delta|_{0,\Gamma}^2 + |\langle u^\delta\rangle|^2 &\le C\left(||u^\delta||_*^2 + |u^\delta|_{0,\Gamma}^2 + |\langle u^\delta\rangle|^2\right) \\ &\le C||u^\delta||_W^2, \end{aligned}$$

so estimate (2.68) leads to

$$||u_1 - u_2||_{L^\infty(0,T;V^*)}^2 + ||u_1 - u_2||_{L^\infty(0,T;H_\Gamma)}^2 \le C_{R,T}||u_1 - u_2||_W^2.$$

However, recalling Remark 2.12, this result can be improved (in the sense of a greater regularity for u^δ), as

$$||u_1 - u_2||_{C^0([0,T];V^*)}^2 + ||u_1 - u_2||_{C^0([0,T];H_\Gamma)}^2 \le C_{R,T}||u_1 - u_2||_W^2. \tag{2.69}$$

Inequality (2.69) is exactly the claim of Corollary 2.5, so the proof of continuous dependence on the initial data is complete.

□

Remark 2.13 This result, in particular, tells us that if $u_{0,1} = u_{0,2}$ we have

$$u_1 = u_2 \text{ in } L^\infty(0,T;V^*), \quad u_1|_\Gamma = u_2|_\Gamma \text{ in } L^\infty(0,T;H_\Gamma),$$

that is, the solution is unique. Hence we completed the proof of Theorem 2.4 too.

□

We conclude this chapter with some observations on the conditions on f and f_Γ. First of all, the above proofs can be adapted to the case $f_\Gamma \in C^{0,1}(\mathbb{R})$: similar, if not easier, arguments apply and lead to the same conclusions.

Moreover, the same techniques can be exploited to generalize both f and f_Γ; it would be sufficient for them to be smooth enough, and satisfy suitable growth conditions as well as coercivity like conditions. For instance, we could ask that $f, f_\Gamma \in C^1(\mathbb{R}, \mathbb{R})$ satisfy (2.7), (2.10) and

$$f(s) = O(|s|^3) \;\text{ as }\; |s| \to +\infty \qquad \text{if }\; d = 3,$$
$$f(s) = O(|s|^p) \;\text{ as }\; |s| \to +\infty \;\text{ with }\; p \geq 1 \qquad \text{if }\; d = 2,$$
$$f_\Gamma(s) = O(|s|^q) \;\text{ as }\; |q| \to +\infty \;\text{ with }\; q \geq 1.$$

Chapter 3

Asymptotic behavior and existence of the global attractor

In this chapter we recall some definitions and classical results from [56] regarding the long time behavior of infinite dimensional dynamical systems; we then apply them to the problem under analysis.

In the upcoming section, (X, d_X) will denote a complete metric space.

3.1 Long time behavior for semidynamical systems

Consider the problem

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{dt}} x(t) = Dx(t) \quad \forall t \geq 0 \\ x(0) = x_0 \end{cases} \tag{3.1}$$

where $D : Y \subset X \to X$ is a, usually differential, operator defined on some dense subset Y of X; a typical choice would be $Y = H^1(\Omega)$, $X = L^2(\Omega)$. If the initial value problem (3.1) possesses a unique solution for every $x_0 \in \Phi \subset Y$ and $S(t)x_0 \in \Phi \ \forall t \geq 0$, one can define the solution operator

$$S(t) : \Phi \to \Phi, \qquad S(t)x_0 = x(t; x_0) \tag{3.2}$$

that satisfies

$$S(0) = I, \qquad S(t)S(s) = S(s)S(t) = S(t+s) \quad \forall t, s \geq 0, \tag{3.3}$$

which means that the family $\{S(t)\}_{t \geq 0}$ forms a semigroup on Φ (also called the *phase space*). A *semidynamical system* is then the couple

$$\left(\Phi, \{S(t)\}_{t \geq 0}\right). \tag{3.4}$$

Such object is the central tool in the long time analysis for evolution PDEs; it indeed forms the right setting in which one should study the asymptotic behavior.

An important concept arising in the analysis of semidynamical systems is that of dissipation. At a first glance one can think of it as the tendency for all the equation's solutions to be eventually uniformly bounded; we however make this idea more precise with the following definitions

Definition 3.1 *S(t) is point dissipative if there exists a bounded set $C \subset \Phi$ such that*

$$S(t)x_0 \in C \qquad \forall x_0 \in \Phi, \quad \forall t \geq t_0(x_0)$$

for every $x_0 \in \Phi$.

Definition 3.2 *S(t) is bounded dissipative if there exists a bounded set $C \subset \Phi$ such that*

$$S(t)B \subset C \qquad \forall t \geq t_0(B),$$

for every bounded set $B \in \Phi$.

These two definitions are equivalent in $\mathbb{R}^N$, but this is not true in general for infinite dimensional spaces. In both cases we say that C is an *absorbing set* for $S(t)$.
The request of C being bounded is quite reasonable; however, in the applications, one usually wants C to be compact too. We will therefore adopt the following definition

Definition 3.3 *S(t) is dissipative if it is bounded dissipative and its absorbing set $C \subset \Phi$ is compact.*

One of the main goals in studying a semidynamical system is to find the set $\mathcal{A} \subset \Phi$ in which the asymptotic dynamics take place: in this way, it is possible to restrict the analysis of $S(t)$ on $\mathcal{A}$. Such object is called the *global attractor*.

Definition 3.4 *The global attractor $\mathcal{A}$ for a semidynamical system $(\Phi, \{S(t)\}_{t\geq 0})$ is the maximal compact invariant set:*

$$S(t)\mathcal{A} = \mathcal{A} \qquad \forall t \geq 0,$$

and the minimal set which attracts bounded sets:

$$\mathrm{dist}(S(t)B, \mathcal{A}) \to 0 \qquad \textit{as } t \to \infty,$$

for every bounded set $B \subset \Phi$, where $\mathrm{dist}(U, V) = \sup_{u\in U} \inf_{v\in V} d_X(u, v)$.

Showing that a semidynamical system possess a global attractor is crucial for systems arising from physics and mechanics. In these cases, one can often prove that such attractor is also finite dimensional (in Hausdorff or fractal sense), showing that in some way the original infinite dimensional system has, in fact, a finite number of degrees of freedom (at least asymptotically).

We now state a classical result regarding the existence of the global attractor.

Theorem 3.5 *If $S(t)$ is dissipative and $S(t)u_0$ is continuous in both t and u_0, then there exists a global attractor $\mathcal{A} = \omega(B)$. If Φ is connected, then so is $\mathcal{A}$.*

Here, $\omega(U)$ is the so-called ω-limit set of U, that is

$$\begin{aligned}\omega(U) &= \{y \in U \mid \exists t_n \to \infty, x_n \in U \text{ such that } S(t_n)x_n \to y\} \\ &= \bigcap_{t\geq 0} \overline{\bigcup_{s\geq t} S(s)U}.\end{aligned}$$

This theorem represents the standard approach in proving the existence of a global attractor; nonetheless there are situations in which it is not of great help, namely when the continuity of $S(t)u_0$ with respect to u_0 cannot be established.

We remark that the problem we are analyzing falls into this category, since Corollary 2.5 gives us only

$$||S(t)u_{0,1} - S(t)u_{0,2}||_{V^*} + ||S(t)u_{0,1} - S(t)u_{0,2}||_{H_\Gamma} \leq C||u_{0,1} - u_{0,2}||_W,$$

instead of

$$||S(t)u_{0,1} - S(t)u_{0,2}||_W \leq C||u_{0,1} - u_{0,2}||_W.$$

In other words, the continuity is obtained only with respect to a weaker metric. To overcome this problem, Pata and Zelik proved in [57] that the continuity condition on the semigroup can be substituted with a, weaker, closedness condition. We recall the authors' result in the following

Theorem 3.6 *Let $S(t)$ be such that*

$$x_n \to x \text{ and } S(t)x_n \to y \quad \Rightarrow \quad S(t)x = y \tag{3.5}$$

that is, $S(t)$ is a closed operator. If $S(t)$ has a connected compact absorbing set $\mathcal{K}$ such that $S(t)\mathcal{K} \subset \mathcal{K}$ for every $t \geq t_0$, then $S(t)$ possesses a connected global attractor $\mathcal{A} = \omega(\mathcal{K})$.

This is the result that we will use to prove the existence of a global attractor for problem (2.29)-(2.30).

3.2 The semidynamical system

In the following, in order to prove some fundamental results, we will assume two more hypothesis (which seem quite reasonable, and are common in literature [31], [45]), in addition to the ones of the previous chapter; that is, we require a greater regularity for the sources g, g_Γ

$$g \in L^\infty(\Omega), \quad g_\Gamma \in L^\infty(\Gamma). \tag{3.6}$$

Notice that we also dropped the dependence on time, which is clearly necessary for $S(t)$ to define a semigroup in the sense we specified.

Recalling the results of the previous chapter, and assuming (3.6), the solution operator $S(t)$ is well defined for every $t \geq 0$. Therefore, if we fix $m \geq 0$, the natural phase space for $S(t)$ is

$$\Phi_m := \{u \in W \mid |\langle u_0 \rangle| \leq m\},$$
$$S(t) : \Phi_m \to \Phi_m \quad \forall t \geq 0.$$

The semidynamical system is then

$$\left(\Phi_m, \{S(t)\}_{t\geq 0}\right). \tag{3.7}$$

We finally have all the elements to state the main result of the chapter

Theorem 3.7 *Let the assumptions of Theorem 2.4 hold. Moreover, assume* (3.6)*. Then, problem* (2.29)-(2.30) *defines the semidynamical system* (3.7)*, and* Φ_m *possesses a connected global attractor* $\mathcal{A}_m$ *which is compact in* $H^1(\Omega) \times H^1(\Gamma)$*.*

3.2.1 Energy estimate

In the following we will operate in a formal way, that is, differentiating (2.29)-(2.30) and using non-admittable test functions; the results could however be obtained in a rigorous way using the discretized version of the equations and then letting $n \to \infty$; nonetheless we avoid such procedure in order not to make the text too heavy.

We take $y = \mathcal{N}(\partial_t \overline{u} + \sigma \overline{u})$ in (2.29) and $y = \partial_t \overline{u} + \sigma \overline{u}$ in (2.30). With such a choice, and using $\mathcal{N}$ properties, the two equations read

$$||\partial_t \overline{u}||_*^2 + \sigma \frac{\mathrm{d}}{\mathrm{dt}} ||\overline{u}||_*^2 + \sigma^2 ||\overline{u}||_*^2 + \int_\Omega \nabla w \cdot \nabla \mathcal{N}(\partial_t \overline{u} + \sigma \overline{u}) = 0,$$

and

$$\begin{aligned}\int_\Omega w(\partial_t\overline{u}+\sigma\overline{u}) &= \frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}|\overline{u}|_1^2+\sigma|\overline{u}|_1^2+\int_\Omega (f(u)-g)(\partial_t u+\sigma u)\\ &+|\partial_t\overline{u}|_{0,\Gamma}^2+\frac{\sigma}{2}\frac{\mathrm{d}}{\mathrm{dt}}|\overline{u}|_{0,\Gamma}^2+\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}|\overline{u}|_{1,\Gamma}^2+\sigma|\overline{u}|_{1,\Gamma}^2\\ &+\frac{\sigma_\Gamma}{2}\frac{\mathrm{d}}{\mathrm{dt}}|\overline{u}|_{0,\Gamma}^2+\sigma_\Gamma\sigma|\overline{u}|_{0,\Gamma}^2+\int_\Gamma (f_\Gamma(u)-g_\Gamma)(\partial_t u+\sigma u)\\ &-(\sigma-\sigma_\Gamma)\langle u_0\rangle\int_\Gamma e^{-\sigma t}(\partial_t\overline{u}+\sigma\overline{u}),\end{aligned}$$

where we also used (2.22) in the integrals with f and f_Γ. Then, we substitute these equations one into the other; we get, after reordering

$$\begin{aligned}&||\partial_t\overline{u}||_*^2+|\partial_t\overline{u}|_{0,\Gamma}^2+\sigma\left(\sigma||\overline{u}||_*^2+|\overline{u}|_1^2+|\overline{u}|_{1,\Gamma}^2+\sigma_\Gamma|\overline{u}|_{0,\Gamma}^2\right)\\ &\quad+\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\left(2\sigma||\overline{u}||_*^2+|\overline{u}|_1^2+|\overline{u}|_{1,\Gamma}^2+(\sigma_\Gamma+\sigma)|\overline{u}|_{0,\Gamma}^2\right)\\ &\quad+\int_\Omega (f(u)-g)\partial_t u+\sigma\int_\Omega (f(u)-g)u+\int_\Gamma (f_\Gamma(u)-g_\Gamma)\partial_t u+\sigma\int_\Gamma (f_\Gamma(u)-g_\Gamma)u\\ &=(\sigma-\sigma_\Gamma)\langle u_0\rangle\int_\Gamma e^{-\sigma t}(\partial_t\overline{u}+\sigma\overline{u}).\end{aligned} \tag{3.8}$$

We need to treat the last four terms on the left hand side; we only show the procedure for the integrals on Ω, as the same arguments apply to those on Γ.

First of all, it clearly holds

$$\int_\Omega (f(u)-g)\partial_t u=\frac{\mathrm{d}}{\mathrm{dt}}\int_\Omega (F(u)-gu).$$

Then, in order to deal with the second term, we fix C_F to be such that

$$F(s)-g(\mathbf{x})s\geq 0 \qquad \forall s\in\mathbb{R},\ \text{ a.e. } \mathbf{x}\in\Omega, \tag{3.9}$$

which is always possible due to (3.6). We now need the following inequality

Lemma 3.8 *There exist constants $C_1, C_2>0$ such that*

$$(f(s)-g(\mathbf{x}))s\geq C_1(F(s)-g(\mathbf{x})s)-C_2 \qquad \forall s\in\mathbb{R},\quad \textit{a.e. } \mathbf{x}\in\Omega,$$

Proof We exploit f and F definitions to rewrite the above inequality as

$$\sum_{j=2}^{2p} b_j(j-C_1)s^j+C_2\geq (1-C_1)g(\mathbf{x})s+C_1C_F,$$

and we see that it is trivially satisfied by choosing $C_1<2p$, and a consequently large enough C_2, due to the boundedness of g.

□

Taking into account these results, and the correspondent ones for f_Γ, we apply the Cauchy–Schwarz and Young inequalities on the right hand side, getting

$$\begin{aligned}
&||\partial_t \overline{u}||_*^2 + |\partial_t \overline{u}|_{0,\Gamma}^2 + \sigma \left(\sigma ||\overline{u}||_*^2 + |\overline{u}|_1^2 + |\overline{u}|_{1,\Gamma}^2 + \sigma_\Gamma |\overline{u}|_{0,\Gamma}^2 + C_1 \int_\Omega (F(u) - gu) \right. \\
&\quad \left. + C_{1,\Gamma} \int_\Gamma (F_\Gamma(u) - g_\Gamma u) \right) + \frac{1}{2} \frac{\mathrm{d}}{\mathrm{dt}} \Big(2\sigma ||\overline{u}||_*^2 + |\overline{u}|_1^2 + |\overline{u}|_{1,\Gamma}^2 + (\sigma_\Gamma + \sigma) |\overline{u}|_{0,\Gamma}^2 \\
&\quad + 2 \int_\Omega (F(u) - gu) + 2 \int_\Gamma (F_\Gamma(u) - g_\Gamma u) \Big) \\
&\leq C \left(1 + |\langle u_0 \rangle|^2 \right) + \frac{1}{2} |\partial_t \overline{u}|_{0,\Gamma}^2 + \frac{\sigma \sigma_\Gamma}{2} |\overline{u}|_{0,\Gamma}^2,
\end{aligned} \tag{3.10}$$

which we recall that is valid for almost every positive t. We then define the energy

$$\begin{aligned}
E(t) := 2\sigma ||\overline{u}(t)||_*^2 + |\overline{u}(t)|_1^2 + 2 \int_\Omega (F(u(t)) - gu(t)) \\
+ (\sigma + \sigma_\Gamma) |\overline{u}(t)|_{0,\Gamma}^2 + |\overline{u}(t)|_{1,\Gamma}^2 + 2 \int_\Gamma (F_\Gamma(u(t)) - g_\Gamma u(t)) .
\end{aligned} \tag{3.11}$$

$E(t)$ is clearly non-negative due to (3.9). Using definition (3.11), we can rewrite (3.10) as

$$\frac{\mathrm{d}}{\mathrm{dt}} E(t) + \alpha E(t) + ||\partial_t \overline{u}||_*^2 + |\partial_t \overline{u}|_{0,\Gamma}^2 \leq C \qquad \text{a.a. } t \geq 0, \tag{3.12}$$

for suitable positive constants α, C; then, eliminating the last two terms on the left hand side, and integrating in $[0, t]$, where $t \geq 0$, we easily see that the solution to the correspondent integral equation is

$$E(t) = \left(E(0) - \frac{C}{\alpha} \right) e^{-\alpha t} + \frac{C}{\alpha} \qquad \forall t \geq 0,$$

thus, by a simple comparison argument, we get

$$E(t) \leq E(0) e^{-\alpha t} + C_0 \qquad \forall t \geq 0. \tag{3.13}$$

3.2.2 Bounded absorbing sets

We notice that, by definition, E must satisfy

$$E(t) \leq C \left(||u(t)||_V^2 + ||u(t)||_{L^{2p}(\Omega)}^{2p} + ||u(t)||_{V_\Gamma}^2 + ||u(t)||_{L^{2q}(\Gamma)}^{2q} + 1 \right), \quad \forall t \geq 0. \tag{3.14}$$

and

$$||u(t)||_V^2 + ||u(t)||_{V_\Gamma}^2 \le c\,(E(t)+1)\,, \quad \forall t \ge 0, \tag{3.15}$$

where we have omitted the dependence on $\langle u_0\rangle$ as this term is trivially bounded, since $u_0 \in \Phi_m$. Indeed C depends on g, m, σ, σ_Γ and the coefficients of F and F_Γ, while c depends on Ω (through the Poincaré inequality), σ, σ_Γ and m.

According to Definition 3.3, let now B be a bounded subset of Φ_m: this means that there exists $R > 0$ such that

$$||u_0||_W \le R \quad \Rightarrow \quad ||u_0||_V^2 + ||u_0||_{L^{2p}(\Omega)}^{2p} + ||u_0||_{V_\Gamma}^2 + ||u_0||_{L^{2q}(\Gamma)}^{2q} \le C_R, \tag{3.16}$$

for every $u_0 \in B$. Therefore, due to (3.13), (3.14) and (3.15)

$$E(t) \le E(0)e^{-\alpha t} + C_0 \le C_R e^{-\alpha t} + C \qquad \forall\, t \ge 0$$

$$||u(t)||_V^2 + ||u(t)||_{V_\Gamma}^2 \le C_R e^{-\alpha t} + C \qquad \forall\, t \ge 0. \tag{3.17}$$

This is all we need to prove the existence of an absorbing set. Indeed a direct consequence of (3.17) is that if C_1 is a positive, large enough constant and we define

$$\mathcal{C} := \left\{ v \in W \,\middle|\, ||v||_W^2 \le C_1 \right\}, \tag{3.18}$$

then

$$u \in \mathcal{C} \qquad \forall t \ge t_1(R), \tag{3.19}$$

That is, there exists a bounded set in which $S(t)$ maps every bounded subset of Φ_m, after a sufficiently long time; however, $\mathcal{C}$ clearly cannot be compact. Thus, using a standard approach, we will need to find another absorbing set in some subset of Φ_m, containing more regular functions.

3.3 Higher-order estimates

A priori estimate for $\partial_t u$ (1)

Eliminating the non-negative term αE from (3.12) and integrating the resulting inequality in $(t, t+1)$, we easily get

$$E(t+1) + \int_t^{t+1} (||\partial_t \overline{u}||_*^2 + |\partial_t \overline{u}|_{0,\Gamma}^2) \le E(t) + C \le E(0)e^{-\alpha t} + C$$

which gives us

$$\int_t^{t+1} (||\partial_t u||_*^2 + |\partial_t u|_{0,\Gamma}^2) \leq C_R e^{-\alpha t} + C \quad \forall t \geq 0.$$

So, if C_2 is large enough

$$\int_t^{t+1} (||\partial_t u||_*^2 + |\partial_t u|_{0,\Gamma}^2) \leq C_2 \quad \forall t \geq t_2(R). \tag{3.20}$$

A priori estimate for $\partial_t u$ (2)

We formally differentiate (2.29)-(2.30) with respect to t

$$\begin{cases} \langle \partial_t^2 \overline{u}, y \rangle_{V^*} + \sigma \int_\Omega \partial_t \overline{u} y + \int_\Omega \nabla \partial_t w \cdot \nabla y = 0 & (3.21) \\ \int_\Omega \partial_t w y = \int_\Omega \nabla \partial_t \overline{u} \cdot \nabla y + \int_\Omega f'(u) \partial_t u y + \int_\Gamma \partial_t^2 \overline{u} y + \int_\Gamma \nabla_\Gamma \partial_t \overline{u} \cdot \nabla_\Gamma y & \\ \qquad + \sigma_\Gamma \int_\Gamma \partial_t \overline{u} y + \int_\Gamma f'_\Gamma(u) \partial_t u y + \sigma(\sigma - \sigma_\Gamma) \langle u_0 \rangle \int_\Gamma e^{-\sigma t} y, & (3.22) \end{cases}$$

and choose $y = \mathcal{N}(\partial_t \overline{u})$ in (3.21), $y = \partial_t \overline{u}$ in (3.22). Applying the usual results, and writing $\partial_t \overline{u} = \partial_t u + \sigma \langle u_0 \rangle e^{-\sigma t}$ in the integrals with $f'(u)$ and $f'_\Gamma(u)$, we get

$$\begin{aligned} &\frac{1}{2} \frac{\mathrm{d}}{\mathrm{dt}} ||\partial_t \overline{u}||_*^2 + \sigma ||\partial_t \overline{u}||_*^2 + |\partial_t \overline{u}|_1^2 + \int_\Omega f'(u) |\partial_t u|^2 + \sigma \langle u_0 \rangle e^{-\sigma t} \int_\Omega f'(u) \partial_t u \\ &\quad + \frac{1}{2} \frac{\mathrm{d}}{\mathrm{dt}} |\partial_t \overline{u}|_{0,\Gamma}^2 + |\partial_t \overline{u}|_{1,\Gamma}^2 + \sigma_\Gamma |\partial_t \overline{u}|_{0,\Gamma}^2 + \int_\Gamma f'_\Gamma(u) |\partial_t u|^2 + \sigma \langle u_0 \rangle e^{-\sigma t} \int_\Gamma f'_\Gamma(u) \partial_t u \\ &= -\sigma(\sigma - \sigma_\Gamma) \langle u_0 \rangle \int_\Gamma e^{-\sigma t} \partial_t \overline{u}. \end{aligned} \tag{3.23}$$

Then, we eliminate the second and the eighth terms; moreover, we estimate the fourth from below, using (2.7), as

$$\int_\Omega f'(u) |\partial_t u|^2 \geq -c_0 |\partial_t u|_0^2.$$

An analogous inequality holds for f_Γ; therefore we get, upon reordering,

$$\begin{aligned} &\frac{1}{2} \frac{\mathrm{d}}{\mathrm{dt}} \left(||\partial_t \overline{u}||_*^2 + |\partial_t \overline{u}|_{0,\Gamma}^2 \right) + |\partial_t \overline{u}|_1^2 + |\partial_t \overline{u}|_{1,\Gamma}^2 \\ &\leq c_0 |\partial_t u|_0^2 + c_{0,\Gamma} |\partial_t u|_{0,\Gamma}^2 - \sigma \langle u_0 \rangle e^{-\sigma t} \left(\int_\Omega f'(u) \partial_t u + \int_\Gamma f'_\Gamma(u) \partial_t u \right) \\ &\quad - \sigma(\sigma - \sigma_\Gamma) \langle u_0 \rangle \int_\Gamma e^{-\sigma t} \partial_t \overline{u}. \end{aligned} \tag{3.24}$$

We now apply once again the Cauchy-Schwarz and Young inequalities, in order to get

$$
\begin{aligned}
&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}(||\partial_t\overline{u}||_*^2 + |\partial_t\overline{u}|_{0,\Gamma}^2) + |\partial_t\overline{u}|_1^2 + |\partial_t\overline{u}|_{1,\Gamma}^2 \\
&\leq c_0|\partial_t u|_0^2 + c_{0,\Gamma}|\partial_t u|_{0,\Gamma}^2 + \sigma|\langle u_0\rangle| \left(|f'(u)|_0|\partial_t u|_0 + |f_\Gamma'(u)|_{0,\Gamma}|\partial_t u|_{0,\Gamma}\right) \\
&\quad + \sigma|\sigma - \sigma_\Gamma||\langle u_0\rangle||\Gamma|^{1/2}|\partial_t\overline{u}|_{0,\Gamma} \\
&\leq C\left(1 + |\partial_t\overline{u}|_0^2 + |\partial_t\overline{u}|_{0,\Gamma}^2 + ||u||_{L^{4p-4}(\Omega)}^{4p-4} + ||u||_{L^{4q-4}(\Gamma)}^{4q-4}\right) \quad \text{a.a. } t \geq 0.
\end{aligned}
$$

Where we also exploited the fact that f' and f_Γ' are, respectively, a $2p-2$ and a $2q-2$ order polynomial. Moreover we notice that, if $d = 3$ and so $p = 2$, the exponent of the second to last term is $4p - 4 = 4$; hence it can be bounded, in both cases (2.8), with $||u||_V^{4p-4}$.

We now use formally (A.13) on $|\partial_t\overline{u}|_0^2$, and write

$$
|\partial_t\overline{u}|_0^2 \leq \frac{1}{2}|\partial_t\overline{u}|_1^2 + C||\partial_t\overline{u}||_*^2,
$$

even if we have no clue that $\partial_t\overline{u} \in V$: again, to be rigorous, we should apply this inequality to $\partial_t\overline{u}^n$.

Using (3.17) too, we conclude

$$
\begin{aligned}
&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\left(||\partial_t\overline{u}||_*^2 + |\partial_t\overline{u}|_{0,\Gamma}^2\right) + \frac{1}{2}|\partial_t\overline{u}|_1^2 + |\partial_t\overline{u}|_{1,\Gamma}^2 \\
&\leq C\left(||\partial_t\overline{u}||_*^2 + |\partial_t\overline{u}|_{0,\Gamma}^2\right) + C_R e^{-\beta t} + C, \quad \text{a.a. } t \geq 0
\end{aligned}
\tag{3.25}
$$

for some positive β depending on α and p. We are hence allowed to apply the Uniform Gronwall Lemma (see, for instance, [58]):

Lemma 3.9 *Let y, g and h be three non-negative, locally integrable functions on $[t_0, +\infty)$ such that*

$$
\frac{\mathrm{d}}{\mathrm{dt}}y(t) \leq g(t)y(t) + h(t) \quad \textit{a.a. } t \geq t_0,
$$

and

$$
\int_t^{t+\tau} y \leq \gamma_1 \qquad \int_t^{t+\tau} g \leq \gamma_2 \qquad \int_t^{t+\tau} h \leq \gamma_3 \qquad \forall t \geq t_0, \tag{3.26}
$$

where τ, γ_1, γ_2 and γ_3 are positive constants. Then

$$
y(t+\tau) \leq \left(\frac{\gamma_1}{\tau} + \gamma_3\right)e^{\gamma_2} \qquad \forall t \geq t_0. \tag{3.27}
$$

We set $\tau = 1$. Then, if $t_0 = t_2(R)$ and $y = ||\partial_t \overline{u}||_*^2 + |\partial_t \overline{u}|_{0,\Gamma}^2$, (3.20) tells us that the first one of (3.26) is verified. The second and the third are trivially satisfied.

So, (3.27) gives

$$||\partial_t \overline{u}||_*^2 + |\partial_t \overline{u}||_{0,\Gamma}^2 \le C_3 \quad \forall t \ge t_3(R) = 1 + t_2(R). \tag{3.28}$$

We now integrate (3.25) in $(t, t+1)$ and forget some positive terms, getting

$$\begin{aligned} \int_t^{t+1} \left(\frac{1}{2} |\partial_t \overline{u}|_1^2 + |\partial_t \overline{u}|_{1,\Gamma}^2 \right) \le C \int_t^{t+1} \left(||\partial_t \overline{u}||_*^2 + |\partial_t \overline{u}|_{0,\Gamma}^2 \right) \\ + \frac{1}{2} \left(||\partial_t \overline{u}||_*^2 + |\partial_t \overline{u}|_{0,\Gamma}^2 \right) + C, \quad \forall\, t \ge 0, \end{aligned} \tag{3.29}$$

and using (3.20) and (3.28) we get

$$\int_t^{t+1} \left(|\partial_t \overline{u}|_1^2 + |\partial_t \overline{u}|_{1,\Gamma}^2 \right) \le C_4 \quad \forall t \ge t_4(R). \tag{3.30}$$

Combining inequalities (3.20) and (3.30) we get the following uniform estimate

$$\begin{aligned} \int_t^{t+1} \left(||\partial_t u||_V^2 + ||\partial_t u||_{V_\Gamma}^2 \right) &\le C \left(1 + \int_t^{t+1} \left(|\partial_t \overline{u}|_1^2 + |\partial_t \overline{u}|_{0,\Gamma}^2 + |\partial_t \overline{u}|_{1,\Gamma}^2 \right) \right) \\ &\le C_5 \quad \forall t \ge t_5(R). \end{aligned} \tag{3.31}$$

A priori estimate for $f(u)$ and $f_\Gamma(u)$

It is almost trivial to check that

$$\begin{aligned} |f(u)|_0^2 \le C \left(1 + ||u||_{L^{4p-2}(\Omega)}^{4p-2} \right) &\le C \left(1 + ||u||_V^{4p-2} \right) \\ &\le C_R e^{-\gamma t} + C, \quad \text{a.a. } t \ge 0 \end{aligned}$$

where γ is a positive constant depending on α and p.
So, for a suitable C_6

$$\int_t^{t+1} |f(u)|_0^2 \le C_6 \quad \forall t \ge t_6(R). \tag{3.32}$$

An analogous estimate for f_Γ is once again straightforward to get.

A priori estimate for w

It only remains to prove an estimate for $w(t)$ in V-norm. This will be obtained, as in the previous chapter, by bounding its gradient and mean value.
So, setting $y(t) = w(t) - \langle w(t) \rangle$ in (2.29)

$$\begin{aligned} |w|_1^2 &= -\langle \partial_t \overline{u}, w - \langle w \rangle \rangle_{V^*} + \sigma \int_\Omega \overline{u}(w - \langle w \rangle) \\ &\leq C(||\partial_t \overline{u}||_* + ||\overline{u}||_V)||w - \langle w \rangle||_V \\ &\leq C(||\partial_t \overline{u}||_*^2 + ||\overline{u}||_V^2) + \frac{1}{2}|w|_1^2, \quad \text{a.a. } t \geq 0 \end{aligned}$$

hence it follows from (3.17) and (3.31)

$$\int_t^{t+1} |w|_1^2 \leq C \int_t^{t+1} \Big(||\partial_t u||_V^2 + ||u||_V^2 + 1 \Big) \leq C_7 \quad \forall t \geq t_7(R). \tag{3.33}$$

In order to estimate the mean value of w, we simply take $y(t) = \frac{1}{|\Omega|}$ in (2.30) and get

$$\begin{aligned} |\langle w \rangle| \leq & C \Big(||f(u)||_{L^1(\Omega)} + ||g||_{L^1(\Omega)} + ||\partial_t \overline{u}||_{L^1(\Gamma)} + ||\overline{u}||_{L^1(\Gamma)} \\ & + ||f_\Gamma(u)||_{L^1(\Gamma)} + ||g_\Gamma||_{L^1(\Gamma)} + 1 \Big) \\ \leq & C \Big(||u||_V^{2p-1} + |\partial_t u|_{0,\Gamma} + ||u||_{V_\Gamma} + 1 \Big), \quad \text{a.a. } t \geq 0 \end{aligned}$$

so that exploiting the previous estimates

$$\int_t^{t+1} |\langle w \rangle|^2 \leq C_8 \quad \forall t \geq t_8(R). \tag{3.34}$$

Summing (3.33) and (3.34), and using the Poincaré inequality, we conclude

$$\int_t^{t+1} ||w||_V^2 \leq C_9 \quad \forall t \geq t_9(R). \tag{3.35}$$

3.4 A compact absorbing set

We will now use the uniform estimates found in the previous section, to construct a compact absorbing set $\mathcal{K}_m$. We start by looking at problem $(\mathrm{CHO} - \mathrm{D})$ from a different point of view: that is, as two different elliptic problems on Ω and Γ

$$\begin{cases} \Delta \overline{u} = g - f(u) - w & \text{in } \Omega, \quad (3.36) \\ \Delta_\Gamma \overline{u} = \partial_t \overline{u} + \partial_n \overline{u} + \sigma_\Gamma \overline{u} + f_\Gamma(u) - g_\Gamma - (\sigma - \sigma_\Gamma)\langle u_0 \rangle e^{-\sigma t} & \text{on } \Gamma, \quad (3.37) \end{cases}$$

where t is fixed.

Owing to the bounds we proved, every term on the right side of (3.36) is at least in $L^2(\Omega)$, hence $\Delta\overline{u}$ must be in this space as well; this in turn implies that $\overline{u} \in H^2(\Omega)$, so $(\partial_n \overline{u})|_\Gamma \in H^{1/2}(\Gamma) \subset L^2(\Gamma)$. Therefore we are allowed to proceed with a similar argument on (3.37), getting $\overline{u}|_\Gamma \in H^2(\Gamma)$.

It is hence natural to look for an upper bound for the solution in H^2-norms. We start by observing that

$$||u||^2_{H^2(\Omega)} + ||u||^2_{H^2(\Gamma)} \le C\left(||\overline{u}||^2_{H^2(\Omega)} + |\overline{u}|^2_{2,\Gamma} + |\overline{u}|^2_{0,\Gamma} + 1\right),$$

since, as well known, $|\cdot|_{2,\Gamma} + |\cdot|_{0,\Gamma}$ is equivalent to the standard $H^2(\Gamma)$ norm.

Then we use (3.37) and get

$$||u||^2_{H^2(\Omega)} + ||u||^2_{H^2(\Gamma)} \le C\left(||\overline{u}||^2_{H^2(\Omega)} + |\partial_t\overline{u}|^2_{0,\Gamma} + |\partial_n\overline{u}|^2_{0,\Gamma} + |\overline{u}|^2_{0,\Gamma} + |f_\Gamma(u)|^2_{0,\Gamma} + 1\right).$$

Exploiting the continuity of the trace operator, that is $|\partial_n\overline{u}|_{0,\Gamma} \le C_T||\overline{u}||_{H^2(\Omega)}$, we obtain

$$||u||^2_{H^2(\Omega)} + ||u||^2_{H^2(\Gamma)} \le C\left(||\overline{u}||^2_{H^2(\Omega)} + |\partial_t\overline{u}|^2_{0,\Gamma} + |\overline{u}|^2_{0,\Gamma} + |f_\Gamma(u)|^2_{0,\Gamma} + 1\right).$$

Finally, using (3.36), we get

$$||u||^2_{H^2(\Omega)} + ||u||^2_{H^2(\Gamma)} \le C\left(|w|^2_0 + |f(u)|^2_0 + |\partial_t u|^2_{0,\Gamma} + |u|^2_{0,\Gamma} + |f_\Gamma(u)|^2_{0,\Gamma} + 1\right). \tag{3.38}$$

We can now integrate (3.38) in $(t, t+1)$ and set $\overline{t}(R) = \max_{i=1,\dots,9} \overline{t}_i(R)$; owing to the previous estimates, we conclude

$$\int_t^{t+1} (||u||^2_{H^2(\Omega)} + ||v||^2_{H^2(\Gamma)}) \le \overline{C} \quad \forall t \ge \overline{t}(R), \tag{3.39}$$

for a suitable $\overline{C} > 0$. At this point, as we want to prove a compactness result, we need to squeeze as much regularity as possible for u; to this aim, we will exploit some classical results on interpolation theory and Bochner spaces (see, for instance, [59]).

Let $s > 0$. We then define the space Z as

$$Z = \left\{ z \in L^2(s,\infty; H^2(\Omega)) \;\middle|\; z' \in L^2(s,\infty; H^1(\Omega)) \right\},$$

where the (time) derivative z' has to be intended in the usual, distributional, sense. It is shown in [59] that the space of traces of Z, which we shall denote by T, can be characterized in the following way

$$||v||_T = \inf_{\substack{z\in Z\\ z(s)=v}} ||z||^{1/2}_{L^2(s,\infty;H^2(\Omega))}||z'||^{1/2}_{L^2(s,\infty;H^1(\Omega))}. \tag{3.40}$$

For such a choice of the exponents on the right hand side of (3.40), it can also be proven that T is an interpolation space between $H^1(\Omega)$ and $H^2(\Omega)$, that is, $H^{3/2}(\Omega)$. So, using the Young inequality, we can write

$$||v||_{H^{3/2}(\Omega)} \le C \inf_{\substack{z\in Z\\ z(s)=v}} \Big(||z||_{L^2(s,\infty;H^2(\Omega))} + ||z'||_{L^2(s,\infty;H^1(\Omega))}\Big).$$

We now choose $t > s$ and set $z = u\,\chi_{[t,t+1]}$. Thus we have

$$\begin{aligned}||u(s)||^2_{H^{3/2}(\Omega)} &\le C\Big(\int_s^\infty ||u(r)\chi_{[t,t+1]}(r)||^2_{H^2(\Omega)}\mathrm{dr} + \int_s^\infty ||\partial_r u(r)\chi_{[t,t+1]}(r)||^2_{H^1(\Omega)}\mathrm{dr}\\ &\quad + \int_s^\infty ||u(r)\delta_t(r)||^2_{H^1(\Omega)}\mathrm{dr} + \int_s^\infty ||u(r)\delta_{t+1}(r)||^2_{H^1(\Omega)}\mathrm{dr}\Big)\\ &\le C\Big(\int_t^{t+1} ||u||^2_{H^2(\Omega)}\mathrm{dr} + \int_t^{t+1} ||\partial_r u||^2_{H^1(\Omega)}\mathrm{dr}\\ &\quad + ||u(t)||^2_{H^1(\Omega)} + ||u(t+1)||^2_{H^1(\Omega)}\Big),\end{aligned}$$

and exploiting (3.17), (3.31) and (3.39), we conclude (using the same argument for $u|_\Gamma$) that

$$||u||^2_{H^{3/2}(\Omega)} + ||u||^2_{H^{3/2}(\Gamma)} \le C_* \quad \forall\, t \ge t_*(R).$$

Therefore we can define the absorbing set

$$\mathcal{K}_m := \Big\{v \in \Phi_m \;\Big|\; ||v||_{H^{3/2}(\Omega)} + ||v||_{H^{3/2}(\Gamma)} \le C\Big\}. \tag{3.41}$$

$\mathcal{K}_m$ is clearly connected and, since $H^{3/2}(\Omega) \subset\subset H^1(\Omega)$ and $H^{3/2}(\Gamma) \subset\subset H^1(\Gamma)$, compact in Φ_m; in other words, $S(t)$ is dissipative in the sense of Definition 3.3. Moreover, it follows from the definition that $S(t)\mathcal{K}_m \subset \mathcal{K}_m$ after a sufficiently long time.

3.5 Proof of Theorem 3.7

Since we want to use Theorem 3.6, we just need to show that $S(t)$ is a closed operator, as the other hypothesis have already been proved; to this aim, we fix $\tau \in \mathbb{R}^+$ and let v_k be a sequence in W such that

$$\begin{cases} v_k \xrightarrow{W} v & (3.42)\\ S(\tau)v_k \xrightarrow{W} y. & (3.43)\end{cases}$$

We then need to prove that $y = S(\tau)u$ in W. Corollary 2.5, together with (3.42), tells us in particular that

$$\begin{cases} S(\tau)v_k \xrightarrow{V^*} S(\tau)v \\ S(\tau)v_k|_\Gamma \xrightarrow{H_\Gamma} S(\tau)v|_\Gamma. \end{cases}$$

At the same time, (3.43) gives us

$$\begin{cases} S(\tau)v_k \xrightarrow{V} y \quad \Rightarrow \quad S(\tau)v_k \xrightarrow{V^*} y \\ S(\tau)v_k|_\Gamma \xrightarrow{V_\Gamma} y|_\Gamma \quad \Rightarrow \quad S(\tau)v_k|_\Gamma \xrightarrow{H_\Gamma} y|_\Gamma, \end{cases}$$

Hence the uniqueness of the limit implies the closedness of $S(t)$. From Theorem 3.6, we get the existence of a connected global attractor $\mathcal{A}_m$ such that

$$\mathcal{A}_m = \omega(\mathcal{K}_m),$$

which in turn implies that $\mathcal{A}_m \subset \mathcal{K}_m$, since $S(t)\mathcal{K}_m \subset \mathcal{K}_m$ after a sufficiently long time; we conclude that $\mathcal{A}_m$ is compact too in $H^1(\Omega) \times H^1(\Gamma)$, and Theorem 3.7 is proved.

□

Remark 3.10 The results of this Chapter too can be extended to the case f_Γ Lipschitz; however, it seems that the additional hypothesis $f_\Gamma \in L^\infty(\mathbb{R})$ is needed (see [45]). Nonetheless, in this case, we remark that the presence of a linear term on the boundary (as it is usually asked for in the applications) is still guaranteed by the term $\sigma_\Gamma u$.

Chapter 4

Numerical analysis

In this chapter we will study the behavior of a $\mathbb{P}^1$ finite elements approximation for our system; the arguments here presented are mainly based on the work of Cherfils and Petcu (see [60], [61]), and the results of the simulations are compared to those obtained in these papers.
Among the vast literature devoted to the numerical analysis of CH-type equations, we cite [17], [62], [63] and [64] dealing with generic degree finite elements. Splitting schemes are quite popular too because of the higher-order nature of the system: we cite, for instance, [65], [66], [67].

In order to simplify the presentation, while maintaining a significant formulation, we consider a slightly modified version of the problem: the domain Ω will now be a 2 or 3 dimensional slab endowed with dynamic boundaries conditions on two opposite sides, and periodic on the rest of the boundary. Clearly, while the first appear explicitly in the problem's formulation, the second will be part of the function spaces definition. So, we now set

$$\Omega = \left(\prod_{i=1}^{d-1} (\mathbb{R} \backslash k L_i) \right) \times (0, L_d) \quad \forall k \in \mathbb{Z},$$

and

$$\Gamma = \left(\prod_{i=1}^{d-1} (\mathbb{R} \backslash k L_i) \right) \times \{0, L_d\} \quad \forall k \in \mathbb{Z},$$

where $L_i > 0 \;\; i = 1, \ldots, d$. As already pointed out, in order to take into account the periodic conditions, we redefine the function space V in the following way

$$V = \left\{ v \in H^1(\Omega) \;\middle|\; v(\cdot, 0) \in H^1_p(0, L_1) \;\text{ and }\; v(\cdot, L_2) \in H^1_p(0, L_1) \right\},$$

if $d = 2$, and similarly if $d = 3$.

This choice does not affect the analysis of the previous chapters: using this notation, the same results can be proven. Moreover, we have the advantage of dealing both with a regular boundary and a polygonal domain.

4.1 Galerkin $\mathbb{P}^1$ semidiscretization

We choose a quasi-uniform family $\{\Omega_h\}$ of triangulations of $\prod_{i=1}^{d}[0, L_i]$, composed by d-simplexes, which takes into account the periodic conditions; as customary, h represents the maximum diameter of the elements. Ω_h is then a decomposition of $\overline{\Omega}$, and it induces naturally the triangulation (of $(d-1)$-simplexes) Γ_h of Γ. Then, we define the $\mathbb{P}^1$ finite elements space X_h as

$$X_h = \left\{ v \in C^0(\overline{\Omega}) \;\middle|\; v|_T \in \mathbb{P}^1 \;\; \forall T \in \Omega_h \right\}.$$

Remark 4.1 In contrast with the previous chapters, we will use the original formulation of problem (that is, without operating the substitution $\overline{u}(t) = u(t) - \langle u(t) \rangle$); this choice is caused by the simple observation that it is more significant to estimate the difference $u_h - u$ rather than $\overline{u}_h - \overline{u}$, as the mean value of the solution and its discretization is not guaranteed to be the same. We remark that equations (2.29)-(2.30) then read

$$\begin{cases} \displaystyle\int_\Omega \partial_t u y + \sigma \int_\Omega u y + \int_\Omega \nabla w \cdot \nabla y = 0 \qquad \forall y \in V, & (4.1) \\ \displaystyle\int_\Omega w y = \int_\Omega \nabla u \cdot \nabla y + \int_\Omega (f(u) - g)\, y + \int_\Gamma \partial_t u y & \\ \displaystyle\qquad + \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma y + \sigma_\Gamma \int_\Gamma u y + \int_\Gamma (f_\Gamma(u) - g_\Gamma)\, y \qquad \forall y \in W. & (4.2) \end{cases}$$

for a.a. $t \in (0, T)$, and with the initial condition $u(0) = u_0$.

With this remark in mind, the Galerkin formulation is:

we look for a couple (u_h, w_h) such that

$$u_h \in H^1(0, T; X_h), \quad w_h \in L^2(0, T; X_h), \tag{4.3}$$

$$u_h(0) = u_{0,h}, \tag{4.4}$$

and satisfying for a.a. $t \in (0, T)$

$$\begin{cases} \displaystyle\int_\Omega \partial_t u_h y + \sigma \int_\Omega u_h y + \int_\Omega \nabla w_h \cdot \nabla y = 0 \qquad \forall y \in X_h, & (4.5) \\ \displaystyle\int_\Omega w_h y = \int_\Omega \nabla u_h \cdot \nabla y + \int_\Omega (f(u_h) - g)\, y + \int_\Gamma \partial_t u_h y & \\ \displaystyle\qquad + \int_\Gamma \nabla_\Gamma u_h \cdot \nabla_\Gamma y + \sigma_\Gamma \int_\Gamma u_h y + \int_\Gamma (f_\Gamma(u_h) - g_\Gamma)\, y \qquad \forall y \in X_h. & (4.6) \end{cases}$$

Here $u_{0,h}$ is a suitable approximation of u_0, the properties of which will be specified later on. We skip the proof of existence of a unique solution of problem (4.3)-(4.6), as it is essentially the same as in Chapter 2; we will thus focus on the error estimates of such discretization.

Remark 4.2 In the following, we will make use of the operator

$$\mathcal{N}_h : X_{h,0} \to X_{h,0}, \quad X_{h,0} = \{v_h \in X_h \mid \langle v_h \rangle = 0\}$$

which is the discrete version of $\mathcal{N}$ (see Appendix A.2). Clearly, $\mathcal{N}_h$ shares all of $\mathcal{N}$ properties, as long as we deal with functions belonging to the discretized space. Moreover, we denote by $||\cdot||_{*,h}$ the norm induced by this operator.

We now state the main result of this chapter:

Theorem 4.3 *Let* (u, w) *be a solution of* (4.1)-(4.2)*, corresponding to the initial datum* u_0*, such that*

$$u,\ \partial_t u,\ \partial_t^2 u,\ w,\ \partial_t w \in L^2(0,T;H^2(\Omega)), \tag{4.7}$$

$$u|_\Gamma,\ \partial_t u|_\Gamma,\ \partial_t^2 u|_\Gamma \in L^2(0,T;H^2(\Gamma)), \tag{4.8}$$

and let (u_h, w_h) *be a solution of* (4.3)-(4.6) *where* $u_{0,h}$ *is a proper approximation of* u_0*. Then, if* h *is small enough, the following error estimates hold*

$$\sup_{[0,T]} (|u_h - u|_0 + |u_h - u|_{0,\Gamma} + ||\partial_t u_h - \partial_t u||_{*,h} + |\partial_t u_h - \partial_t u|_{0,\Gamma}) \le Ch^2, \tag{4.9}$$

$$\left(\int_0^T |w_h - w|_0^2\right)^{1/2} \le Ch^2, \tag{4.10}$$

$$\sup_{[0,T]} ||u_h - u||_W \le Ch^2, \tag{4.11}$$

$$\left(\int_0^T ||w_h - w||_V^2 + ||\partial_t u_h - \partial_t u||_V^2 + ||\partial_t u_h - \partial_t u||_{V_\Gamma}^2\right)^{1/2} \le Ch^2, \tag{4.12}$$

where the constant $C > 0$ *is independent on* h*.*

Remark 4.4 The conditions asked for in (4.7) and (4.8) are rather strong; indeed, using only the results of the previous chapter, we are not allowed to assume such regularity in time for the solutions. However, because of the parabolic nature of the problem on both Ω and Γ, it is expected that (4.7) and (4.8) are satisfied if u_0, f, f_Γ, g and g_Γ are smooth enough.

4.2 Auxiliary results

In this section, we develop some results which we will use in order to prove Theorem 4.3.
We use a standard approach and we write

$$u_h - u = \alpha^u + \beta^u \qquad \alpha^u = u_h - \widetilde{u}_h, \quad \beta^u = \widetilde{u}_h - u, \tag{4.13}$$
$$w_h - w = \alpha^w + \beta^w \qquad \alpha^w = w_h - \widetilde{w}_h, \quad \beta^w = \widetilde{w}_h - w, \tag{4.14}$$

where $\widetilde{u}_h$ and $\widetilde{w}_h$ are the so-called elliptic projections of u and w, defined as

$$\begin{aligned} &\int_\Omega \nabla\widetilde{u}_h \cdot \nabla y + \sigma_\Gamma \int_\Gamma \widetilde{u}_h y + \int_\Gamma \nabla_\Gamma \widetilde{u}_h \cdot \nabla_\Gamma y \\ &= \int_\Omega \nabla u \cdot \nabla y + \sigma_\Gamma \int_\Gamma u y + \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma y, \qquad \forall y \in X_h, \end{aligned} \tag{4.15}$$

and

$$\begin{cases} \langle \widetilde{w}_h \rangle = \langle w \rangle, & (4.16) \\ \displaystyle\int_\Omega \nabla\widetilde{w}_h \cdot \nabla y = \int_\Omega \nabla w \cdot \nabla y \qquad \forall y \in X_h. & (4.17) \end{cases}$$

The well-posedness of (4.15)-(4.17) is easy to show; indeed problem (4.15) possesses a unique solution, as it can be easily seen recalling that $|\cdot|_1 + |\cdot|_{0,\Gamma}$ is an equivalent norm on V, since the bilinear form

$$a(\phi,\psi) = \int_\Omega \nabla\phi \cdot \nabla\psi + \sigma_\Gamma \int_\Gamma \phi\psi + \int_\Gamma \nabla\phi \cdot \nabla\psi$$

is coercive and continuous on W (and hence on X_h). Therefore the conclusion follows from the Lax-Milgram Lemma.
Moreover, we observe that (4.17) defines a solution which is unique up to an additive constant; so, together with (4.16), we get the uniqueness.

Remark 4.5 We now clarify what we mean by "proper approximation" of the initial datum (as requested in Theorem 4.3). Once u_0 is given, we will ask that

$$\alpha^u(0) = u_{0,h} - \widetilde{u}_h(0) = 0, \quad \alpha^w(0) = w_h(0) - \widetilde{w}_h(0) = 0, \tag{4.18}$$

are satisfied. This is not a real limitation in practice, as it only requires to solve the linear elliptic equation (4.15), with u_0 as the projected function; as of $w_h(0)$, its choice doesn't really affect the simulation, since the solution at the time step $n+1$ will depend on the previous step only through u^n (since no time derivative of w appears in the problem). The only reason why one should be interested in calculating $w_h(0)$, would be in order to apply an iterative method with an initial datum close to the real solution; however, a simple interpolation should work fine for most applications.

Requests (4.18) are due to technical reason, and the reason will be evident from the proof of Theorem 4.3. Executing these operation prior than solving the real problem adds however just a little computational expense; on the other hand, getting a prescription on how to build $u_{0,h}$ might even be advantageous.

We start by estimating the error relative to the elliptic projections. Regarding β^w, it is well-known (due to (4.16)-(4.17) and standard numerical results for elliptic problems) that, as $w \in H^2(\Omega)$, it holds

$$|\widetilde{w}_h - w|_0 + h|\widetilde{w}_h - w|_1 \leq Ch^2|w|_2, \tag{4.19}$$

where C depends on Ω_h only. A little more work is needed to get a similar estimate for β^u, which will be proved in the following

Lemma 4.6 *Let $u \in H^2(\Omega)$ such that $u|_\Gamma \in H^2(\Gamma)$, and let $\widetilde{u}_h$ be the unique solution of* (4.15). *Then*

$$|\widetilde{u}_h - u|_0 + |\widetilde{u}_h - u|_{0,\Gamma} + h|\widetilde{u}_h - u|_1 + h|\widetilde{u}_h - u|_{1,\Gamma} \leq Ch^2(|u|_2 + |u|_{2,\Gamma}). \tag{4.20}$$

Proof First, we denote by I_h the interpolation operator

$$I_h : C^0(\overline{\Omega}) \to X_h.$$

We recall that $I_h u$ is the unique function belonging to X_h that takes the same values as $u \in C^0(\overline{\Omega})$ on the nodes of the triangulation.

Clearly $\widetilde{u}_h - I_h u \in X_h$, so we can write

$$a(\widetilde{u}_h - u, \widetilde{u}_h - u) = a(\widetilde{u}_h - u, \widetilde{u}_h - I_h u) + a(\widetilde{u}_h - u, I_h\overline{u} - u),$$

and the first term on the right hand side is zero by definition. Hence, exploiting the coercivity and continuity of $a(\cdot,\cdot)$

$$C_0||\widetilde{u}_h - u||_W^2 \leq (2 + \sigma_\Gamma)||\widetilde{u}_h - u||_W||I_h u - u||_W,$$

and we conclude, due to Lemma A.5, that

$$||\widetilde{u}_h - u||_W \leq Ch(|u|_2 + |u|_{2,\Gamma}). \tag{4.21}$$

In order to get the whole estimate (4.20), we will now use what is known in literature as the Aubin-Nitsche duality trick. So let ϕ be the unique solution of

$$a(\phi, y) = \int_\Omega \chi y + \int_\Gamma \psi y \qquad \forall y \in X_h, \tag{4.22}$$

where $\chi \in L^2(\Omega)$, $\psi \in L^2(\Gamma)$. Then, by elliptic regularity, we have $\phi \in H^2(\Omega)$ and

$\phi|_\Gamma \in H^2(\Gamma)$; moreover it holds

$$|\phi|_2 + |\phi|_{2,\Gamma} \leq C(|\chi|_0 + |\psi|_{0,\Gamma}). \tag{4.23}$$

If we now set $y = \widetilde{u}_h - u$ in (4.22), we obtain

$$\begin{aligned}\int_\Omega \chi(\widetilde{u}_h - u) + \int_\Gamma \psi(\widetilde{u}_h - u) = a(\phi, \widetilde{u}_h - u) = a(\phi - I_h\phi, \widetilde{u}_h - u) \\ \leq C||\phi - I_h\phi||_W||\widetilde{u}_h - u||_W.\end{aligned} \tag{4.24}$$

Finally we set $\chi = \widetilde{u}_h - u$, $\psi = (\widetilde{u}_h - u)|_\Gamma$, thus getting

$$\begin{aligned}|\widetilde{u}_h - u|_0^2 + |\widetilde{u}_h - u|_{0,\Gamma}^2 &\leq Ch^2(|\phi|_2 + |\phi|_{2,\Gamma})(|u|_2 + |u|_{2,\Gamma}) \\ &\leq Ch^2(|\widetilde{u}_h - u|_0 + |\widetilde{u}_h - u|_{0,\Gamma})(|u|_2 + |u|_{2,\Gamma}),\end{aligned}$$

where we used (4.21), (4.23) and once more Lemma A.5. Simplifying and using the resulting inequality with (4.21), we get (4.20).

□

We now prove an estimate for α^u and α^w.

Lemma 4.7 *Let (u, w) be a solution of* (4.1)-(4.2) *corresponding to initial datum u_0, and (u_h, w_h) be a solution of* (4.5)-(4.6) *corresponding to initial datum $u_{0,h}$ satisfying* (4.18)*. Moreover, assume that*

$$||u||_{C^0([0,T];C^0(\overline{\Omega}))} < R \qquad ||\partial_t u||_{C^0([0,T];C^0(\overline{\Omega}))} \leq R \qquad ||u_{0,h}||_{C^0(\overline{\Omega})} < R, \tag{4.25}$$

where $R \in (0, +\infty)$, and let $T_h \in (0, T]$ be the maximal number satisfying

$$||u_h(t)||_{L^\infty(\Omega)} \leq R \quad \forall t \in [0, T_h]. \tag{4.26}$$

Then there exist constants $C_i^* > 0$, independent on h, u, u_h, such that the following estimates hold:

$$\begin{aligned}&\Phi(t) + \int_0^t \left(|\alpha^w|_1^2 + |\partial_t\alpha^u|_{0,\Gamma}^2 + |\partial_t\alpha^u|_1^2 + |\partial_t\alpha^u|_{1,\Gamma}^2\right) \\ &\leq C_1^*\Phi(0) + C_2^*\int_0^t \Big(|\beta^w|_0^2 + |\partial_t\beta^w|_0^2 + |\beta^u|_0^2 + |\beta^u|_{0,\Gamma}^2 \\ &\quad + |\partial_t\beta^u|_0^2 + |\partial_t\beta^u|_{0,\Gamma}^2 + |\partial_t^2\beta^u|_0^2 + |\partial_t^2\beta^u|_{0,\Gamma}^2\Big) + t\, C_3^*|\beta^u(0)|_0^2 \quad \forall t \in [0, T_h],\end{aligned} \tag{4.27}$$

and

$$|\langle\alpha^w\rangle| \leq C_4^*\left(\Phi^{1/2}(t) + |\beta^u|_0^2 + |\beta^u|_{0,\Gamma}^2 + |\partial_t\beta^u|_0^2 + |\partial_t\beta^u|_{0,\Gamma}^2 + |\beta^u(0)|_0^2\right) \quad \forall t \in [0, T_h], \tag{4.28}$$

where

$$\Phi(t) = |\alpha^u|_1^2 + \sigma_\Gamma |\alpha^u|_{0,\Gamma}^2 + |\alpha^u|_{1,\Gamma}^2 + ||\partial_t \alpha^u - \langle \partial_t \alpha^u \rangle||_{*,h}^2 + |\partial_t \alpha^u - \langle \partial_t \alpha^u \rangle|_{0,\Gamma}^2. \quad (4.29)$$

Furthermore

$$|\langle \partial_t \alpha^u \rangle| \le C_5^* (|\beta^u(0)|_0 + |\partial_t \beta^u|_0) \quad \forall t \in [0,T]. \quad (4.30)$$

Proof We start by subtracting (4.1) from (4.5). What we get is

$$\int_\Omega \partial_t(\alpha^u + \beta^u) y + \sigma \int_\Omega (\alpha^u + \beta^u) y + \int_\Omega \nabla(\alpha^w + \beta^w) \cdot \nabla y = 0 \quad \forall y \in X_h, \quad (4.31)$$

which becomes, choosing $y = \frac{1}{|\Omega|}$

$$\frac{\mathrm{d}}{\mathrm{dt}} \langle \alpha^u + \beta^u \rangle = -\sigma \langle \alpha^u + \beta^u \rangle.$$

Similarly as we did in the first Chapter we can easily solve this ODE, and recalling the first one of (4.18) yields to

$$\langle \alpha^u \rangle = \langle \beta^u(0) \rangle e^{-\sigma t} - \langle \beta^u \rangle,$$

so that

$$|\langle \alpha^u \rangle| \le |\Omega|^{-1/2} (|\beta^u(0)|_0 + |\beta^u|_0) \quad \forall t \in [0,T], \quad (4.32)$$

Differentiating (4.31) with respect to time, and using the same arguments, we also get

$$|\langle \partial_t \alpha^u \rangle| \le |\Omega|^{-1/2} (\sigma |\beta^u(0)|_0 + |\partial_t \beta^u|_0) \quad \forall t \in [0,T], \quad (4.33)$$

$$|\langle \partial_t^2 \alpha^u \rangle| \le |\Omega|^{-1/2} (\sigma^2 |\beta^u(0)|_0 + |\partial_t^2 \beta^u|_0) \quad \forall t \in [0,T], \quad (4.34)$$

the first one being (4.30).

We now subtract (4.6) from (4.2) and find, after reordering

$$\begin{aligned} &\int_\Omega \nabla \alpha^u \cdot \nabla y + \int_\Gamma \nabla_\Gamma \alpha^u \cdot \nabla_\Gamma y + \sigma_\Gamma \int_\Gamma \alpha^u y + \int_\Gamma \partial_t \alpha^u y = \\ &\int_\Omega (\alpha^w + \beta^w) y - \int_\Omega (f(u_h) - f(u))\, y - \int_\Gamma (f_\Gamma(u_h) - f_\Gamma(u))\, y - \int_\Gamma \partial_t \beta^u y, \end{aligned} \quad (4.35)$$

for every $y \in X_h$, where we eliminated some terms due to definition (4.15). Choosing $y = \partial_t \alpha^u$ in (4.35) leads to

$$
\begin{aligned}
&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\left(|\alpha^u|_1^2+\sigma_\Gamma|\alpha^u|_{0,\Gamma}^2+|\alpha^u|_{1,\Gamma}^2\right)+|\partial_t\alpha^u|_{0,\Gamma}^2=\\
&\int_\Omega \alpha^w\partial_t\alpha^u+\int_\Omega \beta^w\partial_t\alpha^u-\int_\Omega\left(f(u_h)-f(u)\right)\partial_t\alpha^u\\
&-\int_\Gamma\left(f_\Gamma(u_h)-f_\Gamma(u)\right)\partial_t\alpha^u-\int_\Gamma \partial_t\beta^u\partial_t\alpha^u.
\end{aligned}
$$

On the other hand, setting $y=\alpha^w$ in (4.31) we get

$$
|\alpha^w|_1^2=-\int_\Omega \partial_t(\alpha^u+\beta^u)\alpha^w-\sigma\int_\Omega(\alpha^u+\beta^u)\alpha^w,
$$

because of (4.17). Summing the last two equations and simplifying the term in common yields to

$$
\begin{aligned}
&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\left(|\alpha^u|_1^2+\sigma_\Gamma|\alpha^u|_{0,\Gamma}^2+|\alpha^u|_{1,\Gamma}^2\right)+|\partial_t\alpha^u|_{0,\Gamma}^2+|\alpha^w|_1^2\\
&=-\int_\Omega(\partial_t\beta^u+\sigma\alpha^u+\sigma\beta^u)\alpha^w+\int_\Omega \beta^w\partial_t\alpha^u-\int_\Omega\left(f(u_h)-f(u)\right)\partial_t\alpha^u\\
&\quad-\int_\Gamma\left(f_\Gamma(u_h)-f_\Gamma(u)\right)\partial_t\alpha^u-\int_\Gamma \partial_t\beta^u\partial_t\alpha^u.
\end{aligned}
$$

We can then use the Cauchy-Schwarz and Poincaré inequalities on the terms on the right hand side, in order to get

$$
\begin{aligned}
&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\left(|\alpha^u|_1^2+\sigma_\Gamma|\alpha^u|_{0,\Gamma}^2+|\alpha^u|_{1,\Gamma}^2\right)+|\partial_t\alpha^u|_{0,\Gamma}^2+|\alpha^w|_1^2\\
&\le C(|\partial_t\beta^u|_0+|\alpha^u|_0+|\beta^u|_0)(|\langle\alpha^w\rangle|+|\alpha^w|_1)+|\beta^w|_0|\partial_t\alpha^u|_0\\
&\quad+L(|\alpha^u|_0+|\beta^u|_0)|\partial_t\alpha^u|_0+L_\Gamma(|\alpha^u|_{0,\Gamma}+|\beta^u|_{0,\Gamma})|\partial_t\alpha^u|_{0,\Gamma}+|\partial_t\beta^u|_{0,\Gamma}|\partial_t\alpha^u|_{0,\Gamma},
\end{aligned}
\tag{4.36}
$$

where L and L_Γ are the Lipschitz constants for f and f_Γ, since we assumed (4.25), (4.26) and the nonlinearities are at least locally Lipschitz: hence, this inequality holds for every $t\in[0,T_h]$.

We see that an estimate for $|\langle\alpha^w\rangle|$ is needed; we get it, recalling definition (4.16), by choosing $y=\frac{1}{|\Omega|}$ in (4.35)

$$
\begin{aligned}
|\langle\alpha^w\rangle|&\le C(||\alpha^u||_{L^1(\Gamma)}+||\partial_t\alpha^u||_{L^1(\Gamma)}+||\alpha^u||_{L^1(\Omega)}+||\beta^u||_{L^1(\Omega)}\\
&\quad+||\alpha^u||_{L^1(\Gamma)}+||\beta^u||_{L^1(\Gamma)}+||\partial_t\beta^u||_{L^1(\Gamma)})\\
&\le C(|\alpha^u|_{0,\Gamma}+|\partial_t\alpha^u|_{0,\Gamma}+|\alpha^u|_0+|\beta^u|_0+|\beta^u|_{0,\Gamma}+|\partial_t\beta^u|_{0,\Gamma})\quad \forall t\in[0,T_h],
\end{aligned}
\tag{4.37}
$$

where we exploited again the lipschitzianity of the nonlinearities. From (4.37), in particular, we prove (4.28) using the triangular and the Poincaré inequalities, in addition to (4.32), (4.33); indeed we get

$$|\langle\alpha^w\rangle| \le C(|\alpha^u|_{0,\Gamma} + |\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|_{0,\Gamma} + |\beta^u(0)|_0 + |\alpha^u|_0 + |\beta^u|_0 + |\beta^u|_{0,\Gamma} + |\partial_t\beta^u|_{0,\Gamma}),$$

for every $t \in [0, T_h]$; so, (4.28) follows from the definition of $\Phi(t)$.

We conclude the first part of the proof using (4.37) back into (4.36); we do not write every passage because of the length of the resulting inequality, it however suffices to repeatedly use the Young inequality. A little care in choosing the multiplicative coefficients is needed only for the terms containing $|\alpha^w|_1$ and $|\partial_t\alpha^u|_{0,\Gamma}$, in order to simplify them with the homologous on the left hand side. So we get, upon reordering,

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{dt}}\left(|\alpha^u|_1^2 + |\alpha^u|_{1,\Gamma}^2 + \sigma_\Gamma|\alpha^u|_{0,\Gamma}^2\right) + |\partial_t\alpha^u|_{0,\Gamma}^2 + |\alpha^w|_1^2 \\
&\le C_1(|\partial_t\beta^u|_0^2 + |\beta^u|_0^2 + |\beta^u|_{0,\Gamma}^2 + |\partial_t\beta^u|_{0,\Gamma}^2 + |\beta^w|_0^2) + C_2(|\alpha^u|_0^2 + |\alpha^u|_{0,\Gamma}^2 + |\partial_t\alpha^u|_0^2),
\end{aligned} \tag{4.38}$$

for every $t \in [0, T_h]$.

We now look for an estimate for the derivatives of α^u, α^w. We differentiate (4.31) and (4.35); then, choosing respectively $y = \mathcal{N}_h(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle)$ and $y = \partial_t\alpha^u - \langle\partial_t\alpha^u\rangle$ and summing the resulting inequalities yields to

$$\begin{aligned}
&\int_\Omega \partial_t^2\alpha^u\mathcal{N}_h(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) + \sigma\int_\Omega \partial_t\alpha^u\mathcal{N}_h(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) + |\partial_t\alpha^u|_1^2 \\
&\quad + |\partial_t\alpha^u|_{1,\Gamma}^2 + \sigma_\Gamma\int_\Gamma \partial_t\alpha^u(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) + \int_\Gamma \partial_t^2\alpha^u(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) \\
&= -\int_\Omega \partial_t^2\beta^u\mathcal{N}_h(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) - \sigma\int_\Omega \partial_t\beta^u\mathcal{N}_h(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) \\
&\quad + \int_\Omega \partial_t\beta^w(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) - \int_\Omega \left(f'(u_h)\partial_t u_h - f'(u)\partial_t u\right)(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) \\
&\quad - \int_\Gamma \left(f_\Gamma'(u_h)\partial_t u_h - f_\Gamma'(u)\partial_t u\right)(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) - \int_\Gamma \partial_t^2\beta^u(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle),
\end{aligned}$$

where, again, we eliminated some terms using the definition of elliptic projection. We then write

$$\partial_t\alpha^u = (\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) + \langle\partial_t\alpha^u\rangle, \tag{4.39}$$

$$\partial_t^2\alpha^u = (\partial_t^2\alpha^u - \langle\partial_t^2\alpha^u\rangle) + \langle\partial_t^2\alpha^u\rangle, \tag{4.40}$$

for the first, second, fifth and sixth terms on the left hand side. We then use the properties of $\mathcal{N}_h$, and in particular the definition of $||\cdot||_{*,h}$, to get

$$
\begin{aligned}
&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}||\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle||^2_{*,h} + \sigma||\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle||^2_{*,h} + |\partial_t\alpha^u|^2_1 \\
&\quad + |\partial_t\alpha^u|^2_{1,\Gamma} + \sigma_\Gamma|\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|^2_{0,\Gamma} + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}|\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|^2_{0,\Gamma} \\
&= -\int_\Omega (\partial_t^2\beta^u + \langle\partial_t^2\alpha^u\rangle + \sigma\partial_t\beta^u + \sigma\langle\partial_t\alpha^u\rangle)\mathcal{N}_h(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) \\
&\quad - \sigma_\Gamma\int_\Gamma \langle\partial_t\alpha^u\rangle(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) - \int_\Gamma \langle\partial_t^2\alpha^u\rangle(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) \\
&\quad + \int_\Omega \partial_t\beta^w(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) - \int_\Omega \left(f'(u_h)\partial_t u_h - f'(u)\partial_t u\right)(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) \\
&\quad - \int_\Gamma \left(f'_\Gamma(u_h)\partial_t u_h - f'_\Gamma(u)\partial_t u\right)(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle) - \int_\Gamma \partial_t^2\beta^u(\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle).
\end{aligned}
\tag{4.41}
$$

We start dealing with the nonlinear terms; to this aim, we write

$$
\begin{aligned}
|f'(u_h)\partial_t u_h - f'(u)\partial_t u| &\leq |f'(u_h)(\partial_t u_h - \partial_t u)| + |(f'(u_h) - f'(u))\partial_t u| \\
&\leq L'|\partial_t\alpha^u + \partial_t\beta^u| + 2RL'|\alpha^u + \beta^u|,
\end{aligned}
\tag{4.42}
$$

which makes sense for $t \in [0, T_h]$. L' is the Lipschitz constant for f', and f_Γ is treated analogously. We can hence use (4.42) in (4.41) and write, upon reordering

$$
\begin{aligned}
&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\left(||\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle||^2_{*,h} + |\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|^2_{0,\Gamma}\right) + \sigma||\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle||^2_{*,h} \\
&\quad + |\partial_t\alpha^u|^2_1 + |\partial_t\alpha^u|^2_{1,\Gamma} + \sigma_\Gamma|\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|^2_{0,\Gamma} \\
&\leq |\partial_t^2\beta^u + \langle\partial_t^2\alpha^u\rangle + \sigma\partial_t\beta^u + \sigma\langle\partial_t\alpha^u\rangle|_0||\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle||_{*,h} \\
&\quad + |\sigma_\Gamma\langle\partial_t\alpha^u\rangle + \partial_t^2\beta^u + \langle\partial_t^2\alpha^u\rangle|_{0,\Gamma}|\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|_{0,\Gamma} + |\partial_t\beta^w|_0|\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|_0 \\
&\quad + \left(L'|\partial_t\alpha^u + \partial_t\beta^u|_0 + 2RL'|\alpha^u + \beta^u|_0\right)|\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|_0 \\
&\quad + \left(L'_\Gamma|\partial_t\alpha^u + \partial_t\beta^u|_{0,\Gamma} + 2RL'_\Gamma|\alpha^u + \beta^u|_{0,\Gamma}\right)|\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|_{0,\Gamma},
\end{aligned}
\tag{4.43}
$$

for every $t \in [0, T_h]$, where we have also used the Poincaré inequality together with (A.8), in order to get the $||\cdot||_{*,h}$ norm on the right hand side.

To deduce a bound for the first three terms on the right, we exploit the triangular, the Poincaré and Young inequalities, in addition to (4.33), (4.34) and (A.13), obtaining

$$
\begin{aligned}
&C\Big(|\partial_t^2\beta^u|^2_0 + |\partial_t\beta^u|^2_0 + |\beta^u(0)|^2_0 + ||\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle||^2_{*,h} \\
&\quad + |\partial_t^2\beta^u|^2_{0,\Gamma} + |\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|^2_{0,\Gamma} + |\partial_t\beta^w|^2_0\Big) + \frac{1}{4}|\partial_t\alpha^u|^2_1.
\end{aligned}
$$

Then, the second to last must be smaller than

$$C\left(|\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|_0 + |\langle\partial_t\alpha^u\rangle|_0 + |\partial_t\beta^u|_0 + |\alpha^u|_0 + |\beta^u|_0\right)|\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|_0$$
$$\leq C\left(|\beta^u(0)|_0^2 + |\partial_t\beta^u|_0^2 + |\alpha^u|_0^2 + |\beta^u|_0^2 + ||\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle||_{*,h}^2\right) + \frac{1}{4}|\partial_t\alpha^u|_1^2.$$

Then we observe that the last term is bounded by

$$C\left(|\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|_{0,\Gamma}^2 + |\beta^u(0)|_0^2 + |\partial_t\beta^u|_0^2 + |\partial_t\beta^u|_{0,\Gamma}^2 + |\alpha^u|_{0,\Gamma}^2 + |\beta^u|_{0,\Gamma}^2\right).$$

Again, we used all the aforementioned inequalities. Exploiting these results, we conclude

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{dt}}(||\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle||_{*,h}^2 + |\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|_{0,\Gamma}^2) + \sigma||\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle||_{*,h}^2 \\
&\quad + |\partial_t\alpha^u|_1^2 + |\partial_t\alpha^u|_{1,\Gamma}^2 + \sigma_\Gamma|\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|_{0,\Gamma}^2 \\
&\leq C_1\left(|\partial_t\beta^w|_0^2 + |\beta^u|_0^2 + |\partial_t\beta^u|_0^2 + |\partial_t^2\beta^u|_0^2 + |\beta^u|_{0,\Gamma}^2 + |\partial_t\beta^u|_{0,\Gamma}^2 + |\partial_t^2\beta^u|_{0,\Gamma}^2\right) \\
&\quad + C_2\left(|\alpha^u|_{0,\Gamma}^2 + |\alpha^u|_0^2 + |\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|_{0,\Gamma}^2 + ||\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle||_{*,h}^2\right) + C_3|\beta^u(0)|_0^2.
\end{aligned} \tag{4.44}$$

It is now just a matter of summing (4.38) and (4.44); using (A.13), the Poincaré, triangular, and Young inequalities, we get

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{dt}}\Phi(t) + \sigma||\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle||_{*,h}^2 + \sigma_\Gamma|\partial_t\alpha^u - \langle\partial_t\alpha^u\rangle|_{0,\Gamma}^2 \\
&\quad + |\partial_t\alpha^u|_{0,\Gamma}^2 + |\alpha^w|_1^2 + |\partial_t\alpha^u|_1^2 + |\partial_t\alpha^u|_{1,\Gamma}^2 \\
&\leq C_4\Phi(t) + C_5\left(|\beta^w|_0^2 + |\partial_t\beta^w|_0^2 + |\beta^u|_0^2 + |\partial_t\beta^u|_0^2 + |\partial_t^2\beta^u|_0^2\right. \\
&\quad \left.+|\beta^u|_{0,\Gamma}^2 + |\partial_t\beta^u|_{0,\Gamma}^2 + |\partial_t^2\beta^u|_{0,\Gamma}^2\right) + C_3|\beta^u(0)|_0^2 \quad \forall t\in[0,T_h].
\end{aligned} \tag{4.45}$$

Finally we integrate (4.45) in $(0,t)$, with $t\in[0,T_h]$; applying Gronwall's Lemma to the resulting inequality, and substituting it back into (4.45), we get (4.7) and this concludes the proof.

□

4.3 Proof of Theorem 4.3

We are now ready to complete the proof of the error estimates. We first notice that we can differentiate (4.15)-(4.17) and get a version of inequalities (4.19)-(4.20) involving the derivatives of β^u and β^w, that is,

$$|\partial_t\beta^u|_0 + |\partial_t\beta^u|_{0,\Gamma} + h|\partial_t\beta^u|_1 + h|\partial_t\beta^u|_{1,\Gamma} \leq Ch^2(|\partial_t u|_2 + |\partial_t u|_{2,\Gamma}) \tag{4.46}$$

$$|\partial_t^2\beta^u|_0 + |\partial_t^2\beta^u|_{0,\Gamma} + h|\partial_t^2\beta^u|_1 + h|\partial_t^2\beta^u|_{1,\Gamma} \leq Ch^2(|\partial_t^2 u|_2 + |\partial_t^2 u|_{2,\Gamma}), \tag{4.47}$$

and

$$|\partial_t\beta^w|_0 + h|\partial_t\beta^w|_1 \leq Ch^2|\partial_t w|_2. \tag{4.48}$$

Then, because of the regularity hypothesis (4.7), (4.8), and due to the embedding $H^2(\Omega) \hookrightarrow C^0(\overline{\Omega})$, we infer that there must exists $R \in (0, +\infty)$ such that

$$||u||_{C^0([0,T];C^0(\overline{\Omega}))} < R \quad ||\partial_t u||_{C^0([0,T];C^0(\overline{\Omega}))} \leq R \tag{4.49}$$

We now deal with the initial datum $u_{0,h}$; using Lemma A.6 and Lemma A.7, we obtain

$$\begin{aligned} ||u_{0,h} - u_0||_{C^0(\overline{\Omega})} &\leq ||u_{0,h} - I_h u_0||_{C^0(\overline{\Omega})} + ||I_h u_0 - u_0||_{C^0(\overline{\Omega})} \\ &\leq C_1 h^{-d/2}(|u_{0,h} - u_0|_0 + |u_0 - I_h u_0|_0) + C_2 h^\gamma |u_0|_2 \end{aligned} \tag{4.50}$$

where the Hölder exponent $\gamma \in (0,1)$ is such that $H^2(\Omega) \hookrightarrow C^{0,\gamma}(\Omega)$, and depends on the dimension d. Therefore, recalling (4.18), using (4.20) and Lemma A.5, we get

$$||u_{0,h} - u_0||_{C^0(\overline{\Omega})} \leq C\left(h^{2-d/2}(|u_0|_2 + |u_0|_{2,\Gamma}) + h^\gamma |u_0|_2\right).$$

This means that, if h is chosen small enough, it must hold

$$||u_{0,h}||_{C^0(\overline{\Omega})} < R.$$

Thus, together with (4.49), this tells us that the hypothesis of Lemma 4.7 are satisfied.

Let us now show that

$$\Phi(0) \leq Ch^4,$$

and then prove that the same result holds for $\Phi(t)$, $t \in [0, T]$.
By the definition of Φ and on account of (4.18), we have

$$\Phi(0) = ||\partial_t\alpha^u(0) - \langle\partial_t\alpha^u(0)\rangle||^2_{*,h} + |\partial_t\alpha^u(0) - \langle\partial_t\alpha^u(0)\rangle|^2_{0,\Gamma},$$

thus we only need to estimate these two terms. We do so by writing (4.31), (4.35) at $t = 0$, and choosing $y = \mathcal{N}_h(\partial_t\alpha^u(0) - \partial_t\langle\alpha^u(0)\rangle)$, $y = \partial_t\alpha^u(0) - \langle\partial_t\alpha^u(0)\rangle$, respectively. Summing these inequalities, using $\mathcal{N}_h$ definition, we get

$$
\begin{aligned}
&||\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle||^2_{*,h}+|\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle|^2_{0,\Gamma}\\
&=\int_\Omega(\langle\partial_t\alpha^u(0)\rangle+\partial_t\beta^u(0)+\sigma\beta^u(0))\mathcal{N}_h(\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle)\\
&\quad+\int_\Omega(f(u_{0,h}))-f(u_0))(\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle)\\
&\quad+\int_\Gamma(f_\Gamma(u_{0,h})-f_\Gamma(u_0))(\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle)\\
&\quad-\int_\Gamma(\langle\partial_t\alpha^u(0)\rangle+\beta^u(0))(\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle),
\end{aligned}
\tag{4.51}
$$

where we have also rewritten $\partial_t\alpha^u(0)$ as in (4.39).
The need for condition (4.18) will now be clear; in fact, exploiting also (4.33) and the Cauchy-Schwarz and Poincaré inequalities, (4.51) yields

$$
\begin{aligned}
&||\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle||^2_{*,h}+|\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle|^2_{0,\Gamma}\\
&\le C_1(|\beta^u(0)|_0+|\partial_t\beta^u(0)|_0)||\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle||^2_{*,h}\\
&\quad+C_2|\beta^u(0)|_0|\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle|_0\\
&\quad+C_3(|\beta^u(0)|_{0,\Gamma}+|\partial_t\beta^u(0)|_{0,\Gamma})|\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle|_{0,\Gamma}.
\end{aligned}
\tag{4.52}
$$

We now use the Young inequality on the terms on the right hand side; clearly, the only term which needs particular care is the $L^2(\Omega)$ norm of $\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle$, for which we need an upper bound.
Such bound is obtained by writing (4.31) at $t=0$, and then choosing $y=\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle$; using once more (4.17) and (4.18), we then get

$$
\begin{aligned}
&\int_\Omega\partial_t(\alpha^u(0)-\langle\alpha^u(0)\rangle+\langle\alpha^u(0)\rangle+\beta^u(0))(\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle)\\
&\quad+\sigma\int_\Omega\beta^u(0)(\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle)=0,
\end{aligned}
$$

so

$$
\begin{aligned}
|\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle|^2_0\le{}&C|\langle\partial_t\alpha^u(0)\rangle+\partial_t\beta^u(0)+\sigma\beta^u(0)|^2_0\\
&+\frac{1}{2}|\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle|^2_0,
\end{aligned}
$$

and, owing to (4.33), we conclude

$$
|\partial_t\alpha^u(0)-\langle\partial_t\alpha^u(0)\rangle|^2_0\le C(|\beta^u(0)|^2_0+|\partial_t\beta^u(0)|^2_0).
\tag{4.53}
$$

Finally, summing (4.52) and (4.53), it is now easy to show that it holds

$$
\begin{aligned}
\Phi(0) &= ||\partial_t\alpha^u(0) - \langle\partial_t\alpha^u(0)\rangle||^2_{*,h} + |\partial_t\alpha^u(0) - \langle\partial_t\alpha^u(0)\rangle|^2_{0,\Gamma} \\
&\le C(|\beta^u(0)|^2_0 + |\partial_t\beta^u(0)|^2_0 + |\beta^u(0)|^2_{0,\Gamma} + |\partial_t\beta^u(0)|^2_{0,\Gamma}) \\
&\le Ch^4(|u|^2_2 + |u|^2_{2,\Gamma}),
\end{aligned} \tag{4.54}
$$

as it follows from (4.20) and (4.46); thus, $\Phi(0) \le Ch^4$ as claimed.

Examining estimate (4.27), we notice that the whole right hand side is now bounded by a term of the form Ch^4; hence, this immediately implies

$$
\Phi(t) \le Ch^4, \quad \forall t \in [0, T_h]. \tag{4.55}
$$

In order to extend this result to the whole $[0, T]$, we first notice that (4.55) implies $|\alpha^u|_0 \le Ch^2$, $\forall t \in [0, T_h]$; then, using the same argument showed in (4.50), we get

$$
\begin{aligned}
||u_h(t) - u(t)||_{C^0(\overline{\Omega})} &\le C_1 h^{-d/2}(|u_h(t) - u(t)|_0 + |u(t) - I_h u(t)|_0) + C_2 h^\gamma |u(t)|_2 \\
&= C_1 h^{-d/2}(|\alpha^u(t) + \beta^u(t)|_0 + |u(t) - I_h u(t)|_0) + C_2 h^\gamma |u(t)|_2 \\
&\le C(h^{2-d/2} + h^\gamma).
\end{aligned}
$$

for every $t \in [0, T_h]$; however, this means that

$$
\sup_{t\in[0,T_h]} ||u_h(t) - u(t)||_{C^0(\overline{\Omega})} \to 0 \;\text{ as }\; h \to 0. \tag{4.56}
$$

Hence, by the definition of T_h, we can choose h small enough in order to get $T_h = T$. Estimates (4.9)-(4.12) then follow immediately using the definition of $\Phi(t)$ and (4.55).

□

4.4 Fully discrete scheme

We now know that a $\mathbb{P}^1$ finite elements semidiscretization is a "good" choice: at this point, we need to choose how to approximate the time derivatives. In [60] both a semi-implicit (with an explicit treatment of the nonlinearities) Euler method, and a linearized Crank-Nicolson are used; the same authors suggested a completely implicit Euler scheme in [61], and this will be our approach too.

To this aim, we first fix a time step Δt, and consequently we set $t^n = n\Delta t$, $N_T = \frac{T}{\Delta t}$. Hence, $u_h^n(\mathbf{x}) \approx u(\mathbf{x}, t^n)$ and $w_h^n(\mathbf{x}) \approx w(\mathbf{x}, t^n)$ will be the approximations of the real solution at time t^n. With these conventions, we write the fully discretized system as

$$
\begin{cases}
\dfrac{1}{\Delta t}\displaystyle\int_\Omega (u_h^{n+1}-u_h^n)y+\sigma\int_\Omega u_h^{n+1}y+\int_\Omega \nabla w_h^{n+1}\cdot\nabla y=0 \qquad \forall y\in X_h, & (4.57)\\
\displaystyle\int_\Omega w_h^{n+1}y=\int_\Omega \nabla u_h^{n+1}\cdot\nabla y+\int_\Omega \Big(f(u_h^{n+1})-g(t^{n+1})\Big)\,y & \\
\qquad\qquad +\dfrac{1}{\Delta t}\displaystyle\int_\Gamma (u_h^{n+1}-u_h^n)y+\int_\Gamma \nabla_\Gamma u_h^{n+1}\cdot\nabla_\Gamma y & \\
\qquad\qquad +\sigma_\Gamma\displaystyle\int_\Gamma u_h^{n+1}y+\int_\Gamma \Big(f_\Gamma(u_h^{n+1})-g_\Gamma(t^{n+1}\Big)\,y \qquad \forall y\in X_h. & (4.58)
\end{cases}
$$

where $n=0,\dots,N_T-1$ and u_h^0 is the approximation of the initial datum, as explained in Remark 4.5.

Denoting by N_h the number of degrees of freedom (that is, the number of points) of X_h, we write (4.57), (4.58) in monolithic matrix form as

$$
\begin{bmatrix} A & B\\ C & D\end{bmatrix}\begin{bmatrix}\mathbf{U}^{n+1}\\ \mathbf{W}^{n+1}\end{bmatrix}+\begin{bmatrix}\mathbf{0}\\ \mathbf{H}(\mathbf{U}^{n+1})\end{bmatrix}=\begin{bmatrix}\mathbf{G}_1^{n+1}\\ \mathbf{G}_2^{n+1}\end{bmatrix} \qquad n=0,\dots,N_T-1, \tag{4.59}
$$

where the unknowns are $\mathbf{U}^{n+1}=(u_i^{n+1})_{i=1}^{N_h}$, $\mathbf{W}^{n+1}=(w_i^{n+1})_{i=1}^{N_h}$ and the matrix blocks are defined as follows

$$
\begin{gathered}
A_{ij}=(1+\sigma\Delta t)\int_\Omega \phi_j\phi_i \quad B_{ij}=\Delta t\int_\Omega \nabla\phi_j\cdot\nabla\phi_i,\\
C_{ij}=\Delta t\int_\Omega \nabla\phi_j\cdot\nabla\phi_i+(1+\sigma_\Gamma\Delta t)\int_\Gamma \phi_j\phi_i+\Delta t\int_\Gamma \nabla_\Gamma\phi_j\cdot\nabla_\Gamma\phi_i\\
D_{ij}=-\Delta t\int_\Omega \phi_j\phi_i.
\end{gathered}
$$

Similarly, the vectors are defined as follows

$$
\begin{gathered}
H_i(\mathbf{U}^{n+1})=\Delta t\int_\Omega f\Big(\sum_{k=1}^{N_h}u_k^{n+1}\phi_k\Big)\phi_i+\Delta t\int_\Gamma f_\Gamma\Big(\sum_{k=1}^{N_h}u_k^{n+1}\phi_k\Big)\phi_i\\
G_{1,i}^{n+1}=\int_\Omega u_i^n\phi_i \quad G_{2,i}^{n+1}=\Delta t\int_\Omega g(t^{n+1})\phi_i+\Delta t\int_\Gamma g_\Gamma(t^{n+1})\phi_i+\int_\Gamma u_i^n\phi_i.
\end{gathered}
$$

In the above definitions, the indexes i, j vary between 1 and N_h, and $(\phi_i)_{i=1}^{N_h}$ is a base for X_h.
In order to solve the nonlinear system (4.59), we use a Newton iterative method, at each time step, to solve it. To this aim, we rewrite it as

$$
\mathbf{\Phi}(\mathbf{P}^{n+1})=M\mathbf{P}^{n+1}+\widetilde{\mathbf{H}}(\mathbf{P}^{n+1})-\mathbf{G}^{n+1}=\mathbf{0}, \tag{4.60}
$$

with an obvious meaning for the new letters, and define the flux

$$J_{\mathbf{\Phi}}(\mathbf{P}) = \left(\frac{\partial \Phi_i}{\partial p_j}\right)(\mathbf{P}) = M + \widetilde{N}(\mathbf{P}),$$

where

$$\widetilde{N}(\mathbf{P}) = \begin{bmatrix} 0 & 0 \\ N(\mathbf{P}) & 0 \end{bmatrix} \qquad N(\mathbf{P})_{ij} = \int_\Omega f'\Big(\sum_{k=1}^{N_h} p_k\phi_k\Big)\phi_j\phi_i.$$

Therefore, given an initial vector $\mathbf{P}_0^{n+1}$, the Newton method prescribes to solve the system

$$\begin{cases} J_{\mathbf{\Phi}}(\mathbf{P}_k^{n+1})\,\delta\mathbf{P}_k^{n+1} = \mathbf{\Phi}(\mathbf{P}_k^{n+1}) \\ \mathbf{P}_{k+1}^{n+1} = \mathbf{P}_k^{n+1} + \delta\mathbf{P}_k^{n+1}, \end{cases}$$

until some convergence criterion is met, for each $n = 0, \dots, N_T - 1$.

4.5 Numerical simulations

We chose to solve (4.59) with the aid of the FreeFem++ software, on a $L_x \times L_y = 50 \times 25$ rectangle. Periodic conditions were imposed on the left and right sides, and dynamic boundaries conditions on the top and bottom sides. The uniform mesh was set to be composed of 250×125 points, hence with spatial steps $h_x = h_y = 0.2$; moreover we set the time step to $\Delta t = 0.001$. A very generic version of code that was used is reported in Appendix B, and covers the simulations which we now discuss.

Remark 4.8 As one could choose to vary many different parameters of the problem, we make a simple observation: the maximum/minimum of u_0, the reaction coefficient σ and the final time T are linked each other, as it is clear recalling the decay law for $\langle u \rangle$. Experimental tests show that, once u_0 is fixed, the behavior after a long time with a small σ are qualitatively the same as after a shorter time, with a larger value for σ. We chose the second approach, which is the same as in [66].

For all the simulations f and f_Γ were taken as follows

$$f(s) = s^3 - s \qquad f_\Gamma(s) = s,$$

and the initial datum was chosen randomly, with fluctuations of $\pm\,0.5$. For each set, we show the distribution of u at $t = 0.002,\ 0.005,\ 0.01$, while varying the reaction coefficients, a stable state being attained before $t = 0.01$; for each of these times, the solution was saved and turned into a black and white image, where black areas correspond to negative values of u.
We now examine in detail the different configurations that were considered.

Initial datum with null average
The first set of simulations is characterized by an initial datum satisfying $\langle u_0 \rangle = 0$, and different values of $\sigma = \sigma_\Gamma$. Hence, this configuration fits the phenomenon of phase separation of diblock copolimers.

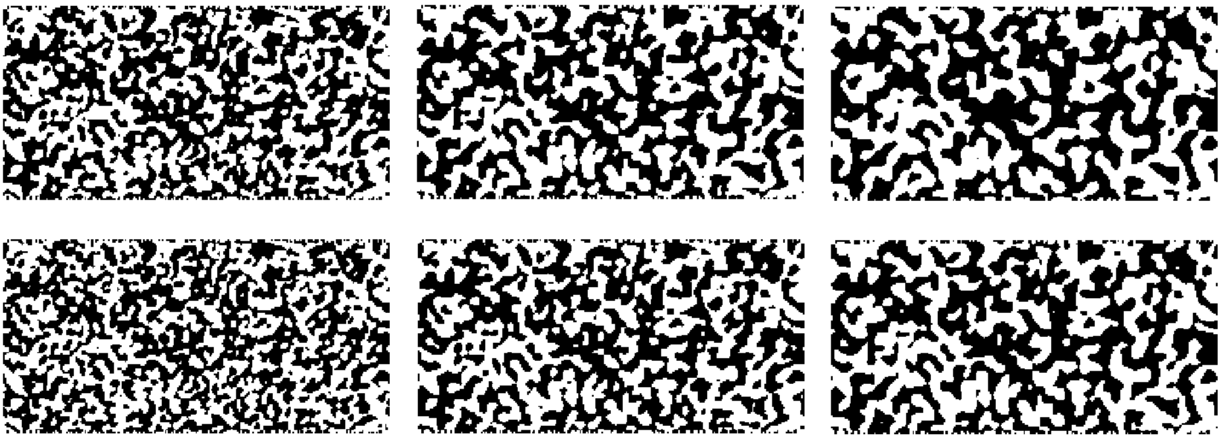

Figure 4.1: Evolution of the same initially homogeneous distribution satisfying $\langle u_0 \rangle = 0$. In the first row, $\sigma = \sigma_\Gamma = 100$, in the second one $\sigma = \sigma_\Gamma = 1000$. Each column represents respectively the times $t = 0.002$, $t = 0.005$, $t = 0.01$

We immediately notice how, even after a small time, the reaction parameters influence the evolution of the mixture. Indeed, even if a similar pattern emerges at the final time $t = 0.1$, the formation of big structures is inhibited in the case of larger σ, σ_Γ (see Figure 4.1).

This fact gets even more evident if we increase such values, as in Figure 4.2; on the other hand, no sensible difference was perceived in the range $\sigma \in (0, 100)$.
We moreover remark that the same effect is present at the boundary, where the distribution gets somehow more discontinuous for larger values of σ_Γ.
It is also clear that the dynamic boundaries condition, as explained in the Introduction, does not force the interface between the two components to be orthogonal to the wall.

The results are qualitatively the same as the ones in [60], [61].

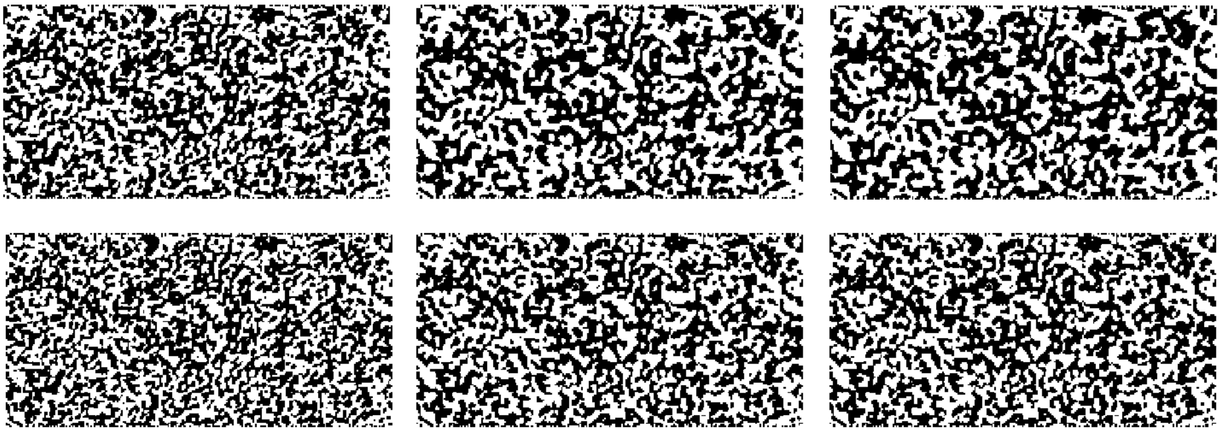

Figure 4.2: Evolution of the same initially homogeneous distribution satisfying $\langle u_0 \rangle = 0$. In the first row, $\sigma = \sigma_\Gamma = 5000$, in the second one $\sigma = \sigma_\Gamma = 10000$. Each column represents respectively the times $t = 0.002$, $t = 0.005$, $t = 0.01$

Initial datum with non-null average

The natural subsequent simulations regard the case where the initial datum is characterized by a non-null average. The fluctuations of u_0 are the same as before, but now $\langle u_0 \rangle \approx -0.15$, so we can think of this configuration as that of two reacting substances in an initially homogeneous alloy.

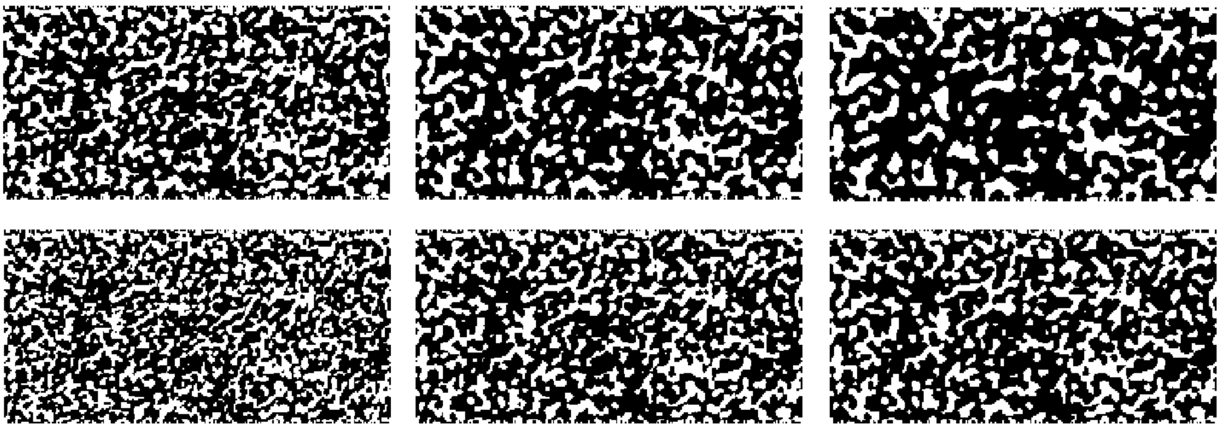

Figure 4.3: Evolution of the same initially homogeneous distribution, with $\langle u_0 \rangle \approx -0.15$. In the first row, $\sigma = \sigma_\Gamma = 1000$, in the second one $\sigma = \sigma_\Gamma = 5000$. Each column represents respectively the times $t = 0.002$, $t = 0.005$, $t = 0.01$

Similar arguments to those of the null-average case hold here too; indeed, even if the steady states seem to contain more "black" component because of the loss of information in the conversion to a black and white image, numerically computing the average shows that it follows the exponential decay law.

A part from this the qualitative analysis, including the behavior at the boundary, is the same as in the previous case.

Source on Γ

We now want to investigate what happens if the PDE on Γ is non-homogeneous, that is if $g_\Gamma \neq 0$; in particular, we set $g_\Gamma = -0.5$.

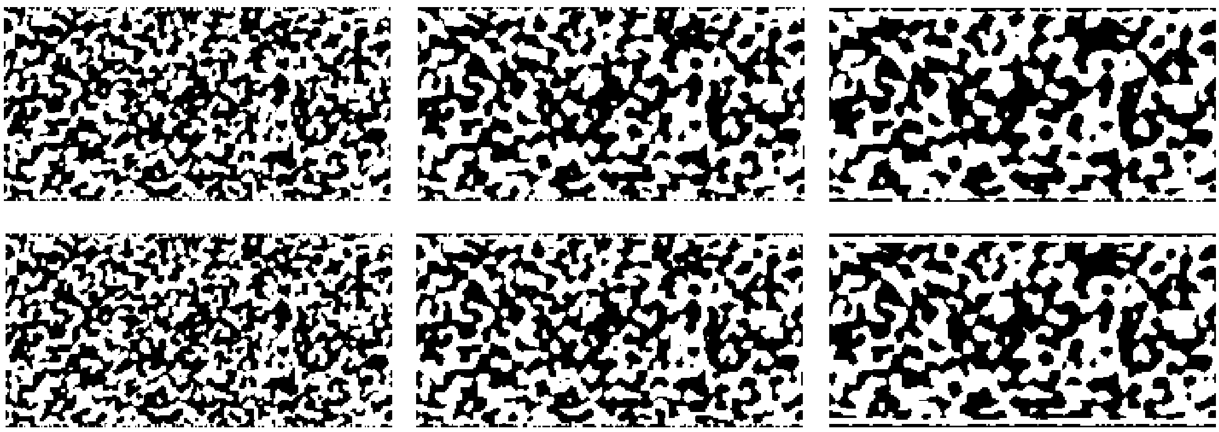

Figure 4.4: Evolution of the same initially homogeneous distribution, with $g_\Gamma = -0.5$. In the first row, $\sigma = \sigma_\Gamma = 100$, in the second one $\sigma = \sigma_\Gamma = 500$. Each column represents respectively the times $t = 0.002$, $t = 0.005$, $t = 0.01$

The upper and lower sides of the slab clearly show a "preference", which grows as time passes, for negative values of u, and this is again in good agreement with both theory and [60], [61].

We did not report the simulation for larger values of σ, as in this case the same effect happens too quickly to make a qualitative analysis.

Different reaction coefficients on Ω and Γ

In the last set of simulations, we wanted to test the cases where $\sigma \neq \sigma_\Gamma$. As pointed out in Remark 2.1, the effect is that of an additional, time dependent, source on the boundary.

We notice that far from the upper and lower sides, the distribution is almost the same as in the previous tests; however, as the difference in the two values increases, and time passes, some peculiar pattern slowly emerges from Γ (Figure 4.5).

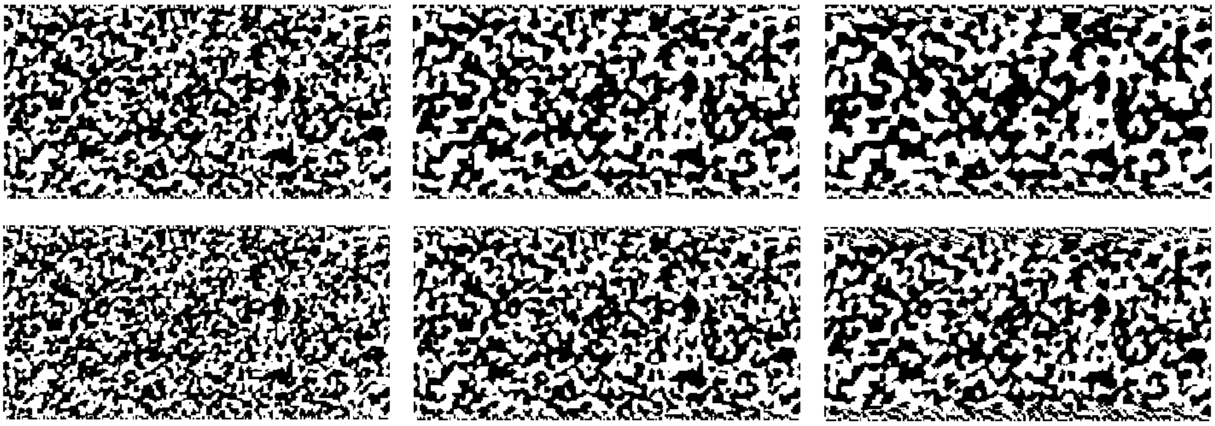

Figure 4.5: Evolution of the same initially homogeneous distribution, with $g_\Gamma = -0.5$. In the first row, $\sigma = 2000$, $\sigma_\Gamma = 1000$, in the second one $\sigma = 5000$, $\sigma_\Gamma = 2500$. Each column represents respectively the times $t = 0.002$, $t = 0.005$, $t = 0.01$

We however remark that it is not clear if such a case corresponds to a significant physical situation; indeed this should be one of the topics for future works.

Conclusions and future work

In this thesis, we have analyzed different properties of the Cahn-Hilliard-Oono equation with dynamic boundary conditions. We proved that, under reasonable assumptions, the correspondent problem is well posed and possesses a connected global attractor. Moreover, we showed that a $\mathbb{P}^1$ finite elements discretization, with an implicit treatment of the time derivatives, can be used to perform numerical simulations which are in good agreement with the theory.

There are still, however, many other aspects of this system whose investigation should be of great interest.

First of all, a significant generalization would be that of dealing with a singular potential. It is expected that in this case a sign compatibility condition on f_Γ will be needed to prove the existence of a distributional solution; on the other hand, if such condition is not assumed, it should be possible to obtain the existence of a weaker solution satisfying a variational inequality, instead of an equality (see [68]).

In Chapter 2, we mentioned that a desirable property for the global attractor is that of being finite dimensional, in Hausdorff or fractal sense. This result, in CHO related equations, is often achieved obtaining estimates independent on σ and then letting such value go to zero; examining our problem formulation, it is evident that we would need better estimates than the ones we proved. Moreover, there is an additional difficulty due to the presence of the parameter σ_Γ.

As a related topic, it seems that a deeper analysis on the link between σ and σ_Γ could lead to significant conclusions; indeed, the numerical simulations suggested that the phenomenon of reacting substances in binary alloys confined in non-permeable walls is greatly influenced by the difference in these two values.

Finally, an analysis of the system coupled with the Navier-Stokes equations could be performed: this should lead to a physically relevant model for reacting substances in liquid mixtures, even close to the boundary (on this topic see, for instance, [69]).

Appendix A

Results used in the paper

In this Appendix we state some results that were recurrently used throughout the text, although non-essential to comprehend the work at a first read.

A.1 Function spaces

We recall how we relabeled the most used function spaces:

$$
\begin{gathered}
V = H^1(\Omega), \quad H = L^2(\Omega), \\
V_\Gamma = H^1(\Gamma), \quad H_\Gamma = L^2(\Gamma), \\
W = \{u \in V \mid u|_\Gamma \in V_\Gamma\}, \\
V_0 = \{v \in V \mid \langle v \rangle = 0\}, \quad V_0^* = \{v^* \in V^* \mid \langle v^* \rangle = 0\}.
\end{gathered}
$$

Let $\{\mu_k\}_{k\in\mathbb{N}}$ and $\{e_k\}_{k\in\mathbb{N}}$ be the set of ordered eigenvalues and the set of the correspondent eigenfunctions for the Laplace operator on Ω with homogeneous Neumann boundary condition, i.e. the countable set of couples (μ, e), $\mu \in \mathbb{R}$ and $e \in V\backslash\{0\}$ solving

$$\int_\Omega \nabla e \cdot \nabla z = \mu \int_\Omega ez \quad \forall z \in V.$$

It is well-know that $\mu_1 = 0$ and $\mu_k > 0\ \forall k > 1$. Moreover, $\{e_k\}_{k\in\mathbb{N}}$ forms an orthonormal base for H. We then set $V_n = \mathrm{span}\{e_1, \dots, e_n\}\ \forall n \geq 1$.

We now cite and prove three Lemmas regarding density results, taken from [44].

Lemma A.1 *Let $z \in Z = \{z \in H^2(\Omega) \mid \partial_n z = 0 \text{ on } \Gamma\}$. If we set*

$$z^n = \sum_{k=1}^{n} (z, e_k)_H e_k, \tag{A.1}$$

that is, z^n is the $L^2(\Omega)$-projection of z on V_n, then

$$||z^n - z||_W \to 0 \quad \text{as } n \to +\infty. \tag{A.2}$$

Proof If we set $a_k := (z, e_k)_H$, it is clear that we can write

$$z = \sum_{k=1}^{\infty} a_k e_k, \quad z - z^n = \sum_{k=n+1}^{\infty} a_k e_k,$$

so that

$$-\Delta z = \sum_{k=1}^{\infty} \mu_k a_k e_k, \quad -\Delta(z - z^n) = \sum_{k=n+1}^{\infty} \mu_k a_k e_k.$$

Obviously $\{a_k\}_{k=1}^{\infty}$, $\{\mu_k a_k\}_{k=1}^{\infty} \subset l^2(\mathbb{N})$. Then, exploiting the continuity of the trace operator and the equivalence of norm $||\cdot||_H + ||-\Delta \cdot||_H$ in $H^2(\Omega)$

$$\begin{aligned} ||z^n - z||_W^2 = ||z^n - z||_V^2 + ||z^n|_\Gamma - z|_\Gamma||^2|_{V_\Gamma} \le c||z^n - z||_{H^2(\Omega)}^2 \\ \le c\Big\{||z^n - z||_H^2 + ||-\Delta(z^n - z)||_H^2\Big\} = c \sum_{k=n+1}^{\infty} (a_k^2 + \mu_k^2 a_k^2) < \infty, \end{aligned}$$

and (A.2) is proved.

□

Lemma A.2 *Z (as defined in Lemma A.1) is dense in W.*

Proof Clearly $Z \subset W$. We then choose $v \in W$ such that $v \perp Z$, that is:

$$(v, z)_W = \int_\Omega vz + \int_\Omega \nabla v \cdot \nabla z + \int_\Gamma v|_\Gamma z|_\Gamma + \int_\Gamma \nabla_\Gamma v|_\Gamma \cdot \nabla_\Gamma z|_\Gamma = 0 \quad \forall z \in Z. \quad \text{(A.3)}$$

If now $z \in C_0^\infty(\Omega)$, it is clear that

$$\int_\Omega vz - \int_\Omega \Delta v z = 0 \quad \Rightarrow \quad v - \Delta v = 0 \ \text{ in } \mathcal{D}'(\Omega),$$

hence

$$\int_\Omega vz + \int_\Omega \nabla v \cdot \nabla z = \langle \partial_n v|_\Gamma, z|_\Gamma \rangle_{H^{-1/2}(\Gamma)\times H^{1/2}(\Gamma)} \quad \forall z \in V. \quad \text{(A.4)}$$

Since $Z \subset V$, we can substitute this last equation in (A.3) and thus obtain

$$\langle \partial_n v|_\Gamma, z|_\Gamma \rangle_{H^{-1/2}(\Gamma)\times H^{1/2}(\Gamma)} + \int_\Gamma v|_\Gamma z|_\Gamma + \int_\Gamma \nabla_\Gamma v|_\Gamma \cdot \nabla_\Gamma z|_\Gamma = 0 \quad \forall z \in Z,$$

and owing to the surjectivity of operator $|_\Gamma$

$$|_\Gamma : H^2(\Omega) \to H^{1/2}(\Gamma) \times H^{3/2}(\Gamma), \quad |_\Gamma : z \mapsto (\partial_n z|_\Gamma, z|_\Gamma),$$

we conclude that

$$\langle \partial_n v|_\Gamma, z_\Gamma \rangle_{H^{-1/2}(\Gamma)\times H^{1/2}(\Gamma)} + \int_\Gamma v|_\Gamma z_\Gamma + \int_\Gamma \nabla_\Gamma v|_\Gamma \cdot \nabla_\Gamma z_\Gamma = 0 \quad \forall z_\Gamma \in H^{3/2}(\Gamma). \quad \text{(A.5)}$$

Equation (A.5) actually holds for every $z_\Gamma \in V_\Gamma$ since $H^{3/2}(\Gamma)$ is dense in $H^1(\Gamma)$. Hence we can combine (A.4) with (A.5) to see that (A.3) holds for every $z \in W$; in order to conclude the proof, it suffices to set $z = v$ to get $v = 0$ in W.

□

Lemma A.3 *Let* $V_\infty = \bigcup_{n=1}^{\infty} V_n$. *Then,* V_∞ *is dense in* W.

Proof Let $v \in W$. We set

$$v_m := \sum_{k=1}^{m} (v, e_k)_H e_k.$$

Lemma A.1 tells us that $||v_m - v||_W \to 0$ since $v \in Z$. Moreover, $v_m \in V_\infty \; \forall m \in \mathbb{N}$, and this concludes the proof.

□

A.2 The operator $\mathcal{N}$

Consider the problem

$$\int_\Omega \nabla u \cdot \nabla z = \langle g, z \rangle_{V^*} \quad \forall z \in V_0 \tag{A.6}$$

where $g \in V_0^*$ is given. Clearly, (A.6) is nothing but the weak formulation of Poisson's problem with homogeneus Neumann condition on the border Γ and datum g; since this problem is well posed, we can define the operator $\mathcal{N} : V_0^* \to V_0$, which maps any given function $g \in V_0^*$ to the corresponding solution $u = \mathcal{N}(g) \in V_0$ of (A.6).

$\mathcal{N} \in \mathcal{L}(V_0^*, V_0)$ is clearly invertible, so it defines an isomorphism between V_0^* and V_0 due to the bounded inverse theorem. Furthermore, it is self-adjoint and positive semidefinite on V_0^*, since

$$\int_\Omega f\mathcal{N}(g) = \int_\Omega \nabla\mathcal{N}(f) \cdot \nabla\mathcal{N}(g) = \int_\Omega \mathcal{N}(f)g \quad \forall f, g \in V_0^*,$$

and

$$\int_\Omega f\mathcal{N}(f) = \int_\Omega \nabla\mathcal{N}(f) \cdot \nabla\mathcal{N}(f) \geq 0 \quad \forall f \in V_0^*.$$

If we now define

$$\begin{gathered} || \cdot ||_* : V^* \to [0, +\infty), \\ ||v^*||_*^2 := ||\nabla\mathcal{N}(v^* - \langle v^* \rangle)||_H^2 + |\langle v^* \rangle|^2 \quad \forall v^* \in V^*, \end{gathered} \tag{A.7}$$

it is easy to see that $||\cdot||_*$ is a norm that makes V^* a complete space, since convergence in the norms on the right hand side forces convergence in $||\cdot||_*$. It then follows from the theory that $||\cdot||_*$ is an equivalent norm in V^*, i.e. there exist $m_*, M_* > 0$ such that

$$m_*||v^*||_{V^*} \le ||v^*||_* \le M_*||v^*||_{V^*} \quad \forall v^* \in V^*.$$

Moreover, we notice that in particular

$$\langle v^*, \mathcal{N}(v^*)\rangle_{V^*} = \int_\Omega |\nabla \mathcal{N}(v^*)|^2 = ||v^*||_*^2 \quad \forall v^* \in V_0^*, \tag{A.8}$$

and, if $v^*(t) \in H^1(0,T;V_0^*)$

$$\begin{aligned}\langle \partial_t v^*(t), \mathcal{N}(v^*(t))\rangle_{V^*} &= \int_\Omega \nabla \mathcal{N}(\partial_t v^*(t)) \cdot \nabla \mathcal{N}(v^*(t)) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\int_\Omega |\nabla \mathcal{N}(v^*(t))|^2 \\ &= \frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}||v^*(t)||_*^2 \quad \text{a.a. } t \in (0,T).\end{aligned} \tag{A.9}$$

A.3 Inequalities

We first recall the Poincaré inequality

$$||v||_H \le C||\nabla v||_H \quad \Rightarrow \quad ||\nabla v||_H^2 \le ||v||_V^2 \le C||\nabla v||_H^2 \quad \forall v \in V_0,$$

with, as a consequence

$$C_1(||\nabla v||_H^2 + |\langle v\rangle|^2) \le ||v||_V^2 \le C_2\left(||\nabla v||_H^2 + |\langle v\rangle|^2\right) \quad \forall v \in V, \tag{A.10}$$

where all the positive constants depend on Ω only.

Then

$$ab \le \frac{\varepsilon}{2}a^2 + \frac{1}{2\varepsilon}b^2 \qquad \forall \varepsilon > 0, \quad a,b \in \mathbb{R}.$$

which is the well-known Young inequality.
We now use these results to write

$$\begin{aligned}||v(t)||_H^2 &= ||v(0)||_H^2 + \int_0^t \frac{\mathrm{d}}{\mathrm{ds}}||v(s)||_H^2 = ||v(0)||_H^2 + 2\int_0^t \langle \partial_s v(s), v(s)\rangle \\ &\le ||v(0)||_H^2 + \varepsilon\int_0^t ||\partial_s v(s)||_{V^*}^2 + \frac{1}{\varepsilon}\int_0^t ||v(s)||_V^2 \quad \forall \varepsilon > 0,\end{aligned} \tag{A.11}$$

which clearly hold for a.a. $t \in (0,T)$ whenever $v(t) \in L^2(0,T;V) \cap H^1(0,T;V^*)$. Similarly we have

$$||v(t)||^2_{H_\Gamma} \leq ||v(0)||^2_{H_\Gamma} + \varepsilon \int_0^t ||\partial_s v(s)||^2_{H_\Gamma} + \frac{1}{\varepsilon} \int_0^t ||v(s)||^2_{H_\Gamma} \quad \forall \varepsilon > 0 \tag{A.12}$$

for a.a. $t \in (0,T)$ whenever $v \in H^1(0,T;H_\Gamma)$.

Finally, there holds

$$\begin{aligned} ||v||^2_H \leq ||v||^2_V = (v,v)_V = \langle v,v \rangle_{V^*} \leq ||v||_{V^*}||v||_V \\ \leq C||v||_{V^*}||\nabla v||_H \leq \varepsilon ||\nabla v||^2_H + \frac{C^2}{4\varepsilon}||v||^2_{V^*} \quad \forall \varepsilon > 0, \end{aligned} \tag{A.13}$$

for every $v \in V_0$. As a natural, more general, consequence

$$||v||^2_H \leq \varepsilon ||\nabla v||^2_H + \frac{C^2}{4\varepsilon}||v - \langle v \rangle||^2_{V^*} + |\Omega||\langle v \rangle|^2 \quad \forall \varepsilon > 0 \tag{A.14}$$

for every $v \in V$.

We conclude this section stating the version of Gronwall inequality which was used throughout the text

Lemma A.4 *Let $I = (a,b)$ be an interval on the real line, and α, β, v three real-valued functions defined on I. Assume that β and v are continuous, and that α is a non-decreasing function with integrable negative part on every compact subset of I. If it holds*

$$v(t) \leq \alpha(t) + \int_a^t \beta(s) v(s) \quad \forall t \in I,$$

then

$$v(t) \leq \alpha(t) \exp\left(\int_a^t \beta(s) \right) \quad \forall t \in I,$$

A.4 Error estimates

In the following, V_h will denote a Galerkin $\mathbb{P}^1$ approximation of V on a family of triangulations $\{\Omega_h\}$ of a domain $\Omega \subset \mathbb{R}^d$, and I_h the interpolation operator on V_h.

We recall three well-known results, a proof of which can be easily found in the literature (see, e.g., [70]).

Lemma A.5 *There exists a positive constant C, depending on $\{\Omega_h\}$ only (and in particular, independent on h), such that*

$$||u - I_h u||_H + h||\nabla (u - I_h u)||_H \leq Ch^2||\Delta u||_H \quad \forall u \in H^2(\Omega), \tag{A.15}$$

$$||v - I_h v||_{H_\Gamma} + h||\nabla_\Gamma (v - I_h v)||_{H_\Gamma} \leq Ch^2||\Delta_\Gamma v||_{H_\Gamma} \quad \forall v \in H^2(\Gamma), \tag{A.16}$$

Lemma A.6 *There exists a positive constant C, depending on $\{\Omega_h\}$ only (and in particular, independent on h), such that*

$$||\phi_h||_{C^0(\overline{\Omega})} \leq Ch^{-d/2}||\phi_h||_H \quad \forall \phi_h \in V_h. \tag{A.17}$$

Lemma A.7 *Let $\gamma \in (0,1)$ such that $H^2(\Omega) \hookrightarrow C^{0,\gamma}(\overline{\Omega})$. Then there exists a positive constant C depending on $\{\Omega_h\}$ only (and in particular, independent on h), such that*

$$||u - I_h u||_{C^0(\overline{\Omega})} \leq Ch^\gamma||\Delta u||_H \quad \forall u \in H^2(\Omega). \tag{A.18}$$

Appendix B

FreeFem++ code

```
real Lx = 50, Ly = 25;       // Domain size
real nx = 250, ny = 125;     // Number of elements in x and y direction


mesh Th = square(nx, ny, [Lx * x, Ly * y]);          // Mesh definition
fespace Vh(Th, P1, periodic = [[2, y], [4, y]]);     // FE space definition


Vh w, wold, u, u0, uold, utemp, phi, chi, feval, fgammaeval, dfeval,
    dfgammaeval, geval, ggammaeval;    // Finite elements functions

real dt = 0.001;                      // Time step
real T = 0.01;                        // Final time
int nsaveT = 2;
real[int] saveT = [0.002, 0.005];     // Save times
real curtime;                         // Current time
real sigma = 1000;                    // Reaction coefficient on Omega
real sigmagamma = 1000;               // Reaction coefficient on Gamma
real dimVh = Vh.ndof;
real dimTot = 2 * dimVh;
int j = 0;                            // GMRES iteration number


func real f(real u) {                 // Non-linearity on Omega
   return u^3 - u;
}

func real df(real u) {                // Derivative of the non-linearity
   return 3 * u^2 - 1;                // on Omega
}

func real fgamma(real u) {            // Non-linearity on Gamma
   return u;
}

func real dfgamma(real u) {           // Derivative of the non-linearity
   return 1;                          // on Gamma
}

func real g(real t) {                 // Source term on Omega
   return 0;
}

func real ggamma(real t) {            // Source term on Gamma
   return 0;
}

```

```
// Variational forms

varf a(u, chi) = int2d(Th)((1 + sigma * dt) * u * chi);

varf b(w, chi) = int2d(Th)(dt * (dx(w) * dx(chi) + dy(w) * dy(chi)));

varf g1(phi, chi) = int2d(Th)(uold * chi);


varf c(u, chi) = int2d(Th)(dt * (dx(u) * dx(chi) + dy(u) * dy(chi))) + int1d(
    Th, 1, 3)((1 + sigmagamma * dt) * u * chi) + int1d(Th, 1, 3)(dt * dx(u) *
    dx(chi));

varf d(w, chi) = - int2d(Th)(dt * w * chi);

varf g2(phi, chi) =  int2d(Th)(dt * geval * chi) + int1d(Th, 1, 3)(dt *
    ggammaeval * chi) + int1d(Th, 1, 3)(uold * chi);



varf h(phi, chi) = int2d(Th)(dt * feval * chi) + int1d(Th, 1, 3)(dt *
    fgammaeval * chi);

varf dh(phi, chi) = int2d(Th)(dt * dfeval * phi * chi) + int1d(Th, 1, 3)(dt *
    dfgammaeval * phi * chi);



// Vectors definition

real[int] G1(dimVh), G2(dimVh), G(dimTot), H(dimVh), Htemp(dimVh), dH(dimVh),
    P(dimTot), deltaP(dimTot), Pold(dimTot), U(dimVh), Psi(dimTot), Psitemp(
    dimTot);



// Matrices definition

matrix A = a(Vh, Vh);
matrix B = b(Vh, Vh);
matrix C = c(Vh, Vh);
matrix D = d(Vh, Vh, solver = UMFPACK);

matrix M = [[A, B], [C, D]];
matrix N, J, Prec = [[A, 0], [0, D]];
set(Prec, solver = UMFPACK);

real[int, int] empty(dimVh, dimVh);
empty = 0;



// Function that return the residual of the linear system (required by
    LinearGMRES)

func real[int] Jmult(real[int] &xx) {

   j++;
   cout << "GMRES iteration n. " << j << endl;

   real[int] rr(dimTot);
   rr = J * xx;

   return rr;

```

```
}



// Initialization of u0 with elliptic projection

randinit(42);

real func initialize() {

    real expvalue = 0.5, fluctuation = 0.5;

    if (randreal1() > expvalue) return fluctuation * randreal1();
    else return -1 * fluctuation * randreal1();

}

Vh uinit;

uinit = initialize();

solve ellproju(u0, chi) = int2d(Th)(dx(u0) * dx(chi) + dy(u0) * dy(chi)) +
    int1d(Th, 1, 3)(sigmagamma * u0 * chi) + int1d(Th, 1, 3)(dx(u0) * dx(chi))
     - int2d(Th)(dx(uinit) * dx(chi) + dy(uinit) * dy(chi)) - int1d(Th, 1, 3)(
    sigmagamma * uinit * chi) - int1d(Th, 1, 3)(dx(uinit) * dx(chi));



// Initialization of w0

feval = f(uold);
fgammaeval = fgamma(uold);
geval = g(0);
ggammaeval = ggamma(0);

real[int] Hinit(dimVh), Ginit(dimVh), tmp1(dimVh), tmp2(dimVh), tmp3(dimVh),
    tmp4(dimVh);

Hinit = h(0, Vh);
Ginit = g2(0, Vh);

tmp1 = Ginit - Hinit;
tmp2 = C * uold[];
tmp3 = tmp1 - tmp2;
tmp4 = D^-1 * tmp3;

wold[] = tmp4;
uold = u0;


// Time iterations

for (int i = 0; i < (T / dt) ; i++) {

    curtime = (i + 1) * dt;
    cout << "CHO with dynamic boundaries condition - t = " << curtime << endl;

    geval = g(curtime);
    ggammaeval = ggamma(curtime);
    G1 = g1(0, Vh);
    G(0 : dimVh - 1) = G1;
    G2 = g2(0, Vh);
    G(dimVh : dimTot - 1) = G2;

    Pold(0 : dimVh - 1) = uold[];
    Pold(dimVh : dimTot - 1) = wold[];
    P = Pold;
```

```


    // Computing initial residual

    feval = f(uold);
    fgammaeval = f(uold);
    H = h(0, Vh);

    real residual = 0;
    real[int] y1(dimTot);
    y1 = M * P;
    real[int] y2(dimTot);
    y2 = 0;
    y2(0 : dimVh - 1) = H;
    real[int] resz(dimTot);
    resz = y1 + y2;
    resz = resz - G;

    for(int q = 0; q < dimTot; q++) residual += resz[q] * resz[q];
    cout << "***Newton method initial residual = " << sqrt(residual) << "***"
        << endl;

    int k = 0;



    // Newton iterations

    while (sqrt(residual) > 1e-6) {

       uold[] = P(0 : dimVh - 1);

       feval = f(uold);
       fgammaeval = f(uold);
       dfeval = df(uold);
       dfgammaeval = df(uold);

       matrix Ntemp = dh(Vh, Vh);

       N = [
            [empty, empty],
            [Ntemp, empty]
           ];

       J = M + N;

       Htemp = h(0, Vh);
       H = 0;
       H(0 : dimTot - 1) = Htemp;

       Psitemp = M * P;
       Psitemp = Psitemp + H;
       Psi = G - Psitemp;


       j = 0;

       LinearGMRES(Jmult, deltaP, Psi, eps = 1e-5, nbiter = 1000);
       P = P + deltaP;



       // Computing residual

       uold[] = P(0 : dimVh - 1);
       feval = f(uold);
       fgammaeval = f(uold);
```

```
        H = h(0, Vh);

        residual = 0;
        real[int] x1(dimTot);
        x1 = M * P;
        real[int] x2(dimTot);
        x2 = 0;
        x2(0 : dimVh - 1) = H;
        real[int] res(dimTot);
        res = x1 + x2;
        res = res - G;

        for(int q = 0; q < dimTot; q++) residual += res[q] * res[q];

        ++k;

        cout << "***Newton iteration: " << k << " residual = " << sqrt(residual)
             << "***" << endl;

    }

    u[] = P(0 : dimVh - 1);
    w[] = P(dimVh : dimTot - 1);


    string title = "Cahn-Hilliard-Oono with dynamic boundaries condition, t = "
         + curtime + " sigma = " + sigma;
    plot(u, wait = 0, fill = 1, value = 1, cmm = title);

    uold = u;
    wold = w;


    // Saving solutions at prescribed times

    for (int l = 0; l < nsaveT; l++) {

        if (curtime == saveT(l) || curtime == T) {

            string filenameu = "chod_u_t" + curtime + "_s" + sigma + ".txt";
            string filenamew = "chod_w_t" + curtime + "_s" + sigma + ".txt";

            ofstream fu(filenameu);
            ofstream fw(filenamew);

            for (int j = ny; j >= 0; j--) {

                for (int i = 0; i < nx; i++) {

                    fu << u(i * (Lx / nx), j * (Ly / ny)) << " ";
                    fw << w(i * (Lx / nx), j * (Ly / ny)) << " ";

                }

                fu << u(Lx, j * (Ly / ny)) << "\n";
                fw << w(Lx, j * (Ly / ny)) << "\n";

            }

        }

    }

}
```

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