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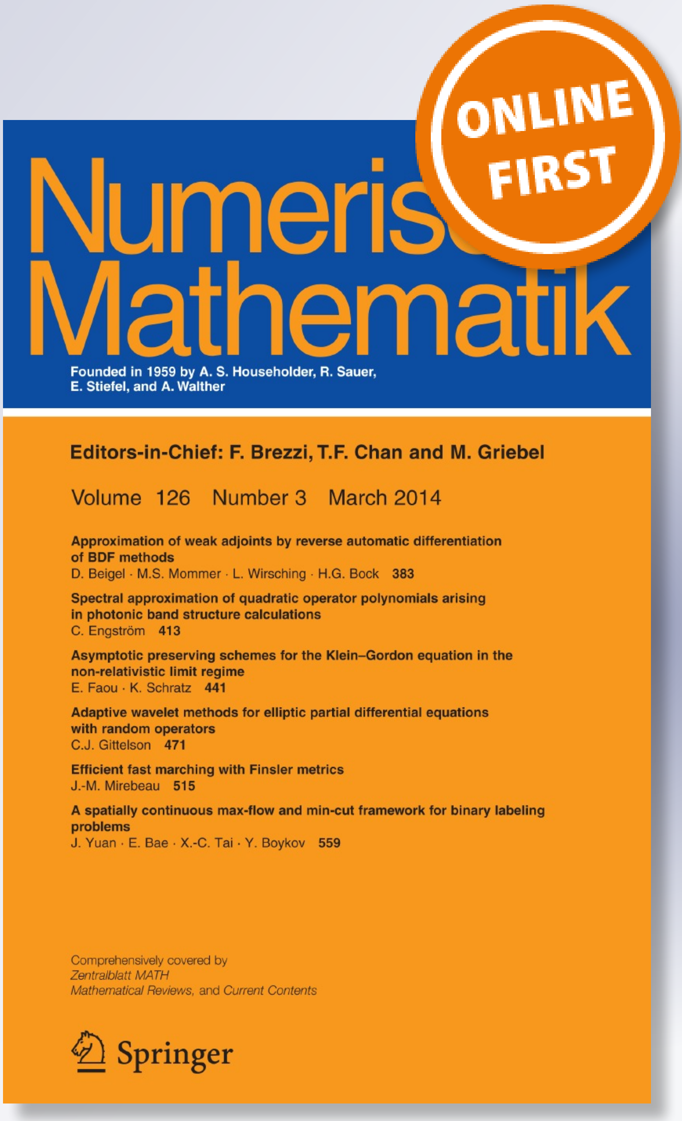

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A numerical analysis of the Cahn–Hilliard equation with non-permeable walls

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Abstract In this article we consider the numerical analysis of the Cahn–Hilliard equation in a bounded domain with non-permeable walls, endowed with dynamic-type boundary conditions. The dynamic-type boundary conditions that we consider here have been recently proposed in Ruiz Goldstein et al. (Phys D 240(8):754–766, 2011) in order to describe the interactions of a binary material with the wall. The equation is semi-discretized using a finite element method for the space variables and error estimates between the exact and the approximate solution are obtained. We also prove the stability of a fully discrete scheme based on the backward Euler scheme for the time discretization. Numerical simulations sustaining the theoretical results are presented.

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1 Setting of the problem

We consider in this paper the Cahn–Hilliard equation with the dynamic boundary conditions introduced in [14]:

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$$\begin{cases} \rho_t = \Delta\mu, \quad t>0, & x\in\Omega,\\ \mu = -\Delta\rho + f(\rho), \quad t>0, & x\in\Omega,\\ \rho_t = \delta\Delta_\Gamma\mu - \partial_n\mu, \quad t>0, & x\in\Gamma,\\ \mu = -\sigma\Delta_\Gamma\rho + \lambda\rho + g(\rho) + \partial_n\rho, \quad t>0, & x\in\Gamma, \end{cases} \tag{1.1}$$

where Ω is a $2d$ or $3d$ slab, i.e.

$$\Omega = \Pi_{i=1}^{d-1}\left(\mathbb{R}/(L_i\mathbb{Z})\right)\times(0,L_d), \qquad L_i>0,\ i=1,\ldots,d, \quad d=2 \text{ or } 3,$$

with smooth boundary

$$\Gamma = \partial\Omega = \Pi_{i=1}^{d-1}\big(\mathbb{R}/(L_i\mathbb{Z})\big)\times\{0,L_d\};$$

in other words, when $d=2$, Ω is the rectangle $(0,L_1)\times(0,L_2)$, ρ and μ are periodic in the x_1-direction and the boundary conditions are valid for $x_2=0$ and $x_2=L_2$; when $d=3$, Ω is the parallelepiped $(0,L_1)\times(0,L_2)\times(0,L_3)$, ρ and μ are periodic in the x_1 and x_2-directions, and the boundary conditions are valid for $x_3=0$ and $x_3=L_3$. The functions f and g belong to $C^2(\mathbb{R},\mathbb{R})$ and satisfy the following standard dissipativity assumptions:

$$\liminf_{|v|\to\infty} f'(v) > 0, \qquad \liminf_{|v|\to\infty} g'(v) > 0, \tag{1.2}$$

which imply the existence of two constants $c_1>0$, $c_2\geq 0$ such that

$$F(v)\geq c_1(v)^2 - c_2 \quad \text{and} \quad G(v)\geq c_1(v)^2-c_2, \tag{1.3}$$

where F and G are antiderivatives of the functions f and g. Typical choices are

$$f(v)=v^3-v \quad \text{and} \quad g(v)=a_\Gamma v - b_\Gamma, \quad v\in\mathbb{R}, a_\Gamma>0, b_\Gamma\in\mathbb{R}. \tag{1.4}$$

In (1.1), Δ_Γ is the Laplace–Beltrami operator on Γ and ∂_n is the outward normal derivative. The evolution boundary value problem (1.1) is completed by an initial condition $u(0)=u_0$. We remark that in the particular case that we consider here, when the domain is a slab, the Laplace–Bertrami operator on Γ reduces to $\partial^2_{x_1x_1}$ for the case $d=2$ and to $\partial^2_{x_1x_1}+\partial^2_{x_2x_2}$ for the case $d=3$.

The Cahn–Hilliard equation (1.1) is derived from the free energy

$$\mathcal{E}(\rho) = \frac{1}{2}\|\nabla\rho\|^2_\Omega + \int_\Omega F(\rho)\,dx + \frac{\sigma}{2}\|\nabla_\Gamma\rho\|^2_\Gamma + \frac{\lambda}{2}\|\rho\|^2_\Gamma + \int_\Gamma G(\rho)\,d\Gamma, \tag{1.5}$$

where $\|\cdot\|_\Omega$ (resp. $\|\cdot\|_\Gamma$) designates the norm on $L^2(\Omega)$ (resp. on $L^2(\Gamma)$) and ∇_Γ is the tangential gradient operator in Γ.

The first two terms from (1.5) represent the Ginsburg–Landau (bulk) free energy, and the remaining terms represent the surface energy. If (ρ,μ) is a regular solution of (1.1), then ρ dissipates $\mathcal{E}$ since

$$\frac{\mathrm{d}}{\mathrm{dt}}\mathcal{E}(\rho(t)) = -\|\nabla\mu\|_\Omega^2 - \delta\|\nabla_\Gamma\mu\|_\Gamma^2 \leq 0, \quad t \geq 0. \tag{1.6}$$

Moreover, the above dynamic boundary conditions ensure the conservation of the total (i.e. bulk plus boundary) mass, since

$$\frac{\mathrm{d}}{\mathrm{dt}}\left(\int_\Omega \rho dx + \int_\Gamma \rho d\Gamma\right) = 0, \quad t \geq 0,$$

which is immediately obtained by integrating $(1.1)_1$ and $(1.1)_3$ respectively over Ω and Γ.

In [14] the authors proved the existence and uniqueness of solutions in certain function spaces and they studied the asymptotic behavior of the solution as time goes to infinity. Our purpose is to provide a numerical study of this model, proving the convergence of the approximate solution, obtained by discretizing the equations, to the exact solution of (1.1).

We introduce the space $H = L^2(\Omega) \times L^2(\Gamma)$ and we endow the space H with the scalar product $(v, w)_H = (v_1, w_1)_\Omega + (v_2, w_2)_\Gamma$, for all $v = (v_1, v_2)$ and $w = (w_1, w_2)$ in H; the corresponding norm is $\|\cdot\|_H = (\cdot,\cdot)_H^{\frac{1}{2}}$.

We also introduce the space $V = \{ v \in H_p^1(\Omega),\ v_{|\Gamma} \in H_{\mathrm{per}}^1(\Gamma) \}$, which is a Hilbert space for the norm $\|v\|_V = (\|v\|_{H^1(\Omega)}^2 + \|v\|_{H^1(\Gamma)}^2)^{1/2}$ and the space $V_2 = \{ v \in H_p^2(\Omega),\ v_{|\Gamma} \in H_{\mathrm{per}}^2(\Gamma) \}$.

By $H_p^m(\Omega)$, with $m \geq 1$, we understand the functions that belong to $H^m(\Omega)$ and which are periodic in the $x_1, \ldots, x_{d-1}$-directions. More precisely, when $d = 2$, a function $v \in V$ is a function belonging to $H^1(\Omega)$, which is periodic in the x_1-direction and for which we have that $v(\cdot, 0) \in H_{\mathrm{per}}^1(0, L_1)$ and $v(\cdot, L_2) \in H_{\mathrm{per}}^1(0, L_1)$, where

$$H_{\mathrm{per}}^1(0, L_1) = \left\{ v \in H^1(0, L_1), \quad v \text{ is } L_1\text{-periodic} \right\}.$$

A similar definition holds for $d = 3$ and for V_2.

We will use also the notation $m(v) = \frac{1}{|\Omega|+|\Gamma|}(v, \mathbf{1})_H$, where $\mathbf{1} = (1, 1)$, and $\dot{H} = \{v \in H\,;\, m(v) = 0\}$. More generally, for an arbitrary set W, we will note $\dot{W} = W \cap \dot{H}$. We also denote by V' the dual space of V.

We will often use the Poincaré inequality in the form (see [25])

$$\|v - m(v)\|_H \leq c_p\,|v|_{1,V} \quad \forall\, v \in V, \tag{1.7}$$

with $|v|_{1,V}^2 = \|\nabla v\|_\Omega^2 + \|\nabla_\Gamma v\|_\Gamma^2$,

as well as the following inequality:

$$\|v\|_\Omega^2 \leq C_p(\|\nabla v\|_\Omega^2 + \|v\|_\Gamma^2), \quad \forall v \in H_p^1(\Omega). \tag{1.8}$$

Inequality (1.8) ensures the fact that $(\|\nabla v\|_\Omega^2 + \|v\|_\Gamma^2)^{1/2}$ is a norm on $H_p^1(\Omega)$, equivalent to the usual one.

The Cahn–Hilliard equations with different dynamic boundary conditions were introduced in [9,10,18] and a large literature on the mathematical study of these models is available (see, for example, [4,11–13,21–24,27]). The numerical analysis of the Cahn–Hilliard equation with different boundary conditions was considered in [3], while the numerical study of phase field models with classical (non-dynamical) boundary conditions can be found, for instance, in [2,6,7,16,17]. In this article, we start with the same approach as in [3] but the differences between the models and the boundary conditions lead to some different treatments. In Sects. 2 and 3 we suppose the constants σ and δ from (1.1) to be strictly positive, while in Sect. 4 we study the case $\sigma = 0$ and in Sect. 5 we consider the case where $\delta = 0$. In Sect. 6 we study the stability of the backward Euler scheme. In the last section of this article we provide the results of some numerical simulations which, apart from their intrinsic interest in illustrating the results presented above, also show that the model with the boundary conditions that we consider produces a different behavior at the boundary, as compared to [3] but the patterns at the interior of the domain are rather similar both here and in [3].

2 The space semidiscrete scheme

The variational formulation of (1.1) reads:

For f and g satisfying (1.2) and $\rho_0 \in V$, find $\rho \in L^\infty(0, T, V)$ and $\mu \in L^2(0, T, V)$ such that $\rho(0) = \rho_0$ and:

$$\begin{cases} (\rho_t, \psi)_H + (\nabla\mu, \nabla\psi)_\Omega + \delta(\nabla_\Gamma\mu, \nabla_\Gamma\psi)_\Gamma = 0, \\ (\mu, \phi)_H = (\nabla\rho, \nabla\phi)_\Omega + \sigma(\nabla_\Gamma\rho, \nabla_\Gamma\phi)_\Gamma + (f(\rho), \phi)_\Omega + \lambda(\rho, \phi)_\Gamma + (g(\rho), \phi)_\Gamma, \end{cases} \tag{2.1}$$

for all ϕ and $\psi \in V$.

For the space discretization of these equations, we consider a quasiuniform family of decompositions $\{\Omega^h\}$ of $\Pi_{i=1}^d [0, L_i]$ into d-simplices which take into account the periodic boundary conditions on Ω, so that $\{\Omega^h\}$ is also a triangulation of $\overline{\Omega}$. The triangulation Ω^h of $\overline{\Omega}$ induces a triangulation Γ^h of Γ into $d-1$ simplices in a natural way. For a given triangulation $\Omega^h = \cup_{T\in\Omega^h} T$, we define V^h as the usual P^1 conforming finite element space

$$V^h = \left\{ v^h \in C^0(\overline{\Omega}),\ v^h_{|T} \text{ is affine } \quad \forall T \in \Omega^h \right\}.$$

Note that for every $v^h \in V^h$, the restriction $\varphi^h = v^h_{|\Gamma}$ on the boundary is a P^1 finite element on the $(d-1)$-dimensional domain Γ. In fact, the space of such functions φ^h is the usual P^1 conforming finite element discretization of the space $H^1_{\text{per}}(\Gamma)$ built on the triangulation Γ^h. Thus, $V^h \subset V$ and V^h can be seen as a conforming discretization of V. Note that the same space V^h is used for both the discretization of $H^1_p(\Omega)$ and that of V.

For $u \in C^0(\overline{\Omega})$, let $I^h u$ denote the P^1 interpolate of u on Ω^h, i.e. $I^h u$ is the unique function in V^h which takes the same values as u on the nodes of the triangulation. Note that $(I^h u)_{|\Gamma}$ is the P^1 interpolate of $u_{|\Gamma}$ on Γ^h. We have the following standard approximation results (see also [5]), where C is a strictly positive constant:

$$\forall u \in H^2_p(\Omega), \quad \|u - I^h u\|_\Omega + h|u - I^h u|_{1,\Omega} \leq Ch^2 |u|_{2,\Omega}, \tag{2.2}$$

$$\forall \varphi \in H^2_{\text{per}}(\Gamma), \quad \|\varphi - I^h \varphi\|_\Gamma + h|\varphi - I^h \varphi|_{1,\Gamma} \leq Ch^2 |\varphi|_{2,\Gamma}, \tag{2.3}$$

where $|u|_{m,\Omega}$ and $|u|_{m,\Gamma}$ are the seminorms associated with respectively the $H^m_p(\Omega)$ and $H^m_{\text{per}}(\Gamma)$ norms, for $m \in \mathbb{N}^*$.

Moreover, the following inverse estimate holds (see for instance [8]):

$$\forall v^h \in V^h, \quad \|v^h\|_{C^0(\overline{\Omega})} \leq Ch^{-d/2} \|v^h\|_\Omega, \tag{2.4}$$

where $d = 2$ or 3 is the dimension of the space Ω. Here and thereafter C or c will denote constants independent of h which may vary at different occurrences.

The semidiscrete version of (2.1) reads:

Find $(\rho^h, \mu^h) : [0, T] \to V^h \times V^h$ *such that*:

$$\begin{cases} (\rho^h_t, \psi)_H + (\nabla \mu^h, \nabla \psi)_\Omega + \delta(\nabla_\Gamma \mu^h, \nabla_\Gamma \psi)_\Gamma = 0, \\ (\mu^h, \phi)_H = (\nabla \rho^h, \nabla \phi)_\Omega + (f(\rho^h), \phi)_\Omega + \sigma(\nabla_\Gamma \rho^h, \nabla_\Gamma \phi)_\Gamma \\ \qquad\qquad +\lambda(\rho^h, \phi)_\Gamma + (g(\rho^h), \phi)_\Gamma, \end{cases} \tag{2.5}$$

for all $\phi, \psi \in V^h$.

Taking $\psi = \mathbf{1}$ in (2.5), we find

$$m(\rho^h_t(t)) = 0 \quad \text{and} \quad m(\rho^h(t)) = cst \quad \forall\, t \geq 0. \tag{2.6}$$

Theorem 2.1 *For every* $\rho^h_0 \in V^h$, *problem* (2.5) *has a unique solution*

$$(\rho^h, \mu^h) \in \mathcal{C}^1([0, +\infty);\ V^h \times V^h)$$

such that $\rho^h(0) = \rho^h_0$. *Moreover, the following energy estimate holds:*

$$\mathcal{E}(\rho^h(t)) + \int_0^t \delta \|\nabla_\Gamma \mu^h(s)\|^2_\Gamma + \|\nabla \mu^h(s)\|^2_\Omega \, ds \ \leq\ \mathcal{E}(\rho^h_0), \quad \forall t \geq 0, \tag{2.7}$$

where $\mathcal{E}$ *is defined in* (1.5).

Proof Let $(\varphi_1, \ldots, \varphi_M)$ be an orthonormal basis of V^h for the $L^2(\Omega)$-scalar product and such that $\varphi_1 \equiv cst$. We seek for $\rho^h(t) = \sum_{i=1}^M \rho_i(t)\varphi_i$ and $\mu^h(t) = \sum_{i=1}^M \mu_i(t)\varphi_i$. We define the matrices

$$(A)_{ij} = (\nabla \varphi_i, \nabla \varphi_j)_\Omega, \quad (M_\Gamma)_{ij} = (\varphi_i, \varphi_j)_\Gamma \text{ and } (A_\Gamma)_{ij} = (\nabla_\Gamma \varphi_i, \nabla_\Gamma \varphi_j)_\Gamma, \quad 1 \leq i, j \leq M,$$

the vectors

$$U = \begin{pmatrix} \rho_1 \\ \vdots \\ \rho_M \end{pmatrix}, \quad W = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_M \end{pmatrix},$$

and the functions

$$F^h(U) = \begin{pmatrix} (f(\rho^h), \varphi_1)_\Omega \\ \vdots \\ (f(\rho^h), \varphi_M)_\Omega \end{pmatrix}, \quad G^h(U) = \begin{pmatrix} (\lambda\rho^h + g(\rho^h), \varphi_1)_\Gamma \\ \vdots \\ (\lambda\rho^h + g(\rho^h), \varphi_M)_\Gamma \end{pmatrix}.$$

Then (2.5) can be written as

$$\begin{cases} (I_M + M_\Gamma)\, W = \sigma A_\Gamma U + AU + F^h(U) + G^h(U), \\ (I_M + M_\Gamma)\, U' + (A + \delta A_\Gamma) W = 0. \end{cases} \tag{2.8}$$

We easily check that the matrix $I + M_\Gamma$ is invertible. Therefore we have:

$$W = (I_M + M_\Gamma)^{-1} (\sigma A_\Gamma U + AU + F^h(U) + G^h(U)),$$

and thus

$U' = -(I_M + M_\Gamma)^{-1}\, (\delta A_\Gamma + A)\, (I_M + M_\Gamma)^{-1} (\sigma A_\Gamma U + AU + F^h(U) + G^h(U))$.

Therefore, by the Cauchy–Lipschitz theorem, problem (2.5) has a unique maximal solution $(\rho^h, \mu^h) \in \mathcal{C}^1([0, T^+);\ V^h \times V^h)$ such that $\rho^h(0) = \rho_0^h$.

Taking $\psi = \mu^h$ (resp. $\phi = \rho_t^h$) in the first (resp. the second) equation of (2.5) and summing the two corresponding equations, we get

$$\frac{\mathrm{d}}{\mathrm{dt}} \{\mathcal{E}(\rho^h)\} + \delta \|\nabla_\Gamma \mu^h\|_\Gamma^2 + \|\nabla \mu^h\|_\Omega^2 = 0,$$

so (ρ^h, μ^h) satisfies the energy estimate (2.7) of Theorem 2.1. Therefore, using (1.3), we find $\rho^h \in L^\infty(0, T^+, V)$ and we conclude that $T^+ = +\infty$ (i.e. the solution is global). □

Definition 2.1 A steady state for (2.5) with initial condition ρ_0^h is a pair $(\bar\rho^h, \bar\mu^h) \in V^h \times \mathbb{R}$ such that $\forall \phi \in V^h$,

$$\begin{cases} (\bar\rho^h, \mathbf{1})_H = (\rho_0^h, \mathbf{1})_H, \\ (\bar\mu^h, \phi)_H = \sigma(\nabla_\Gamma \bar\rho^h, \nabla_\Gamma \phi)_\Gamma + (\nabla \bar\rho^h, \nabla\phi)_\Omega + \lambda(\bar\rho^h, \phi)_\Gamma + (g(\bar\rho^h), \phi)_\Gamma + (f(\bar\rho^h), \phi)_\Omega. \end{cases}$$

Corollary 2.1 *The flow $S^h(t)\rho_0^h = \rho^h(t)$ defined in Theorem 2.1 is a gradient flow for $\mathcal{E}$ in the affine space $\tilde V^h = \{v^h \in V^h \,:\, m(v^h) = m(\rho_0^h)\}$, i.e.*

$$\langle \rho_t^h, \varphi^h \rangle^h = -\frac{d\mathcal{E}}{d\alpha} (\rho^h(t) + \alpha\varphi^h)_{|\alpha=0} \quad \forall \varphi^h \in \tilde V^h,$$

where $\langle .,. \rangle^h$ is a scalar product on $\tilde{V}^h$ given by (2.12). In particular, if f and g are real analytic functions, there exists a steady state $(\bar{\rho}^h, \bar{\mu}^h) \in V^h \times \mathbb{R}$ such that $(\rho^h(t), \mu^h(t)) \to (\bar{\rho}^h, \bar{\mu}^h)$ as $t \to +\infty$.

Proof The matrix $A + \delta A_\Gamma$ is not invertible, we can easily notice that since $\varphi_1 = cst$ then the first line and the first column of this matrix are filled only with null elements. For this reason, for a vector $X = (x_i)_{1 \le i \le M} \in \mathbb{R}^M$, we write $\dot{X} = (x_i)_{2 \le i \le M} \in \mathbb{R}^{M-1}$ (recall that the first component x_1 is associated to the constant φ_1). For a square matrix $C = (c_{ij})_{1 \le i,j \le M}$ of size M, we write $\dot{C} = (c_{ij})_{2 \le i,j \le M}$. Equation (2.8) without the two lines corresponding to φ_1 becomes

$$\begin{cases} (I_{M-1} + \dot{M}_\Gamma)\, \dot{U}' = -(\delta \dot{A}_\Gamma + \dot{A})\dot{W}, \\ (I_{M-1} + \dot{M}_\Gamma)\, \dot{W} = \sigma \dot{A}_\Gamma \dot{U} + \dot{A}\dot{U} + \dot{F}^h(\rho_1, \dot{U}) + \dot{G}^h(\rho_1, \dot{U}). \end{cases} \tag{2.9}$$

Now, the matrix $\dot{A} + \delta \dot{A}_\Gamma$ is invertible, thus we can eliminate $\dot{W}$ and obtain

$$\begin{aligned} &(I_{M-1} + \dot{M}_\Gamma)(\delta \dot{A}_\Gamma + \dot{A})^{-1}(I_{M-1} + \dot{M}_\Gamma)\, \dot{U}' = -(\sigma \dot{A}_\Gamma \dot{U} + \dot{A}\dot{U} \\ &\quad + \dot{F}^h(\rho_1, \dot{U}) + \dot{G}^h(\rho_1, \dot{U})). \end{aligned} \tag{2.10}$$

This is a gradient flow for the function

$$\mathbb{R}^{M-1} \ni \dot{v} \to \mathcal{E}\left(\rho_1 \varphi_1 + \sum_{i=2}^{M} v_i \varphi_i \right) \in \mathbb{R}, \tag{2.11}$$

with respect to the scalar product on $\tilde{V}^h$

$$\langle .,. \rangle^h = \left((I_{M-1} + \dot{M}_\Gamma)(\delta \dot{A}_\Gamma + \dot{A})^{-1}(I_{M-1} + \dot{M}_\Gamma) \cdot, \cdot \right) \tag{2.12}$$

and with $\rho_1 = (\rho^h(0), \varphi_1)_\Omega$. Since f and g are assumed to be real analytic and $V^h \subset \mathcal{C}^0(\bar{\Omega})$, the function defined by (2.11) is also analytic on $\mathbb{R}^{M-1}$. Then the Łojasiewicz inequality [19] implies the convergence to a steady state as $t \to +\infty$. □

For the next result (and only for this result), we have to assume that f and g have a subcritical growth. More precisely, we assume that there exists a positive constant c_3 such that

$$|f(\sigma)| \le c_3(1 + |\sigma|^{p-1}), \quad \forall \sigma \in \mathbb{R}, \tag{2.13}$$

with $p \in [2, 6]$ when $d = 3$ and $p \ge 2$ arbitrary when $d = 2$. When $d = 3$, we also assume that there exists a positive constant c_4 such that

$$|g(\sigma)| \le c_4(1 + |\sigma|^{q-1}), \quad \forall \sigma \in \mathbb{R}, \tag{2.14}$$

with $q \ge 2$ arbitrary. We note that the nonlinearities defined by (1.4) satisfy these assumptions with $p = 4$ and $q = 2$.

Theorem 2.2 *Assume that* $f,\ g \in \mathcal{C}^1(\mathbb{R}, \mathbb{R})$ *satisfy* (1.2), (2.13) *and* (2.14). *Let* $\rho_0 \in V$ *and let* $\rho_0^h \in V^h$ *such that* $\rho_0^h \to \rho_0$ *in* V *as* $h \to 0$. *Then, for all* $T > 0$,

$$\begin{cases} \rho^h \to \rho \ \text{ weak } * \text{ in } L^\infty(0, T; V) \quad \text{and strongly in } \mathcal{C}^0([0, T]; L^2(\Omega)), \\ \rho_t^h \to \rho_t \text{ weakly in } L^2(0, T; V'), \\ \rho_{|\Gamma}^h \to \rho_{|\Gamma} \text{ strongly in } \mathcal{C}^0([0, T]; L^2(\Gamma)), \\ \mu^h \to \mu \text{ weakly in } L^2(0, T; V), \end{cases}$$

where (ρ, μ) *is the unique solution of the continuous problem* (2.1) *such that* $\rho(0) = \rho_0$.

Proof By (2.13) and (2.14), there exist positive constants $c_5, \ldots, c_8$ such that

$$\forall \sigma \in \mathbb{R},\ |F(\sigma)| \leq c_5|\sigma|^p + c_6 \quad \text{and} \quad |G(\sigma)| \leq c_7|\sigma|^q + c_8.$$

Since $H_p^1(\Omega) \hookrightarrow L^p(\Omega)$, $H^1_{\text{per}}(\Gamma) \hookrightarrow L^q(\Gamma)$ and $\rho_0^h \to \rho_0$ in V as $h \to 0$, we infer that the energy $\mathcal{E}(\rho_0^h)$ is bounded by a constant independent of h. Hence the discrete energy estimate (2.7) together with (1.3) imply that $(\rho^h)_h$ is bounded in $L^\infty(0, T; V)$, that $(\nabla \mu^h)_h$ is bounded in $L^2(0, T; L^2(\Omega))$ and $(\nabla_\Gamma \mu^h_{|\Gamma})_h$ is bounded in $L^2(0, T; L^2(\Gamma))$. Moreover, choosing $\phi = \mathbf{1}$ in the second equation of (2.5), we also have

$$(\mu^h, \mathbf{1})_H = (f(\rho^h), 1)_\Omega + \lambda(\rho^h, 1)_\Gamma + (g(\rho^h), 1)_\Gamma,$$

which implies that $(\mu^h, \mathbf{1})_H$ is bounded in $L^2(0, T)$. From these estimates, we obtain that, up to a subsequence, $\rho^h \longrightarrow \rho$ weak $*$ in $L^\infty(0, T; V)$ and $\mu^h \longrightarrow \mu$ weakly in $L^2(0, T; V)$.

Finally, for the strong convergence of $(\rho^h)_h$, we use the fact that for all $0 \leq s \leq t \leq T$,

$$\begin{aligned} &\|\rho^h(t) - \rho^h(s)\|_\Omega^2 + \|\rho^h(t) - \rho^h(s)\|_\Gamma^2 \\ &= 2\int_s^t (\rho_t^h(\sigma), \rho^h(\sigma) - \rho^h(s))_\Omega \, d\sigma + 2\int_s^t (\rho_t^h(\sigma), \rho^h(\sigma) - \rho^h(s))_\Gamma \, d\sigma \\ &= -2\int_s^t (\nabla \mu^h(\sigma), \nabla(\rho^h(\sigma) - \rho^h(s)))_\Omega \, d\sigma - 2\delta \int_s^t (\nabla_\Gamma \mu^h(\sigma), \nabla_\Gamma(\rho^h(\sigma) \\ &\quad -\rho^h(s)))_\Gamma \, d\sigma \leq c\|\mu^h\|_{L^2(0,T;V)} \, \|\rho^h\|_{L^\infty(0,T,V)} \, |t - s|^{1/2}. \end{aligned}$$

As a consequence, $(\rho^h)_h$ is uniformly equicontinuous in $\mathcal{C}^0([0, T]; L^2(\Omega))$ and $(\rho_h)_{|\Gamma}$ is uniformly equicontinuous in $\mathcal{C}^0([0, T]; L^2(\Gamma))$. Since $(\rho^h)_h$ is bounded in $L^\infty(0, T; V)$, we deduce from the Ascoli theorem that $\rho^h \longrightarrow \rho$ strongly in $\mathcal{C}^0([0, T]; L^2(\Omega))$ and $\rho^h_{|\Gamma} \longrightarrow \rho_{|\Gamma}$ strongly in $\mathcal{C}^0([0, T]; L^2(\Gamma))$. We can also see that (ρ, μ) satisfies (2.1). From the uniqueness of the solution in the continuous case (see [14]), we conclude that the whole sequence converges to (ρ, μ). □

3 Error estimates for the space semidiscrete scheme

In order to estimate the errors $\rho^h - \rho$ and $\mu^h - \mu$, we write, following a standard approach (see, for instance [7,15,26]):

$$\begin{aligned} \rho^h(t) - \rho(t) &= v^\rho(t) + w^\rho(t) \quad \text{with} \quad v^\rho = \rho^h - \tilde{\rho}^h, \quad w^\rho = \tilde{\rho}^h - \rho, \\ \mu^h(t) - \mu(t) &= v^\mu(t) + w^\mu(t) \quad \text{with} \quad v^\mu = \mu^h - \tilde{\mu}^h, \ \ w^\mu = \tilde{\mu}^h - \mu, \end{aligned} \tag{3.1}$$

with $\tilde{\rho}^h$, $\tilde{\mu}^h$ the elliptic projections of ρ, μ in V^h, defined by

$$\begin{cases} (\nabla\tilde{\rho}^h, \nabla\phi)_\Omega + \sigma(\nabla_\Gamma\tilde{\rho}^h, \nabla_\Gamma\phi)_\Gamma + \lambda(\tilde{\rho}^h, \phi)_\Gamma = (\nabla\rho, \nabla\phi)_\Omega + \sigma(\nabla_\Gamma\rho, \nabla_\Gamma\phi)_\Gamma + \lambda(\rho, \phi)_\Gamma, \\ (\nabla\tilde{\mu}^h, \nabla\phi)_\Omega + \delta(\nabla_\Gamma\tilde{\mu}^h, \nabla_\Gamma\phi)_\Gamma = (\nabla\mu, \nabla\phi)_\Omega + \delta(\nabla_\Gamma\mu, \nabla_\Gamma\phi)_\Gamma, \\ (\tilde{\mu}^h, \mathbf{1})_H = (\mu, \mathbf{1})_H, \end{cases} \tag{3.2}$$

for all $\phi \in V^h$.

We first estimate w^ρ and w^μ. We state the

Lemma 3.1 *For all ρ, $\mu \in V^2$, the functions $\tilde{\rho}^h$, $\tilde{\mu}^h$ defined by (3.2) satisfy*

$$\begin{aligned} \|\tilde{\rho}^h - \rho\|_H + h|\tilde{\rho}^h - \rho|_{1,V} &\le ch^2\,(|\rho|_{2,\Omega} + |\rho|_{2,\Gamma}), \\ \|\tilde{\mu}^h - \mu\|_H + h|\tilde{\mu}^h - \mu|_{1,V} &\le ch^2\,(|\mu|_{2,\Omega} + |\mu|_{2,\Gamma}), \end{aligned} \tag{3.3}$$

with c a positive constant independent of h.

Proof We only detail the proof of the estimate for $\tilde{\mu}^h$, the one for $\tilde{\rho}^h$ being similar.

Let us define the bilinear function $a_\delta(\phi, \psi) = (\nabla\phi, \nabla\psi)_\Omega + \delta(\nabla_\Gamma\phi, \nabla_\Gamma\psi)_\Gamma$. This function is continuous on $V \times V$ and c_0-coercive on $\dot{V} \times \dot{V}$ with $\dot{V} = \{v \in V; m(v) = 0\}$. The existence of $\tilde{\mu}^h$ is ensured by the Lax–Milgram theorem.

The second and the third equations of (3.2) read as $a_\delta(\tilde{\mu}^h - \mu, \phi) = 0 \quad \forall\phi \in V^h$, and $\tilde{\mu}^h - \mu \in \dot{V}$. Since $\tilde{\mu}^h - I^h\mu \in V^h$, we infer:

$$\begin{aligned} a_\delta(\tilde{\mu}^h - \mu, \tilde{\mu}^h - \mu) &= a_\delta(\tilde{\mu}^h - \mu, \tilde{\mu}^h - I^h\mu) + a_\delta(\tilde{\mu}^h - \mu, I^h\mu - \mu) \\ &= a_\delta(\tilde{\mu}^h - \mu, I^h\mu - \mu). \end{aligned}$$

Using (2.2), (2.3) we obtain:

$$c_0\|\tilde{\mu}^h - \mu\|_V \le (1+\delta)\,\|I^h\mu - \mu\|_V \le ch(|\mu|_{2,\Omega} + |\mu|_{2,\Gamma}), \tag{3.4}$$

that is the H^1 estimate for $\tilde{\mu}^h - \mu$. In order to have the L^2-estimates, we use a duality argument (see [5]). For $(z, \psi) \in L^2(\Omega) \times L^2(\Gamma)$, let $\varphi \in \dot{V}$ be the unique solution of the problem

$$a_\delta(\varphi, \xi) = (z, \xi)_\Omega + (\psi, \xi)_\Gamma, \quad \forall\xi \in \dot{V}. \tag{3.5}$$

Then, $\varphi \in V^2$ and an elliptic regularity result holds (see [21]):

$$|\varphi|_{2,\Omega} + |\varphi|_{2,\Gamma} \le C\,(\|z\|_\Omega + \|\psi\|_\Gamma), \tag{3.6}$$

for some constant $C > 0$ independent of z and ψ.

Choosing $\xi = \tilde{\mu}^h - \mu$ in (3.5), we find (using $I^h\varphi \in V^h$)

$$\begin{aligned}(z, \tilde{\mu}^h - \mu)_\Omega + (\psi, \tilde{\mu}^h - \mu)_\Gamma &= a_\delta(\varphi, \tilde{\mu}^h - \mu) = a_\delta(\varphi - I^h\varphi, \tilde{\mu}^h - \mu)\\ &\le (1+\delta)\|\varphi - I^h\varphi\|_V\,\|\tilde{\mu}^h - \mu\|_V\\ &\le c\,h^2\,(|\varphi|_{2,\Omega} + |\varphi|_{2,\Gamma})\,(|\mu|_{2,\Omega} + |\mu|_{2,\Gamma})\\ &\le c\,h^2\,(\|z\|_\Omega + \|\psi\|_\Gamma)\,(|\mu|_{2,\Omega} + |\mu|_{2,\Gamma}).\end{aligned}$$

Now, setting $z = \tilde{\mu}^h - \mu$ and $\psi = (\tilde{\mu}^h - \mu)_{|\Gamma}$, we obtain

$$\begin{aligned}\|\tilde{\mu}^h - \mu\|_\Omega^2 + \|\tilde{\mu}^h - \mu\|_\Gamma^2 &\le ch^2(\|\tilde{\mu}^h - \mu\|_\Omega + \|\tilde{\mu}^h - \mu\|_\Gamma)\,(|\mu|_{2,\Omega} + |\mu|_{2,\Gamma})\\ &\le ch^2\,(\|\tilde{\mu}^h - \mu\|_\Omega^2 + \|\tilde{\mu}^h - \mu\|_\Gamma^2)^{1/2}\,(|\mu|_{2,\Omega} + |\mu|_{2,\Gamma}).\end{aligned}$$

Hence we conclude that $(\|\tilde{\mu}^h - \mu\|_\Omega^2 + \|\tilde{\mu}^h - \mu\|_\Gamma^2)^{1/2} \le ch^2(|\mu|_{2,\Omega} + |\mu|_{2,\Gamma})$, which is equivalent to

$$\|\tilde{\mu}^h - \mu\|_H \le ch^2(|\mu|_{2,\Omega} + |\mu|_{2,\Gamma}).$$

We thus obtained the L^2-part of the estimate for $w^\mu = \tilde{\mu}^h - \mu$ in (3.3). The proof for $w^\rho = \tilde{\rho}^h - \rho$ is similar and is then omitted. □

Now, we need to estimate $v^\rho = \rho^h - \tilde{\rho}^h$ and $v^\mu = \mu^h - \tilde{\mu}^h$. We start by introducing the following definition.

Definition 3.1 We set $T^h : \dot{H} \to \dot{V}^h, \quad f \mapsto T^h f$, where $T^h f$ is the unique solution of the problem:

$$(\nabla T^h f, \nabla \chi^h)_\Omega + \delta(\nabla_\Gamma T^h f, \nabla_\Gamma \chi^h)_\Gamma = (f, \chi^h)_H \quad \forall \chi^h \in \dot{V}^h. \tag{3.7}$$

Furthermore, we introduce the discrete negative seminorm:

$$|f|_{-1,h} = (T^h f, f)_H^{1/2} = \left(\|\nabla T^h f\|_\Omega^2 + \delta\,\|\nabla_\Gamma T^h f\|_\Gamma^2\right)^{1/2} \quad \forall f \in \dot{H}.$$

We remark that (3.7) is still valid for $\chi^h \in V^h$, thanks to the fact that $f \in \dot{H}$.

Lemma 3.2 *The operator T^h is self-adjoint, positive, semi-definite on $\dot{H}$. Moreover, the following interpolation inequality holds, for all $v^h \in \dot{V}^h$,*

$$\|v^h\|_H^2 \le c\,|v^h|_{-1,h}\,|v^h|_{1,V}, \tag{3.8}$$

and

$$|f|_{-1,h} \leq c\,\|f\|_H \quad \forall f \in \dot{H}, \tag{3.9}$$

with c a positive constant independent of h.

Proof Choosing $\chi^h = T^h f$ in (3.7), we obtain

$$(f, T^h f)_H = \|\nabla T^h f\|_\Omega^2 + \delta \|\nabla_\Gamma T^h f\|_\Gamma^2 \geq 0.$$

Moreover,

$$(g, T^h f)_H = (\nabla T^h g, \nabla T^h f)_\Omega + \delta(\nabla_\Gamma T^h g, \nabla_\Gamma T^h f)_\Gamma = (f, T^h g)_H$$

for all $f, g \in \dot{H}$, and we conclude that T^h is self-adjoint, positive semi-definite on $\dot{H}$.
In order to check (3.8), we write:

$$\begin{aligned}
\|v^h\|_H^2 &= (\nabla T^h v^h, \nabla v^h)_\Omega + \delta(\nabla_\Gamma T^h v^h, \nabla_\Gamma v^h)_\Gamma \\
&\leq \|\nabla T^h v^h\|_\Omega \,\|\nabla v^h\|_\Omega + \delta \|\nabla_\Gamma T^h v^h\|_\Gamma \,\|\nabla_\Gamma v^h\|_\Gamma \\
&\leq (\|\nabla T^h v^h\|_\Omega^2 + \delta^2 \|\nabla_\Gamma T^h v^h\|_\Gamma^2)^{\frac{1}{2}} \,(\|\nabla v^h\|_\Omega^2 + \|\nabla_\Gamma v^h\|_\Gamma^2)^{\frac{1}{2}} \\
&\leq \sqrt{\max(1,\delta)}\,(\|\nabla T^h v^h\|_\Omega^2 + \delta \|\nabla_\Gamma T^h v^h\|_\Gamma^2)^{\frac{1}{2}} \,(\|\nabla v^h\|_\Omega^2 + \|\nabla_\Gamma v^h\|_\Gamma^2)^{\frac{1}{2}} \\
&\leq \sqrt{\max(1,\delta)}\,|v^h|_{-1,h}\,|v^h|_{1,V} \quad \forall v^h \in \dot{V}^h,
\end{aligned}$$

and we have obtained (3.8) with $c = \sqrt{\max(1,\delta)}$. In order to prove (3.9) we use

$$|f|_{-1,h}^2 = (T^h f, f)_H \leq \|T^h f\|_H \,\|f\|_H,$$

and the Poincaré inequality (1.7). It yields

$$\begin{aligned}
\|T^h f\|_H^2 &\leq c_p\,(\|\nabla T^h f\|_\Omega^2 + \|\nabla_\Gamma T^h f\|_\Gamma^2) \\
&\leq c_p \max\left(1, \frac{1}{\delta}\right)(\|\nabla T^h f\|_\Omega^2 + \delta \|\nabla_\Gamma T^h f\|_\Gamma^2) \\
&\leq c_p \max\left(1, \frac{1}{\delta}\right)|f|_{-1,h}^2.
\end{aligned}$$

Combining the last two inequalities, we obtain (3.9) with $c = \sqrt{c_p \max(1, \frac{1}{\delta})}$ and the proof is complete. □

We will now estimate $v^\rho = \rho^h - \tilde{\rho}^h$ and $v^\mu = \mu^h - \tilde{\mu}^h$. First of all, since ρ^h is solution of $(2.5)_2$ and $\tilde{\rho}^h$ is solution of $(3.2)_1$, we infer that $v^\rho = \rho^h - \tilde{\rho}^h$ is solution of the following equation:

$$\begin{aligned}
&(\nabla v^\rho, \nabla \phi)_\Omega + \sigma(\nabla_\Gamma v^\rho, \nabla_\Gamma \phi)_\Gamma + \lambda(v^\rho, \phi)_\Gamma + (f(\rho^h), \phi)_\Omega + (g(\rho^h), \phi)_\Gamma \\
&\quad = (\mu^h, \phi)_H - ((\nabla \rho, \nabla \phi)_\Omega + \sigma(\nabla_\Gamma \rho, \nabla_\Gamma \phi)_\Gamma + \lambda(\rho, \phi)_\Gamma)\,.
\end{aligned}$$

Then, using the fact that ρ is solution to (2.1) and $\mu^h - \mu = v^\mu + w^\mu$, this yields

$$(\nabla v^\rho, \nabla\phi)_\Omega + \sigma(\nabla_\Gamma v^\rho, \nabla_\Gamma\phi)_\Gamma + \lambda(v^\rho, \phi)_\Gamma + (g(\rho^h) - g(\rho), \phi)_\Gamma \\ +(f(\rho^h) - f(\rho), \phi)_\Omega - (v^\mu, \phi)_H = (w^\mu, \phi)_H, \tag{3.10}$$

for all $\phi \in V^h$. From $(2.5)_1$, $(2.1)_1$ and $(3.2)_2$, we infer

$$(\rho_t^h - \rho_t, \psi)_H + (\nabla v^\mu, \nabla\psi)_\Omega + \delta(\nabla_\Gamma v^\mu, \nabla_\Gamma\psi)_\Gamma = 0.$$

Thus, since $\rho^h - \rho = v^\rho + w^\rho$, we get:

$$(v_t^\rho, \psi)_H + (\nabla v^\mu, \nabla\psi)_\Omega + \delta(\nabla_\Gamma v^\mu, \nabla_\Gamma\psi)_\Gamma = -(w_t^\rho, \psi)_H, \quad \psi \in V^h. \tag{3.11}$$

Taking $\psi = \mathbf{1}$ in (3.11) yields to

$$(v_t^\rho, \mathbf{1})_H = -(w_t^\rho, \mathbf{1})_H,$$

which means that

$$m(v_t^\rho(t)) = -m(w_t^\rho(t)) \quad \forall t \geq 0. \tag{3.12}$$

Lemma 3.3 *Let (ρ, μ) be a solution of the continuous problem (2.1) supposed here to be regular enough and (ρ^h, μ^h) a solution of (2.5). Assume that*

$$\sup_{t\in[0,T]} \|\rho(t)\|_{\mathcal{C}^0(\bar\Omega)} \leq R, \quad \sup_{t\in[0,T]} \|\rho_t(t)\|_{\mathcal{C}^0(\bar\Omega)} \leq R, \quad \|\rho^h(0)\|_{\mathcal{C}^0(\bar\Omega)} < R, \tag{3.13}$$

for some constant $R < +\infty$, and let $T^h \in (0, T]$ be the maximal time such that $\|\rho^h(t)\|_{L^\infty(\Omega)} \leq R$ for all $t \in [0, T^h]$. Then, for all $t \in [0, T^h]$

$$\mathcal{N}(t) + \int_0^t (\sigma\|\nabla_\Gamma v_t^\rho\|_\Gamma^2 + \|\nabla v_t^\rho\|_\Omega^2 + \|\nabla v^\mu\|_\Omega^2 + \delta\|\nabla_\Gamma v^\mu\|_\Gamma^2)\, ds \\ \leq c\mathcal{N}(0) + c\int_0^t (\|w_{tt}^\rho\|_H^2 + \|w_t^\rho\|_H^2 + \|w^\rho\|_H^2 + \|w_t^\mu\|_H^2 + \|w^\mu\|_H^2)\, ds, \tag{3.14}$$

with

$$\mathcal{N}(t) = |v_t^\rho - m(v_t^\rho)|_{-1,h}^2 + \|\nabla v^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v^\rho\|_\Gamma^2 + \lambda\|v^\rho\|_\Gamma^2. \tag{3.15}$$

Moreover, it holds

$$|(v^\mu, \mathbf{1})_H| \leq C\left(\mathcal{N}(t)^{\frac{1}{2}} + \|w^\rho\|_H\right), \quad \forall t \in [0, T^h]. \tag{3.16}$$

Proof We take $\phi = v_t^\rho$ in (3.10) and $\psi = v^\mu$ in (3.11) and add the resulting equations. We obtain

$$\begin{aligned}&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\left\{\|\nabla v^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v^\rho\|_\Gamma^2 + \lambda\|v^\rho\|_\Gamma^2\right\} + \|\nabla v^\mu\|_\Omega^2 \\ &\quad + \delta\|\nabla_\Gamma v^\mu\|_\Gamma^2 + (g(\rho^h) - g(\rho), v_t^\rho)_\Gamma + (f(\rho^h) - f(\rho), v_t^\rho)_\Omega \\ &\quad = -(w_t^\rho, v^\mu)_H + (w^\mu, v_t^\rho)_H. \end{aligned} \tag{3.17}$$

We have the following estimates on the nonlinear terms:

$$\begin{cases} \|f(\rho^h) - f(\rho)\|_\Omega \le L_f\|\rho^h - \rho\|_\Omega \le L_f(\|v^\rho\|_\Omega + \|w^\rho\|_\Omega), \\ \|g(\rho^h) - g(\rho)\|_\Gamma \le L_g\|\rho^h - \rho\|_\Gamma \le L_g(\|v^\rho\|_\Gamma + \|w^\rho\|_\Gamma), \end{cases} \tag{3.18}$$

for all $t \in [0, T^h]$, where L_f and L_g are respectively the Lipschitz constants of f and g on $[-R, R]$.

Combining (3.17) and (3.18), we get

$$\begin{aligned}&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\left\{\|\nabla v^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v^\rho\|_\Gamma^2 + \lambda\|v^\rho\|_\Gamma^2\right\} + \|\nabla v^\mu\|_\Omega^2 + \delta\|\nabla_\Gamma v^\mu\|_\Gamma^2 \\ &\quad \le L_f(\|v^\rho\|_\Omega + \|w^\rho\|_\Omega)\|v_t^\rho\|_\Omega + L_g(\|v^\rho\|_\Gamma + \|w^\rho\|_\Gamma)\|v_t^\rho\|_\Gamma \\ &\quad\quad + \|w_t^\rho\|_H\|v^\mu\|_H + \|w^\mu\|_H\|v_t^\rho\|_H, \end{aligned} \tag{3.19}$$

which further implies:

$$\begin{aligned}&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\left\{\|\nabla v^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v^\rho\|_\Gamma^2 + \lambda\|v^\rho\|_\Gamma^2\right\} + \|\nabla v^\mu\|_\Omega^2 + \delta\|\nabla_\Gamma v^\mu\|_\Gamma^2 \\ &\quad \le c(\|v^\rho\|_H\|v_t^\rho\|_H + \|w^\rho\|_H\|v_t^\rho\|_H) + \|w_t^\rho\|_H\|v^\mu\|_H + \|w^\mu\|_H\|v_t^\rho\|_H. \end{aligned} \tag{3.20}$$

We take $\phi = \mathbf{1}$ in (3.10). This yields, applying (3.18) and $(3.2)_3$, that we can estimate the mass of v^μ as follows:

$$|(v^\mu, \mathbf{1})_H| \le c(\|v^\rho\|_H + \|w^\rho\|_H) + \lambda|(v^\rho, 1)_\Gamma| \le c(\|v^\rho\|_H + \|w^\rho\|_H). \tag{3.21}$$

Now, we apply the Poincaré inequality (1.7) to v^μ:

$$\begin{aligned}\|v^\mu\|_H &\le c(\|\nabla v^\mu\|_\Omega^2 + \|\nabla_\Gamma v^\mu\|_\Gamma^2)^{\frac{1}{2}} + c|(v^\mu, \mathbf{1})_H| \\ &\le c(\|\nabla v^\mu\|_\Omega^2 + \delta\|\nabla_\Gamma v^\mu\|_\Gamma^2)^{\frac{1}{2}} + c|(v^\mu, \mathbf{1})_H|. \end{aligned} \tag{3.22}$$

Combining (3.20) and (3.22), we obtain:

$$\begin{aligned}&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\left\{\|\nabla v^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v^\rho\|_\Gamma^2 + \lambda\|v^\rho\|_\Gamma^2\right\} + \|\nabla v^\mu\|_\Omega^2 + \delta\|\nabla_\Gamma v^\mu\|_\Gamma^2 \\ &\quad \le c(\|v^\rho\|_H\|v_t^\rho\|_H + \|w^\rho\|_H\|v_t^\rho\|_H) + c\|w_t^\rho\|_H(\|\nabla v^\mu\|_\Omega^2 + \delta\|\nabla_\Gamma v^\mu\|_\Gamma^2)^{\frac{1}{2}} \\ &\quad\quad + c\|w_t^\rho\|_H|(v^\mu, \mathbf{1})_H| + \|w^\mu\|_H\|v_t^\rho\|_H. \end{aligned} \tag{3.23}$$

Then,

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}\left\{\|\nabla v^\rho\|_\Omega^2+\sigma\|\nabla_\Gamma v^\rho\|_\Gamma^2+\lambda\|v^\rho\|_\Gamma^2\right\}+\frac{1}{2}\|\nabla v^\mu\|_\Omega^2+\frac{\delta}{2}\|\nabla_\Gamma v^\mu\|_\Gamma^2$$
$$\le c(\|v^\rho\|_H\|v_t^\rho\|_H+\|w^\rho\|_H\|v_t^\rho\|_H)+c\|w_t^\rho\|_H^2$$
$$+c\|w_t^\rho\|_H(\|v^\rho\|_H+\|w^\rho\|_H)+\|w^\mu\|_H\|v_t^\rho\|_H.$$

We finally get the following differential inequality:

$$\frac{\mathrm{d}}{\mathrm{dt}}\left\{\|\nabla v^\rho\|_\Omega^2+\sigma\|\nabla_\Gamma v^\rho\|_\Gamma^2+\lambda\|v^\rho\|_\Gamma^2\right\}+\|\nabla v^\mu\|_\Omega^2+\delta\|\nabla_\Gamma v^\mu\|_\Gamma^2$$
$$\le c(\|v^\rho\|_H^2+\|v_t^\rho\|_H^2+\|w^\rho\|_H^2+\|w_t^\rho\|_H^2+\|w^\mu\|_H^2). \tag{3.24}$$

Now it remains to estimate v_t^ρ in order to be able to use the Gronwall Lemma for (3.24). We differentiate (3.10) and (3.11) with respect to time. We get:

$$(v_{tt}^\rho,\psi)_H+(\nabla v_t^\mu,\nabla\psi)_\Omega+\delta(\nabla_\Gamma v_t^\mu,\nabla_\Gamma\psi)_\Gamma+(w_{tt}^\rho,\psi)_H=0,\quad\forall\,\psi\in V^h, \tag{3.25}$$

and

$$(\nabla v_t^\rho,\nabla\phi)_\Omega+\sigma(\nabla_\Gamma v_t^\rho,\nabla_\Gamma\phi)_\Gamma+\lambda(v_t^\rho,\phi)_\Gamma+(g'(\rho^h)\rho_t^h-g'(\rho)\rho_t,\phi)_\Gamma$$
$$+(f'(\rho^h)\rho_t^h-f'(\rho)\rho_t,\phi)_\Omega-(v_t^\mu,\phi)_H=(w_t^\mu,\phi)_H,\quad\forall\,\phi\in V^h. \tag{3.26}$$

In (3.25) we take the test function $\psi=T^h(v_t^\rho-m(v_t^\rho))$. Using (3.7), we get:

$$(v_{tt}^\rho,T^h(v_t^\rho-m(v_t^\rho)))_H+(v_t^\rho-m(v_t^\rho),v_t^\mu)_H=-(w_{tt}^\rho,T^h(v_t^\rho-m(v_t^\rho)))_H,$$

which implies:

$$(v_{tt}^\rho-m(v_{tt}^\rho),T^h(v_t^\rho-m(v_t^\rho)))_H+(m(v_{tt}^\rho),T^h(v_t^\rho-m(v_t^\rho)))_H$$
$$+(v_t^\rho-m(v_t^\rho),v_t^\mu)_H=-(w_{tt}^\rho,T^h(v_t^\rho-m(v_t^\rho)))_H.$$

Since $m(w_{tt}^\rho)=-m(v_{tt}^\rho)$, the following relation holds:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}|v_t^\rho-m(v_t^\rho)|_{-1,h}^2+(v_t^\rho-m(v_t^\rho),v_t^\mu)_H=-(w_{tt}^\rho-m(w_{tt}^\rho),T^h(v_t^\rho-m(v_t^\rho)))_H. \tag{3.27}$$

We also take the test function $\phi=v_t^\rho-m(v_t^\rho)$ in (3.26). We obtain:

$$\|\nabla v_t^\rho\|_\Omega^2+\sigma\|\nabla_\Gamma v_t^\rho\|_\Gamma^2+\lambda(v_t^\rho,v_t^\rho-m(v_t^\rho))_\Gamma+(g'(\rho^h)\rho_t^h-g'(\rho)\rho_t,v_t^\rho-m(v_t^\rho))_\Gamma$$
$$+(f'(\rho^h)\rho_t^h-f'(\rho)\rho_t,v_t^\rho-m(v_t^\rho))_\Omega-(v_t^\mu,v_t^\rho-m(v_t^\rho))_H=(w_t^\mu,v_t^\rho-m(v_t^\rho))_H. \tag{3.28}$$

Since $f'(\rho^h)\rho_t^h - f'(\rho)\rho_t = f'(\rho^h)(\rho_t^h - \rho_t) + (f'(\rho^h) - f'(\rho))\rho_t$, this yields:

$$|(f'(\rho^h)\rho_t^h - f'(\rho)\rho_t, v_t^\rho - m(v_t^\rho))_\Omega| \leq \sup_{[-R,R]} |f'| \|\rho_t^h - \rho_t\|_\Omega \, \|v_t^\rho - m(v_t^\rho)\|_\Omega + L_{f'} \, R \, \|\rho^h - \rho\|_\Omega \, \|v_t^\rho - m(v_t^\rho)\|_\Omega, \tag{3.29}$$

where $L_{f'}$ is the Lipschitz constant of f' on $[-R, R]$.

By the same reasoning applied to the function g, we obtain:

$$|(g'(\rho^h)\rho_t^h - g'(\rho)\rho_t, v_t^\rho - m(v_t^\rho))_\Gamma| \leq \sup_{[-R,R]} |g'| \|\rho_t^h - \rho_t\|_\Gamma \, \|v_t^\rho - m(v_t^\rho)\|_\Gamma + L_{g'} \, R \, \|\rho^h - \rho\|_\Gamma \, \|v_t^\rho - m(v_t^\rho)\|_\Gamma, \tag{3.30}$$

where $L_{g'}$ is the Lipschitz constant of g' on $[-R, R]$.

Hence, from (3.28) we obtain:

$$\begin{aligned}
&\|\nabla v_t^\rho\|_\Omega^2 + \sigma \|\nabla_\Gamma v_t^\rho\|_\Gamma^2 + \lambda(v_t^\rho, v_t^\rho - m(v_t^\rho))_\Gamma - (v_t^\mu, v_t^\rho - m(v_t^\rho))_H \\
&\quad \leq \sup_{[-R,R]} |f'| \|\rho_t^h - \rho_t\|_\Omega \, \|v_t^\rho - m(v_t^\rho)\|_\Omega + L_{f'} \, R \, \|\rho^h - \rho\|_\Omega \, \|v_t^\rho - m(v_t^\rho)\|_\Omega \\
&\qquad + \sup_{[-R,R]} |g'| \|\rho_t^h - \rho_t\|_\Gamma \, \|v_t^\rho - m(v_t^\rho)\|_\Gamma + L_{g'} \, R \, \|\rho^h - \rho\|_\Gamma \, \|v_t^\rho - m(v_t^\rho)\|_\Gamma \\
&\qquad + |(w_t^\mu, v_t^\rho - m(v_t^\rho))_H|.
\end{aligned} \tag{3.31}$$

This implies, adding (3.27) and (3.31),

$$\begin{aligned}
&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}|v_t^\rho - m(v_t^\rho)|_{-1,h}^2 + \|\nabla v_t^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v_t^\rho\|_\Gamma^2 \leq |(w_{tt}^\rho - m(w_{tt}^\rho), T^h(v_t^\rho - m(v_t^\rho)))_H| \\
&\quad + |(w_t^\mu, v_t^\rho - m(v_t^\rho))_H| + c(\|\rho_t^h - \rho_t\|_\Omega \|v_t^\rho - m(v_t^\rho)\|_\Omega + \|\rho^h - \rho\|_\Omega \|v_t^\rho - m(v_t^\rho)\|_\Omega \\
&\quad + \|\rho_t^h - \rho_t\|_\Gamma \|v_t^\rho - m(v_t^\rho)\|_\Gamma + \|\rho^h - \rho\|_\Gamma \|v_t^\rho - m(v_t^\rho)\|_\Gamma) + \lambda|(v_t^\rho, v_t^\rho - m(v_t^\rho))_\Gamma|,
\end{aligned} \tag{3.32}$$

where the constant c depends on $R, L_{f'}, L_{g'}$. Moreover, since $m(w_t^\rho) = -m(v_t^\rho)$ and $\rho^h - \rho = v^\rho + w^\rho$, we have:

$$\begin{aligned}
|(w_{tt}^\rho - m(w_{tt}^\rho), T^h(v_t^\rho - m(v_t^\rho)))_H| &\leq c|w_{tt}^\rho - m(w_{tt}^\rho)|_{-1,h} \, |v_t^\rho - m(v_t^\rho)|_{-1,h} \\
&\leq c(|w_{tt}^\rho - m(w_{tt}^\rho)|_{-1,h}^2 + |v_t^\rho - m(v_t^\rho)|_{-1,h}^2), \\
\|\rho_t^h - \rho_t\|_\Omega \, \|v_t^\rho - m(v_t^\rho)\|_\Omega &\leq c\|v_t^\rho - m(v_t^\rho)\|_\Omega \, \|v_t^\rho + w_t^\rho\|_\Omega \\
&\leq c(\|v_t^\rho - m(v_t^\rho)\|_\Omega^2 + \|w_t^\rho\|_\Omega^2 + |m(w_t^\rho)|^2) \\
&\leq c(\|v_t^\rho - m(v_t^\rho)\|_H^2 + \|w_t^\rho\|_H^2), \\
\|\rho_t^h - \rho_t\|_\Gamma \, \|v_t^\rho - m(v_t^\rho)\|_\Gamma &\leq c\|v_t^\rho - m(v_t^\rho)\|_\Gamma \, \|v_t^\rho + w_t^\rho\|_\Gamma \\
&\leq c(\|v_t^\rho - m(v_t^\rho)\|_\Gamma^2 + \|w_t^\rho\|_\Gamma^2 + |m(w_t^\rho)|^2) \\
&\leq c(\|v_t^\rho - m(v_t^\rho)\|_H^2 + \|w_t^\rho\|_H^2), \\
\|\rho^h - \rho\|_\Omega \, \|v_t^\rho - m(v_t^\rho)\|_\Omega &\leq c\,(\|v_t^\rho - m(v_t^\rho)\|_\Omega^2 + \|v^\rho\|_\Omega^2 + \|w^\rho\|_\Omega^2), \\
\|\rho^h - \rho\|_\Gamma \, \|v_t^\rho - m(v_t^\rho)\|_\Gamma &\leq c\,(\|v_t^\rho - m(v_t^\rho)\|_\Gamma^2 + \|v^\rho\|_\Gamma^2 + \|w^\rho\|_\Gamma^2), \\
|(w_t^\mu, v_t^\rho - m(v_t^\rho))_H| &\leq \|w_t^\mu\|_H^2 + \|v_t^\rho - m(v_t^\rho)\|_H^2,
\end{aligned}$$

$$
\begin{aligned}
|(v_t^\rho, v_t^\rho - m(v_t^\rho))_\Gamma| &\le \|v_t^\rho - m(v_t^\rho)\|_\Gamma^2 + |(m(w_t^\rho), v_t^\rho - m(v_t^\rho))_\Gamma| \\
&\le c(\|v_t^\rho - m(v_t^\rho)\|_H^2 + \|w_t^\rho\|_H^2).
\end{aligned}
$$

Taking into account all these, (3.32) becomes:

$$
\begin{aligned}
&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{dt}}|v_t^\rho - m(v_t^\rho)|_{-1,h}^2 + \|\nabla v_t^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v_t^\rho\|_\Gamma^2 \le c(|w_{tt}^\rho - m(w_{tt}^\rho)|_{-1,h}^2 \\
&\quad + |v_t^\rho - m(v_t^\rho)|_{-1,h}^2 + \|v_t^\rho - m(v_t^\rho)\|_H^2 + \|w_t^\rho\|_H^2 + \|w^\rho\|_H^2 + \|v^\rho\|_H^2 + \|w_t^\mu\|_H^2).
\end{aligned} \tag{3.33}
$$

Now, applying the interpolation inequality (3.8), we get

$$
\begin{aligned}
\|v_t^\rho - m(v_t^\rho)\|_H^2 &\le c|v_t^\rho - m(v_t^\rho)|_{-1,h}\,|v_t^\rho - m(v_t^\rho)|_{1,V} \\
&\le c|v_t^\rho - m(v_t^\rho)|_{-1,h}\,(\|\nabla v_t^\rho\|_\Omega^2 + \|\nabla_\Gamma v_t^\rho\|_\Gamma^2)^{\frac{1}{2}} \\
&\le c|v_t^\rho - m(v_t^\rho)|_{-1,h}\,(\|\nabla v_t^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v_t^\rho\|_\Gamma^2)^{\frac{1}{2}} \\
&\le \frac{1}{2}(\|\nabla v_t^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v_t^\rho\|_\Gamma^2) + c\,|v_t^\rho - m(v_t^\rho)|_{-1,h}^2.
\end{aligned}
$$

We also use the fact that, thanks to (3.9), $|w_{tt}^\rho - m(w_{tt}^\rho)|_{-1,h} \le c\|w_{tt}^\rho - m(w_{tt}^\rho)\|_H \le c\|w_{tt}^\rho\|_H$.

Finally, we find

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{dt}}|v_t^\rho - m(v_t^\rho)|_{-1,h}^2 + \sigma\|\nabla_\Gamma v_t^\rho\|_\Gamma^2 + \|\nabla v_t^\rho\|_\Omega^2 \le c|v_t^\rho - m(v_t^\rho)|_{-1,h}^2 \\
&\quad + c(\|w_{tt}^\rho\|_H^2 + \|w_t^\rho\|_H^2 + \|w^\rho\|_H^2 + \|v^\rho\|_H^2 + \|w_t^\mu\|_H^2).
\end{aligned} \tag{3.34}
$$

We sum (3.24) and (3.34). This yields:

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{dt}}\left\{|v_t^\rho - m(v_t^\rho)|_{-1,h}^2 + \|\nabla v^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v^\rho\|_\Gamma^2 + \lambda\|v^\rho\|_\Gamma^2\right\} \\
&\quad + \|\nabla v_t^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v_t^\rho\|_\Gamma^2 + \|\nabla v^\mu\|_\Omega^2 + \delta\|\nabla_\Gamma v^\mu\|_\Gamma^2 \\
&\le c(|v_t^\rho - m(v_t^\rho)|_{-1,h}^2 + \|v^\rho\|_H^2 + \|v_t^\rho\|_H^2 + \|w_{tt}^\rho\|_H^2 \\
&\quad + \|w_t^\rho\|_H^2 + \|w^\rho\|_H^2 + \|w_t^\mu\|_H^2 + \|w^\mu\|_H^2).
\end{aligned} \tag{3.35}
$$

Moreover, we have

$$
\begin{aligned}
c\|v_t^\rho\|_H^2 &\le c(\|v_t^\rho - m(v_t^\rho)\|_H^2 + |m(v_t^\rho)|^2) \\
&\le c(|v_t^\rho - m(v_t^\rho)|_{-1,h}\,|v_t^\rho - m(v_t^\rho)|_{1,V} + |m(v_t^\rho)|^2) \\
&\le \frac{1}{2}\{\|\nabla v_t^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v_t^\rho\|_\Gamma^2\} + c|v_t^\rho - m(v_t^\rho)|_{-1,h}^2 + c\|w_t^\rho\|_H^2,
\end{aligned}
$$

and

$$
\begin{aligned}
\|v^\rho\|_H^2 &= \|v^\rho\|_\Omega^2 + \|v^\rho\|_\Gamma^2 \\
&\le c(\|\nabla v^\rho\|_\Omega^2 + \|v^\rho\|_\Gamma^2) \quad \text{(Generalized Poincaré inequality (1.8))}.
\end{aligned}
$$

Hence we obtain

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{dt}}\left\{|v_t^\rho - m(v_t^\rho)|_{-1,h}^2 + \|\nabla v^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v^\rho\|_\Gamma^2 + \lambda\|v^\rho\|_\Gamma^2\right\}\\
&\quad+\frac{\sigma}{2}\|\nabla_\Gamma v_t^\rho\|_\Gamma^2 + \frac{1}{2}\|\nabla v_t^\rho\|_\Omega^2 + \|\nabla v^\mu\|_\Omega^2 + \delta\|\nabla_\Gamma v^\mu\|_\Gamma^2\\
&\le c(|v_t^\rho - m(v_t^\rho)|_{-1,h}^2 + \|\nabla v^\rho\|_\Omega^2 + \sigma\|\nabla_\Gamma v^\rho\|_\Gamma^2 + \lambda\|v^\rho\|_\Gamma^2)\\
&\quad+c(\|w^\rho\|_H^2 + \|w_t^\rho\|_H^2 + \|w_{tt}^\rho\|_H^2 + \|w^\mu\|_H^2 + \|w_t^\mu\|_H^2). \qquad (3.36)
\end{aligned}$$

Applying the Gronwall lemma to (3.36) and using (3.15), we derive (3.14).

Finally, we apply the generalized Poincaré inequality to (3.21) and (3.15) leads to (3.16). □

Theorem 3.1 *Let (ρ, μ) be the solution of (2.1) with $\rho(0) = \rho_0$ such that*

$$\rho,\ \rho_t,\ \rho_{tt}, \mu,\ \mu_t \in L^2(0, T; V_2), \qquad (3.37)$$

and let (ρ^h, μ^h) be the solution of the discrete problem (2.5) with $\rho^h(0) = \rho_0^h$. If

$$v^\rho(0) = 0 \quad \textit{and} \quad v^\mu(0) = 0, \qquad (3.38)$$

then the following error estimates hold, for h small enough:

$$\sup_{[0,T]} (\|\rho^h - \rho\|_H + |\rho_t^h - \rho_t|_{-1,h}) \le ch^2,$$

$$\sup_{[0,T]} (|\rho^h - \rho|_{1,V}) \le ch,$$

$$\left(\int_0^T \|\mu^h - \mu\|_H^2\, ds\right)^{\frac{1}{2}} \le ch^2,$$

$$\left(\int_0^T |\rho_t^h - \rho_t|_{1,V}^2 + |\mu^h - \mu|_{1,V}^2\, ds\right)^{\frac{1}{2}} \le ch,$$

with c a positive constant independent of h.

Proof The regularity required on ρ implies, by classical arguments (see, for instance, [25]), that $\rho \in \mathcal{C}^1([0, T]; V_2)$ and by the Sobolev continuous injection $H_p^2(\Omega) \subset \mathcal{C}^0(\bar{\Omega})$, we have $\rho, \rho_t \in \mathcal{C}^0([0, T]; \mathcal{C}^0(\bar{\Omega}))$. Thus

$$\sup_{t\in[0,T]} \|\rho(t)\|_{\mathcal{C}^0(\bar{\Omega})} < R, \quad \sup_{t\in[0,T]} \|\rho_t(t)\|_{\mathcal{C}^0(\bar{\Omega})} \le R, \qquad (3.39)$$

for some fixed $R > 0$. In order to apply Lemma 3.3, we also need to prove that $\|\rho^h(0)\|_{\mathcal{C}^0(\bar{\Omega})} < R$. Indeed, we have

$$\begin{aligned}\|\rho^h(0) - \rho(0)\|_{\mathcal{C}^0(\bar{\Omega})} &\leq \|\rho^h(0) - I^h\rho(0)\|_{\mathcal{C}^0(\bar{\Omega})} + \|I^h\rho(0) - \rho(0)\|_{\mathcal{C}^0(\bar{\Omega})} \\ &\leq c\, h^{-\frac{d}{2}} \left\{\|\rho^h(0) - \rho(0)\|_\Omega + \|\rho(0) - I^h\rho(0)\|_\Omega\right\} + c\, h^\gamma \|\rho(0)\|_{H^2_p(\Omega)},\end{aligned}$$

where we have used the inverse estimate (2.4), together with the Sobolev injection $H^2_p(\Omega) \subset \mathcal{C}^\gamma(\bar{\Omega})$, with $0 < \gamma < 1$ and the fact that $\|I^h\rho(0) - \rho(0)\|_{\mathcal{C}^0(\bar{\Omega})} \leq Ch^\gamma\|\rho(0)\|_{\mathcal{C}^\gamma(\bar{\Omega})}$. Furthermore, we infer from (3.1), (3.3) and (3.38) that

$$\begin{aligned}\|\rho^h(0) - \rho(0)\|_\Omega \;&\leq\; c\,(\|\rho^h(0) - \tilde{\rho}^h(0)\|_\Omega + \|\tilde{\rho}^h(0) - \rho(0)\|_\Omega) \\ &\leq ch^2\{|\rho(0)|_{2,\Omega} + |\rho(0)|_{2,\Gamma}\},\end{aligned}$$

and from (2.2) we get

$$\|\rho(0) - I^h\rho(0)\|_\Omega \leq ch^2|\rho(0)|_{2,\Omega}.$$

Thus, combining the three above estimates, we finally obtain

$$\|\rho^h(0) - \rho(0)\|_{\mathcal{C}^0(\bar{\Omega})} \;\leq\; ch^{2-\frac{d}{2}}\{|\rho(0)|_{2,\Omega} + |\rho(0)|_{2,\Gamma}\} + ch^\gamma\, \|\rho(0)\|_{H^2_p(\Omega)}, \tag{3.40}$$

which, together with (3.39), implies that $\|\rho^h(0)\|_{\mathcal{C}^0(\bar{\Omega})} < R$ for sufficiently small h. Thus we can apply Lemma 3.3.

We note that, differentiating equations (3.2) with respect to t, we obtain that the elliptic projections of ρ_t and μ_t are respectively $\tilde{\rho}^h_t$ and $\tilde{\mu}^h_t$. A similar statement holds for ρ_{tt}. Therefore, by linearity, Lemma 3.1 applies to ρ replaced by ρ_t or ρ_{tt}, and μ replaced by μ_t. In particular, the following estimates hold:

$$\begin{aligned}\|w^\rho\|_H \;&\leq\; ch^2\,(|\rho|_{2,\Omega} + |\rho|_{2,\Gamma}),\\ \|w^\mu\|_H \;&\leq\; ch^2\,(|\mu|_{2,\Omega} + |\mu|_{2,\Gamma}),\\ \|w^\rho_t\|_H \;&\leq\; ch^2\,(|\rho_t|_{2,\Omega} + |\rho_t|_{2,\Gamma}),\\ \|w^\mu_t\|_H \;&\leq\; ch^2\,(|\mu_t|_{2,\Omega} + |\mu_t|_{2,\Gamma}),\\ \|w^\rho_{tt}\|_H \;&\leq\; ch^2\,(|\rho_{tt}|_{2,\Omega} + |\rho_{tt}|_{2,\Gamma}).\end{aligned} \tag{3.41}$$

It remains to prove that $\mathcal{N}(0) \leq ch^4$. We first notice that, by (3.15) and (3.38), $\mathcal{N}(0)$ reduces to

$$\mathcal{N}(0) = |v^\rho_t(0) - m(v^\rho_t)(0)|^2_{-1,h}.$$

We also infer from (3.11) and (3.38) that

$$(v^\rho_t(0), \psi)_H \;=\; -(w^\rho_t(0), \psi)_H \quad \forall\psi \in V^h,$$

or, equivalently,

$$(v_t^\rho(0) - m(v_t^\rho)(0), \psi)_H = -(w_t^\rho(0) + m(v_t^\rho)(0), \psi)_H \quad \forall \psi \in V^h, \quad (3.42)$$

the terms $v_t^\rho(0) - m(v_t^\rho)(0)$ and $w_t^\rho(0) + m(v_t^\rho)(0)$ having null average by (3.12). Then, choosing $\psi = T^h(v_t^\rho - m(v_t^\rho)(0))$ in (3.42), we obtain:

$$|v_t^\rho(0) - m(v_t^\rho)(0)|^2_{-1,h} \le |w_t^\rho(0) + m(v_t^\rho)(0)|_{-1,h}\, |v_t^\rho(0) - m(v_t^\rho)(0)|_{-1,h}.$$

Hence we deduce (using (3.9) and (3.41))

$$\begin{aligned} |v_t^\rho(0) - m(v_t^\rho)(0)|_{-1,h} &\le |w_t^\rho(0) + m(v_t^\rho)(0)|_{-1,h} \le c\|w_t^\rho(0) + m(v_t^\rho)(0)\|_H \\ &\le c\|w_t^\rho(0)\|_H \le ch^2 (|\rho_t(0)|_{2,\Omega} + |\rho_t(0)|_{2,\Gamma}), \end{aligned}$$

and, finally, we get that $\mathcal{N}(0) \le c\, h^4$ as claimed. Hence we conclude from (3.14) and (3.41) that $\mathcal{N}(t) \le c\, h^4 \quad \forall t \in [0, T^h]$.

Arguing as in (3.40), we also deduce that

$$\sup_{t \in [0, T^h]} \|\rho^h(t) - \rho(t)\|_{\mathcal{C}^0(\bar{\Omega})} \to 0 \quad \text{as } h \to 0.$$

Thus, for h small enough, $T^h = T$. The conclusion follows from Lemma 3.1, Lemma 3.3 and (3.22). □

Remark 3.1 We remark here that the regularity required in (3.37) is a strong one, this is due to the fact that we need strong regularity results in order to estimate the term v_t^ρ. Taking into account the parabolic nature of system (1.1), we expect that the solutions are regular enough provided that the initial data ρ_0 is also regular enough.

4 The case $\sigma = 0$

In this section we are interested in studying the numerical analysis of the initial model when in (1.1) we take $\sigma = 0$. The variational formulation (2.1) now reads:

For f and g satisfying (1.2) and $\rho_0 \in H^1_p(\Omega)$, find $\rho \in L^\infty(0, T, H^1_p(\Omega))$ and $\mu \in L^2(0, T, V)$ such that $\rho(0) = \rho_0$ and satisfying:

$$\begin{cases} (\rho_t, \psi)_H + (\nabla\mu, \nabla\psi)_\Omega + \delta(\nabla_\Gamma\mu, \nabla_\Gamma\psi)_\Gamma = 0, \\ (\mu, \phi)_H = (\nabla\rho, \nabla\phi)_\Omega + (f(\rho), \phi)_\Omega + \lambda(\rho, \phi)_\Gamma + (g(\rho), \phi)_\Gamma, \end{cases} \quad (4.1)$$

for all ϕ and $\psi \in V$.

The free energy is:

$$\mathcal{E}(\rho) = \frac{1}{2}\|\nabla\rho\|^2_\Omega + \int_\Omega F(\rho)dx + \frac{\lambda}{2}\|\rho\|^2_\Gamma + \int_\Gamma G(\rho)d\Gamma. \quad (4.2)$$

The semidiscrete version of (4.1) reads:
Find $(\rho^h, \mu^h) : [0, T] \to V^h \times V^h$ *such that:*

$$\begin{cases} (\rho_t^h, \psi)_H + (\nabla\mu^h, \nabla\psi)_\Omega + \delta(\nabla_\Gamma\mu^h, \nabla_\Gamma\psi)_\Gamma = 0, \\ (\mu^h, \phi)_H = (\nabla\rho^h, \nabla\phi)_\Omega + (f(\rho^h), \phi)_\Omega + \lambda(\rho^h, \phi)_\Gamma + (g(\rho^h), \phi)_\Gamma, \end{cases} \tag{4.3}$$

for all $\phi, \psi \in V^h$.

In this new context, Theorem 2.1 and Corollary 2.1 are unchanged, but the Theorem 2.2 now reads:

Theorem 4.1 *Assume that* $f, g \in \mathcal{C}^1(\mathbb{R}, \mathbb{R})$ *satisfy* (1.2), (2.13) *and* (2.14). *Let* $\rho_0 \in H_p^1(\Omega)$ *and let* $\rho_0^h \in V^h$ *such that* $\rho_0^h \to \rho_0$ *in* $H_p^1(\Omega)$ *as* $h \to 0$. *Then, for all* $T > 0$,

$$\begin{cases} \rho^h \to \rho \ \textit{weak} * \textit{ in } L^\infty(0, T; H_p^1(\Omega)) \ \textit{ and strongly in } \mathcal{C}^0([0, T]; L^2(\Omega)), \\ \rho_t^h \to \rho_t \textit{ weakly in } L^2(0, T; V'), \\ \mu^h \to \mu \textit{ weakly in } L^2(0, T; V), \end{cases}$$

where (ρ, μ) *is the unique solution of the continuous problem* (4.1) *with* $\rho(0) = \rho_0$.

Proof Mimicking the proof of Theorem 2.2, we infer that $\rho^h \to \rho$ weak $*$ in $L^\infty(0, T; H_p^1(\Omega))$ and $\mu^h \to \mu$ weakly in $L^2(0, T; V)$.

Then, we infer from the first equations of (4.1) and (4.3) that $\rho_t^h \to \rho_t$ weakly in $L^2(0, T; V')$ and we conclude with the Aubin–Lions compactness theorem that $\rho^h \to \rho$ strongly in $\mathcal{C}^0([0, T]; L^2(\Omega))$. □

We argue as in Sect. 3 and decompose $\rho^h - \rho$ and $\mu^h - \mu$ as in (3.1), the elliptic projections $\tilde{\rho}^h, \tilde{\mu}^h$ in V^h respectively of ρ, μ being now defined by:

$$\begin{cases} (\nabla\tilde{\rho}^h, \nabla\phi)_\Omega + \lambda(\tilde{\rho}^h, \phi)_\Gamma = (\nabla\rho, \nabla\phi)_\Omega + \lambda(\rho, \phi)_\Gamma, \\ (\nabla\tilde{\mu}^h, \nabla\phi)_\Omega + \delta(\nabla_\Gamma\tilde{\mu}^h, \nabla_\Gamma\phi)_\Gamma = (\nabla\mu, \nabla\phi)_\Omega + \delta(\nabla_\Gamma\mu, \nabla_\Gamma\phi)_\Gamma, \\ (\tilde{\mu}^h, \mathbf{1})_H = (\mu, \mathbf{1})_H, \end{cases} \tag{4.4}$$

for all $\phi \in V^h$.

We first estimate $w^\rho = \tilde{\rho}^h - \rho$ and $w^\mu = \tilde{\mu}^h - \mu$. We state the following result (compare to Lemma 3.1):

Lemma 4.1 *For all* $\rho \in H_p^2(\Omega)$, $\mu \in V_2$, *the functions* $\tilde{\rho}^h, \tilde{\mu}^h$ *defined by* (4.4) *satisfy*

$$\begin{aligned} &\|\tilde{\rho}^h - \rho\|_\Omega + h|\tilde{\rho}^h - \rho|_{1,\Omega} \le ch^2|\rho|_{2,\Omega}, \\ &\|\tilde{\mu}^h - \mu\|_H + h|\tilde{\mu}^h - \mu|_{1,V} \le ch^2(|\mu|_{2,\Omega} + |\mu|_{2,\Gamma}), \\ &\|\tilde{\rho}^h - \rho\|_\Gamma \le c(\varepsilon)h^{\frac{3}{2}-\varepsilon}|\rho|_{2,\Omega}, \quad \varepsilon \in (0, 1/2), \end{aligned} \tag{4.5}$$

with $c(\varepsilon)$ *a positive constant depending on* ε *and* c *a positive constant independent of* h.

Proof The proof for the first two statements is very similar to the one of Lemma 3.1 and is thus omitted. (For the estimation of $\tilde{\rho}^h - \rho$, we use the fact that the bilinear form $\hat{a}(\phi, \psi) = (\nabla\phi, \nabla\psi)_\Omega + \lambda(\phi, \psi)_\Gamma$ is continuous and coercive on $H^1_p(\Omega)$ and thus the estimate is standard). For the last statement, we use the continuous injection $H_p^{\frac{1}{2}+\varepsilon}(\Omega) \subset L^2(\Gamma)$, as well as the interpolation of $H_p^{\frac{1}{2}+\varepsilon}(\Omega)$ between $L^2(\Omega)$ and $H^1_p(\Omega)$, namely

$$\|\tilde{\rho}^h - \rho\|_\Gamma \le c(\varepsilon)\|\tilde{\rho}^h - \rho\|_{H_p^{\frac{1}{2}+\varepsilon}(\Omega)} \le c(\varepsilon)\|\tilde{\rho}^h - \rho\|_\Omega^{\frac{1}{2}-\varepsilon}\,\|\tilde{\rho}^h - \rho\|_{H^1_p(\Omega)}^{\frac{1}{2}+\varepsilon} \le c(\varepsilon)h^{\frac{3}{2}-\varepsilon}|\rho|_{2,\Omega}.$$

□

Lemma 4.2 *The following estimate holds:*

$$\|v\|_{V'} \le c(|v|_{-1,h} + h\|v\|_H) \quad \forall v \in \dot{H}, \tag{4.6}$$

with $|\cdot|_{-1,h}$ *the seminorm defined in Definition 3.1 and c independent of h.*

Proof We set $T : \dot{H} \to \dot{V},\ f \mapsto Tf$, where Tf is the unique solution of the problem

$$(\nabla Tf, \nabla\chi)_\Omega + \delta\,(\nabla_\Gamma Tf, \nabla_\Gamma\chi)_\Gamma = (f, \chi)_H \quad \forall\chi \in \dot{V}.$$

Following the arguments of [26], more precisely noticing that:

$$\begin{aligned}
&(\nabla T^h f, \nabla\chi^h)_\Omega + \delta(\nabla_\Gamma T^h f, \nabla_\Gamma\chi^h)_\Gamma = (f, \chi^h)_H\\
&\quad = (\nabla Tf, \nabla\chi^h)_\Omega + \delta\,(\nabla_\Gamma Tf, \nabla_\Gamma\chi^h)_\Gamma\\
&\quad = (\nabla R^h Tf, \nabla\chi^h)_\Omega + \delta\,(\nabla_\Gamma R^h Tf, \nabla_\Gamma\chi^h)_\Gamma, \quad \forall\,\chi^h \in \dot{V}^h,
\end{aligned} \tag{4.7}$$

we deduce that we have $T^h = R^h T$, with R^h the elliptic projection operator defined in $(4.4)_2$, namely $\tilde{\mu}^h = R^h(\mu)$. Using (4.5) and the elliptic regularity (3.6), we obtain

$$\|T^h f - Tf\|_H = \|(R^h - I)Tf\|_H \le ch^2\,(|Tf|_{2,\Omega} + |Tf|_{2,\Gamma}) \le ch^2\|f\|_H.$$

Let us take $v \in \dot{V}$. Then the above estimate implies:

$$\begin{aligned}
\|v\|^2_{V'} = (Tv,\ v)_H &= (T^h v, v)_H + ((T - T^h)v, v)_H,\\
&= |v|^2_{-1,h} + \|(T - T^h)v\|_H\,\|v\|_H,\\
&\le |v|^2_{-1,h} + ch^2\|v\|^2_H,
\end{aligned}$$

and (4.6) is proven. □

Theorem 4.2 *Let* (ρ, μ) *be a solution of* (4.1) *such that*

$$\rho,\ \rho_t,\ \rho_{tt}, \in L^2(0, T; H^2_p(\Omega)) \quad \textit{and} \quad \mu,\ \mu_t \in L^2(0, T; V_2), \tag{4.8}$$

and let (ρ^h, μ^h) *be a solution of* (4.3). *If we assume that*

$$v^\rho(0) = 0 \quad and \quad v^\mu(0) = 0, \tag{4.9}$$

then for every $\varepsilon \in (0, \frac{1}{2})$ *the following estimates hold provided that h is sufficiently small:*

$$\sup_{[0,T]} (\|\rho^h - \rho\|_\Omega + |\rho_t^h - \rho_t|_{-1,h}) \le c(\varepsilon)\, h^{\frac{3}{2}-\varepsilon},$$

$$\sup_{[0,T]} (|\rho^h - \rho|_{1,\Omega}) \le c(\varepsilon)\, h,$$

$$\left(\int_0^T \|\mu^h - \mu\|_H^2\, ds\right)^{\frac{1}{2}} \le c(\varepsilon)\, h^{\frac{3}{2}-\varepsilon},$$

$$\left(\int_0^T |\rho_t^h - \rho_t|_{1,\Omega}^2 + |\mu^h - \mu|_{1,V}^2\, ds\right)^{\frac{1}{2}} \le c(\varepsilon)\, h,$$

with $c(\varepsilon)$ *a positive constant depending on* ε.

Proof We argue as in the proof of Theorem 3.1. Thus, we need to prove an a priori estimate similar to the one in Lemma 3.3. Mimicking the previous computations, we obtain:

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{dt}}\left\{|v_t^\rho - m(v_t^\rho)|_{-1,h}^2 + \|\nabla v^\rho\|_\Omega^2 + \lambda\|v^\rho\|_\Gamma^2\right\} + \|\nabla v_t^\rho\|_\Omega^2 + \|\nabla v^\mu\|^2 + \delta\|\nabla_\Gamma v^\mu\|_\Gamma^2\\
&\quad \le c(\|v^\rho\|_H^2 + |v_t^\rho - m(v_t^\rho)|_{-1,h}^2 + \|v_t^\rho - m(v_t^\rho)\|_H^2 + \|w^\rho\|_H^2\\
&\qquad + \|w_t^\rho\|_H^2 + \|w_{tt}^\rho\|_H^2 + \|w^\mu\|_H^2 + \|w_t^\mu\|_H^2).
\end{aligned} \tag{4.10}$$

The term $\|v^\rho\|_H$ is handled with the Poincaré inequality (1.8). The actual difference with the computations of Sect. 3 is that in (4.10), the term $\|\nabla v_t^\rho\|_\Gamma^2$ is missing in the left hand side, thus we have to change the way we deal with the term $\|v_t^\rho - m(v_t^\rho)\|_H$. For every $\varepsilon \in (0, 1/2)$, we have:

$$\begin{aligned}
c\|v_t^\rho - m(v_t^\rho)\|_H^2 &\le c'(\varepsilon)\,\|v_t^\rho - m(v_t^\rho)\|_{H_p^{1/2+\varepsilon}}^2\\
&\le \frac{1}{4}\|\nabla v_t^\rho\|_\Omega^2 + c'(\varepsilon)\,\|v_t^\rho - m(v_t^\rho)\|_{H^{-1}}^2\\
&\le \frac{1}{4}\|\nabla v_t^\rho\|_\Omega^2 + c'(\varepsilon)\,\|v_t^\rho - m(v_t^\rho)\|_{V'}^2,
\end{aligned}$$

where $c'(\varepsilon)$ denotes a positive constant, depending on ε, that can change at different occurrences.

The above computations are due to a proper $H^1_p(\Omega) - H^{-1}(\Omega)$ interpolation resulting from the chains of continuous embeddings (see [14])

$$H^1_0(\Omega) \subset H^1_p(\Omega) \subset H_p^{\frac{1}{2}+\varepsilon}(\Omega) \subset L^2(\Omega) \subset (H^1_p(\Omega))' \subset H^{-1}(\Omega),$$

and

$$H^1_0(\Omega) \subset V \subset H \subset V' \subset H^{-1}(\Omega).$$

Applying Lemma 4.2, we write:

$$\|v_t^\rho - m(v_t^\rho)\|^2_{V'} \le c\,|v_t^\rho - m(v_t^\rho)|^2_{-1,h} + c\,h^2\,\|v_t^\rho - m(v_t^\rho)\|^2_H,$$

and then we obtain

$$c\|v_t^\rho - m(v_t^\rho)\|^2_H \;\le\; \frac{1}{4}\|\nabla v_t^\rho\|^2_\Omega + c'(\varepsilon)\,|v_t^\rho - m(v_t^\rho)|^2_{-1,h} + c'(\varepsilon)\,h^2\|v_t^\rho - m(v_t^\rho)\|^2_H.$$

Thus, provided h is chosen small enough ($c - c'(\varepsilon)\,h^2 \ge \frac{c}{2}$), we infer that

$$c\|v_t^\rho - m(v_t^\rho)\|^2_H \;\le\; \frac{1}{2}\|\nabla v_t^\rho\|^2_\Omega + c'(\varepsilon)\,|v_t^\rho - m(v_t^\rho)|^2_{-1,h}. \tag{4.11}$$

Finally, we derive

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{dt}}\left\{|v_t^\rho - m(v_t^\rho)|^2_{-1,h} + \|\nabla v^\rho\|^2_\Omega + \lambda\|v^\rho\|^2_\Gamma\right\} + \frac{1}{2}\|\nabla v_t^\rho\|^2_\Omega + \|\nabla v^\mu\|^2 + \delta\|\nabla_\Gamma v^\mu\|^2_\Gamma\\ &\le c(\varepsilon)\,(|v_t^\rho - m(v_t^\rho)|^2_{-1,h} + \|\nabla v^\rho\|^2_\Omega + \lambda\|v^\rho\|^2_\Gamma)\\ &\quad + c(\|w^\rho\|^2_H + \|w_t^\rho\|^2_H + \|w_{tt}^\rho\|^2_H + \|w^\mu\|^2_H + \|w_t^\mu\|^2_H).\end{aligned} \tag{4.12}$$

An application of the Gronwall lemma leads to

$$\begin{aligned}\mathcal{N}(t) &+ \int_0^t (\|\nabla v_t^\rho\|^2_\Omega + \|\nabla v^\mu\|^2_\Omega + \delta\|\nabla_\Gamma v^\mu\|^2_\Gamma)\,ds \le c(\varepsilon)\,\mathcal{N}(0)\\ &+ c(\varepsilon)\int_0^t (\|w_{tt}^\rho\|^2_H + \|w_t^\rho\|^2_H + \|w^\rho\|^2_H + \|w_t^\mu\|^2_H + \|w^\mu\|^2_H)\,ds,\end{aligned} \tag{4.13}$$

where we now have:

$$\mathcal{N}(t) = |v_t^\rho - m(v_t^\rho)|^2_{-1,h} + \|\nabla v^\rho\|^2_\Omega + \lambda\|v^\rho\|^2_\Gamma. \tag{4.14}$$

Arguing as in Sect. 3 and using (4.9) and (4.5), we find that

$$\mathcal{N}(0)=|v_t^\rho(0)-m(v_t^\rho)(0)|_{-1,h}^2 \le c\|w_t^\rho(0)\|_H^2 \le c(\varepsilon)\,h^{3-2\varepsilon}\,|\rho_t(0)|_{2,\Omega}^2 \quad (4.15)$$

and

$$\int_0^t (\|w_{tt}^\rho\|_H^2+\|w_t^\rho\|_H^2+\|w^\rho\|_H^2+\|w_t^\mu\|_H^2+\|w^\mu\|_H^2)\,ds \le c(\varepsilon)\,h^{3-2\varepsilon}, \quad \forall\, t\in[0,T^h]. \quad (4.16)$$

Therefore, applying (4.15) and (4.16) into (4.13), we obtain the estimates claimed in Theorem 4.2. Notice that for the third estimate, we use (3.21) and the Poincaré inequality (1.8) in order to estimate $\|v^\mu\|_H$. □

5 The case $\delta = 0$

In this section we are interested in studying the case when $\delta = 0$. The semidiscrete version of (2.1) now reads:

Find $(\rho^h, \mu^h) : [0, T] \to V^h \times V^h$ *such that:*

$$\begin{cases} (\rho_t^h, \psi)_H + (\nabla\mu^h, \nabla\psi)_\Omega = 0, \\ (\mu^h, \phi)_H = (\nabla\rho^h, \nabla\phi)_\Omega + (f(\rho^h), \phi)_\Omega + \sigma(\nabla_\Gamma\rho^h, \nabla_\Gamma\phi)_\Gamma \\ \qquad +\lambda(\rho^h, \phi)_\Gamma + (g(\rho^h), \phi)_\Gamma, \end{cases} \quad (5.1)$$

for all $\phi, \psi \in V^h$.

The results of Theorem 2.1 and Corollary 2.1 can be extended without any difficulty to the case $\delta = 0$. Moreover, Theorem 2.2 now reads (the proof is very similar to the one of Theorem 2.2 and is omitted):

Theorem 5.1 *Assume that* $f, g \in \mathcal{C}^1(\mathbb{R}, \mathbb{R})$ *satisfy* (1.2), (2.13) *and* (2.14). *Let* $\rho_0 \in V$ *and let* $\rho_0^h \in V^h$ *such that* $\rho_0^h \to \rho_0$ *in* V *as* $h \to 0$. *Then, for all* $T > 0$,

$$\begin{cases} \rho^h \to \rho \;\; weak * \;\; in\; L^\infty(0, T; V) \quad and\ strongly\ in\; \mathcal{C}^0([0, T]; L^2(\Omega)), \\ \rho_t^h \to \rho_t \; weakly\;\; in\; L^2(0, T; V'), \\ \rho^h|_\Gamma \to \rho|_\Gamma \quad strongly\ in\; \mathcal{C}^0([0, T]; L^2(\Gamma)), \\ \mu^h \to \mu \;\; weakly\ in\; L^2(0, T; H_p^1(\Omega)), \end{cases}$$

where (ρ, μ) *is the unique solution of the continuous problem* (2.1) *with* $\delta = 0$, *satisfying* $\rho(0) = \rho_0$.

The main difference, compared to the cases considered in the previous sections, concerns the error estimates for the space semidiscrete scheme. We again use the decomposition (3.1) and introduce $\tilde{\rho}^h$, $\tilde{\mu}^h$ the elliptic projections of ρ, μ in V^h, defined by:

$$\begin{cases} (\nabla\tilde{\rho}^h, \nabla\phi)_\Omega + \sigma(\nabla_\Gamma\tilde{\rho}^h, \nabla_\Gamma\phi)_\Gamma + \lambda(\tilde{\rho}^h, \phi)_\Gamma = (\nabla\rho, \nabla\phi)_\Omega + \sigma(\nabla_\Gamma\rho, \nabla_\Gamma\phi)_\Gamma \\ \quad +\lambda(\rho, \phi)_\Gamma, \\ (\nabla\tilde{\mu}^h, \nabla\phi)_\Omega = (\nabla\mu, \nabla\phi)_\Omega, \\ (\tilde{\mu}^h, \mathbf{1})_H = (\mu, \mathbf{1})_H, \end{cases} \tag{5.2}$$

for all $\phi \in V^h$.

The estimates for $w^\rho = \tilde{\rho}^h - \rho$ and $w^\mu = \tilde{\mu}^h - \mu$ now read:

Lemma 5.1 *For all $\rho \in V_2$ and $\mu \in H^2_p(\Omega)$, the functions $\tilde{\rho}^h$, $\tilde{\mu}^h$ defined by (5.2) satisfy*

$$\begin{aligned} \|\tilde{\rho}^h - \rho\|_H + h|\tilde{\rho}^h - \rho|_{1,V} &\le ch^2\,(|\rho|_{2,\Omega} + |\rho|_{2,\Gamma}), \\ \|\tilde{\mu}^h - \mu\|_\Omega + h|\tilde{\mu}^h - \mu|_{1,\Omega} &\le ch^2\,|\mu|_{2,\Omega}, \end{aligned} \tag{5.3}$$

with c a positive constant independent of h.

Proof For the estimate for $\tilde{\mu}^h$, we mimick the proof of Lemma 3.1, except that we use the bilinear function $a_0(\phi, \psi) = (\nabla\phi, \nabla\psi)_\Omega$, which is continuous on $H^1_p(\Omega)\times H^1_p(\Omega)$ and coercive on $\dot{H}^1_p(\Omega) \times \dot{H}^1_p(\Omega)$, where $\dot{H}^1_p(\Omega) = \{v \in H^1_p(\Omega);\ m(v) = 0\}$. □

As in Sect. 3, we now define the (new) discrete negative seminorm as:

Definition 5.1 We set $\tilde{T}^h : \dot{H} \to \dot{V}^h$, $f \mapsto \tilde{T}^h f$, where $\tilde{T}^h f$ is the unique solution of the problem:

$$(\nabla\tilde{T}^h f, \nabla\chi^h)_\Omega = (f, \chi^h)_H \quad \forall\chi^h \in V^h. \tag{5.4}$$

Furthermore, we introduce the discrete negative seminorm:

$$|f|_{-\tilde{1},h} = (\tilde{T}^h f, f)_H^{1/2} = \|\nabla\tilde{T}^h f\|_\Omega \quad \forall f \in \dot{H}.$$

Lemma 5.2 *The operator $\tilde{T}^h$ is self-adjoint, positive, semi-definite on $\dot{H}$. Moreover, the following interpolation inequality holds, for all $v^h \in \dot{V}^h$,*

$$\|v^h\|^2_H \le c\,|v^h|_{-\tilde{1},h}\,|v^h|_{1,\Omega}, \tag{5.5}$$

and

$$|f|_{-\tilde{1},h} \le c\,\|f\|_H \quad \forall f \in \dot{H}, \tag{5.6}$$

with c a positive constant independent of h.

We can now state the main results of this section (compare to the results of Theorem 3.1):

Theorem 5.2 *Let* (ρ, μ) *be a solution of* ((2.1), $\delta = 0$) *such that*

$$\rho,\ \rho_t,\ \rho_{tt}\ \in L^2(0,T;V_2),\ \mu,\ \mu_t\ \in L^2(0,T;H^2_p(\Omega)) \tag{5.7}$$

and let (ρ^h, μ^h) *be a solution of the discrete problem* (5.1). *If*

$$v^\rho(0) = 0 \quad and \quad v^\mu(0) = 0, \tag{5.8}$$

then for every $\varepsilon \in (0, \frac{1}{2})$ *the following error estimates hold, provided that* h *is small enough:*

$$\sup_{[0,T]} (\|\rho^h - \rho\|_H + |\rho^h_t - \rho_t|_{-\tilde{1},h}) \le c(\varepsilon)\, h^{3/2-\varepsilon},$$

$$\sup_{[0,T]} (|\rho^h - \rho|_{1,V}) \le c(\varepsilon)\, h,$$

$$\left(\int_0^T \|\mu^h - \mu\|^2_H\, ds\right)^{\frac{1}{2}} \le c(\varepsilon)\, h^{3/2-\varepsilon},$$

$$\left(\int_0^T |\rho^h_t - \rho_t|^2_{1,V} + |\mu^h - \mu|^2_{1,\Omega}\, ds\right)^{\frac{1}{2}} \le c(\varepsilon)\, h,$$

where $c(\varepsilon)$ *is a positive constant depending on* ε.

Proof Mimicking the proof of Lemma 3.3, we obtain

$$\mathcal{N}(t) + \int_0^t (\sigma \|\nabla_\Gamma v^\rho_t\|^2_\Gamma + \|\nabla v^\rho_t\|^2_\Omega + \|\nabla v^\mu\|^2_\Omega) ds$$
$$\le c\mathcal{N}(0) + c\int_0^t (\|w^\rho_{tt}\|^2_H + \|w^\rho_t\|^2_H + \|w^\rho\|^2_H + \|w^\mu_t\|^2_H + \|w^\mu\|^2_H)\, ds, \tag{5.9}$$

where

$$\mathcal{N}(t) = |v^\rho_t - m(v^\rho_t)|^2_{-\tilde{1},h} + \|\nabla v^\rho\|^2_\Omega + \sigma\|\nabla_\Gamma v^\rho\|^2_\Gamma + \lambda\|v^\rho\|^2_\Gamma.$$

From Lemma 5.1, we infer that:

$$\begin{aligned} \|w^\rho\|_H &\le ch^2(|\rho|_{2,\Omega} + |\rho|_{2,\Gamma}),\\ \|w^\rho_t\|_H &\le ch^2(|\rho_t|_{2,\Omega} + |\rho_t|_{2,\Gamma}),\\ \|w^\rho_{tt}\|_H &\le ch^2(|\rho_{tt}|_{2,\Omega} + |\rho_{tt}|_{2,\Gamma}). \end{aligned} \tag{5.10}$$

Moreover, interpolating $H_p^{\frac{1}{2}+\varepsilon}(\Omega)$ between $L^2(\Omega)$ and $H_p^1(\Omega)$ and applying Lemma 5.1 again, we get (compare with Lemma 3.1 and Lemma 4.1):

$$\begin{aligned}\|w^\mu\|_H^2 &\le \|w^\mu\|_\Omega^2 + \|w^\mu\|_\Gamma^2 \le \|w^\mu\|_\Omega^2 + c(\varepsilon)\,\|w^\mu\|^2_{H_p^{1/2+\varepsilon}(\Omega)} \\ &\le \|w^\mu\|_\Omega^2 + c(\varepsilon)\,\|w^\mu\|_\Omega^{1-2\varepsilon}\,\|w^\mu\|^{1+2\varepsilon}_{H_p^1(\Omega)} \le ch^4|\mu|^2_{2,\Omega} + c(\varepsilon)\,h^{3-2\varepsilon}|\mu|^2_{2,\Omega} \\ &\le c(\varepsilon)\,h^{3-2\varepsilon}|\mu|^2_{2,\Omega}. \end{aligned} \tag{5.11}$$

Similarly, we have

$$\|w_t^\mu\|_H \le c(\varepsilon)\,h^{3/2-\varepsilon}|\mu_t|_{2,\Omega}.$$

Finally, we argue as in Theorem 3.1 in order to check that $\mathcal{N}(0) \le ch^4$ and the conclusion follows from (5.9), (5.10) and (5.11). □

Remark 5.1 We remark that in this section we considered the case $\delta = 0$, $\sigma > 0$ but the case $\delta = \sigma = 0$ can be treated similarly.

6 Stability of the backward Euler scheme

For the space and time discretization of (2.1), we consider the backward Euler scheme applied to the space semidiscrete scheme (2.5). The time step $\tau > 0$ is fixed. Hence the total discretization reads:

Let $\rho_h^0 \in V^h$. For $n \ge 1$ find $(\rho_h^n, \mu_h^n) \in V^h \times V^h$ such that

$$\begin{cases} \frac{1}{\tau}(\rho_h^n,\psi)_H + (\nabla\mu_h^n,\nabla\psi)_\Omega + \delta(\nabla_\Gamma\mu_h^n,\nabla_\Gamma\psi)_\Gamma = \frac{1}{\tau}(\rho_h^{n-1},\psi)_H \\ (\mu_h^n,\phi)_H = (\nabla\rho_h^n,\nabla\phi)_\Omega + \sigma(\nabla_\Gamma\rho_h^n,\nabla_\Gamma\phi)_\Gamma + (f(\rho_h^n),\phi)_\Omega + \lambda(\rho_h^n,\phi)_\Gamma \\ \qquad\qquad +(g(\rho_h^n),\phi)_\Gamma \end{cases} \tag{6.1}$$

for all $\phi, \psi \in V^h$.

The dissipativity property (1.2) on the functions f and g imply the existence of some positive constants $C_f \ge 0$ and $C_g \ge 0$ such that:

$$f'(v) \ge -C_f, \quad g'(v) \ge -C_g, \quad \forall\, v \in \mathbb{R}. \tag{6.2}$$

In what follows we prove the existence, uniqueness and stability of the sequences of solutions (ρ_h^n, μ_n^h) of problem (6.1):

Theorem 6.1 *Let us suppose $\sigma > 0$. If $\rho_h^0 \in V^h$, there exists a sequence $(\rho_h^n,\ \mu_h^n)_{n\ge1}$ generated by (6.1) and satisfying the following discrete energy inequality:*

$$\mathcal{E}(\rho_h^n) + \frac{1}{2\tau}|\rho_h^n - \rho_h^{n-1}|^2_{-1,h} \le \mathcal{E}(\rho_h^{n-1}), \quad \forall\, n \ge 1. \tag{6.3}$$

Furthermore, if the time step τ *is small enough, more exactly if* $\tau < \dfrac{4}{\max^2(C_f,\ C_g)} \min(\frac{\sigma}{\delta}, 1)$*, then the sequence is uniquely defined.*

Proof In order to prove the existence of solutions for problem (6.1), we consider the following variational problem:

$$\mathcal{J}^h(u) = \inf_{v \in K^h} \mathcal{J}^h(v), \tag{6.4}$$

where

$$\mathcal{J}^h(v) = \mathcal{E}(v) + \frac{1}{2\tau}|v - \rho_h^{n-1}|^2_{-1,h},$$

and

$$K^h = \{v \in V^h;\ (v - \rho_h^{n-1}, \mathbf{1})_H = 0\}. \tag{6.5}$$

Taking into account (1.5) as well as (1.3), we can easily see that:

$$\mathcal{J}^h(v) \geq \frac{1}{2}(\min(1,\sigma)|v|^2_{1,V} + 2c_1\|v\|^2_H + \lambda\|v\|^2_\Gamma) - c_2(|\Omega| + |\Gamma|), \quad \forall v \in V^h.$$

The functional $\mathcal{J}^h$ is continuous, so we deduce that problem (6.4) has a solution which satisfies the following Euler-Lagrange equation:

$$\begin{aligned}(\nabla u, \nabla\psi)_\Omega &+ (f(u), \psi)_\Omega + \sigma(\nabla_\Gamma u, \nabla_\Gamma \psi)_\Gamma + \lambda(u,\psi)_\Gamma \\ &+ (g(u), \psi)_\Gamma + \frac{1}{\tau}(T^h(u - \rho_h^{n-1}), \psi)_H - \alpha(\mathbf{1}, \psi)_H = 0, \quad \forall\, \psi \in V^h,\end{aligned} \tag{6.6}$$

with α the Lagrange multiplier for the constraint (6.5).

Setting $u = \rho_h^n$ and $\mu_h^n = \alpha - 1/\tau T^h(\rho_h^n - \rho_h^{n-1})$ in (6.6), we see that (ρ_h^n, μ_h^n) is a solution of problem (6.1). By construction $\mathcal{J}^h(\rho_h^n) \leq \mathcal{J}^h(\rho_h^{n-1}) = \mathcal{E}(\rho_h^{n-1})$ and we thus deduce the energy inequality (6.3). We remark that the case $\sigma = 0$ is included in the arguments above, the only difference appearing in the definition of the energy. For the case $\delta = 0$, we use $\tilde{T}^h$ instead of T^h in the definition of μ_h^n and the existence is similarly obtained.

In order to prove the uniqueness of solutions of problem (6.1), we assume that there exist two solutions $(\rho_{h,1}^n, \mu_{h,1}^n)$ and $(\rho_{h,2}^n, \mu_{h,2}^n)$ originating from the same initial data $(\rho_h^{n-1}, \mu_h^{n-1})$ and set $\theta_h = \rho_{h,1}^n - \rho_{h,2}^n$ and $\zeta_h = \mu_{h,1}^n - \mu_{h,2}^n$. Then (θ_h, μ_h) is solution to the following problem:

$$\begin{aligned}&\frac{1}{\tau}(\theta_h, \psi)_H + (\nabla\zeta_h, \nabla\psi)_\Omega + \delta(\nabla_\Gamma\zeta_h, \nabla_\Gamma\psi)_\Gamma = 0,\\ &\quad(\zeta_h, \phi)_H = (\nabla\theta_h, \nabla\phi)_\Omega + \sigma(\nabla_\Gamma\theta_h, \nabla_\Gamma\phi)_\Gamma + (f(\rho_{h,1}^n) - f(\rho_{h,2}^n), \phi)_\Omega\\ &\qquad + \lambda(\theta_h, \phi)_\Gamma + (g(\rho_{h,1}^n) - g(\rho_{h,2}^n), \phi)_\Gamma.\end{aligned} \tag{6.7}$$

We choose $\psi = \zeta_h$ and $\phi = \theta_h$ in (6.7) and subtract the two resulting equations. This yields

$$\begin{aligned}
&\delta\tau\|\nabla_\Gamma\zeta_h\|_\Gamma^2 + \tau\|\nabla\zeta_h\|_\Omega^2 + \sigma\|\nabla_\Gamma\theta_h\|_\Gamma^2 + \|\nabla\theta_h\|_\Omega^2 + \lambda\|\theta_h\|_\Gamma^2\\
&\quad = -(f(\rho_{h,1}^n) - f(\rho_{h,2}^n), \theta_h)_\Omega - (g(\rho_{h,1}^n) - g(\rho_{h,2}^n), \theta_h)_\Gamma\\
&\quad \le C_f\|\theta_h\|_\Omega^2 + C_g\|\theta_h\|_\Gamma^2\\
&\quad \le \max(C_f,\ C_g)\,\|\theta_h\|_H^2.
\end{aligned}$$

Now, we choose $\psi = \theta_h$ in the first equation of (6.7). We obtain:

$$\begin{aligned}
\|\theta_h\|_H^2 &= -\delta\,\tau\,(\nabla_\Gamma\zeta_h, \nabla_\Gamma\theta_h)_\Gamma - \tau(\nabla\zeta_h, \nabla\theta_h)_\Omega\\
&\le \delta\,\tau\|\nabla_\Gamma\zeta_h\|_\Gamma\|\nabla_\Gamma\theta_h\|_\Gamma + \tau\|\nabla\zeta_h\|_\Omega\|\nabla\theta_h\|_\Omega.
\end{aligned}$$

Thus,

$$\begin{aligned}
&\max(C_f,\ C_g)\,\|\theta_h\|_H^2 \ \le\ \delta\tau\|\nabla_\Gamma\zeta_h\|_\Gamma^2 + \frac{\delta\tau}{4}\max{}^2(C_f,\ C_g)\,\|\nabla_\Gamma\theta_h\|_\Gamma^2\\
&\quad + \tau\|\nabla\zeta_h\|_\Omega^2 + \frac{\tau}{4}\max{}^2(C_f,\ C_g)\,\|\nabla\theta_h\|_\Omega^2.
\end{aligned}$$

Collecting the above estimates, we conclude that

$$\sigma\|\nabla_\Gamma\theta_h\|_\Gamma^2 + \|\nabla\theta_h\|_\Omega^2 + \lambda\|\theta_h\|_\Gamma^2 \le \frac{\tau}{4}\max{}^2(C_f,\ C_g)\,(\delta\|\nabla_\Gamma\theta_h\|_\Gamma^2 + \|\nabla\theta_h\|_\Omega^2),$$

and

$$\left(\sigma - \frac{\delta\tau}{4}\max{}^2(C_f,\ C_g)\right)\|\nabla_\Gamma\theta_h\|_\Gamma^2 + \left(1 - \frac{\tau}{4}\max{}^2(C_f,\ C_g)\right)\|\nabla\theta_h\|_\Omega^2 + \lambda\|\theta_h\|_\Gamma^2 \ \le 0.$$

Therefore, provided $\tau < \dfrac{4}{\max^2(C_f,\ C_g)}\min(\dfrac{\sigma}{\delta}, 1)$, this yields $\theta_h = 0$ and, by (6.7), $\zeta_h = 0$. ◻

Remark 6.1 When $\sigma = 0$ we can still prove the uniqueness of the solution; the difference (θ^h, ψ^h) of two solutions satisfy the following variational formulation:

$$\begin{aligned}
&\frac{1}{\tau}(\theta_h, \psi)_H + (\nabla\zeta_h, \nabla\psi)_\Omega + \delta(\nabla_\Gamma\zeta_h, \nabla_\Gamma\psi)_\Gamma = 0,\\
&\quad(\zeta_h, \phi)_H = (\nabla\theta_h, \nabla\phi)_\Omega + (f(\rho_{h,1}^n) - f(\rho_{h,2}^n), \phi)_\Omega\\
&\qquad\qquad + \lambda(\theta_h, \phi)_\Gamma + (g(\rho_{h,1}^n) - g(\rho_{h,2}^n), \phi)_\Gamma.
\end{aligned} \tag{6.8}$$

We choose $\psi = T^h\theta_h$ in the first equation of (6.8) and $\phi = \theta_h$ in the second, we get, arguing as in (4.11):

$$
\begin{aligned}
&\frac{1}{\tau}|\theta_h|^2_{-1,h} + \|\nabla\theta_h\|^2_\Omega + \lambda\|\theta_h\|^2_\Gamma \\
&\quad = -(f(\rho^n_{h,1}) - f(\rho^n_{h,2}), \theta_h)_\Omega + (g(\rho^n_{h,1}) - g(\rho^n_{h,2}), \theta_h)_\Gamma \\
&\quad \leq C_f\|\theta_h\|^2_\Omega + C_g\|\theta_h\|^2_\Gamma \\
&\quad \leq \max(C_f, C_g)\,\|\theta_h\|^2_H \\
&\quad \leq \frac{1}{2}\|\nabla\theta_h\|^2_\Omega + c'|\theta_h|^2_{-1,h},
\end{aligned} \tag{6.9}
$$

provided that h is chosen small enough.

Thus, we obtain

$$
\left(\frac{1}{\tau} - c'\right)|\theta_h|^2_{-1,h} + \frac{1}{2}\|\nabla\theta_h\|^2_\Omega + \|\theta_h\|^2_\Gamma \leq 0,
$$

which implies the uniqueness as long as the time step τ satisfies $\tau < 1/c'$.

We can also obtain a fully discrete version of Corollary 2.1:

Corollary 6.1 *If f and g are real analytic functions, then for all $\rho^0_h \in V^h$, any sequence (ρ^n_h, μ^n_h) generated by (6.1) and satisfying the energy estimate (6.3) converges to a steady state $(\bar\rho_h, \bar\mu_h)$ as $n \to \infty$.*

Proof The proof of this result is based on the Łojasiewicz gradient inequality (see [1,20]) and it follows very closely the main lines of the proof in [3]. We thus skip this proof referring the interested reader to [3]. □

7 Numerical results

In this section we present several numerical simulations in two space dimensions, using the FreeFem++ software.[1] We first solve the fully discrete scheme (6.1) to illustrate the solution on the slab $[0, L_x] \times [0, L_y] = [0, 80] \times [0, 40]$. The triangulation Ω^h was obtained by dividing the domain into 200×100 rectangles, each rectangle being divided among the same diagonal into two triangles. The functions f and g are considered as:

$$
f(v) = v^3 - v, \quad g(v) = g_s v - h_s;
$$

for Figs. 1, 2, and 3 we write $\tilde g_s = g_s + \lambda$ and we use $\tilde g_s = -4$ and h_s=0.

Although in the previous sections we studies the case $g_s > 0$, the case $g_s < 0$ is still pertinent and we refer the interested reader to [9] where the authors explain that this situation appears in practical cases, for example in f.c.c. binary alloys with competing interactions in the bulk. The time step $\tau = 0.01$ and the initial value of ρ^h is an uniformly distributed random fluctuation of amplitude ± 0.01. In each figure, we represent the solution ρ on the left hand side and the solution μ on the right hand side

[1] FreeFem++ is freely available at http://www.freefem.org/ff++.

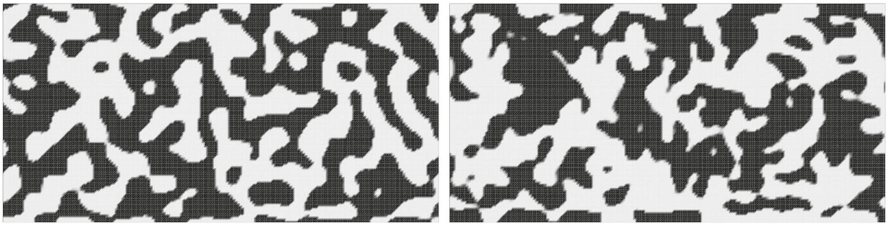

Fig. 1 $\tilde{g}_s = -4$, $\sigma = 5$, $\delta = 5$, on the *left* the solution ρ and on the *right* the solution μ

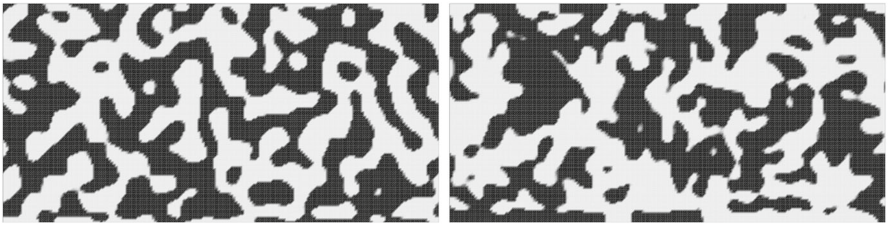

Fig. 2 $\tilde{g}_s = -4$, $\sigma = 5$, $\delta = 0$, on the *left* the solution ρ and on the *right* the solution μ

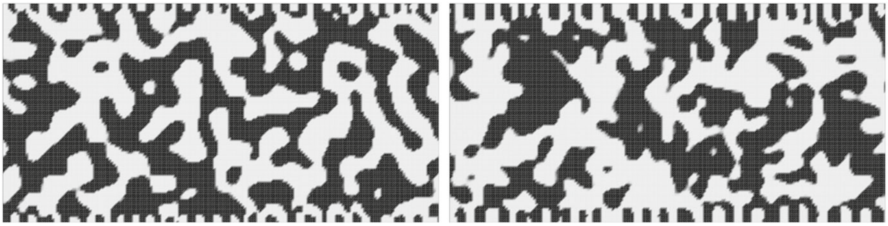

Fig. 3 $\tilde{g}_s = -4$, $\sigma = 0$, $\delta = 1$, on the *left* the solution ρ and on the *right* the solution μ

picture; the negative and the positive values of the solution are respectively represented in white and black. Since in Figs. 1, 2, 3 we considered the parameter $h_s = 0$, none of the components is preferentially attracted by the walls, which is visible on the fact that both white and black zones appear at the boundary. We also remark that away from the boundary, Figs. 1, 2, 3 present the same patterns. In these numerical simulations, we chose the same parameters as in [3] in order to be able to compare the behavior of the solutions when different type of dynamic boundary conditions are considered. We notice that the choice of the boundary conditions significantly modify the behavior of the solution near the boundary (compare to [3] and [9]).

In Figs. 4 and 5 we see the results produced by the implicit scheme (6.1) with the nonlinearities:

$$f(v) = v^3 - v, \quad g(v) = g_s v - h_s,$$

for $\tilde{g}_s = 4$ and $h_s = 0$ or $h_s = 0.1$. In these two figures the domain Ω is a disk of radius 80 centered at $(0, 0)$ from which we cut off a disk of radius 40 and centered at $(20, 0)$. The exterior boundary is divided into 400 intervals and the internal boundary

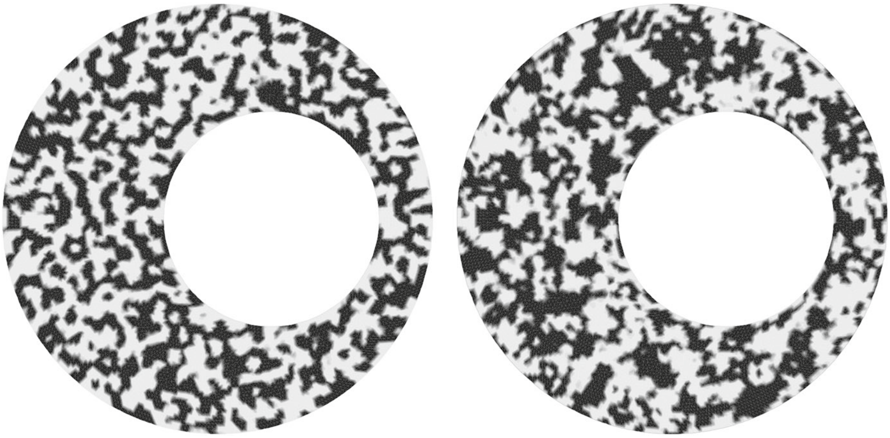

Fig. 4 $\tilde{g}_s = 4$, $\sigma = 5$, $\delta = 1$, $h_s = 0$, on the *left* the solution ρ and on the *right* the solution μ

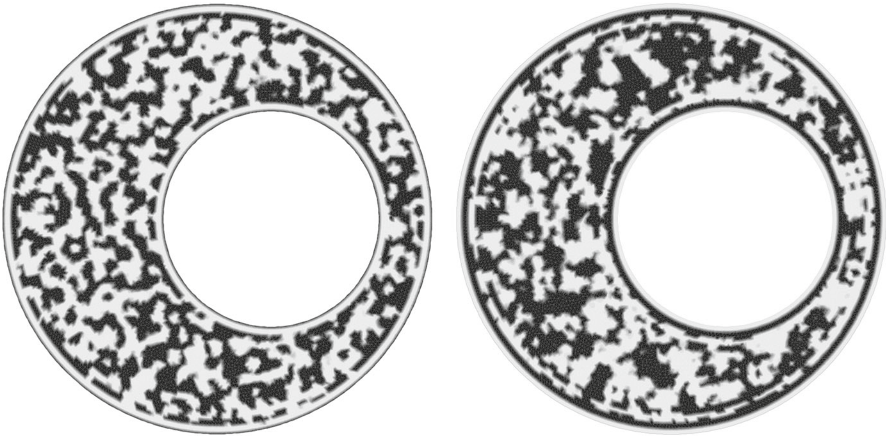

Fig. 5 $\tilde{g}_s = 4$, $\sigma = 5$, $\delta = 1$, $h_s = 0.1$, on the *left* the solution ρ and on the *right* the solution μ

is divided into 200 intervals. The time step is $\tau = 0.01$. For $h_s = 0$, we illustrate the case when no phase is preferentially attracted by the walls, while for $h_s = 0.1$ we see that one of the phases is preferentially attracted by the walls. We also remark that away from the boundary, Figs. 4 and 5 present the same patterns.

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