ANALYSIS OF A TIME DISCRETIZATION SCHEME FOR A NONSTANDARD VISCOUS CAHN–HILLIARD SYSTEM[1]

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Zusammenfassung

In this paper we propose a time discretization of a system of two parabolic equations describing diffusion-driven atom rearrangement in crystalline matter. The equations express the balances of microforces and microenergy; the two phase fields are the order parameter and the chemical potential. The initial and boundary-value problem for the evolutionary system is known to be well posed. Convergence of the discrete scheme to the solution of the continuous problem is proved by a careful development of uniform estimates, by weak compactness and a suitable treatment of nonlinearities. Moreover, for the difference of discrete and continuous solutions we prove an error estimate of order one with respect to the time step.

1 Introduction

This paper deals with a time discretization of a PDE system arising from a mechanical model for phase segregation by atom rearrangement on a lattice. The model was proposed by one of us in [29]; the resulting system has been analyzed in a recent and intensive research work by four of the present authors (see, in particular, [16] and [17], both for well-posedness results and for a detailed presentation of the model).

The initial and boundary value problem we consider consists in looking for two *fields*, the *chemical potential* $\mu > 0$ and the *order parameter* $\rho \in (0,1)$, solving

$$(1+2g(\rho))\partial_t\mu + \mu\,\partial_t g(\rho) - \Delta\mu = 0 \qquad \text{in } \Omega\times(0,T), \tag{1.1}$$

$$\partial_t\rho - \Delta\rho + f'(\rho) = \mu g'(\rho) \qquad \text{in } \Omega\times(0,T), \tag{1.2}$$

$$\partial_\nu\mu = \partial_\nu\rho = 0 \qquad \text{on } \Gamma\times(0,T), \tag{1.3}$$

$$\mu|_{t=0} = \mu_0 \quad \text{and} \quad \rho|_{t=0} = \rho_0 \qquad \text{in } \Omega; \tag{1.4}$$

here Ω denotes a bounded domain of $\mathbb{R}^3$ with conveniently smooth boundary Γ, $T > 0$ stands for some final time, and ∂_ν denotes differentiation in the direction of the outward normal ν.

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Problem (1.1)–(1.4) is parameterized by two nonlinear scalar-valued functions, g and f, which enter into the definition of the system's *free energy*:

$$\psi = \widehat{\psi}(\rho, \nabla\rho, \mu) = -\left(\frac{1}{2} + g(\rho)\right)\mu + f(\rho) + \frac{1}{2}|\nabla\rho|^2. \tag{1.5}$$

We point out that in (1.1)–(1.5) all physical constants have been set equal to 1. We also note that the last two terms in (1.5) favor phase segregation, the former because it introduces local energy minima, the latter because it penalizes spatial changes of the order parameter. For g, one can take any smooth function, provided it is nonnegative in the physically admissible domain:

$$g(\rho) \geq 0 \quad \text{for all } \rho \in (0,1); \tag{1.6}$$

accordingly, the coefficient $1/2$ of μ in (1.5) should be regarded as a prescribed material bound. As to the possibly multi-well potential f, we take it to be the sum of two functions:

$$f(\rho) = f_1(\rho) + f_2(\rho);$$

the one, f_1, is convex over $(0,1)$, and such that its derivative f_1' (and possibly also f_1) is singular at the endpoints 0 and 1 (cf. (2.3)); the other is required to be smooth over the entire interval $[0,1]$, but not to have any convexity property, so that in equation (1.2) f_2' may serve as a non-monotone perturbation of the increasing function f_1'.

As to the parameter functions, in [16] the choice made for g was:

$$g(\rho) = \rho, \tag{1.7}$$

while the assumptions on f were compatible with choosing a double-well potential:

$$f(\rho) = \alpha_1 \{\rho \ln(\rho) + (1-\rho)\ln(1-\rho)\} + \alpha_2\, \rho\,(1-\rho) + \alpha_3\rho, \tag{1.8}$$

for some non-negative constants α_1, α_2, α_3. Note that, if α_3 is taken null, then, according to whether or not $2\alpha_1 \geq \alpha_2$, f turns out to be convex in the whole of $[0,1]$ or it exhibits two wells, with a local maximum at $\rho = 1/2$; moreover, for $\alpha_3 > 0$, the combined function:

$$-g(\rho)\mu + f(\rho) \quad \text{(a part of } \psi)$$

shows one global minimum in all cases, and it depends on the sign of $(\alpha_3 - \mu)$ which minimum actually occurs. On the other hand, the framework of paper [17] allows for much more general choices of g and f, as well as for nonlinear diffusion of μ. Existence and uniqueness results were proved in both [16] and [17], with different approaches. Here, we take inspiration from arguments developed either in the one or in the other of those papers.

We introduce a time discretization of system (1.1)–(1.4) which is implicit with respect to the principal terms and tries to handle very carefully the nonlinearities. Namely, we address the recursive sequence of the elliptic problems:

$$(1+2\gamma_n)\,\delta_h\mu_n + \mu_{n+1}\,\delta_h\gamma_n - \Delta\mu_{n+1} = 0 \qquad \text{in } \Omega, \tag{1.9}$$

$$\delta_h\rho_n - \Delta\rho_{n+1} + f'(\rho_{n+1}) = \mu_n g'(\rho_n) \qquad \text{in } \Omega, \tag{1.10}$$

$$\partial_\nu\mu_{n+1} = \partial_\nu\rho_{n+1} = 0 \qquad \text{on } \Gamma, \tag{1.11}$$

for $n = 0, 1, \ldots, N$, where $h = T/N$ is the time step, $\gamma_n := g(\rho_n)$ and, for any $(N+1)$-tuple $z_0, z_1, \ldots, z_N$, we let

$$\delta_h z_n := (z_{n+1} - z_n)/h \quad \text{for } n = 0, \ldots, N-1.$$

After showing the existence of a discrete solution at any step, we carry out a number of uniform estimates on the time-discrete solution which allow us to prove convergence to the unique solution (μ, ρ) of the continuous problem (1.1)–(1.4), as h tends to 0 (or, equivalently, N goes to $+\infty$). Then, we estimate certain norms of the difference between the piecewise-linear-in-time interpolants of the discrete solutions and the continuous solution: more precisely, the first error estimate we prove is of order $h^{1/2}$; the second, which holds under stronger regularity assumptions on the initial data, is of order h.

We regard our results as a cornerstone in the construction of a time-and-space discretization of problem (1.1)–(1.4). With reference to such a complete discretization of Cahn-Hilliard and viscous Cahn-Hilliard systems, we quote papers [1, 2, 3, 4, 5, 6, 7, 8, 22, 21, 23]. Some recent efforts can be found in the literature with the aim of analyzing other classes of phase transition problems, either to show existence via time discretization [9, 14, 15, 19, 20, 27, 30, 35, 36] or to prove numerical results such as special convergence properties, stability or error estimates [11, 12, 13, 18, 25, 28, 31, 33, 34] (cf. also [26] for a recent review on phase-field models). We dare say that our contribution goes deeply into the structure of the mathematical problem, because, as is not the case for many other similar investigations, we succeed in showing a linear order of convergence.

Our paper is organized as follows. In the next section, we list and discuss our assumptions, formulate the continuous and discrete problems precisely, and state our main results. Section 3 is devoted to proving that there is a discrete solution. The convergence result is proved in the long and articulate Section 4. Finally, the last two Sections 5 and 6 contain detailed proofs of the two error estimates.

2 Main results

In this section, we describe the mathematical problem under investigation, introduce the time discretization scheme, make our assumptions precise, and state our results.

First of all, we assume Ω to be a bounded connected open set in $\mathbb{R}^3$ with smooth boundary Γ. For convenience, we set

$$V := H^1(\Omega), \quad H := L^2(\Omega), \quad \text{and} \quad W := \{v \in H^2(\Omega) : \partial_\nu v = 0, \text{ on } \Gamma\}, \tag{2.1}$$

and we endow these spaces with their standard norms, for which we use a self-explanatory notation like $\|\cdot\|_V$. The notation $\|\cdot\|_p$ $(1 \le p \le +\infty)$ stands for the standard L^p-norm in $L^p(\Omega)$; for short, we sometimes do not distinguish between a space (or its norm) and a power thereof.

As to the parameter functions f and g, we assume that

$$f = f_1 + f_2, \quad \text{where} \tag{2.2}$$

$$f_1 : (0,1) \to [0,+\infty) \text{ is a convex } C^2 \text{ function satisfying}$$

$$\lim_{r \searrow 0} f_1'(r) = -\infty\,, \quad \text{and} \quad \lim_{r \nearrow 1} f_1'(r) = +\infty, \tag{2.3}$$

$$f_2 : [0,1] \to \mathbb{R} \quad \text{is of class } C^2; \tag{2.4}$$

$$g : [0,1] \to \mathbb{R} \quad \text{is of class } C^2 \text{ and nonnegative.} \tag{2.5}$$

For the initial data, we require that

$$\mu_0 \in V \cap L^\infty(\Omega) \quad \text{and} \quad \mu_0 \geq 0 \quad \text{a.e. in } \Omega; \tag{2.6}$$

$$\rho_0 \in W \subset C^0(\overline{\Omega}) \quad \text{and} \quad \inf \rho_0 > 0, \ \sup \rho_0 < 1. \tag{2.7}$$

We stress that conditions (2.7) actually imply that ρ_0 is $1/2$-Hölder continuous: indeed, as Ω is a three-dimensional domain, W is continuosly embedded in $C^{0,1/2}(\overline{\Omega})$. As a consequence, also $f(\rho_0)$ and $f'(\rho_0)$ are $1/2$-Hölder continuous, since f and f' are smooth in $(0,1)$. On the other hand, we point out that in the sequel we will mostly exploit the compactness of the embedding $W \subset C^0(\overline{\Omega})$; Hölder continuity will play no role.

As recalled in the Introduction, in papers [16] and [17] two versions of problem (1.1)–(1.4) were solved over an arbitrary time interval $[0,T]$ in a rather strong sense, because the solution pairs (μ,ρ) were required to satisfy

$$\mu \in H^1(0,T;H) \cap L^2(0,T;W), \tag{2.8}$$

$$\rho \in W^{1,\infty}(0,T;H) \cap H^1(0,T;V) \cap L^\infty(0,T;W), \tag{2.9}$$

$$\mu \geq 0 \quad \text{a.e. in } Q, \tag{2.10}$$

$$0 < \rho < 1 \quad \text{a.e. in } Q \quad \text{and} \quad f'(\rho) \in L^\infty(0,T;H). \tag{2.11}$$

Note that the boundary conditions (1.3) follow from (2.8)–(2.9), due to the definition of W in (2.1). Accordingly, the solutions to the problems of type (1.1)–(1.4) studied in [16] and [17] were pairs (μ,ρ) satisfying, in addition to (2.8)–(2.11), the system

$$\big(1 + 2g(\rho)\big)\partial_t \mu + \mu\, \partial_t g(\rho) - \Delta \mu = 0 \qquad \text{a.e. in } Q, \tag{2.12}$$

$$\partial_t \rho - \Delta \rho + f'(\rho) = \mu g'(\rho) \qquad \text{a.e. in } Q, \tag{2.13}$$

$$\mu(0) = \mu_0 \quad \text{and} \quad \rho(0) = \rho_0 \qquad \text{a.e. in } \Omega. \tag{2.14}$$

Some of the results proved in the quoted papers are summarized in the following theorem.

Theorem 2.1. *Let assumptions* (2.2)–(2.7) *hold. Then, there exists a unique pair* (μ,ρ) *satisfying* (2.8)–(2.11) *and solving problem* (2.12)–(2.14)*. Moreover,* $\mu \in L^\infty(Q)$*, and there exist* $\rho_*, \rho^* \in (0,1)$ *such that* $\rho_* \leq \rho \leq \rho^*$ *a.e. in* Q*.*

The main aim of the present paper is to show that, given the time-discretization scheme introduced here below, the discrete solution converges to the solution (μ,ρ) as the time step h tends to zero.

Notation 2.2. Assume that N is a positive integer, and let Z be any normed space. We define $\delta_h : Z^{N+1} \to Z^N$ as follows:

$$\begin{aligned} &\text{for } z = (z_0, z_1, \dots, z_N) \in Z^{N+1} \text{ and } w = (w_0, \dots, w_{N-1}) \in Z^N, \\ &\delta_h z_n = w \quad \text{means that} \quad w_n = \frac{z_{n+1} - z_n}{h} \quad \text{for } n = 0, \dots, N-1. \end{aligned} \tag{2.15}$$

We can also iterate the discretization procedure, and define, e.g.,

$$\delta_h^2 z_n := \frac{\delta_h z_{n+1} - \delta_h z_n}{h} = \frac{z_{n+2} - 2z_{n+1} + z_n}{h^2} \quad \text{for } n = 0, \dots, N-2. \tag{2.16}$$

Next, by setting $h := T/N$ (without stressing the dependence of h on N) and $I_n := ((n-1)h, nh)$ for $n = 1, \dots, N$, we introduce the interpolation maps from Z^{N+1} into either $L^\infty(0,T;Z)$ or $W^{1,\infty}(0,T;Z)$ as follows: for $z = (z_0, z_1, \dots, z_N) \in Z^{N+1}$, we set

$$\overline{z}_h,\, \underline{z}_h \in L^\infty(0,T;Z) \quad \text{and} \quad \widehat{z}_h \in W^{1,\infty}(0,T;Z)\,, \tag{2.17}$$

$$\overline{z}_h(t) = z_n \quad \text{and} \quad \underline{z}_h(t) = z_{n-1} \quad \text{for a.a. } t \in I_n,\ n = 1, \dots, N, \tag{2.18}$$

$$\widehat{z}_h(0) = z_0 \quad \text{and} \quad \partial_t \widehat{z}_h(t) = \delta_h z_{n-1} \quad \text{for a.a. } t \in I_n,\ n = 1, \dots, N. \tag{2.19}$$

These maps yield the backward/forward piecewise-constant and piecewise-linear interpolants of the discrete vectors. We obviously have:

$$\|\overline{z}_h\|_{L^\infty(0,T;Z)} = \max_{n=1,\dots,N} \|z_n\|_Z\,, \quad \|\underline{z}_h\|_{L^\infty(0,T;Z)} = \max_{n=0,\dots,N-1} \|z_n\|_Z, \tag{2.20}$$

$$\|\overline{z}_h\|^2_{L^2(0,T;Z)} = h \sum_{n=1}^{N} \|z_n\|_Z^2\,, \quad \|\underline{z}_h\|^2_{L^2(0,T;Z)} = h \sum_{n=0}^{N-1} \|z_n\|_Z^2\,. \tag{2.21}$$

Moreover, as $\widehat{z}_h(t)$ is a convex combination of z_{n-1} and z_n for $t \in I_n$, we also have

$$\|\widehat{z}_h\|_{L^\infty(0,T;Z)} = \max_{n=1,\dots,N} \max\{\|z_{n-1}\|_Z, \|z_n\|_Z\} = \max\{\|z_0\|_Z, \|\overline{z}_h\|_{L^\infty(0,T;Z)}\}, \tag{2.22}$$

$$\|\widehat{z}_h\|^2_{L^2(0,T;Z)} \le h \sum_{n=1}^{N} \bigl(\|z_{n-1}\|_Z^2 + \|z_n\|_Z^2\bigr) \le h\|z_0\|_Z^2 + 2\|\overline{z}_h\|^2_{L^2(0,T;Z)}\,. \tag{2.23}$$

Finally, by a direct computation, it is straightforward to prove that

$$\|\overline{z}_h - \widehat{z}_h\|_{L^\infty(0,T;Z)} = \max_{n=0,\dots,N-1} \|z_{n+1} - z_n\|_Z = h\,\|\partial_t \widehat{z}_h\|_{L^\infty(0,T;Z)}, \tag{2.24}$$

$$\|\overline{z}_h - \widehat{z}_h\|^2_{L^2(0,T;Z)} = \frac{h}{3} \sum_{n=0}^{N-1} \|z_{n+1} - z_n\|_Z^2 = \frac{h^2}{3}\,\|\partial_t \widehat{z}_h\|^2_{L^2(0,T;Z)}, \tag{2.25}$$

and that the same identities hold for the difference $\underline{z}_h - \widehat{z}_h$.

At this point, we can write the discrete scheme presented in the Introduction in a precise form. For any positive integer N, we look for two vectors $(\mu_n)_{n=0}^N$ and $(\rho_n)_{n=0}^N$ satisfying the following conditions:

$i)$ *the first components* μ_0 *and* ρ_0 *coincide with the initial data;*

$ii)$ *for* $n = 0, \dots, N-1$, *we have that*

$$\mu_{n+1}\,,\ \rho_{n+1} \in W, \quad \mu_{n+1} \geq 0 \quad \textit{and} \quad 0 < \rho_{n+1} < 1 \quad \textit{in } \Omega, \quad f'(\rho_{n+1}) \in H; \tag{2.26}$$

$iii)$ *if* $(\gamma_n)_{n=0}^N$ *is the vector whose components are* $\gamma_n := g(\rho_n)$, *there hold*

$$(1 + 2\gamma_n)\,\delta_h\mu_n + \mu_{n+1}\,\delta_h\gamma_n - \Delta\mu_{n+1} = 0, \tag{2.27}$$

$$\delta_h\rho_n - \Delta\rho_{n+1} + f'(\rho_{n+1}) = \mu_n g'(\rho_n), \tag{2.28}$$

for $n = 0, \dots, N-1$.

Also in this case, the homogenous Neumann boundary conditions are implicit in the regularity requirements (see (2.26) and (2.1)).

Clearly, the "true" problem consists in finding (μ_{n+1}, ρ_{n+1}) once (ρ_n, μ_n) is given. Here is our result in this direction.

Theorem 2.3. *Assume* (2.2)–(2.7). *Then, there exists* $h_0 > 0$ *such that, for* $h < h_0$ *and* $n = 0, \dots, N-1$, *problem* (2.27)–(2.28) *has a unique solution* (μ_{n+1}, ρ_{n+1}) *satisfing* (2.26).

Our next results concern firstly convergence of interpolants for vectors (ρ_n) and (μ_n) to the solution (μ, ρ) to problem (2.12)–(2.14), then error estimates. We point out that, for simplicity, the convergence theorem here below is not stated in a precise form: the topological setting will be specified later, by means of relations (4.34)-(4.38).

Theorem 2.4. *Assume* (2.2)–(2.7). *Then, in accord with Notation 2.2, the sequences of interpolants for the discrete solutions given by Theorem 2.3 converge to the solution* (μ, ρ) *given by Theorem 2.1 as* h *tends to* 0, *in a suitable topology.*

Theorem 2.5. *In addition to* (2.2)–(2.7), *assume that*

$$\rho_0 \in H^3(\Omega). \tag{2.29}$$

Then, for sufficiently small $h > 0$, *the following error estimate holds:*

$$\|\widehat{\rho}_h - \rho\|_{H^1(0,T;H)\cap L^\infty(0,T;V)} + \|\widehat{\mu}_h - \mu\|_{L^\infty(0,T;H)\cap L^2(0,T;V)} \leq c\,h^{1/2}, \tag{2.30}$$

where c *depends only on the structural assumptions and the data.*

Theorem 2.6. *In addition to* (2.2)–(2.7), *assume* (2.29) *and*

$$\mu_0 \in W. \tag{2.31}$$

Then, for sufficiently small $h > 0$, *the following error estimate holds:*

$$\|\widehat{\rho}_h - \rho\|_{H^1(0,T;H)\cap L^\infty(0,T;V)} + \|\widehat{\mu}_h - \mu\|_{L^\infty(0,T;H)\cap L^2(0,T;V)} \leq c\,h, \tag{2.32}$$

where c *depends only on the structural assumptions and the data.*

Remark 2.7. It is easy to see that our assumptions (2.2)–(2.7) ensure that both $f'(\rho_0)$ and $\mu_0 g'(\rho_0)$ belong to V. It follows that (2.29) is equivalent to

$$-\Delta\rho_0 + f'(\rho_0) - \mu_0 g'(\rho_0) \in V. \tag{2.33}$$

We also notice that the assumptions (2.29) and (2.31) ensure further regularity for the solution (μ, ρ) to the continuous problem (see the forthcoming Remark 6.1).

We prove Theorem 2.3 in Section 3 and Theorem 2.4 in Section 4; the last two sections are devoted to proving, respectively, Theorems 2.5 and 2.6.

Throughout the paper, we account for the well-known embeddings $V \subset L^q(\Omega)$ $(1 \le q \le 6)$ and $W \subset C^0(\overline{\Omega})$, and for the related Sobolev inequalities:

$$\|v\|_q \le C\|v\|_V \quad \text{and} \quad \|v\|_\infty \le C\|v\|_W, \tag{2.34}$$

for $v \in V$ and $v \in W$, respectively, where C depends on Ω only, since sharpness is not needed. We remark that these embeddings are compact. In particular, the following compactness inequality holds:

$$\|v\|_4 \le \sigma\|\nabla v\|_H + C_\sigma\|v\|_H, \quad \text{for every } v \in V \text{ and } \sigma > 0; \tag{2.35}$$

in (2.35), C_σ is a constant that depends only on Ω and σ. Furthermore, we make repeated use of Hölder's inequality, of the following elementary identity:

$$(a-b)a = \frac{1}{2}\,a^2 - \frac{1}{2}b^2 + \frac{1}{2}\,(a-b)^2, \quad \text{for every } a, b \in \mathbb{R}, \tag{2.36}$$

and of Young's inequality

$$ab \le \sigma a^2 + \frac{1}{4\sigma}\,b^2, \quad \text{for every } a, b \ge 0 \text{ and } \sigma > 0. \tag{2.37}$$

Moreover, we use the discrete Gronwall lemma in the following form (see, e.g., [24, Prop. 2.2.1]): if $(a_0, \ldots, a_N) \in [0, +\infty)^{N+1}$ and $(b_1, \ldots, b_N) \in [0, +\infty)^N$ satisfy

$$\begin{aligned} &a_m \le a_0 + \sum_{n=1}^{m-1} b_n a_n \quad \text{for } m = 1, \ldots, N, \quad \text{then} \\ &a_m \le a_0 \exp\Big(\sum_{n=1}^{m-1} b_n\Big) \quad \text{for } m = 1, \ldots, N. \end{aligned} \tag{2.38}$$

Finally, throughout the paper we use a small-case italic c for a number of different constants that may only depend on Ω, the final time T, the shape of f, the properties of the data involved in the statements at hand; those constants we need to refer to are always denoted by capital letters, just like C in (2.34). Moreover, a notation like c_σ signals a constant that depends also on the parameter σ. The reader should keep in mind that the meaning of c and c_σ might change from line to line and even in the same chain of inequalities and that their values never depend on the time step h.

3 Existence

In this section, we prove Theorem 2.3. We argue inductively with respect to n, i.e., by assuming that a pair (μ_n, ρ_n) satisfying (2.26) with n in place of $n+1$ is given, we prove that problem (2.27)–(2.28) has a unique solution (μ_{n+1}, ρ_{n+1}) satisfying (2.26). More precisely, as is going to be clear from the proof, we need less regularity for μ_n, e.g., $\mu_n \in V$. In particular, our assumptions on μ_0 are sufficient to start. We rewrite (2.27)–(2.28) in the form

$$\big(1+\gamma_n+\gamma_{n+1}\big)\mu_{n+1} - h\Delta\mu_{n+1} = \big(1+2\gamma_n\big)\mu_n, \tag{3.1}$$

$$\rho_{n+1} - h\Delta\rho_{n+1} + hf'(\rho_{n+1}) = \rho_n + h\mu_n g'(\rho_n), \tag{3.2}$$

and solve (3.2) first for ρ_{n+1} (so that γ_{n+1} is also known), then (3.1). In order to solve both problems, it is expedient to replace each equation by a minimum problem, at least for h small enough. We consider the functionals:

$$J_1 : V \to \mathbb{R} \quad \text{and} \quad J_2 : V \to (-\infty, +\infty], \quad \text{defined by, respectively,}$$

$$J_1(v) := \frac{h}{2}\int_\Omega |\nabla v|^2 + \frac{1}{2}\int_\Omega \big(1+\gamma_n+\gamma_{n+1}\big)v^2 - \int_\Omega \big(1+2\gamma_n\big)\mu_n\, v \quad \text{and} \tag{3.3}$$

$$J_2(v) := \frac{h}{2}\int_\Omega |\nabla v|^2 + \frac{1}{2}\int_\Omega v^2 + h\int_\Omega \tilde f(v) - \int_\Omega \big(\rho_n + h\mu_n g'(\rho_n)\big)\, v. \tag{3.4}$$

In (3.4), we have $\tilde f = \tilde f_1 + \tilde f_2$, where $\tilde f_2$ is any smooth extension of f_2 to the whole of $\mathbb{R}$ and $\tilde f_1$ is the unique convex and lower semicontinuous extension of f_1 that satisfies $\tilde f(r) = +\infty$ if $r \notin [0,1]$. By the way, it is understood that the corresponding integral that appears in (3.4) is infinite if $\tilde f(v)$ does not belong to $L^1(\Omega)$. Therefore, both functionals are well-defined and proper whenever $\mu_n \in V$ and $\rho_n \in W$ (and this implies boundedness of $g(\rho_n)$ and $g'(\rho_n)$). Moreover, in view of the above remarks, J_1 is continuous, and J_2 lower semicontinuous, on V.

Now, we observe that equations (3.1) and (3.2), when complemented by the regularity requirements in (2.26) (which yield the homogeneous Neumann boundary conditions), are the strong forms of the Euler-Lagrange variational equations for the stationary points of J_1 and J_2, respectively. More precisely, the strong form (3.1) follows from the variational formulation thanks to the regularity theory of elliptic equations. As far as (3.2) is concerned, the function f' should be replaced – in principle, at least – by the sum $\partial\tilde f_1 + \tilde f_2'$, where $\partial\tilde f_1$ is the subdifferential of $\tilde f_1$. However, once an $L^2(\Omega)$-estimate is obtained for the subdifferential (and standard arguments of the theory of maximal monotone operators (see, e.g., [10]), easily yield such an estimate), the variational Euler-Lagrange equation can be written exactly in the form (3.2), because $\partial\tilde f_1$ is single-valued due to our assumptions on f_1 (see (2.3), in particular). Consequently, existence and uniqueness of the solution (μ_n, ρ_n) follow if the functionals (3.3) and (3.4) are convex, so that each of the correponding minimum problems has a unique solution. This is granted for the first problem: indeed, J_1 is strictly convex and coercive, because g is nonnegative. The same holds for J_2, provided that the second derivative of function $r \mapsto r^2/2 + hf_2(r)$ is strictly positive on $[0,1]$, which is the case if $h \sup |f_2''| < 1$.

It remains to prove that $\mu_{n+1} \geq 0$. To this end, we multiply (3.1) by $-\mu_{n+1}^-$, where $v^- =$

$\max\{-v,0\}$ denotes the negative part of v, and integrate over Ω. We obtain:

$$\int_\Omega \big(1+g(\rho_n)+g(\rho_{n+1})\big)|\mu_{n+1}^-|^2 + h\int_\Omega |\nabla \mu_{n+1}^-|^2 = -\int_\Omega \big(1+2g(\rho_n)\big)\mu_n\mu_{n+1}^- \le 0,$$

because both g and μ_n are nonnegative. This implies that $\mu_{n+1}^- = 0$, and hence that $\mu_{n+1} \ge 0$.

4 Convergence

In this section, we prove Theorem 2.4. For convenience, we introduce one more vector, $(\xi_n)_{n=0}^N$, and recall the definition of $(\gamma_n)_{n=0}^N$:

$$\xi_n := f_1'(\rho_n) \quad \text{and} \quad \gamma_n := g(\rho_n) \quad \text{for } n = 0,\dots,N. \tag{4.1}$$

Later on, we also use the interpolants of these vectors according to Notation 2.2. Our argument uses compactness and monotonicity methods.

First a priori estimate. We multiply (3.1) by μ_{n+1} and integrate over Ω. By accounting for the elementary identity (2.36), we obtain

$$\begin{aligned}&\frac12\int_\Omega \mu_{n+1}^2 - \frac12\int_\Omega \mu_n^2 + \frac12\int_\Omega |\mu_{n+1}-\mu_n|^2 + h\int_\Omega |\nabla\mu_{n+1}|^2\\ &+\int_\Omega \big(\gamma_n\mu_{n+1}^2 + \gamma_{n+1}\mu_{n+1}^2 - 2\gamma_n\mu_n\mu_{n+1}\big) = 0.\end{aligned}$$

As $\gamma_n\mu_{n+1}^2 + \gamma_{n+1}\mu_{n+1}^2 - 2\gamma_n\mu_n\mu_{n+1} = \gamma_{n+1}\mu_{n+1}^2 - \gamma_n\mu_n^2 + \gamma_n(\mu_{n+1}-\mu_n)^2$, we derive that

$$\begin{aligned}&\int_\Omega \Big(\frac12+\gamma_{n+1}\Big)\mu_{n+1}^2 - \int_\Omega \Big(\frac12+\gamma_n\Big)\mu_n^2 + \int_\Omega \Big(\frac12+\gamma_n\Big)|\mu_{n+1}-\mu_n|^2\\ &\quad + h\int_\Omega |\nabla\mu_{n+1}|^2 = 0.\end{aligned}$$

On summing over $n = 0,\dots,m-1$ with $1 \le m \le N$, we conclude that

$$\begin{aligned}&\int_\Omega \Big(\frac12+\gamma_m\Big)\mu_m^2 + h^2\sum_{n=0}^{m-1}\int_\Omega \Big(\frac12+\gamma_n\Big)|\delta_h\mu_n|^2 + h\sum_{n=0}^{m-1}\int_\Omega |\nabla\mu_{n+1}|^2\\ &= \int_\Omega \Big(\frac12+\gamma_0\Big)\mu_0^2 \quad \text{for } m = 1,\dots,N.\end{aligned}$$

As g is nonnegative and hence $\gamma_i \ge 0$, this implies that $\|\mu_m\|_H \le c$ for $m = 1,\dots,N$. Thus, the above estimate also yields

$$\max_{m=1,\dots,N}\|\mu_m\|_H^2 + h^2\sum_{n=0}^{N-1}\|\delta_h\mu_n\|_H^2 + h\sum_{n=1}^{N}\|\mu_n\|_V^2 \le c. \tag{4.2}$$

In terms of the interpolants introduced in Notation 2.2, with the help of $\mu_0 \in V$, (2.20)–(2.21), and (2.24)–(2.25) we have that

$$\|\overline{\mu}_h\|^2_{L^\infty(0,T;H)\cap L^2(0,T;V)} + \|\underline{\mu}_h\|^2_{L^\infty(0,T;H)\cap L^2(0,T;V)} + \|\widehat{\mu}_h\|^2_{L^\infty(0,T;H)\cap L^2(0,T;V)} + h\|\partial_t \widehat{\mu}_h\|^2_{L^2(0,T;H)} \le c. \tag{4.3}$$

Second a priori estimate. In (3.2), we move ρ_n to the left-hand side. Then, we multiply by $\rho_{n+1} - \rho_n$ and integrate over Ω. We obtain

$$\int_\Omega |\rho_{n+1} - \rho_n|^2 + \frac{h}{2}\int_\Omega |\nabla \rho_{n+1}|^2 - \frac{h}{2}\int_\Omega |\nabla \rho_n|^2 + \frac{h}{2}\int_\Omega |\nabla \rho_{n+1} - \nabla \rho_n|^2 + h\int_\Omega f'(\rho_{n+1})(\rho_{n+1} - \rho_n) = h\int_\Omega \mu_n g'(\rho_n)(\rho_{n+1} - \rho_n). \tag{4.4}$$

Now, we consider the last integral on the left-hand side of (4.4). We split $f' = f_1' + f_2'$ and use the convexity assumption of f_1 and boundedness for f_2'. We get

$$\int_\Omega f'(\rho_{n+1})(\rho_{n+1} - \rho_n) \ge \int_\Omega \big(f_1(\rho_{n+1}) - f_1(\rho_n)\big) - c\int_\Omega |\rho_{n+1} - \rho_n|.$$

Since also g' is bounded, we infer from (4.4) that

$$\begin{aligned}
&\int_\Omega |\rho_{n+1} - \rho_n|^2 + \frac{h}{2}\int_\Omega |\nabla \rho_{n+1}|^2 - \frac{h}{2}\int_\Omega |\nabla \rho_n|^2 + \frac{h}{2}\int_\Omega |\nabla \rho_{n+1} - \nabla \rho_n|^2 \\
&\quad + h\int_\Omega \big(f_1(\rho_{n+1}) - f_1(\rho_n)\big) \le c\,h\int_\Omega (1 + \mu_n)|\rho_{n+1} - \rho_n| \\
&\le \frac{1}{2}\int_\Omega |\rho_{n+1} - \rho_n|^2 + c\,h^2\int_\Omega (1 + \mu_n^2) \le \frac{1}{2}\int_\Omega |\rho_{n+1} - \rho_n|^2 + c\,h^2,
\end{aligned}$$

the last inequality being due to (4.3). By dividing by h, summing over $n = 0, \dots, m-1$, and owing to the obvious inequality $mh \le c$, we conclude that

$$h\sum_{n=0}^{m-1}\int_\Omega |\delta_h \rho_n|^2 + \frac{1}{2}\int_\Omega |\nabla \rho_{m+1}|^2 + h^2\sum_{n=0}^{m-1}\int_\Omega |\delta_h(\nabla \rho_n)|^2 + \int_\Omega f_1(\rho_{m+1}) \le c \tag{4.5}$$

for $m = 0, \dots, N-1$. As the term involving the difference quotient $\delta_h \rho_{N-1}$ is missing in the first sum since $m \le N-1$, we estimate it directly. We multiply (2.28), written for $n = N-1$, by $h\delta_h \rho_{N-1}$ and integrate over Ω. We have

$$h\int_\Omega |\delta_h \rho_{N-1}|^2 + \int_\Omega (\nabla \rho_N - \nabla \rho_{N-1}) \cdot \nabla \rho_N + \int_\Omega f_1'(\rho_N)(\rho_N - \rho_{N-1}) = h\int_\Omega \phi\, \delta_h \rho_{N-1},$$

where we have set $\phi := \mu_{N-1}\, g'(\rho_{N-1}) - f_2'(\rho_{N-1})$. Owing to the elementary identity (2.36) and to the convexity of f_1 as before, we have

$$\begin{aligned}
&h\|\delta_h \rho_{N-1}\|_H^2 + \frac{1}{2}\|\nabla \rho_N\|_H^2 + \frac{1}{2}\|\nabla \rho_N - \nabla \rho_{N-1}\|_H^2 + \int_\Omega f_1(\rho_N) \\
&\le \frac{1}{2}\|\nabla \rho_{N-1}\|_H^2 + \int_\Omega f_1(\rho_{N-1}) + h\|\phi\|_H\, \|\delta_h \rho_{N-1}\|_H \\
&\le \frac{1}{2}\|\nabla \rho_{N-1}\|_H^2 + \int_\Omega f_1(\rho_{N-1}) + \frac{h}{2}\|\phi\|_H^2 + \frac{h}{2}\|\delta_h \rho_{N-1}\|_H.
\end{aligned}$$

Now, we observe that the first two terms of the last line are bounded by (4.5) written with $m = N-2$ and that ϕ is estimated in H thanks to (4.2) and our assumptions of g and f_2. Moreover, the last term of the first line can be ignored since f_1 is nonnegative. Hence, we get the desired bound for the first term. At this point, we can easily derive an estimate for $\|\rho_m\|_H$ for $m = 1, \ldots, N$. By using the obvious identity $\rho_m = \rho_0 + h \sum_{n=0}^{m-1} \delta_h \rho_n$ and the euclidean Schwarz and Young inequalities, we see that

$$\|\rho_m\|_H \le \|\rho_0\|_H + h \sum_{n=0}^{m-1} \|\delta_h \rho_n\|_H \le c + \frac{h}{2} \Big(m + \sum_{n=0}^{m-1} \|\delta_h \rho_n\|_H^2 \Big) \le c.$$

Hence, by recalling (4.5) and our last estimates, we conclude that

$$h \sum_{n=0}^{N-1} \|\delta_h \rho_n\|_H^2 + \max_{m=1,\ldots,N} \|\rho_m\|_V^2 + h^2 \sum_{n=0}^{N-2} \|\delta_h(\nabla \rho_n)\|_H^2 \le c. \tag{4.6}$$

In terms of the interpolants, (4.6) reads (thanks also to $\rho_0 \in V$ and to (2.20)–(2.21) and (2.24))

$$\begin{aligned} &\|\partial_t \widehat{\rho}_h\|_{L^2(0,T;H)}^2 + \|\overline{\rho}_h\|_{L^\infty(0,T;V)}^2 + \|\underline{\rho}_h\|_{L^\infty(0,T;V)}^2 \\ &\qquad + \|\widehat{\rho}_h\|_{L^\infty(0,T;V)}^2 + h \|\partial_t \nabla \widehat{\rho}_h\|_{L^2(0,T-h;H)}^2 \le c. \end{aligned} \tag{4.7}$$

Third a priori estimate. We come back to (2.28) and rewrite it as (recall (4.1))

$$-\Delta \rho_{n+1} + \xi_{n+1} = -\delta_h \rho_n + \mu_n g'(\rho_n) - f_2'(\rho_{n+1}).$$

Hence, a standard argument (multiplying by $-\Delta \rho_{n+1}$ and by ξ_{n+1}) shows that the following estimate holds true

$$\|\Delta \rho_{n+1}\|_H + \|\xi_{n+1}\|_H \le c \|-\delta_h \rho_n + \mu_n g'(\rho_n) - f_2'(\rho_{n+1})\|_H \,.$$

Thus, we infer that

$$\|\Delta \rho_{n+1}\|_H^2 + \|\xi_{n+1}\|_H^2 \le c \big(\|\delta_h \rho_n\|_H^2 + \|\mu_n\|_H^2 + 1 \big) \quad \text{for } n = 0, \ldots, N-1. \tag{4.8}$$

Moreover, by using the regularity theory of elliptic equations, we deduce that

$$\|\rho_{n+1}\|_W^2 + \|\xi_{n+1}\|_H^2 \le c \big(\|\rho_{n+1}\|_V^2 + \|\delta_h \rho_n\|_H^2 + \|\mu_n\|_H^2 + 1 \big). \tag{4.9}$$

Now, we multiply (4.8) by h and sum over $n = 0, \ldots, m-1$. By accounting for (4.2) and (4.6), we conclude that

$$h \sum_{n=0}^{N-1} \|\rho_{n+1}\|_W^2 + h \sum_{n=0}^{N-1} \|\xi_{n+1}\|_H^2 \le c. \tag{4.10}$$

In terms of the interpolants, (4.10) yields (by accounting for $\rho_0 \in W$)

$$\|\overline{\rho}_h\|_{L^2(0,T;W)}^2 + \|\underline{\rho}_h\|_{L^2(0,T;W)}^2 + \|\widehat{\rho}_h\|_{L^2(0,T;W)}^2 \le c \tag{4.11}$$

besides an estimate for, e.g., $\|\overline{\xi}_h\|$ in $L^2(0,T;H)$.

Fourth a priori estimate. We write (2.28) with $n+1$ in place of n and take the difference between the obtained equality and (2.28) itself. Then we multiply this difference by $\delta_h\rho_{n+1}$ and integrate over Ω. We have

$$\int_\Omega (\delta_h\rho_{n+1} - \delta_h\rho_n)\delta_h\rho_{n+1} + \int_\Omega (\nabla\rho_{n+2} - \nabla\rho_{n+1}) \cdot \delta_h\nabla\rho_{n+1} + \int_\Omega \big(f'(\rho_{n+2}) - f'(\rho_{n+1})\big)\delta_h\rho_{n+1} = \int_\Omega \big(\mu_{n+1}g'(\rho_{n+1}) - \mu_n g'(\rho_n)\big)\delta_h\rho_{n+1}. \quad (4.12)$$

By accounting for the elementary identity (2.36), we get

$$\int_\Omega (\delta_h\rho_{n+1} - \delta_h\rho_n)\delta_h\rho_{n+1} = \frac{1}{2}\int_\Omega |\delta_h\rho_{n+1}|^2 - \frac{1}{2}\int_\Omega |\delta_h\rho_n|^2 + \frac{1}{2}\int_\Omega |\delta_h\rho_{n+1} - \delta_h\rho_n|^2.$$

Moreover, the second integral on the left-hand side of (4.12) can be written in terms of $\delta_h\rho_{n+1}$ in an obvious way. Finally, by splitting f' into $f_1' + f_2'$, observing that the contribution due to the terms involving f_1' is nonnegative since f_1' is monotone and moving the other ones to the right-hand side, we see that (4.12) yields the inequality

$$\frac{1}{2}\int_\Omega |\delta_h\rho_{n+1}|^2 - \frac{1}{2}\int_\Omega |\delta_h\rho_n|^2 + \frac{1}{2}\int_\Omega |\delta_h\rho_{n+1} - \delta_h\rho_n|^2 + h\int_\Omega |\delta_h\nabla\rho_{n+1}|^2 \le -\int_\Omega \big(f_2'(\rho_{n+2}) - f_2'(\rho_{n+1})\big)\delta_h\rho_{n+1} + \int_\Omega \big(\mu_{n+1}g'(\rho_{n+1}) - \mu_n g'(\rho_n)\big)\delta_h\rho_{n+1}. \quad (4.13)$$

The first term on the right-hand side of (4.13) is easily treated in the following way:

$$-\int_\Omega \big(f_2'(\rho_{n+2}) - f_2'(\rho_{n+1})\big)\delta_h\rho_{n+1} \le c\,h\int_\Omega |\delta_h\rho_{n+1}|^2. \quad (4.14)$$

On the other hand, we have

$$\begin{aligned}
&\int_\Omega \big(\mu_{n+1}g'(\rho_{n+1}) - \mu_n g'(\rho_n)\big)\delta_h\rho_{n+1} \\
&= \int_\Omega \mu_{n+1}\big(g'(\rho_{n+1}) - g'(\rho_n)\big)\delta_h\rho_{n+1} + \int_\Omega \big(\mu_{n+1} - \mu_n\big)g'(\rho_n)\delta_h\rho_{n+1} \\
&\le c\,h\int_\Omega \mu_{n+1}|\delta_h\rho_n|\,|\delta_h\rho_{n+1}| + \int_\Omega \big(\mu_{n+1} - \mu_n\big)g'(\rho_n)\delta_h\rho_{n+1}\,.
\end{aligned}$$

Next, we deal with the last integral by using equation (2.27). Owing to our assumptions on g, we obtain

$$\begin{aligned}
&\int_\Omega \big(\mu_{n+1} - \mu_n\big)g'(\rho_n)\delta_h\rho_{n+1} = -h\int_\Omega \frac{g'(\rho_n)}{1+2\gamma_n}\,\big(\mu_{n+1}\,\delta_h\gamma_n - \Delta\mu_{n+1}\big)\delta_h\rho_{n+1} \\
&\le c\,h\int_\Omega \mu_{n+1}\,|\delta_h\rho_n|\,|\delta_h\rho_{n+1}| - h\int_\Omega \nabla\mu_{n+1}\cdot\nabla\Big(\frac{g'(\rho_n)}{1+2\gamma_n}\,\delta_h\rho_{n+1}\Big) \\
&\le c\,h\int_\Omega \mu_{n+1}\,|\delta_h\rho_n|\,|\delta_h\rho_{n+1}| \\
&\quad - h\int_\Omega \frac{g'(\rho_n)}{1+2\gamma_n}\,\nabla\mu_{n+1}\cdot\nabla\delta_h\rho_{n+1} - h\int_\Omega \delta_h\rho_{n+1}\,\nabla\mu_{n+1}\cdot\nabla\frac{g'(\rho_n)}{1+2\gamma_n}\,.
\end{aligned}$$

We treat the last three terms separately. Thanks to the Hölder, Sobolev, and Young inequalities, and our assumption on g, we have for every $\sigma > 0$

$$
\begin{aligned}
& h \int_\Omega \mu_{n+1} \, |\delta_h \rho_n| \, |\delta_h \rho_{n+1}| \le c\, h \, \|\mu_{n+1}\|_4 \, \|\delta_h \rho_n\|_H \, \|\delta_h \rho_{n+1}\|_4 \\
& \le \sigma h \|\delta_h \rho_{n+1}\|_V^2 + \frac{c\, h}{\sigma} \, \|\mu_{n+1}\|_V^2 \, \|\delta_h \rho_n\|_H^2 \qquad (4.15) \\
& -h \int_\Omega \frac{g'(\rho_n)}{1 + 2\gamma_n} \, \nabla \mu_{n+1} \cdot \nabla \delta_h \rho_{n+1} \le c\, h \int_\Omega |\nabla \mu_{n+1}| \, |\nabla \delta_h \rho_{n+1}| \\
& \le \sigma \, h \|\nabla \delta_h \rho_{n+1}\|_H^2 + \frac{c\, h}{\sigma} \|\nabla \mu_{n+1}\|_H^2 \qquad (4.16) \\
& -h \int_\Omega \delta_h \rho_{n+1} \, \nabla \mu_{n+1} \cdot \nabla \frac{g'(\rho_n)}{1 + 2\gamma_n} \le c\, h \int_\Omega |\delta_h \rho_{n+1}| \, |\nabla \mu_{n+1}| \, |\nabla \rho_n| \\
& \le c\, h \|\delta_h \rho_{n+1}\|_4 \, \|\nabla \mu_{n+1}\|_H \, \|\nabla \rho_n\|_4 \\
& \le \sigma h \|\delta_h \rho_{n+1}\|_V^2 + \frac{c\, h}{\sigma} \, \|\nabla \mu_{n+1}\|_H^2 \left(\|\rho_n\|_H^2 + \|\Delta \rho_n\|_H^2 \right). \qquad (4.17)
\end{aligned}
$$

Now, we rewrite (4.8) as

$$
\|\Delta \rho_n\|_H^2 + \|\xi_n\|_H^2 \le c\big(\|\delta_h \rho_{n-1}\|_H^2 + \|\mu_{n-1}\|_H^2 + 1 \big) \quad \text{for } n = 1, \dots, N,
$$

and note that we can allow the choice $n = 0$ provided that we define

$$
\rho_{-1} := \rho_0 \ \text{ and, e.g., } \ \mu_{-1} := 0.
$$

Hence, we can improve (4.17). By using (4.3) and (4.7) as well, we have

$$
\begin{aligned}
& -h \int_\Omega \delta_h \rho_{n+1} \, \nabla \mu_{n+1} \cdot \nabla \frac{g'(\rho_n)}{1 + 2\gamma_n} \\
& \le \sigma h \|\delta_h \rho_{n+1}\|_V^2 + \frac{c\, h}{\sigma} \, \|\nabla \mu_{n+1}\|_H^2 \left(\|\rho_n\|_H^2 + \|\delta_h \rho_{n-1}\|_H^2 + \|\mu_{n-1}\|_H^2 + 1 \right) \\
& \le \sigma h \|\delta_h \rho_{n+1}\|_V^2 + \frac{c\, h}{\sigma} \, \|\nabla \mu_{n+1}\|_H^2 \left(\|\delta_h \rho_{n-1}\|_H^2 + 1 \right). \qquad (4.18)
\end{aligned}
$$

By recalling all these estimates, we see that (4.13) yields

$$
\begin{aligned}
& \frac{1}{2} \int_\Omega |\delta_h \rho_{n+1}|^2 - \frac{1}{2} \int_\Omega |\delta_h \rho_n|^2 + \frac{1}{2} \int_\Omega |\delta_h \rho_{n+1} - \delta_h \rho_n|^2 + h \int_\Omega |\delta_h \nabla \rho_{n+1}|^2 \\
& \le c\, h \int_\Omega |\delta_h \rho_{n+1}|^2 + 3\sigma h \|\delta_h \rho_{n+1}\|_V^2 + \frac{c\, h}{\sigma} \, \|\mu_{n+1}\|_V^2 \, \|\delta_h \rho_n\|_H^2 \\
& \quad + \frac{c\, h}{\sigma} \, \|\nabla \mu_{n+1}\|_H^2 \left(\|\delta_h \rho_{n-1}\|_H^2 + 1 \right).
\end{aligned}
$$

Now, just by changing the value of the constant c in front of the first integral on the right-hand side, we can replace the last integral on the left-hand side by $\|\delta_h \rho_{n+1}\|_V^2$. Then, we choose

$\sigma = 1/4$ and rearrange. We obtain

$$\frac{1}{2}\int_\Omega |\delta_h\rho_{n+1}|^2 - \frac{1}{2}\int_\Omega |\delta_h\rho_n|^2 + \frac{1}{2}\int_\Omega |\delta_h\rho_{n+1} - \delta_h\rho_n|^2 + \frac{h}{4}\,\|\delta_h\rho_{n+1}\|_V^2$$
$$\le c\,h\int_\Omega |\delta_h\rho_{n+1}|^2 + c\,h\,\|\mu_{n+1}\|_V^2\,\|\delta_h\rho_n\|_H^2 + c\,h\,\|\nabla\mu_{n+1}\|_H^2\,\big(\|\delta_h\rho_{n-1}\|_H^2 + 1\big)\,.$$

At this point, by assuming $m \le N-1$, we sum over $n = 0, \dots, m-1$ and have

$$\frac{1}{2}\int_\Omega |\delta_h\rho_m|^2 + \frac{1}{2}\sum_{n=0}^{m-1}\int_\Omega |\delta_h\rho_{n+1} - \delta_h\rho_n|^2 + \frac{h}{4}\sum_{n=0}^{m-1}\|\delta_h\rho_{n+1}\|_V^2$$
$$\le \frac{1}{2}\int_\Omega |\delta_h\rho_0|^2 + c\,h\sum_{n=0}^{m-1}\int_\Omega |\delta_h\rho_{n+1}|^2 + c\,h\sum_{n=0}^{m-1}\|\mu_{n+1}\|_V^2\,\|\delta_h\rho_n\|_H^2$$
$$+ c\,h\sum_{n=0}^{m-1}\|\nabla\mu_{n+1}\|_H^2\,\|\delta_h\rho_{n-1}\|_H^2 + c\,h\sum_{n=0}^{m-1}\|\nabla\mu_{n+1}\|_H^2\,. \tag{4.19}$$

The second and the last terms on the right-hand side of (4.19) have been already estimated by (4.6) and (4.2), respectively. To treat the first term, we write (2.28) with $n = 0$ and add $\Delta\rho_0$ to both sides. Then, we multiply the resulting equality by $\delta_h\rho_0$ and integrate over Ω. After a rearrangement, owing to (2.4) and the assumptions on the initial data (see (2.7), in particular), we obtain:

$$\int_\Omega |\delta_h\rho_0|^2 + h\int_\Omega |\nabla\delta_h\rho_0|^2 + \int_\Omega \big(f_1'(\rho_1) - f_1'(\rho_0)\big)\delta_h\rho_0$$
$$= \int_\Omega \big(\Delta\rho_0 + \mu_0 g'(\rho_0) - f_1'(\rho_0) - f_2'(\rho_1)\big)\delta_h\rho_0 \le c\|\delta_h\rho_0\|_H.$$

As $\big(f_1'(\rho_1) - f_1'(\rho_0)\big)\delta_h\rho_0 \ge 0$ due to the monotonicity of f_1', we immediately deduce that

$$\|\delta_h\rho_0\|_H^2 + h\|\nabla\delta_h\rho_0\|_H^2 \le c. \tag{4.20}$$

In particular, the desired estimate for $\|\delta_h\rho_0\|_H$ is achieved. Therefore, on recalling that $\delta_h\rho_{-1} = 0$ because $\rho_{-1} = \rho_0$, we see that (4.19) yields:

$$\|\delta_h\rho_m\|_H^2 + \sum_{n=0}^{m-1}\|\delta_h\rho_{n+1} - \delta_h\rho_n\|_H^2 + h\sum_{n=0}^{m-1}\|\delta_h\rho_{n+1}\|_V^2$$
$$\le c + c\,h\sum_{n=0}^{m-1}\|\mu_{n+1}\|_V^2\,\|\delta_h\rho_n\|_H^2 + c\,h\sum_{n=1}^{m-1}\|\nabla\mu_{n+1}\|_H^2\,\|\delta_h\rho_{n-1}\|_H^2$$
$$\le c + c\,h\sum_{n=0}^{m-1}\|\mu_{n+1}\|_V^2\,\|\delta_h\rho_n\|_H^2 + c\,h\sum_{n=0}^{m-2}\|\nabla\mu_{n+2}\|_H^2\,\|\delta_h\rho_n\|_H^2$$
$$\le C_1 + C_2\,h\sum_{n=0}^{m-1}\big(\|\mu_{n+1}\|_V^2 + \|\mu_{n+2}\|_V^2\big)\,\|\delta_h\rho_n\|_H^2$$

for $m = 0, \dots, N-1$. Hence, we can apply the discrete Gronwall lemma (see (2.38), where N is to be replaced here by $N-1$) and deduce that

$$\|\delta_h \rho_m\|_H^2 + \sum_{n=0}^{m-1} \|\delta_h \rho_{n+1} - \delta_h \rho_n\|_H^2 + h \sum_{n=0}^{m-1} \|\delta_h \rho_{n+1}\|_V^2$$
$$\leq C_1 \exp\Big(C_2 h \sum_{n=0}^{m-1} \big(\|\mu_{n+1}\|_V^2 + \|\mu_{n+2}\|_V^2 \big) \Big)$$

for $m = 0, \dots, N-1$. Owing to (4.2), we infer that

$$\|\delta_h \rho_m\|_H^2 + \sum_{n=0}^{m-1} \|\delta_h \rho_{n+1} - \delta_h \rho_n\|_H^2 + h \sum_{n=0}^{m-1} \|\delta_h \rho_{n+1}\|_V^2 \leq c \quad \text{for } m = 0, \dots, N-1;$$

moreover, on using the estimates of $\delta_h \rho_0$ and $\nabla \delta_h \rho_0$ given by (4.20), we conclude that

$$\max_{m=0,\dots,N-1} \|\delta_h \rho_m\|_H^2 + \sum_{n=0}^{N-1} \|\delta_h \rho_n - \delta_h \rho_{n-1}\|_H^2 + h \sum_{n=0}^{N-1} \|\delta_h \rho_n\|_V^2 \leq c. \tag{4.21}$$

In particular, (4.21) yields:

$$\|\partial_t \widehat{\rho}_h\|_{L^\infty(0,T;H) \cap L^2(0,T;V)} \leq c. \tag{4.22}$$

Fifth a priori estimate. We improve (4.10)–(4.11). Owing to (4.9), on using (4.21) in addition to previous estimates, we immediately obtain (cf. also (2.7)) that

$$\|\rho_m\|_W + \|\xi_m\|_H \leq c \quad \text{for } m = 0, \dots, N, \tag{4.23}$$

$$\|\overline{\rho}_h\|_{L^\infty(0,T;W)}^2 + \|\underline{\rho}_h\|_{L^\infty(0,T;W)}^2 + \|\widehat{\rho}_h\|_{L^\infty(0,T;W)}^2 \leq c\,, \tag{4.24}$$

as well as an estimate for, e.g., $\overline{\xi}_h$ in $L^\infty(0,T;H)$.

Sixth a priori estimate. We rewrite (2.27) in the form

$$\big(1 + \gamma_n + \gamma_{n+1}\big) \delta_h \mu_n - \Delta \mu_{n+1} = -\mu_n\, \delta_h \gamma_n\,.$$

We test this equality by $(\mu_{n+1} - \mu_n)$, and integrate over Ω. We obtain

$$h \int_\Omega \big(1 + \gamma_n + \gamma_{n+1}\big) |\delta_h \mu_n|^2 + \int_\Omega (\nabla \mu_{n+1} - \nabla \mu_n) \cdot \nabla \mu_{n+1} = -h \int_\Omega \mu_n\, \delta_h \gamma_n\, \delta_h \mu_n.$$

As g is nonnegative and Lipschitz continuous, we infer that

$$h \int_\Omega |\delta_h \mu_n|^2 + \frac{1}{2} \int_\Omega |\nabla \mu_{n+1}|^2 - \frac{1}{2} \int_\Omega |\nabla \mu_n|^2 + \frac{1}{2} \int_\Omega |\nabla(\mu_{n+1} - \mu_n)|^2$$
$$\leq c\, h \int_\Omega \mu_n\, |\delta_h \rho_n|\, |\delta_h \mu_n| \leq c\, h\, \|\mu_n\|_4\, \|\delta_h \rho_n\|_4\, \|\delta_h \mu_n\|_2$$
$$\leq \frac{h}{2}\, \|\delta_h \mu_n\|_H^2 + c\, h \|\delta_h \rho_n\|_V^2 \left(\|\nabla \mu_n\|_H^2 + \|\mu_n\|_H^2 \right)$$
$$\leq \frac{h}{2}\, \|\delta_h \mu_n\|_H^2 + c\, h \|\delta_h \rho_n\|_V^2\, \|\nabla \mu_n\|_H^2 + c\, h \|\delta_h \rho_n\|_V^2\,,$$

the last inequality being due to (4.2). By rearranging and summing over $n = 0, \dots, m-1$ with $1 \le m \le N$, we get:

$$\begin{aligned}
&\frac{h}{2} \sum_{n=0}^{m-1} \|\delta_h \mu_n\|_H^2 + \frac{1}{2} \|\nabla \mu_m\|_H^2 + \frac{h^2}{2} \sum_{n=0}^{m-1} \|\nabla \delta_h \mu_n\|_H^2 \\
&\le \frac{1}{2} \|\nabla \mu_0\|_H^2 + c\,h \sum_{n=0}^{m-1} \|\delta_h \rho_n\|_V^2 \, \|\nabla \mu_n\|_H^2 + c\,h \sum_{n=0}^{m-1} \|\delta_h \rho_n\|_V^2 \\
&\le c + c\,h \sum_{n=0}^{m-1} \|\delta_h \rho_n\|_V^2 \, \|\nabla \mu_n\|_H^2 \,,
\end{aligned}$$

where we have used (4.21). Now, we first apply the discrete Gronwall lemma (2.38) and then account for (4.21) once more. We obtain, for $m = 1, \dots, N$,

$$h \sum_{n=0}^{m-1} \|\delta_h \mu_n\|_H^2 + \|\nabla \mu_m\|_H^2 + h^2 \sum_{n=0}^{m-1} \|\nabla \delta_h \mu_n\|_H^2 \le c. \tag{4.25}$$

Next, by (2.27), the Hölder and Sobolev inequalities and the Lipschitz continuity of g, we infer that

$$\begin{aligned}
&\|\Delta \mu_{n+1}\|_H \le c\big(\|\delta_h \mu_n\|_H + \|\mu_{n+1} \delta_h \gamma_n\|_H\big) \le c\big(\|\delta_h \mu_n\|_H + \|\mu_{n+1}\|_4 \, \|\delta_h \gamma_n\|_4\big) \\
&\le c\big(\|\delta_h \mu_n\|_H + \|\mu_{n+1}\|_4 \, \|\delta_h \rho_n\|_4\big) \le c\big(\|\delta_h \mu_n\|_H + \|\mu_{n+1}\|_V \, \|\delta_h \rho_n\|_V\big);
\end{aligned}$$

note that in the last product we can ignore the factor $\|\mu_{n+1}\|_V$, due to (4.3) and (4.25), provided we update the last value of c. By squaring, summing up, and multiplying by h, we thus obtain for $m = 1, \dots, N$ the estimate

$$h \sum_{n=0}^{m-1} \|\Delta \mu_{n+1}\|_H^2 \le c\,h \sum_{n=0}^{m-1} \|\delta_h \mu_n\|_H^2 + c\,h \sum_{n=0}^{m-1} \|\delta_h \rho_n\|_V^2 \,,$$

and we can replace the H-norm of $\Delta \mu_{n+1}$ by the W-norm of μ_{n+1} thanks to (4.2). We collect this and (4.25) and account for (4.21) and $\mu_0 \in V$. We have:

$$h \sum_{n=0}^{N-1} \|\delta_h \mu_n\|_H^2 + \max_{n=0,\dots,N} \|\nabla \mu_n\|_H^2 + h \sum_{n=0}^{N-1} \|\mu_{n+1}\|_W^2 \le c \,, \tag{4.26}$$

so that

$$\|\partial_t \widehat{\mu}_h\|_{L^2(0,T;H)} + \|\overline{\mu}_h\|_{L^\infty(0,T;V) \cap L^2(0,T;W)} + \|\underline{\mu}_h\|_{L^\infty(0,T;V)} + \|\widehat{\mu}_h\|_{L^\infty(0,T;V)} \le c. \tag{4.27}$$

We note that (4.25) also gives the non-sharp estimate

$$h \|\nabla \partial_t \widehat{\mu}_h\|_{L^2(0,T;H)}^2 \le c. \tag{4.28}$$

Limit and conclusion. By standard weak compactness results, we find some convergent subsequence for the interpolants. Therefore, in principle, it is understood that the convergence

that we refer to holds for a subsequence. However, once we prove that the limit we find is the solution (μ, ρ) to problem (2.12)–(2.14), then the whole family of interpolants is convergent, due to uniqueness. For the reader's convenience, we select some estimates among those we have proved in the previous steps. These are:

$$\|\overline{\mu}_h\|_{L^\infty(0,T;V)\cap L^2(0,T;W)} + \|\underline{\mu}_h\|_{L^\infty(0,T;V)} + \|\widehat{\mu}_h\|_{L^\infty(0,T;V)} \le c \tag{4.29}$$

$$\|\overline{\rho}_h\|_{L^\infty(0,T;W)} + \|\underline{\rho}_h\|_{L^\infty(0,T;W)} + \|\widehat{\rho}_h\|_{L^\infty(0,T;W)} \le c \tag{4.30}$$

$$\|\partial_t\widehat{\mu}_h\|_{L^2(0,T;H)} + \|\partial_t\widehat{\rho}_h\|_{L^\infty(0,T;H)\cap L^2(0,T;V)} \le c. \tag{4.31}$$

Now, we observe that (4.31) and (2.25) imply that

$$\|\overline{\mu}_h - \widehat{\mu}_h\|_{L^2(0,T;H)} + \|\underline{\mu}_h - \widehat{\mu}_h\|_{L^2(0,T;H)} \le c\,h \tag{4.32}$$

$$\|\overline{\rho}_h - \widehat{\rho}_h\|_{L^2(0,T;V)} + \|\underline{\rho}_h - \widehat{\rho}_h\|_{L^2(0,T;V)} \le c\,h. \tag{4.33}$$

This yields, in particular, that the weak limits we find for $\overline{\mu}_h$, $\underline{\mu}_h$, and $\widehat{\mu}_h$, by using (4.29) and weak compactness results coincide and that the same happens for $\overline{\rho}_h$, $\underline{\rho}_h$, and $\widehat{\rho}_h$. Therefore, we can conclude that some functions μ and ρ exist such that

$$\overline{\mu}_h,\ \underline{\mu}_h,\ \widehat{\mu}_h \to \mu \qquad \text{weakly star in } L^\infty(0,T;V), \tag{4.34}$$

$$\overline{\mu}_h \to \mu \qquad \text{weakly in } L^2(0,T;W), \tag{4.35}$$

$$\overline{\rho}_h,\ \underline{\rho}_h,\ \widehat{\rho}_h \to \rho \qquad \text{weakly star in } L^\infty(0,T;W), \tag{4.36}$$

$$\partial_t\widehat{\mu}_h \to \partial_t\mu \qquad \text{weakly in } L^2(0,T;H), \tag{4.37}$$

$$\partial_t\widehat{\rho}_h \to \partial_t\rho \qquad \text{weakly star in } L^\infty(0,T;H)\cap L^2(0,T;V)\,. \tag{4.38}$$

Now we prove that (μ, ρ) satisfies (2.8)–(2.11) and solves problem (2.12)–(2.14).

We remark that the topology alluded to in the statement of Theorem 2.4 is precisely the topology associated with the convergences specified in (4.34)–(4.38). Clearly, (2.8)–(2.10) are fulfilled. Moreover, the Cauchy conditions (2.14) are satisfied, because $(\widehat{\mu}_h, \widehat{\rho}_h)$ converges to (μ, ρ) at least weakly in $C^0([0,T];H)$. Therefore, it remains to check that (2.11) holds and that equations (2.12)–(2.13) are satisfied. To do that, we read the discrete problem (2.27)–(2.28) in terms of the interpolants. We have:

$$\bigl(1 + 2\underline{\gamma}_h\bigr)\partial_t\widehat{\mu}_h + \overline{\mu}_h\partial_t\widehat{\gamma}_h - \Delta\overline{\mu}_h = 0, \tag{4.39}$$

$$\partial_t\widehat{\rho}_h - \Delta\overline{\rho}_h + f'(\overline{\rho}_h) = \underline{\mu}_h\, g'(\underline{\rho}_h). \tag{4.40}$$

Hence, the main problem consists in identifying correctly the limits of the nonlinear terms and those of the products. To this end, we recover some strong convergence (without looking for sharpness, since it is not necessary). We first recall that the embeddings $V \subset H$ and $W \subset C^0(\overline{\Omega})$ are compact, so that we can apply [32, Sect. 8, Cor. 4] and deduce that

$$\widehat{\mu}_h \to \mu \quad \text{strongly in } C^0([0,T];H) \text{ and a.e. in } Q, \tag{4.41}$$

$$\widehat{\rho}_h \to \rho \quad \text{strongly in } C^0([0,T];C^0(\overline{\Omega})) = C^0(\overline{Q}). \tag{4.42}$$

By combining this with (4.32) and (4.33), we infer that

$$\overline{\mu}_h,\ \underline{\mu}_h \to \mu \quad \text{and} \quad \overline{\rho}_h,\ \underline{\rho}_h \to \rho \quad \text{strongly in } L^2(0,T;H) \text{ and a.e. in } Q. \tag{4.43}$$

We point out that a.e.-convergence actually holds for a subsequence. Take now $\rho_\bullet \in (0, \rho_*)$ and $\rho^\bullet \in (\rho^*, 1)$, where $\rho_*, \rho^* \in (0,1)$ are given by Theorem 2.1. Then, (4.42) implies that

$$\rho_\bullet \le \widehat{\rho}_h \le \rho^\bullet \quad \text{in } Q, \quad \text{provided that } h \text{ is small enough.} \tag{4.44}$$

This means that the same bounds hold for ρ_n, $n = 0, \dots, N$ (where $(\rho_n)_{n=0}^N$ is the vector associated with $\widehat{\rho}_h$), and hence also for $\overline{\rho}_h$ and $\underline{\rho}_h$. As f', g, and g' are Lipschitz continuous on $[\rho_\bullet, \rho^\bullet]$, we deduce a bound for $\|f'(\overline{\rho}_h)\|_\infty$ and for the L^∞ norm of the other functions we are interested in. By combining this with the a.e.-convergence implied by (4.43), we deduce that

$$\phi(\overline{\rho}_h),\ \phi(\underline{\rho}_h) \to \phi(\rho) \quad \text{strongly in } L^p(Q) \text{ for } p \in [1, +\infty) \text{ and } \phi = f', g, g'. \tag{4.45}$$

In particular, (2.11) holds. On the other hand, we also have

$$|\partial_t \widehat{\gamma}_h| = |\delta_h \gamma_n| = |\delta_h g(\rho_n)| \le c|\delta_h \rho_n| = c|\partial_t \widehat{\rho}_h| \quad \text{a.e. in } I_{n+1}, \text{ for } n = 0, \dots, N-1\,,$$

so that (4.31) yields an estimate of $\partial_t \widehat{\gamma}_h$ in $L^\infty(0,T;H)$. Hence, thanks to (2.24), we have

$$\|\widehat{\gamma}_h - \overline{\gamma}_h\|_{L^\infty(0,T;H)} \le c\,h \|\partial_t \widehat{\gamma}_h\|_{L^\infty(0,T;H)} \le c\,h\,,$$

whence even $\widehat{\gamma}_h$ converges to $g(\rho)$, e.g., strongly in $L^2(Q)$. Therefore, we infer that

$$\partial_t \widehat{\gamma}_h \to \partial_t g(\rho) \quad \text{weakly star in } L^\infty(0,T;H). \tag{4.46}$$

Finally, as to the limits of the products in (4.39)–(4.40), we can infer that

$$\underline{\gamma}_h \partial_t \widehat{\mu}_h \to g(\rho) \partial_t \mu, \quad \overline{\mu}_h \partial_t \widehat{\gamma}_h \to \mu \partial_t g(\rho), \quad \overline{\mu}_h g'(\underline{\rho}_h) \to \mu g'(\rho), \quad \text{weakly in } L^1(Q).$$

Therefore, (2.12)–(2.13) follow from (4.39)–(4.40), and the proof is complete.

5 Proof of Theorem 2.5

In this section, we prove Theorem 2.5. It is understood that h is as small as needed; oftentimes, we do not pause and quantify such smallness precisely. First of all, we remind the reader that the interpolants $\widehat{\rho}_h$, $\underline{\rho}_h$, and $\overline{\rho}_h$ are uniformly far for 0 and 1 (see (4.44) and the subsequent lines). Therefore, without loss of generality, we can assume that the derivative function f' is Lipschitz continuous. We need additional a priori estimates.

Auxiliary a priori estimates. We prepare an estimate for $\|\nabla \delta_h \rho_0\|_H$. To this end, we notice that (2.28) with $n = 0$ can be written as

$$\delta_h \rho_0 - h \Delta \delta_h \rho_0 = f'(\rho_0) - f'(\rho_1) - \psi_0\,, \tag{5.1}$$

where $\psi_0 := -\Delta \rho_0 + f'(\rho_0) - \mu_0 g'(\rho_0)$. As $\psi_0 \in V$ by (2.33), we can test (5.1) by $-\Delta \delta_h \rho_0$ and integrate by parts. In view of the Lipschitz continuity of f', we find out that

$$\begin{aligned}
&\|\nabla \delta_h \rho_0\|_H^2 + h \|\Delta \delta_h \rho_0\|_H^2 \le c\,h \|\delta_h \rho_0\|_H \, \|\Delta \delta_h \rho_0\|_H + \|\nabla \psi_0\|_H \, \|\nabla \delta_h \rho_0\|_H \\
&\le \frac{h}{2} \, \|\Delta \delta_h \rho_0\|_H^2 + c\,h \|\delta_h \rho_0\|_H^2 + \frac{1}{2} \, \|\nabla \delta_h \rho_0\|_H^2 + c.
\end{aligned}$$

By accounting for (4.20), we obtain the desired estimate

$$\|\nabla \delta_h \rho_0\|_H \leq c. \tag{5.2}$$

Let us come now to the basic estimate we need. We write (2.28) with $(n+1)$ in place of n, and take the difference between the so-obtained equality and (2.28) itself. Then, we multiply this difference by $-\Delta \delta_h \rho_{n+1}$ and integrate over Ω. We easily have, for $n = 0, \ldots, N-2$, that

$$\begin{aligned}
&\int_\Omega (\nabla \delta_h \rho_{n+1} - \nabla \delta_h \rho_n) \cdot \nabla \delta_h \rho_{n+1} + \int_\Omega (\Delta \rho_{n+2} - \Delta \rho_{n+1}) \, \Delta \delta_h \rho_{n+1} \\
&= - \int_\Omega \big(f'(\rho_{n+2}) - f'(\rho_{n+1}) \big) (-\Delta \delta_h \rho_{n+1}) \\
&\quad + \int_\Omega \big(\mu_{n+1} g'(\rho_{n+1}) - \mu_n g'(\rho_n) \big) (-\Delta \delta_h \rho_{n+1}).
\end{aligned} \tag{5.3}$$

By the elementary identity (2.36), the first integral is equal to

$$\frac{1}{2} \int_\Omega |\nabla \delta_h \rho_{n+1}|^2 - \frac{1}{2} \int_\Omega |\nabla \delta_h \rho_n|^2 + \frac{1}{2} \int_\Omega |\nabla \delta_h \rho_{n+1} - \nabla \delta_h \rho_n|^2.$$

On the other hand, we obviously have that

$$\int_\Omega (\Delta \rho_{n+2} - \Delta \rho_{n+1}) \, \Delta \delta_h \rho_{n+1} = h \int_\Omega |\Delta \delta_h \rho_{n+1}|^2.$$

Now, we deal with the right-hand side of (5.3). By Lipschitz continuity, we deduce that

$$\begin{aligned}
&- \int_\Omega \big(f'(\rho_{n+2}) - f'(\rho_{n+1}) \big) (-\Delta \delta_h \rho_{n+1}) \leq c \int_\Omega |\rho_{n+2} - \rho_{n+1}| \, |\Delta \delta_h \rho_{n+1}| \\
&= c\, h \int_\Omega |\delta_h \rho_{n+1}| \, |\Delta \delta_h \rho_{n+1}| \leq \frac{h}{4} \int_\Omega |\Delta \delta_h \rho_{n+1}|^2 + c\, h \int_\Omega |\delta_h \rho_{n+1}|^2.
\end{aligned}$$

As far as the last term of (5.3) is concerned, we combine the above elementary argument with the Hölder and Young inequalities and the Sobolev embedding $V \subset L^4(\Omega)$. We find:

$$\begin{aligned}
&\int_\Omega \big(\mu_{n+1} g'(\rho_{n+1}) - \mu_n g'(\rho_n) \big) (-\Delta \delta_h \rho_{n+1}) \\
&\leq c \int_\Omega \big(\mu_{n+1} |\rho_{n+1} - \rho_n| + |\mu_{n+1} - \mu_n| \big) |\Delta \delta_h \rho_{n+1}| \\
&\leq c\, h \big(\|\mu_{n+1}\|_4 \|\delta_h \rho_n\|_4 + \|\delta_h \mu_n\|_H \big) \|\Delta \delta_h \rho_{n+1}\|_H \\
&\leq \frac{h}{4} \int_\Omega |\Delta \delta_h \rho_{n+1}|^2 + ch \|\mu_{n+1}\|_V^2 \, \|\delta_h \rho_n\|_V^2 + ch \|\delta_h \mu_n\|_H^2 \, .
\end{aligned}$$

By collecting the inequalities we have obtained, we see that (5.3) yields:

$$\begin{aligned}
&\frac{1}{2} \int_\Omega |\nabla \delta_h \rho_{n+1}|^2 - \frac{1}{2} \int_\Omega |\nabla \delta_h \rho_n|^2 + \frac{1}{2} \int_\Omega |\nabla \delta_h \rho_{n+1} - \nabla \delta_h \rho_n|^2 + \frac{h}{2} \int_\Omega |\Delta \delta_h \rho_{n+1}|^2 \\
&\leq c\, h \int_\Omega |\delta_h \rho_{n+1}|^2 + ch \|\mu_{n+1}\|_V^2 \, \|\delta_h \rho_n\|_V^2 + ch \|\delta_h \mu_n\|_H^2 \, .
\end{aligned}$$

At this point, we sum over $n = 0, \ldots, m-1$, with $1 \le m \le N-1$, and deduce that

$$\frac{1}{2}\int_\Omega |\nabla \delta_h \rho_m|^2 + \frac{1}{2}\sum_{n=0}^{m-1}\int_\Omega |\nabla \delta_h \rho_{n+1} - \nabla \delta_h \rho_n|^2 + \frac{h}{2}\sum_{n=0}^{m-1}\int_\Omega |\Delta \delta_h \rho_{n+1}|^2$$
$$\le \frac{1}{2}\int_\Omega |\nabla \delta_h \rho_0|^2 + c\,h\sum_{n=0}^{N-2}\|\delta_h \rho_{n+1}\|_H^2$$
$$+ c \max_{n=0,\ldots,N-1}\|\mu_{n+1}\|_V^2 \; h\sum_{n=0}^{N-1}\|\delta_h \rho_n\|_V^2 + c\,h\sum_{n=0}^{N-1}\|\delta_h \mu_n\|_H^2 \,. \tag{5.4}$$

The first term on the right-hand side of (5.4) is estimated by (5.2); all other terms on the right-hand side have been estimated already (cf. (4.22) and (4.27)). Therefore, by recalling also (4.21), we conclude that

$$\max_{m=0,\ldots,N-1}\|\delta_h \rho_m\|_V^2 + h\sum_{n=0}^{N-2}\|\Delta \delta_h \rho_{n+1}\|_H^2 \le c, \tag{5.5}$$

$$\|\partial_t \widehat{\rho}_h\|_{L^\infty(0,T;V)} + \|\Delta \partial_t \widehat{\rho}_h\|_{L^2(0,T;H)} \le c. \tag{5.6}$$

Consequence. In view of the regularity theory for elliptic equations and the continuous embedding $W \subset L^\infty(\Omega)$, we derive from (5.6) that

$$\|\partial_t \widehat{\rho}_h\|_{L^2(0,T;W)} \le c \quad \text{and} \quad \|\partial_t \widehat{\rho}_h\|_{L^2(0,T;L^\infty(\Omega))} \le c. \tag{5.7}$$

Moreover, as the second (5.7) means an estimate of the difference quotients associated to the vector $(\rho_n)_{n=0}^N$, and as g is Lipschitz continuous, a similar estimate holds for the vector $(g(\rho_n))_{n=0}^N$ (see (4.1)), and we infer that

$$\|\partial_t \widehat{\gamma}_h\|_{L^2(0,T;L^\infty(\Omega))} \le c. \tag{5.8}$$

Furthermore, by applying (2.25), we see that (5.6) also implies that

$$\|\Delta(\overline{\rho}_h - \widehat{\rho}_h)\|_{L^2(0,T;H)} \le c\,h. \tag{5.9}$$

Proof of Theorem 2.5. A possible strategy could be the following: to multiply the difference between (4.39) and (2.12) by $(\widehat{\mu}_h - \mu)$, and the difference between (4.40) and (2.13) by $\partial_t(\widehat{\rho}_h - \rho)$; then, to sum up and start estimating. However, in order to split calculations and give more transparence to the proof, we prefer to proceed with those pairs of equation separately, and collect the inequalities we obtain later on. So, we first consider just one couple, for instance, (4.40) and (2.13). We multiply their difference by $\partial_t(\widehat{\rho}_h - \rho)$, integrate over Q_t, where $t \in (0,T)$

is arbitrary, and add the same integral to both sides for convenience. We obtain:

$$
\begin{aligned}
&\int_0^t\!\!\int_\Omega |\partial_t(\widehat{\rho}_h-\rho)|^2+\frac{1}{2}\,\|(\widehat{\rho}_h-\rho)(t)\|_V^2\\
&=\int_0^t\!\!\int_\Omega\Big\{-\Delta(\widehat{\rho}_h-\overline{\rho}_h)-\big(f'(\overline{\rho}_h)-f'(\rho)\big)\\
&\qquad+g'(\underline{\rho}_h)(\underline{\mu}_h-\mu)+\mu\big(g'(\underline{\rho}_h)-g'(\rho)\big)+(\widehat{\rho}_h-\rho)\Big\}\partial_t(\widehat{\rho}_h-\rho)\\
&\le\frac{1}{2}\int_0^t\!\!\int_\Omega|\partial_t(\widehat{\rho}_h-\rho)|^2\\
&\quad+c\int_0^t\!\!\int_\Omega\Big\{|\Delta(\widehat{\rho}_h-\overline{\rho}_h)|^2+|\overline{\rho}_h-\rho|^2+|\underline{\mu}_h-\mu|^2+|\underline{\rho}_h-\rho|^2+|\widehat{\rho}_h-\rho|^2\Big\}. \quad (5.10)
\end{aligned}
$$

In the above inequality, we have used the Lipschitz continuity of f' and g', and the boundedness of μ. Now, we estimate the last integral of (5.10). Thanks to (5.9), we have that

$$
\int_0^t\!\!\int_\Omega|\Delta(\widehat{\rho}_h-\overline{\rho}_h)|^2\le c\,h^2.
$$

On the other hand, owing to (4.33), we obtain:

$$
\begin{aligned}
&\int_0^t\!\!\int_\Omega\big(|\overline{\rho}_h-\rho|^2+|\underline{\rho}_h-\rho|^2+|\widehat{\rho}_h-\rho|^2\big)\\
&\le c\int_0^t\!\!\int_\Omega\big(|\overline{\rho}_h-\widehat{\rho}_h|^2+|\underline{\rho}_h-\widehat{\rho}_h|^2+|\widehat{\rho}_h-\rho|^2\big)\\
&\le c\,h^2+c\int_0^t\!\!\int_\Omega|\widehat{\rho}_h-\rho|^2.
\end{aligned}
$$

Similarly, we have, by (4.32), that

$$
\int_0^t\!\!\int_\Omega|\underline{\mu}_h-\mu|^2\le c\int_0^t\!\!\int_\Omega\big(|\underline{\mu}_h-\widehat{\mu}_h|^2+|\widehat{\mu}_h-\mu|^2\big)\le c\,h^2+c\int_0^t\!\!\int_\Omega|\widehat{\mu}_h-\mu|^2.
$$

By collecting the above inequalities, we see that (5.10) and the Gronwall lemma yield:

$$
\int_0^t\!\!\int_\Omega|\partial_t(\widehat{\rho}_h-\rho)|^2+\|(\widehat{\rho}_h-\rho)(t)\|_V^2\le c\Big\{h^2+\int_0^t\!\!\int_\Omega|\widehat{\rho}_h-\rho|^2+\int_0^t\!\!\int_\Omega|\widehat{\mu}_h-\mu|^2\Big\} \quad (5.11)
$$

for every $t\in[0,T]$. Now, we deal with equations (4.39) and (2.12). For the reader's convenience, by recalling that $\overline{\gamma}_h=g(\overline{\rho}_h)$ and $\underline{\gamma}_h=g(\underline{\rho}_h)$ (see (4.1)), we rewrite the former in a different way, namely,

$$
\big(1+2g(\underline{\rho}_h)\big)\partial_t\widehat{\mu}_h+\overline{\mu}_h\partial_t\widehat{\gamma}_h-\Delta\overline{\mu}_h=0. \quad (5.12)
$$

Next, we take the difference between (5.12) and (2.12) and write it as

$$
\begin{aligned}
&\big(1+2g(\widehat{\rho}_h)\big)\,\partial_t(\widehat{\mu}_h-\mu)-\Delta(\widehat{\mu}_h-\mu)+(\widehat{\mu}_h-\mu)\\
&=-2\partial_t\mu\big(g(\widehat{\rho}_h)-g(\rho)\big)-\partial_t\widehat{\gamma}_h\,(\overline{\mu}_h-\mu)-\mu\,\partial_t\big(\widehat{\gamma}_h-g(\rho)\big)\\
&\quad+2\big(g(\widehat{\rho}_h)-g(\underline{\rho}_h)\big)\partial_t\widehat{\mu}_h-\Delta(\widehat{\mu}_h-\overline{\mu}_h)+(\widehat{\mu}_h-\mu)\,.
\end{aligned}
$$

Finally, we multiply this equality by $(\widehat{\mu}_h - \mu)$ and obtain the following identity:

$$\begin{aligned}
&\partial_t\big\{\big(\tfrac{1}{2} + g(\widehat{\rho}_h)\big)(\widehat{\mu}_h - \mu)^2\big\} - \Delta(\widehat{\mu}_h - \mu)\,(\widehat{\mu}_h - \mu) + (\widehat{\mu}_h - \mu)^2 \\
&= \partial_t g(\widehat{\rho}_h)\,(\widehat{\mu}_h - \mu)^2 - 2\partial_t\mu\,\big(g(\widehat{\rho}_h) - g(\rho)\big)(\widehat{\mu}_h - \mu) \\
&\quad - \partial_t\widehat{\gamma}_h\,(\overline{\mu}_h - \mu)(\widehat{\mu}_h - \mu) - \mu\,\partial_t\big(\widehat{\gamma}_h - g(\rho)\big)(\widehat{\mu}_h - \mu) \\
&\quad + 2\big(g(\widehat{\rho}_h) - g(\underline{\rho}_h)\big)\partial_t\widehat{\mu}_h\,(\widehat{\mu}_h - \mu) - \Delta(\widehat{\mu}_h - \overline{\mu}_h)\,(\widehat{\mu}_h - \mu) + (\widehat{\mu}_h - \mu)^2. \qquad (5.13)
\end{aligned}$$

At this point, we integrate over Q_t. As g is nonnegative, we get:

$$\frac{1}{2}\int_\Omega |(\widehat{\mu}_h - \mu)(t)|^2 + \int_0^t \|(\widehat{\mu}_h - \mu)(s)\|_V^2\,ds \le \sum_{j=1}^7 I_j(t)\,, \qquad (5.14)$$

with an obvious meaning of $I_j(t)$, $j = 1, \dots, 7$. Now, we estimate these integrals, but the last one. By combining Hölder's, Young's, and Sobolev's inequalities, and in view of (5.6), we have that

$$\begin{aligned}
I_1(t) &\le c\int_0^t \|\partial_t\widehat{\rho}_h(s)\|_4\|(\widehat{\mu}_h - \mu)(s)\|_H\|(\widehat{\mu}_h - \mu)(s)\|_4\,ds \\
&\le c\int_0^t \|\partial_t\widehat{\rho}_h(s)\|_V\|(\widehat{\mu}_h - \mu)(s)\|_H\|(\widehat{\mu}_h - \mu)(s)\|_V\,ds \\
&\le \sigma\int_0^t \|(\widehat{\mu}_h - \mu)(s)\|_V^2\,ds + c_\sigma\int_0^t \|(\widehat{\mu}_h - \mu)(s)\|_H^2\,ds\,,
\end{aligned}$$

where $\sigma > 0$ is arbitrary. Similarly, we infer that

$$\begin{aligned}
I_2(t) &\le 2\int_0^t \|\partial_t\mu(s)\|_H\|(\widehat{\rho}_h - \rho)(s)\|_4\|(\widehat{\mu}_h - \mu)(s)\|_4\,ds \\
&\le \sigma\int_0^t \|(\widehat{\mu}_h - \mu)(s)\|_V^2\,ds + c_\sigma\int_0^t \|\partial_t\mu(s)\|_H^2\|(\widehat{\rho}_h - \rho)(s)\|_V^2\,ds.
\end{aligned}$$

Notice that, by means of the Gronwall lemma, we shall be able to control the last integral in terms of the $L^1(0,T)$-norm of the function $s \mapsto \|\partial_t\mu(s)\|_H^2$ (cf. (2.8)). We use a similar procedure for the next integral and notice that the same remark holds, due to (5.8). Indeed, we have that

$$\begin{aligned}
I_3(t) &\le \int_0^t \|\partial_t\widehat{\gamma}_h(s)\|_\infty\|(\widehat{\mu}_h - \mu)(s)\|_H\|(\overline{\mu}_h - \mu)(s)\|_H\,ds \\
&\le \int_0^t \|\partial_t\widehat{\gamma}_h(s)\|_\infty\|(\widehat{\mu}_h - \mu)(s)\|_H\big(\|(\widehat{\mu}_h - \mu)(s)\|_H + \|(\overline{\mu}_h - \widehat{\mu}_h)(s)\|_H\big)\,ds \\
&\le \int_0^t \|\partial_t\widehat{\gamma}_h(s)\|_\infty^2\|(\widehat{\mu}_h - \mu)(s)\|_H^2\,ds + c\int_0^t \big(\|(\widehat{\mu}_h - \mu)(s)\|_H^2 + \|(\overline{\mu}_h - \widehat{\mu}_h)(s)\|_H^2\big)\,ds \\
&\le c\int_0^t \big(\|\partial_t\widehat{\gamma}_h(s)\|_\infty^2 + 1\big)\|(\widehat{\mu}_h - \mu)(s)\|_H^2\,ds + ch^2\,,
\end{aligned}$$

where the last inequality is due to (4.32). In order to treat $I_4(t)$, we prove a preliminary estimate, namely, that

$$|\partial_t\big(\widehat{\gamma}_h - g(\rho)\big)| \le c\,\big\{|\overline{\rho}_h - \widehat{\rho}_h| + |\underline{\rho}_h - \widehat{\rho}_h| + |\widehat{\rho}_h - \rho|\big\}\,|\partial_t\widehat{\rho}_h| + c|\partial_t(\widehat{\rho}_h - \rho)| \qquad (5.15)$$

a.e. in Q. As we argue pointwise, we fix (x,t) a.e. in Q and choose n such that t belongs to the interval $(nh,(n+1)h]$; in order to simplify the notation, we omit writing at what point (x,t) we work. By the mean value theorem, we find r between ρ_n and ρ_{n+1} such that

$$\partial_t\big(\widehat{\gamma}_h - g(\rho)\big) = \frac{g(\rho_{n+1}) - g(\rho_n)}{h} - g'(\rho)\partial_t\rho = g'(r)\,\frac{\rho_{n+1}-\rho_n}{h} - g'(\rho)\partial_t\rho$$
$$= g'(r)\partial_t\widehat{\rho}_h - g'(\rho)\partial_t\rho = \big(g'(r) - g'(\rho)\big)\partial_t\widehat{\rho}_h + g'(\rho)\big(\partial_t\widehat{\rho}_h - \partial_t\rho\big).$$

As g' is bounded and Lipschitz continuous, we infer that

$$|\partial_t\big(\widehat{\gamma}_h - g(\rho)\big)| \le c|r-\rho|\,|\partial_t\widehat{\rho}_h| + c|\partial_t\widehat{\rho}_h - \partial_t\rho|.$$

On the other hand, we have

$$|r-\rho| \le |r-\rho_n| + |\rho_n - \rho| \le |\rho_{n+1} - \rho_n| + |\rho_n - \rho|$$
$$= |\overline{\rho}_h - \underline{\rho}_h| + |\underline{\rho}_h - \rho| \le |\overline{\rho}_h - \widehat{\rho}_h| + 2|\underline{\rho}_h - \widehat{\rho}_h| + |\widehat{\rho}_h - \rho|.$$

Hence, (5.15) follows, and we can use it to estimate $I_4(t)$. We also account for the boundedness of μ and for identity (2.24) and the analogue identity concerning $\underline{z}_h$. We have:

$$I_4(t) \le c\int_0^t\!\!\int_\Omega \big\{|\overline{\rho}_h - \widehat{\rho}_h| + |\underline{\rho}_h - \widehat{\rho}_h| + |\widehat{\rho}_h - \rho|\big\}\,|\partial_t\widehat{\rho}_h|\,|\widehat{\mu}_h - \mu|$$
$$+ c\int_0^t\!\!\int_\Omega |\partial_t(\widehat{\rho}_h - \rho)|\,|\widehat{\mu}_h - \mu|$$
$$\le c\int_0^t \big\{\|\overline{\rho}_h(s) - \widehat{\rho}_h(s)\|_H^2 + \|\underline{\rho}_h(s) - \widehat{\rho}_h(s)\|_H^2 + \|\widehat{\rho}_h(s) - \rho(s)\|_H^2\big\}\,\|\partial_t\widehat{\rho}_h(s)\|_\infty^2\,ds$$
$$+ \frac12\int_0^t \|\partial_t(\widehat{\rho}_h - \rho)(s)\|_H^2\,ds + c\int_0^t \|(\widehat{\mu}_h - \mu)(s)\|_H^2\,ds$$
$$\le c\,h^2\|\partial_t\widehat{\rho}_h\|_{L^\infty(0,T;H)}^2\,\|\partial_t\widehat{\rho}_h\|_{L^2(0,T;L^\infty(\Omega))}^2 + c\int_0^t \|\partial_t\widehat{\rho}_h(s)\|_\infty^2\,\|\widehat{\rho}_h(s) - \rho(s)\|_H^2\,ds$$
$$+ \frac12\int_0^t \|\partial_t(\widehat{\rho}_h - \rho)(s)\|_H^2\,ds + c\int_0^t \|(\widehat{\mu}_h - \mu)(s)\|_H^2\,ds\,;$$

furthermore, estimates (4.31) and (5.7) allow us to infer that

$$I_4(t) \le c\,h^2 + c\int_0^t \|\partial_t\widehat{\rho}_h(s)\|_\infty^2\,\|\widehat{\rho}_h(s) - \rho(s)\|_V^2\,ds + \frac12\int_0^t \|\partial_t(\widehat{\rho}_h - \rho)(s)\|_H^2\,ds$$
$$+ c\int_0^t \big(1 + \|\partial_t\widehat{\rho}_h(s)\|_\infty^2\big)\,\|(\widehat{\mu}_h - \mu)(s)\|_H^2\,ds.$$

Next, we deal with $I_5(t)$. By accounting for (2.25) and (5.7), we deduce that

$$I_5(t) \le c\int_0^t \|(\widehat{\rho}_h - \underline{\rho}_h)(s)\|_\infty \|\partial_t\widehat{\mu}_h(s)\|_H\,\|(\widehat{\mu}_h - \mu)(s)\|_H\,ds$$
$$\le c\,h^2\|\partial_t\widehat{\rho}_h\|_{L^2(0,T;L^\infty(\Omega))}^2 + c\int_0^t \|\partial_t\widehat{\mu}_h(s)\|_H^2\,\|(\widehat{\mu}_h - \mu)(s)\|_H^2\,ds$$
$$\le c\,h^2 + c\int_0^t \|\partial_t\widehat{\mu}_h(s)\|_H^2\,\|(\widehat{\mu}_h - \mu)(s)\|_H^2\,ds.$$

We note at once that we shall be able to control even the last terms of the last two estimates with the help of the Gronwall lemma, in view of (5.7) and (4.31), respectively. Finally, thanks to (2.25) once more, we have:

$$
\begin{aligned}
I_6(t) &= \int_0^t \int_\Omega \nabla(\widehat{\mu}_h - \overline{\mu}_h) \cdot \nabla(\widehat{\mu}_h - \mu) \\
&\le \sigma \int_0^t \int_\Omega |\nabla(\widehat{\mu}_h - \mu)|^2 + c_\sigma \int_0^t \int_\Omega |\nabla(\widehat{\mu}_h - \overline{\mu}_h)|^2 \\
&\le \sigma \int_0^t \int_\Omega |\nabla(\widehat{\mu}_h - \mu)|^2 + c_\sigma \, h^2 \|\nabla \partial_t \widehat{\mu}_h\|^2_{L^2(0,T;H)} \\
&\le \sigma \int_0^t \int_\Omega |\nabla(\widehat{\mu}_h - \mu)|^2 + c_\sigma \, h \,, \qquad (5.16)
\end{aligned}
$$

where the last inequality is a consequence of the non-sharp estimate (4.28). We stress that I_6 is the only term of order h instead of h^2. At this point, we collect all the estimates of the integrals I_j we have obtained, and come back to (5.13)–(5.14). If we choose σ small enough, we conclude that

$$
\begin{aligned}
&\frac{1}{2} \|(\widehat{\mu}_h - \mu)(t)\|^2_H + \frac{1}{2} \int_0^t \|(\widehat{\mu}_h - \mu)(s)\|^2_V \, ds \\
&\le c \Big\{ h + \int_0^t \big(1 + \|\partial_t \widehat{\gamma}_h(s)\|^2_\infty + \|\partial_t \widehat{\mu}_h(s)\|^2_H \big) \|(\widehat{\mu}_h - \mu)(s)\|^2_H \, ds \\
&\quad + \int_0^t \big(\|\partial_t \mu(s)\|^2_H + \|\partial_t \widehat{\rho}_h(s)\|^2_\infty \big) \, \|\widehat{\rho}_h(s) - \rho(s)\|^2_V \, ds \\
&\quad + \int_0^t \int_\Omega |\partial_t(\widehat{\rho}_h - \rho)|^2 \Big\} + \frac{1}{2} \int_0^t \|\partial_t(\widehat{\rho}_h - \rho)(s)\|^2_H \, ds \qquad (5.17)
\end{aligned}
$$

for every $t \in [0,T]$. Now, we revert to (5.11) and add it to (5.17). After rearranging, we apply the Gronwall lemma and obtain (2.30). This concludes the proof.

6 Proof of Theorem 2.6

As is clear from the proof of Theorem 2.5, to obtain estimate (2.32) there is just one step to modify, namely, the estimate of I_6 (see (5.16)), which was based on the non-sharp inequality (4.28). Thus, we only have to prove that our further assumption (2.31) implies that I_6 must be of order h^2, not h. Moreover, it is clear that this is true whenever we improve (4.28) and replace it by

$$
\|\nabla \partial_t \widehat{\mu}_h\|^2_{L^2(0,T;H)} \le c, \quad \text{i.e.,} \quad h \sum_{n=0}^{N-1} \|\nabla \delta_h \mu_n\|^2_H \le c. \qquad (6.1)
$$

Hence, it suffices to prove (6.1). In order to make our argument transparent, we prove some additional estimates, the first of which holds under assumption (2.31).

Further a priori estimates. We prepare an estimate of $\|\delta_h\mu_0\|_H$. In view of (2.31), we write equation (2.27), with $n=0$, in the form:

$$(1+2\gamma_0)\delta_h\mu_0 - h\Delta\delta_h\mu_0 = \Delta\mu_0 - \mu_1\,\delta_h\gamma_0,$$

and test it by $\delta_h\mu_0$. As γ_0 is nonnegative, we immediately arrive at

$$\int_\Omega |\delta_h\mu_0|^2 + h\int_\Omega |\nabla\delta_h\mu_0|^2 \le \bigl(\|\Delta\mu_0\|_H + \|\mu_1\|_4\,\|\delta_h\rho_0\|_4\bigr)\,\|\delta_h\mu_0\|_H\,.$$

Thanks to (2.31), the Sobolev inequality, (4.26), and (5.5), we deduce that

$$\|\delta_h\mu_0\|_H + h\int_\Omega |\nabla\delta_h\mu_0|^2 \le c. \tag{6.2}$$

Let us come to the basic estimate we need. We improve (4.21) and obtain a bound for the second-difference quotients $\delta_h^2\rho_n$ (see (2.16)). We write (2.28), with $(n+1)$ in place of n, and test the difference between the resulting relation and (2.28) itself by $(\delta_h\rho_{n+1} - \delta_h\rho_n)$. We find:

$$\begin{aligned}
&\int_\Omega |\delta_h\rho_{n+1} - \delta_h\rho_n|^2 + h\int_\Omega \nabla\delta_h\rho_{n+1}\cdot\nabla(\delta_h\rho_{n+1} - \delta_h\rho_n)\\
&= -\int_\Omega \bigl(f'(\rho_{n+2}) - f'(\rho_{n+1})\bigr)(\delta_h\rho_{n+1} - \delta_h\rho_n)\\
&\quad + h\int_\Omega \bigl(g'(\rho_{n+1})\delta_h\mu_n + \mu_n\delta_h(g'(\rho_n))\bigr)(\delta_h\rho_{n+1} - \delta_h\rho_n)\\
&\le C\,h\int_\Omega \bigl(|\delta_h\rho_{n+1}| + |\delta_h\mu_n| + |\mu_n|\,|\delta_h\rho_n|\bigr)|\delta_h\rho_{n+1} - \delta_h\rho_n|\,.
\end{aligned} \tag{6.3}$$

By the elementary identity (2.36), we have:

$$\nabla\delta_h\rho_{n+1}\cdot\nabla(\delta_h\rho_{n+1} - \delta_h\rho_n) = \frac{1}{2}|\nabla\delta_h\rho_{n+1}|^2 - \frac{1}{2}|\nabla\delta_h\rho_n|^2 + \frac{1}{2}|\nabla\delta_h\rho_{n+1} - \nabla\delta_h\rho_n|^2.$$

On the other hand, by the Sobolev inequality, (4.26), and (5.5), we infer that

$$\begin{aligned}
&C\,h\int_\Omega \bigl(|\delta_h\rho_{n+1}| + |\delta_h\mu_n| + |\mu_n|\,|\delta_h\rho_n|\bigr)|\delta_h\rho_{n+1} - \delta_h\rho_n|\\
&\le \frac{1}{2}\int_\Omega |\delta_h\rho_{n+1} - \delta_h\rho_n|^2 + c\,h^2\bigl(\|\delta_h\rho_{n+1}\|_H^2 + \|\delta_h\mu_n\|_H^2 + \|\mu_n\|_4^2\,\|\delta_h\rho_n\|_4^2\bigr)\\
&\le \frac{1}{2}\int_\Omega |\delta_h\rho_{n+1} - \delta_h\rho_n|^2 + c\,h^2\bigl(\|\delta_h\rho_{n+1}\|_H^2 + \|\delta_h\mu_n\|_H^2 + \|\mu_n\|_V^2\,\|\delta_h\rho_n\|_V^2\bigr)\\
&\le \frac{1}{2}\int_\Omega |\delta_h\rho_{n+1} - \delta_h\rho_n|^2 + c\,h^2\bigl(\|\delta_h\rho_{n+1}\|_H^2 + \|\delta_h\mu_n\|_H^2 + 1\bigr).
\end{aligned}$$

Now, we combine this estimate, the identity just above, and (6.3). Then, we divide by h and sum over $n=0,\dots,m-1$, where $1\le m\le N-1$. We obtain:

$$\begin{aligned}
&\frac{h}{2}\sum_{n=0}^{m-1}\|\delta_h^2\rho_n\|_H^2 + \frac{1}{2}\,\|\nabla\delta_h\rho_m\|_H^2 + \frac{1}{2}\sum_{n=0}^{m-1}\|\nabla\delta_h\rho_{n+1} - \nabla\delta_h\rho_n\|_H^2\\
&\le \frac{1}{2}\,\|\nabla\delta_h\rho_0\|_H^2 + c\,h\sum_{n=0}^{m-1}\|\delta_h\rho_{n+1}\|_H^2 + c\,h\sum_{n=0}^{m-1}\|\delta_h\mu_n\|_H^2 + c.
\end{aligned}$$

At this point, by (5.5), (4.6), and (4.26), we conclude that

$$h \sum_{n=0}^{N-2} \|\delta_h^2 \rho_n\|_H^2 \le c. \tag{6.4}$$

Consequence. With a view toward deriving an estimate for $\delta_h^2 \gamma_n$, we begin by arguing pointwise. So, for a.a. $(x,t) \in Q$ (once again we omit writing at what point of Q we work) and for suitable r_1 between ρ_{n+2} and ρ_{n+1}, and r_2 between ρ_n and ρ_{n+1}, we have by the Taylor formula:

$$\begin{aligned}
&|\delta_h^2 \gamma_n| = h^{-2} \, |g(\rho_{n+2}) - g(\rho_{n+1}) + g(\rho_n) - g(\rho_{n+1})| \\
&= h^{-2} \, |g'(\rho_{n+1})(\rho_{n+2} - \rho_{n+1}) + \tfrac{1}{2} \, g''(r_1)(\rho_{n+2} - \rho_{n+1})^2 \\
&\quad + g'(\rho_{n+1})(\rho_n - \rho_{n+1}) + \tfrac{1}{2} \, g''(r_2)(\rho_n - \rho_{n+1})^2| \\
&\le c \, |\delta_h^2 \rho_n| + c \, \big(|\delta_h \rho_{n+1}|^2 + |\delta_h \rho_n|^2 \big).
\end{aligned}$$

Now, we square this pointwise estimate, integrate over Ω, sum over n, and deduce that

$$h \sum_{n=0}^{N-2} \|\delta_h^2 \gamma_n\|_H^2 \le c \, h \sum_{n=0}^{N-2} \|\delta_h^2 \rho_n\|_H^2 + c \, h \sum_{n=0}^{N-1} \|\delta_h \rho_n\|_4^4 .$$

Then, (6.4), the Sobolev inequality, and (5.5) yield:

$$h \sum_{n=0}^{N-2} \|\delta_h^2 \gamma_n\|_H^2 \le c. \tag{6.5}$$

Proof of Theorem 2.6. As said before, it suffices to prove (6.1). We reason that, in order to obtain the analogous estimate for the solution to the continuous problem, one first differentiates (2.12) with respect to time and then tests the resulting equality by $\partial_t \mu$; this yields the desired term $\displaystyle\int_0^t \int_\Omega |\nabla \partial_t \mu|^2$ on the left-hand side. The idea is to perform the corresponding procedure on the discrete equation (2.27). However, it turns out that the calculation in the discrete case becomes simpler if one tests by the analogue of the product $(1 + 2g(\rho))\partial_t \mu$. To simplify the notation, we introduce the vector π defined by

$$\pi_n := (1 + 2\gamma_n) \delta_h \mu_n \quad \text{for } n = 0, \dots, N-1. \tag{6.6}$$

We write (2.27) with $(n+1)$ in place of n, and take the difference between the resulting equality and (2.27) itself. Then, we test this difference by π_{n+1} and integrate over Ω. By taking the elementary identity (2.36) into account, we obtain for $n = 0, \dots, N-2$ that

$$\begin{aligned}
&\frac{1}{2} \int_\Omega |\pi_{n+1}|^2 - \frac{1}{2} \int_\Omega |\pi_n|^2 + \frac{1}{2} \int_\Omega |\pi_{n+1} - \pi_n|^2 + h \int_\Omega \nabla \delta_h \mu_{n+1} \cdot \nabla \pi_{n+1} \\
&= - \int_\Omega \big(\mu_{n+2} \, \delta_h \gamma_{n+1} - \mu_{n+1} \, \delta_h \gamma_n \big) \, \pi_{n+1} \, .
\end{aligned}$$

By computing the fourth term on the left-hand side with the help of (6.6), recalling that g is nonnegative, and rearranging, we deduce that

$$\begin{aligned}
&\int_\Omega |\pi_{n+1}|^2 - \int_\Omega |\pi_n|^2 + \int_\Omega |\pi_{n+1} - \pi_n|^2 + 2h \int_\Omega |\nabla \delta_h \mu_{n+1}|^2 \\
&\le -2 \int_\Omega \big(\mu_{n+2}\, \delta_h \gamma_{n+1} - \mu_{n+1}\, \delta_h \gamma_n \big)\, \pi_{n+1} - 4h \int_\Omega \delta_h \mu_{n+1}\, \nabla \delta_h \mu_{n+1} \cdot \nabla \gamma_{n+1} \\
&= -2 \int_\Omega \pi_{n+1} (\mu_{n+2} - \mu_{n+1})\, \delta_h \gamma_{n+1} - 2 \int_\Omega \pi_{n+1}\, \mu_{n+1} \big(\delta_h \gamma_{n+1} - \delta_h \gamma_n \big) \\
&\quad - 4h \int_\Omega \delta_h \mu_{n+1}\, \nabla \delta_h \mu_{n+1} \cdot \nabla \gamma_{n+1} \\
&= -2h \int_\Omega \pi_{n+1}\, \delta_h \mu_{n+1}\, \delta_h \gamma_{n+1} - 2h \int_\Omega \pi_{n+1}\, \mu_{n+1}\, \delta_h^2 \gamma_n \\
&\quad - 4h \int_\Omega \delta_h \mu_{n+1}\, \nabla \delta_h \mu_{n+1} \cdot \nabla \gamma_{n+1} \,. \qquad (6.7)
\end{aligned}$$

Now, we estimate each term of the right-hand side separately, before summing over n, in order to simplify the notation. For the first one, we use Hölder and Sobolev inequalities, and estimates (5.5) and (6.4). We have:

$$\begin{aligned}
&-2h \int_\Omega \pi_{n+1}\, \delta_h \mu_{n+1}\, \delta_h \gamma_{n+1} \\
&\le 2h \|\pi_{n+1}\|_4\, \|\delta_h \mu_{n+1}\|_H\, \|\delta_h \gamma_{n+1}\|_4 \le c\, h \|\delta_h \mu_{n+1}\|_V\, \|\delta_h \mu_{n+1}\|_H\, \|\delta_h \rho_{n+1}\|_V \\
&\le \frac{h}{4} \big(\|\nabla \delta_h \mu_{n+1}\|_H^2 + \|\delta_h \mu_{n+1}\|_H^2 \big) + c\, h \|\delta_h \mu_{n+1}\|_H^2 \\
&\le \frac{h}{4}\, \|\nabla \delta_h \mu_{n+1}\|_H^2 + c\, h\, \|\pi_{n+1}\|_H^2 \\
&\le \frac{h}{4}\, \|\nabla \delta_h \mu_{n+1}\|_H^2 + c\, h\, \|\pi_n\|_H^2 + C\, h\, \|\pi_{n+1} - \pi_n\|_H^2 \,.
\end{aligned}$$

For h small enough, namely, for $h \le 1/(3C)$, we conclude that

$$-2h \int_\Omega \pi_{n+1}\, \delta_h \mu_{n+1}\, \delta_h \gamma_{n+1} \le \frac{h}{4}\, \|\nabla \delta_h \mu_{n+1}\|_H^2 + c\, h\, \|\pi_n\|_H^2 + \frac{1}{3}\, \|\pi_{n+1} - \pi_n\|_H^2 .$$

Next, by (4.26), we similarly have:

$$\begin{aligned}
&-2h \int_\Omega \pi_{n+1}\, \mu_{n+1}\, \delta_h^2 \gamma_n \le c\, h \|\delta_h \mu_{n+1}\|_4\, \|\mu_{n+1}\|_4\, \|\delta_h^2 \gamma_n\|_H \\
&\le \frac{h}{4} \big(\|\nabla \delta_h \mu_{n+1}\|_H^2 + \|\delta_h \mu_{n+1}\|_H^2 \big) + c\, h\, \|\mu_{n+1}\|_V^2\, \|\delta_h^2 \gamma_n\|_H^2 \\
&\le \frac{h}{4}\, \|\nabla \delta_h \mu_{n+1}\|_H^2 + h\, \|\pi_n\|_H^2 + \frac{1}{3}\, \|\pi_{n+1} - \pi_n\|_H^2 + c\, h\, \|\delta_h^2 \gamma_n\|_H^2 \,,
\end{aligned}$$

for sufficiently small h. Finally, by accounting for (4.23), Sobolev inequality, and the compactness

inequality (2.35), we have that, for h small enough,

$$
\begin{aligned}
&-4h \int_\Omega \delta_h\mu_{n+1}\, \nabla\delta_h\mu_{n+1} \cdot \nabla\gamma_{n+1} \le c\,h\|\delta_h\mu_{n+1}\|_4\, \|\nabla\delta_h\mu_{n+1}\|_H\, \|\nabla\rho_{n+1}\|_4 \\
&\le \frac{h}{4}\, \|\nabla\delta_h\mu_{n+1}\|_H^2 + c\,h\|\delta_h\mu_{n+1}\|_4^2\, \|\nabla\rho_{n+1}\|_V^2 \le \frac{h}{4}\, \|\nabla\delta_h\mu_{n+1}\|_H^2 + c\,h\|\delta_h\mu_{n+1}\|_4^2 \\
&\le \frac{h}{4}\, \|\nabla\delta_h\mu_{n+1}\|_H^2 + h\big(\tfrac{1}{4}\, \|\nabla\delta_h\mu_{n+1}\|_H^2 + c\|\delta_h\mu_{n+1}\|_H^2\big) \\
&\le \frac{h}{2}\, \|\nabla\delta_h\mu_{n+1}\|_H^2 + c\,h\|\pi_{n+1}\|_H^2 \le \frac{h}{2}\, \|\nabla\delta_h\mu_{n+1}\|_H^2 + c\,h\|\pi_n\|_H^2 + \frac{1}{3}\, \|\pi_{n+1}-\pi_n\|_H^2 .
\end{aligned}
$$

At this point, we combine the inequalities just obtained with (6.7) and note that the terms involving $\pi_{n+1}-\pi_n$ cancel out. Then, we sum over $n = 0, \dots, (m-1)$, with $1 \le m \le (N-1)$. We obtain:

$$
\|\pi_m\|_H^2 + h\sum_{n=0}^{m-1} \|\nabla\delta_h\mu_{n+1}\|_H^2 \le \|\pi_0\|_H^2 + h\sum_{n=0}^{m-1} \|\pi_n\|_H^2 + h\sum_{n=0}^{m-1} \|\delta_h^2\gamma_n\|_H^2
$$

and the discrete Gronwall lemma allows us to deduce that

$$
\|\pi_m\|_H^2 + h\sum_{n=0}^{m-1} \|\nabla\delta_h\mu_{n+1}\|_H^2 \le c\Big(\|\pi_0\|_H^2 + c\,h\sum_{n=0}^{N-2} \|\delta_h^2\gamma_n\|_H^2\Big)
$$

for $1 \le m \le (N-1)$. From (6.2) and (6.5), we infer that

$$
h\sum_{n=0}^{N-2} \|\nabla\delta_h\mu_{n+1}\|_H^2 \le c.
$$

This and (6.2) yield (6.1), and the proof is complete.

Remark 6.1. As a consequence of estimates (6.1) and (6.4), the solution to the continuous problem enjoys the following additional regularity properties:

$$
\nabla\partial_t\mu \in L^2(Q) \quad \text{and} \quad \partial_t^2\rho \in L^2(Q)\,.
$$

This can give even more: for instance, equation (2.13) can be differentiated with respect to time, to show that $\Delta\partial_t\rho$ belongs to $L^2(Q)$ as well, so as to conclude that

$$
\rho \in H^2(0,T;H) \cap H^1(0,T;W).
$$

However, this regularity result could be proved formally and directly for the continuous problem.

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