Construction of a two-phase flow with singular energy by gradient flow methods

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CONSTRUCTION OF A TWO-PHASE FLOW WITH SINGULAR ENERGY BY GRADIENT FLOW METHODS

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ABSTRACT. We prove the existence of weak solutions to a system of two diffusion equations that are coupled by a pointwise volume constraint. The time evolution is given by gradient dynamics for a free energy functional. Our primary example is a model for the demixing of polymers, the corresponding energy is the one of Flory, Huggins and de Gennes. Due to the non-locality in the equations, the dynamics considered here is qualitatively different from the one found in the formally related Cahn-Hilliard equations.

Our angle of attack is from the theory of optimal mass transport, that is, we consider the evolution equations for the two components as two gradient flows in the Wasserstein distance with one joint energy functional that has the volume constraint built in. The main difference to our previous work [6] is the nonlinearity of the energy density in the gradient part, which becomes singular at the interface between pure and mixed phases, leading to new theoretical difficulties.

1. INTRODUCTION

We show existence of non-negative solutions to the following coupled system of diffusion equations:

$$\partial_t c_1 = \operatorname{div}(m_1 c_1 \nabla \mu_1), \tag{1a}$$

$$\partial_t c_2 = \operatorname{div}(m_2 c_2 \nabla \mu_2), \tag{1b}$$

$$c_1 + c_2 = 1, \tag{1c}$$

$$\mu_1 - \mu_2 = -f'(c_1)\Delta f(c_1) + \chi\big(\tfrac{1}{2} - c_1\big), \tag{1d}$$

on a bounded and convex domain $\Omega \subset \mathbb{R}^d$ in the plane ($d = 2$) or physical space ($d = 3$) with smooth boundary $\partial\Omega$. Solutions are subject to no-flux and homogeneous Neumann boundary conditions

$$\mathbf{n} \cdot (c_1 \nabla \mu_1) = \mathbf{n} \cdot (c_2 \nabla \mu_2) = 0, \tag{2a}$$

$$\mathbf{n} \cdot \nabla c_1 = \mathbf{n} \cdot \nabla c_2 = 0 \tag{2b}$$

on $\partial\Omega$ and to the initial conditions

$$c_1(0) = c_1^0, \quad c_2(0) = c_2^0, \tag{3}$$

with initial data $c_1^0, c_2^0 : \Omega \to [0,1]$ satisfying the constraint (1c). The mobility coefficients $m_1, m_2 > 0$ and the parameter $\chi > 0$ are given constants, and the function $f : [0,1] \to \mathbb{R}$ in (1d) is assumed to satisfy:

Assumption 1. *f is continuous on $[0,1]$, it is smooth on $(0,1)$ with $f'(r) > 0$ there, it satisfies $f'(r) \to +\infty$ for $r \downarrow 0$ and for $r \uparrow 1$, and the function $1/(f')^2$ is concave on $(0,1)$. Moreover, $f(r)$ is point-symmetric about $r = 1/2$, i.e., $f(1-r) = -f(r)$ for all $r \in [0,1]$.*

Systems of the type (1) are widely used as models for spinodal decomposition. Particularly, the choice (4) of f below describes the demixing of two polymers, see e.g. [9, 10, 23]. In the current paper, the example of primary interest is

$$f(r) = \arcsin(2r-1), \quad \text{with} \quad \frac{1}{f'(r)^2} = r(1-r). \tag{4}$$

An alternative admissible choice for f is $f(r) = r^\gamma - (1-r)^\gamma$ with $\frac{1}{2} \leq \gamma < 1$. Note that these functions interpolate between the linear function $f(r) = 2r - 1$ at $\gamma \uparrow 1$, corresponding to the Cahn-Hilliard model, and a function with square-root singularities like in (4) at $\gamma = \frac{1}{2}$.

An f satisfying Assumption 1 is *singular* in the sense that it has infinite slope at the boundary of $[0, 1]$. It is this behaviour which makes the analysis of the problem at hand significantly more challenging than the corresponding Cahn-Hilliard problem with $f(r) = r - \frac{1}{2}$ that the authors have considered recently with Nabet [6]. The additional difficulty enters mainly at two points. First, the relevant a priori estimates are significantly more difficult to obtain, already on the formal level. Our main estimate is a bound on $f(c_1)$ in $L^2(0, T; H^2)$; its proof builds on a variety of non-obvious manipulations and integration by parts, and it is made rigorous using the flow interchange method from [21], see Section 4. Second, on the right-hand side of equation (1d), the pre-factor $f'(c_1)$ is $+\infty$ in the "pure" regions of Ω where either $c_1 \equiv 0$ or $c_2 \equiv 1$. Our global L^2-bound on $\Delta f(c_1)$ is not sufficient to estimate the product with $f'(c_1)$ in a decent way, and thus we have no control on the potentials μ_i near the edges of the pure zones. Our approach, explained in more details in Section 1.4 below, is to rewrite the system in a formally equivalent way avoiding the "bare" potentials μ_i and instead using products $q_i = \omega(c_i)\mu_i$ with a suitable $\omega(c_i)$ vanishing on the pure zones.

The role of f is best understood as follows: there is a dissipated free energy functional for (1), which is given by

$$\mathcal{E}(c_1, c_2) = \frac{1}{4} \int_\Omega \big(|\nabla f(c_1)|^2 + |\nabla f(c_2)|^2 + 2\chi c_1 c_2 \big) \, \mathrm{d}x. \tag{5}$$

Assumption 1 guarantees that the gradient parts, i.e.,

$$c_i \mapsto \int_\Omega |\nabla f(c_i)|^2 \, \mathrm{d}x,$$

are convex functionals. Consequently, $\mathcal{E}$ is of the form "convex plus smooth". With the choice (4), $\mathcal{E}$ is referred to as Flory-Huggins-de Gennes-energy.

We remark that thermal agitation effects can be incorporated into the model by augmenting the energy (5) with the mixing entropy

$$\theta \int_\Omega \big(c_1 \log c_1 + c_2 \log c_2 \big) \, \mathrm{d}x, \qquad \theta \geq 0.$$

Here we are concerned solely with the so-called deep-quench limit $\theta = 0$, which is analytically the most challenging case. Indeed, thermal effects introduce additional diffusion to the problem which provide more regularity.

1.1. **Local versus non-local dynamics.** In dimensions $d > 1$, there is a subtle difference between the "non-local" model under consideration here and its "local" reduction in the sense of de Gennes [9]. That difference, and its consequences on the long time asymptotics of solutions, have been discussed in detail in [23]. For

the local model, one strengthens the constraint (1c) by requiring annihilation of the fluxes of c_1 and c_2 (and not only the divergences of these fluxes), i.e.,

$$m_1 c_1 \nabla \mu_1 + m_2 c_2 \nabla \mu_2 = 0. \tag{6}$$

This condition is stronger than the original constraint (1c) in the sense that the system consisting of (1a), (1b), (1d), and (6) propagates (1c) in time. Moreover, (6) allows to eliminate μ_2 from (1d), and the system then becomes equivalent to one single evolution equation of fourth order for c_1; in the case $m_1 = m_2 = 1$, it reads

$$\partial_t c_1 = -\operatorname{div}\big(c_1(1-c_1)\,\nabla\big[f'(c_1)\Delta f(c_1) + \chi(c_1 - \tfrac{1}{2})\big]\big). \tag{7}$$

There seems to be no way to reduce the original system (1) to a single differential equation in a similar fashion. The reduction that comes closest to (7) — still in the case $m_1 = m_2 = 1$ — is the following non-local equation, taken from [23],

$$\partial_t c_1 = -\operatorname{div}\big(c_1 \mathbf{P}\big\{(1-c_1)\,\nabla\big[f'(c_1)\Delta f(c_1) + \chi(c_1 - \tfrac{1}{2})\big]\big\}\big), \tag{8}$$

in which $\mathbf{P}$ is the Helmholtz projection onto the gradient vector fields. More explicitly, one combines (1a) with the following elliptic equation for μ_1:

$$-\Delta \mu_1 = \operatorname{div}\big((1-c_1)\nabla\big[f'(c_1)\Delta f(c_1) + \chi(c_1 - \tfrac{1}{2})\big]\big), \tag{9}$$

which is easily derived by adding (1a) and (1b), and using that $\partial_t(c_1 + c_2) = 0$ because of (1c). Despite all the advantages that the reduced equation (8) might have, the original two-component formulation (1) is the significant one for our existence analysis.

The less restrictive constraint (1c) provides more flexibility for the fluxes than (6). This effect is measurable on the level of energy decay, which is significantly faster in the non-local model (8) than in the local model (7). Numerical evidence of this fact has been presented in [7, 6] in the Cahn-Hilliard case. On the theoretical side, the dynamics of (7) and of (8) have been compared in [23] in the sharp interface limit: this is where χ is large and the considered time scale is proportional to χ. Then the values of the solution c_1 are concentrated around zero and one, and the interfaces in between these pure phases become sharper the larger χ is. It turns out that the long-time asymptotics of the interfaces in (7) and in (8) are different: while (7) is asymptotically equivalent to (the slower) surface diffusion, (8) leads to (the faster) Hele-Shaw flow. We refer to [13] for a recent mathematical study of the interface dynamics inside the framework of optimal mass transport.

1.2. **Gradient flow structure.** Similarly as in our recent paper [6], we take the interpretation of (1) as a metric gradient flow as starting point for the existence analysis. More specifically, we use the gradient flow structure to construct time-discrete approximations of the true solution $\boldsymbol{c}$ by means of the minimizing movement scheme, derive a priori estimates on the approximation by variational methods, and finally pass to the time-continuous limit. We emphasize that the interpretation of (1) as gradient flow motivates the aforementioned procedure, but we are not going to verify that solutions to (1) are curves of steepest descent in a rigorous way.

The potential $\mathbf{E}$ of the flow under consideration is essentially the system's free energy $\mathcal{E}$ from (5), however, modified such that the volume constraint (1c) is built

in:

$$\begin{aligned} &\mathbf{E}(\boldsymbol{c}) = \mathbf{E}_1(c_1) + \mathbb{I}_{c_1+c_2\equiv 1}(\boldsymbol{c}), \\ &\text{with} \quad \mathbf{E}_1(c_1) = \frac{1}{2}\int_\Omega |\nabla f(c_1)|^2 \,\mathrm{d}x + \frac{\chi}{2}\int_\Omega c_1(1-c_1)\,\mathrm{d}x. \end{aligned} \tag{10}$$

Above, $\mathbb{I}_{c_1+c_2\equiv 1}$ denotes the indicator function that is zero if the constraint $c_1+c_2 \equiv 1$ is satisfied, and is $+\infty$ otherwise. $\mathbf{E}$'s "gradient" is calculated with respect to a metric $\mathbf{d}$ that combines the squared L^2-Wasserstein distances of the components c_1 and c_2. More specifically, on the space

$$\begin{aligned} &\mathbf{X}_{\text{mass}} := \left\{ \boldsymbol{c} : \Omega \to [0,1]^2 \;\middle|\; \fint_\Omega c_1 \,\mathrm{d}x = \rho_1,\ \fint_\Omega c_2 \,\mathrm{d}x = \rho_2 \right\}, \\ &\text{with} \quad \rho_1 = \fint_\Omega c_1^0 \,\mathrm{d}x = 1-\rho_2, \end{aligned} \tag{11}$$

we introduce the metric $\mathbf{d}$ by (see Section 2 below for the definition of $\mathbf{W}$)

$$\mathbf{d}\big(\hat{\boldsymbol{c}}, \check{\boldsymbol{c}}\big)^2 = \frac{\mathbf{W}(\hat{c}_1, \check{c}_1)^2}{m_1} + \frac{\mathbf{W}(\hat{c}_2, \check{c}_2)^2}{m_2}. \tag{12}$$

In the eyes of the metric $\mathbf{d}$, the two components of $\boldsymbol{c}$ are independent, and the constraint $c_1 + c_2 \equiv 1$ is enforced only by means of the energy. This way, the metric $\mathbf{d}$ inherits all of the established properties of the L^2-Wasserstein distance. The analogous idea has been successfully used for analyzing related cross-diffusion models with an inequality constraint $0 \le c_1+c_2 \le 1$ instead of (1c), see e.g. [17, 15]. In comparison, to the best of our knowledge, very little is known about the metric that would result by including the constraint already in its definition; see, however, [3].

1.3. **Estimates.** There are three essential a priori estimates that play a role in our existence proof for (1). The first two are consequences of the gradient flow structure outlined above: first, the energy is non-increasing in time, and in particular, $\mathbf{E}(\boldsymbol{c}(t)) \le \mathbf{E}(\boldsymbol{c}^0)$ for each $t \ge 0$. This ensures validity of the constraint (1c), and provides a priori estimates of c_i and $f(c_i)$ in $L^\infty(0,T;H^1(\Omega))$. Second, the curve $\boldsymbol{c}$ is L^2-absolutely continuous in time with respect to $\mathbf{d}$, that is, both components c_i are absolutely continuous in $\mathbf{W}$. That means that the kinetic energy densities $\frac{m_i}{2}c_i|\nabla\mu_i|^2$ — see the continuity equations (1a)&(1b) — are integrable in space and time. This provides a priori estimate on $\sqrt{c_i}\nabla\mu_i$ in $L^2(\Omega_T)$.

The third estimate is related to the dissipation of an auxiliary functional, namely the entropy:

$$\mathbf{H}(\boldsymbol{c}) = \frac{\tilde{\mathbf{H}}(c_1)}{m_1} + \frac{\tilde{\mathbf{H}}(c_2)}{m_2}, \quad \text{where} \quad \tilde{\mathbf{H}}(c_i) = \int_\Omega c_i(\log c_i - 1) + 1 \,\mathrm{d}x. \tag{13}$$

Indeed, it follows from a formal calculation given below in (38) that $\mathbf{H}$'s dissipation can be estimated in the form

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{H}(\boldsymbol{c}) \ge \frac{1}{2d}\int_\Omega \big(\Delta f(c_1)\big)^2 \,\mathrm{d}x - M, \tag{14}$$

with some constant $M \ge 0$ that is independent of the specific solution $\boldsymbol{c}$. This provides an a priori estimate on $f(c_1)$ in $L^2_{\text{loc}}(\mathbb{R}_{>0}; H^2(\Omega))$, which is our main source of compactness. Notice that thanks to the constraint $c_1 + c_2 = 1$ and the

symmetry $f(r) = f(1-r)$, the dissipation relation (14) can equivalently be written in the symmetric form

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{H}(\boldsymbol{c}) \geq \frac{1}{4d}\int_\Omega \Big[\big(\Delta f(c_1)\big)^2 + \big(\Delta f(c_2)\big)^2\Big]\,\mathrm{d}x - M.$$

1.4. **Reformulation of the equations.** A key element in our existence analysis is a very particular weak formulation of the system (1), which is taylored to the special nonlinearity under consideration. In the Cahn-Hilliard case, where f is smooth up to the boundary, it is possible to define a proper notion of phase chemical potential μ_i even when the corresponding phase vanishes, $c_i = 0$, see [6]. This approach does not extend easily to the case of singular f's considered here. Our ansatz is to substitute the potentials μ_1 and μ_2, which are difficult to analyze, by auxiliary quantites q_1 and q_2 given in (16) below.

Some notation is needed: by Assumption 1 on f, there exists a continuous $\omega : [0,1] \to \mathbb{R}$ with $\omega(0) = 0$ that is smooth and positive on $(0,1]$ such that

$$\frac{1}{f'(r)} = \omega(r)\omega(1-r) \quad \text{for } 0 < r < 1. \tag{15}$$

For notational convenience, we further introduce the continuous function $\alpha : [0,1] \to \mathbb{R}$ with $\alpha(0) = 0$ and $\alpha(r) = r/\omega(r)$ for $r \in (0,1]$; continuity at $r = 0$ is a consequence of the assumed concavity of $r \mapsto \frac{1}{f'(r)^2} = \omega(r)^2\omega(1-r)^2$. For f from (4), one may choose $\omega(r) = \sqrt{r}$, and then finds that $\alpha(r) = \sqrt{r}$ as well.

The auxiliary quantities that replace μ_1 and μ_2 are

$$q_1 = \omega(c_1)\,\mu_1, \quad q_2 = \omega(c_2)\,\mu_2. \tag{16}$$

The q_i are much better behaved than the μ_i, since they vanish by definition when c_i does since $\omega(0) = 0$. Accordingly, the continuity equation (1a) is — formally — interpreted in the following way:

$$\begin{aligned}\partial_t c_1 &= \operatorname{div}\left(m_1 c_1 \nabla\left[\frac{q_1}{\omega(c_1)}\right]\right) = m_1 \operatorname{div}\left(\nabla\left[c_1\frac{q_1}{\omega(c_1)}\right] - \nabla c_1\,\frac{q_1}{\omega(c_1)}\right)\\ &= m_1 \operatorname{div}\big(\nabla[\alpha(c_1)q_1] - \omega(c_2)\nabla f(c_1)\,q_1\big),\end{aligned} \tag{17}$$

and similarly for (1b). Concerning the constitutive relation (1d): after multiplication by $1/f'(c_1)$, it can be reformulated — still formally — in terms of the q_i as

$$\omega(c_1)q_2 - \omega(c_2)q_1 = \mathfrak{F}[c_1] := \Delta f(c_1) + \chi\omega(c_1)\omega(c_2)\left(c_1 - \tfrac{1}{2}\right), \tag{18}$$

which makes perfectly sense in view of the $L^2(\Omega_T)$-regularity of $\Delta f(c_1)$.

The significance of the formulation (17) is that the right-hand side can be interpreted in the sense of distributions as soon the product $q_1\nabla f(c_1)$ is locally integrable. Since $f(c_1) \in L^2(0,T;H^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega))$ thanks to the a priori estimates, we have $\nabla f(c_1) \in L^3(\Omega_T)$ by interpolation (recall that $d \leq 3$), and so it is sufficient that $q_1 \in L^{3/2}(\Omega_T)$. That latter is deduced by means of the representation

$$q_1 = \omega(c_1)\bar{\mu} + \alpha(c_2)\mathfrak{F}[c_1], \tag{19}$$

in which $\bar{\mu} = c_1\mu_1 + c_2\mu_2 = \alpha(c_1)q_1 + \alpha(c_2)q_2$ is an average chemical potential. The quantity $\mathfrak{F}[c_1]$ is bounded in $L^2(\Omega_T)$ thanks to the main a priori estimate; a bound

on $\bar{\mu}$ is obtained from the following representation of $\bar{\mu}$'s gradient:

$$\begin{aligned}\nabla\bar{\mu} &= c_1\nabla\mu_1 + c_2\nabla\mu_2 + \nabla c_1(\mu_1-\mu_2)\\ &= \sqrt{c_1}\big(\sqrt{c_1}\nabla\mu_1\big) + \sqrt{c_2}\big(\sqrt{c_2}\nabla\mu_2\big) + \nabla f(c_1)\,\mathfrak{F}[c_1],\end{aligned} \tag{20}$$

in which the first two terms are controlled thanks to the $L^2(\Omega_T)$-bound on $\sqrt{c_i}\nabla\mu_i$, and the last term is controlled by a combination of the $L^\infty(0,T;H^1(\Omega))$-bound on $f(c_1)$ and the $L^2(\Omega_T)$-bound on $\Delta f(c_1)$. This provides an estimate of $\bar{\mu}$ in $L^2(0,T;W^{1,1}(\Omega)) \hookrightarrow L^{3/2}(\Omega_T)$, and thus also the desired bound on q_i via (19).

Remark 1. *Our approach is bound to fail in high dimensions d. The bottleneck is to ensure local integrability of $q_1\nabla f(c_1)$ to give a meaning to* (17) *in the distributional sense. To indicate the difficulty, let us ignore integrability in time for the moment, i.e., we only want to have $q_1\nabla f(c_1) \in L^1(\Omega)$ at almost every time. The a priori estimate* (14) *will not provide more than $\mathfrak{F}[c_1] \in L^2(\Omega)$ and, via Sobolev embedding, $\nabla f(c_1) \in L^{2d/(d-2)}(\Omega)$ at almost every time. Hence, the best integrability that we could possibly conclude from* (20) *is $\nabla\bar{\mu} \in L^{d/(d-1)}(\Omega)$, and thus $\bar{\mu} \in L^{d/(d-2)}(\Omega)$ by means of Sobolev-Poincaré. In view of* (19)*, also $q_1 \in L^{d/(d-2)}(\Omega)$. In general, the product of $q_1 \in L^{d/(d-2)}(\Omega)$ and $\nabla f \in L^{2d/(d-2)}(\Omega)$ is not integrable in dimensions $d > 6$.*

The admissible integrability exponents are significantly more complicated to compute if integrability in time is taken into account as well, and in any case they will lead to a more restrictive condition on the dimension d. We did not try to determine the maximal possible value of d, but simply restrict attention to the physically relevant dimensions.

1.5. **Main result.** In the following, $C^\infty_{c,n}(\mathbb{R}_{>0}\times\Omega)$ denotes the space of all test functions $\xi \in C^\infty(\mathbb{R}_{\geq 0}\times\overline{\Omega})$ such that $\xi(t,\cdot)\equiv 0$ for all $t \geq 0$ outside of some compact time interval $I \subset \mathbb{R}_{>0}$, and for which $\xi(t;\cdot)$ satisfies homogeneous Neumann boundary conditions at each $t > 0$.

Our main result is the following.

Theorem 1. *Let initial data $\boldsymbol{c}^0 = (c_1^0, c_2^0)$ with $c_1^0 + c_2^0 \equiv 1$ and $f(c_1^0), f(c_2^0) \in H^1(\Omega)$ be given. Then there exists $\boldsymbol{c} = (c_1, c_2) : \mathbb{R}_{\geq 0}\times\Omega \to [0,1]^2$ with the following properties:*

- regularity in time:
  c_1, c_2 *are Hölder continuous with respect to time as a map into* $L^2(\Omega)$.
- regularity in space:
  $c_1, c_2, f(c_1),\ f(c_2) \in L^\infty(\mathbb{R}_{\geq 0}; H^1(\Omega))$ *and* $f(c_1),\ f(c_2) \in L^2_{loc}(\mathbb{R}_{\geq 0}; H^2(\Omega))$
- boundary conditions:
  $c_1(t), c_2(t)$ *satisfy homogenous Neumann conditions* (2b) *at a.e.* $t \geq 0$
- initial conditions:
  $c_1(0) = c_1^0,\ c_2(0) = c_2^0$.

$\boldsymbol{c}$ is accompanied by $\boldsymbol{q} = (q_1, q_2) : \mathbb{R}_{\geq 0} \times \Omega \to \mathbb{R}^2$ with $q_1, q_2 \in L^{3/2}(\Omega_T)$ for each $T > 0$, such that the system (1) is satisfied in the following sense:

$$\text{(21a)}\quad 0 = \int_0^\infty \int_\Omega \big[\partial_t \xi\, c_i + m_i q_i \big(\alpha(c_i)\,\Delta\xi + \omega(1-c_i)\,\nabla f(c_i)\cdot\nabla\xi\big)\big]\,\mathrm{d}x\,\mathrm{d}t$$
$$\text{for } i = 1, 2 \text{ and all test functions } \xi \in C^\infty_{c,n}(\mathbb{R}_{>0} \times \Omega),$$

$$\text{(21b)}\quad 1 = c_1 + c_2 \qquad \text{a.e. on } \mathbb{R}_{\geq 0} \times \Omega,$$

$$\text{(21c)}\quad \omega(c_1)\, q_2 - \omega(c_2)\, q_1 = \Delta f(c_1) + \frac{\chi}{2}(c_1 - c_2)\omega(c_1)\omega(c_2) \qquad \text{a.e. on } \mathbb{R}_{\geq 0} \times \Omega.$$

Notice that the no-flux boundary conditions (2a) are encoded in the weak form (21a) of the continuity equations (1a)&(1b): since the test function ξ is only supposed have vanishing normal derivative, but still may attain arbitrary values on $\partial\Omega$, a formal integration by parts in (21a) produces a weak form of (2a).

1.6. **Plan of the paper.** In Section 2 below, we give a very brief summary of the relevant results from the theory of optimal transportation that are needed in our proof of Theorem 1. In Section 3, we describe the construction of the time-discrete approximate solutions, and we derive a priori estimates in Sections 4 and 5 on the approximate volume fractions $\boldsymbol{c}$ and phase potentials $\boldsymbol{q}$ respectively. Finally, in Section 6, we pass to the time-continuous limit, obtaining a weak solution in the sense of Theorem 1.

1.7. **Notation.** When we write in the following that some constant depends *only on the parameters of the problem*, then we mean that this constant can in principle be expressed in terms of the factor χ, the mobilities m_1, m_2, the averages ρ_1, ρ_2 from (11), properties of the function f, and geometric properties of the domain Ω.

2. Preliminaries from the theory of optimal transportation

In the section, we briefly recall three alternative definitions of the L^2-Wasserstein distance $\mathbf{W}$; in the proof of our main result, we need all three of them. For more information on the mathematical theory of optimal mass transportation, we refer to the monographs [26, 27, 25]. Below, we assume that $\rho_0, \rho_1 : \Omega \to [0, 1]$ are two measurable functions of the same total mass,

$$\int_\Omega \rho_0(x)\,\mathrm{d}x = \int_\Omega \rho_1(x)\,\mathrm{d}x.$$

In this case, the definitions are all equivalent.

2.1. **Monge characterization.** One says that a measurable map $T : \Omega \to \Omega$ pushes ρ_0 forward to ρ_1, written as $T\#\rho_0 = \rho_1$, if

$$\int_\Omega \Theta(x)\rho_1(x)\,\mathrm{d}x = \int_\Omega \Theta \circ T(y)\rho_0(y)\,\mathrm{d}y \quad \text{for all } \Theta \in C^0(\overline{\Omega}).$$

The Monge characterization of the L^2-Wasserstein distance between ρ_0 and ρ_1 is given by

$$\mathbf{W}(\rho_0, \rho_1)^2 = \inf_{T\#\rho_0 = \rho_1} \int_\Omega |T(x) - x|^2 \rho_0(x)\,\mathrm{d}x, \tag{22}$$

where the infimum runs over all measurable maps $T : \Omega \to \Omega$ with $T\#\rho_0 = \rho_1$. In the situation at hand, the infimum in (22) is actually a minimum. It is attained

by an optimal transport map T_{opt}; the optimal map is uniquely determined on the support of ρ_0.

2.2. **Kantorovich characterization.** A Borel measure γ on the product space $\Omega \times \Omega$ is called a transport plan from ρ_0 to ρ_1 if the latter are the marginals of γ, i.e.,

$$\iint_{\Omega\times\Omega} \varphi(x)\,\mathrm{d}\gamma(x,y) = \int_\Omega \varphi(x)\rho_0(x)\,\mathrm{d}x,$$
$$\iint_{\Omega\times\Omega} \psi(y)\,\mathrm{d}\gamma(x,y) = \int_\Omega \psi(y)\rho_1(y)\,\mathrm{d}y,$$

for all $\varphi, \psi \in C^0(\Omega)$. The set of all such transport plans is denoted by $\Gamma(\rho_0, \rho_1)$. The Kantorovich characterization of $\mathbf{W}$ amounts to

$$\mathbf{W}(\rho_0,\rho_1)^2 = \inf_{\gamma\in\Gamma(\rho_0,\rho_1)} \iint_{\Omega\times\Omega} |x-y|^2\,\mathrm{d}\gamma(x,y),$$

and the infimum is attained by some optimal plan γ_{opt}. In the situation at hand, γ_{opt} is unique. Moreover, it is concentrated on a graph: γ_{opt}'s support is contained in $\{(x, T_{\mathrm{opt}}(x)) | x \in \Omega\} \subset \Omega \times \Omega$, where T_{opt} is an optimal map from the Monge characterization.

2.3. **Dual characterization.** The dual characterization of the Wasserstein distance is given by

$$\frac{1}{2}\mathbf{W}(\rho_0,\rho_1)^2 = \sup_{\varphi(x)+\psi(y)\le\frac{1}{2}|x-y|^2} \left(\int_\Omega \varphi(x)\rho_0(x)\,\mathrm{d}x + \int_\Omega \psi(y)\rho_1(y)\,\mathrm{d}y \right), \tag{23}$$

where the supremum runs over all potentials $\phi, \psi \in C^0(\Omega)$ satisfying $\varphi(x)+\psi(y) \le \frac{1}{2}|x-y|^2$. The infimum is attained by a pair of globally Lipschitz functions $(\varphi_{\mathrm{opt}}, \psi_{\mathrm{opt}})$, which are referred to as Kantorovich potentials. The potentials are related to the optimal Monge map T_{opt} via $T_{\mathrm{opt}}(x) = x - \nabla\varphi_{\mathrm{opt}}(x)$ which holds ρ-a.e.

There are always infinitely many pairs of Kantorovich potentials, since the value of the function and the constraint are invariant under the exchange of a global constant, i.e., $\varphi \rightsquigarrow \varphi + C$ and $\psi \rightsquigarrow \psi - C$ for any $C \in \mathbb{R}$. On the other hand, if at least one of the two densities ρ_0 and ρ_1 has full support, then this global constant is the only degree of non-uniqueness.

3. Time-discrete approximation via minimizing movement scheme

As explained in Section 1.2, the problem (1)–(3) can be interpreted as the gradient flow of the singular energy $\mathbf{E}$ with respect to the metric $\mathbf{d}$ on the space $\mathbf{X}_{\mathrm{mass}}$. In view of that structure, a natural approach to construction of solutions to (1) is the time-discrete approximation by means of the minimizing movement scheme. This approach has been proven extremely robust, and has been applied for existence proofs in linear and nonlinear Fokker-Planck equations [14, 2], non-local aggregation-diffusion equations [4, 8, 16, 28], doubly non-linear and flux-limited equations [1, 22], fourth order quantum and lubrication equations [12, 21, 18, 20], multi-phase flows [19, 5, 6], also with volumetric constraints [17, 15], and many more settings.

In addition to approximations of the volume fractions c_1 and c_2, we also need to construct approximations of the auxiliary quantities q_1 and q_2. These will be

obtained from the Kantorovich potentials for the optimal transport of the volume fractions between time steps. In order to ensure that these potentials are well-defined (up to a global additive constant), we regularize the minimizing movement scheme by modifying the volume fractions in the previous time step such that both have full support. This removes the ambiguity in the definition of the Kantorovich potentials, as explained in Section 2.3.

Throughout this section, let two parameters be fixed: a time step size $\tau > 0$, and a positivity parameter $\delta > 0$. We assume that τ and δ are related as follows:

$$\delta \leq \tau^2. \tag{24}$$

Recall the definitions of the energy functional $\mathbf{E}$ from (10) and of the metric $\mathbf{d}$ from (12) on the space $\mathbf{X}_{\mathrm{mass}}$. Recall further the definition of the averages ρ_1 and ρ_2 in (11), and introduce the regularization $[\boldsymbol{c}]_\delta = ([c_1]_\delta, [c_2]_\delta)$ of a $\boldsymbol{c} = (c_1, c_2) \in \mathbf{X}_{\mathrm{mass}}$ by

$$[c_i]_\delta = \delta\rho_i + (1-\delta)c_i. \tag{25}$$

With these notations at hand, define for given $\bar{\boldsymbol{c}} \in \mathbf{X}_{\mathrm{mass}}$ a variational functional in $\boldsymbol{c} \in \mathbf{X}_{\mathrm{mass}}$ by

$$\mathbf{E}_{\tau,\delta}(\boldsymbol{c}; \bar{\boldsymbol{c}}) = \frac{1}{2\tau}\mathbf{d}\big(\boldsymbol{c}, [\bar{\boldsymbol{c}}]_\delta\big)^2 + \mathbf{E}(\boldsymbol{c}). \tag{26}$$

At each instance of discretized time $t = n\tau$, an approximation $(\boldsymbol{c}^n, \boldsymbol{q}^n)$ of $(\boldsymbol{c}(t), \boldsymbol{q}(t))$ is constructed as follows. Starting from the given initial condition $\boldsymbol{c}^0$, each $\boldsymbol{c}^n$ is inductively chosen as a global minimizer of $\mathbf{E}_{\tau,\delta}(\cdot; \boldsymbol{c}^{n-1})$, i.e.,

$$\boldsymbol{c}^n \in \operatorname*{argmin}_{\boldsymbol{c} \in \mathbf{X}_{\mathrm{mass}}} \mathbf{E}_{\tau,\delta}(\boldsymbol{c}; \boldsymbol{c}^{n-1}). \tag{27}$$

Solvability of that minimization problem is shown in Lemma 2 below.

The accompanying auxiliary quantities q_1^n and q_2^n are obtained as follows. First, let (φ_1^n, ψ_1^n) and (φ_2^n, ψ_2^n) be two pairs of Kantorovich potentials for the respective optimal transport of $[c_i^{n-1}]_\delta$ to c_i^n; since $[c_i^{n-1}]_\delta \geq \delta\rho_i$ on Ω, these pairs are unique up to addition of global constants. These constants are normalized by requiring

$$\int_\Omega \left[\frac{c_1^n\psi_1^n}{m_1} + \frac{c_2^n\psi_2^n}{m_2}\right] \mathrm{d}x = 0, \quad \int_\Omega \left[\psi_2^n - \psi_1^n - \chi\left(c_1 - \frac{1}{2}\right)\right] \omega(c_1^n)\omega(c_2^n)\,\mathrm{d}x = 0. \tag{28}$$

From the ψ_i^n, define the rescaled pair of potentials $\boldsymbol{\mu}^n = (\mu_1^n, \mu_2^n)$ via

$$\mu_1^n := \frac{\psi_1^n}{m_1\tau}, \quad \mu_2^n := \frac{\psi_2^n}{m_2\tau},$$

and finally $\boldsymbol{q}^n = (q_1^n, q_2^n)$ is given — as indicated in (16) — by

$$q_1^n := \omega(c_1^n)\mu_1^n, \quad q_2^n := \omega(c_2^n)\mu_2^n.$$

Lemma 2. *Given initial data $\boldsymbol{c}^0$ as in Theorem 1, the minimization problem for $\boldsymbol{c}^n$ can be solved inductively, leading to infinite sequences $(\boldsymbol{c}^n)_{n\in\mathbb{N}}$ and $(\boldsymbol{q}^n)_{n\in\mathbb{N}}$. The $\boldsymbol{c}^n$ satisy the constraint*

$$c_1^n + c_2^n = 1. \tag{29}$$

Proof. Inductive solvability of the minimization problem follows by the direct methods from the calculus of variations. Indeed, it suffices to observe the following about the functional $\mathbf{E}_{\tau,\delta}(\cdot; \boldsymbol{c}^{n-1})$, considered as a map from $\mathbf{X}_{\mathrm{mass}}$ with the topology of $L^2(\Omega; \mathbb{R}^2)$ to the extended non-negative real numbers:

- It is bounded below (in fact: is non-negative) and is not identically $+\infty$ (e.g., is finite at $\boldsymbol{c}^{n-1}$).
- It is coercive: if $\tilde{\boldsymbol{c}}^k$ is a sequence in $\mathbf{X}_{\text{mass}}$ such that $\mathbf{E}_{\tau,\delta}(\tilde{\boldsymbol{c}}^k;\boldsymbol{c}^{n-1})$ is bounded, then in particular $\int_\Omega |\nabla f(\tilde{c}_1^k)|^2\,\mathrm{d}x$ is bounded, i.e., $f(\tilde{c}_1^k)$ is bounded in $H^1(\Omega)$. Rellich's compactness theorem now implies strong convergence of a subsequence $f(\tilde{c}_1^{k'})$ in $L^2(\Omega)$, and thanks to the properties of f, also $\tilde{c}_1^{k'}$ itself converges in $L^2(\Omega)$. Finally, since finiteness of $\mathbf{E}_{\tau,\delta}(\tilde{\boldsymbol{c}}^k;\boldsymbol{c}^{n-1})$ implies that $\tilde{c}_2^k = 1-\tilde{c}_1^k$, convergence of $\tilde{c}_2^{k'}$ follows as well.
- It is lower semi-continuous. To see this, let $\tilde{\boldsymbol{c}}^k$ be a sequence in $\mathbf{X}_{\text{mass}}$ that converges to $\tilde{\boldsymbol{c}}^*$ in $L^2(\Omega;\mathbb{R}^2)$. Convergence of $\mathbf{d}(\tilde{\boldsymbol{c}}^k,\boldsymbol{c}^{n-1})$ and of $\int_\Omega \tilde{c}_1^k(1-\tilde{c}_1^k)\,\mathrm{d}x$ towards their respective limits is immediate. On the other hand, it follows by continuity of f that also $f(\tilde{c}_1^k)$ converges to $f(\tilde{c}_1^*)$ in $L^2(\Omega)$. And so,

$$\liminf_{k\to\infty}\int_\Omega |\nabla f(\tilde{c}_1^k)|^2\,\mathrm{d}x \geq \int_\Omega |\nabla f(\tilde{c}_1^*)|^2\,\mathrm{d}x$$

  is a consequence of the lower semi-continuity of the $H^1(\Omega)$-norm on $L^2(\Omega)$.

The relation (29) holds since each minimizer $\boldsymbol{c}^n$ has a finite energy. □

4. A priori estimates on the volume fractions

The ultimate goal is to obtain solutions $\boldsymbol{c}$ and $\boldsymbol{q}$ of the weak formulation (21) as appropriate limits of the time-discrete quantities $\boldsymbol{c}^n$ and $\boldsymbol{q}^n$ for $\tau\downarrow 0$ and $\delta\downarrow 0$. In this and the next section, we establish the a priori estimates that eventually provide sufficient compactness for performing the limit. As indicated in the introduction, there are three essential estimates: the first two, given in Lemma 3 right below, follow almost immediately from the gradient flow structure. These two estimates are sufficient to conclude the weak convergence of the volume fractions. The third estimate, given in Lemma 5, follows from the control (13) on the dissipation rate of the entropy $\mathbf{H}$. It provides strong convergence of the volume fractions and indirectly — see Section 5 below — also weak convergence of the auxiliary functions.

Lemma 3. *There is a constant K, only depending on the parameters of the problem, such that for all $N=1,2,\dots$*

$$\mathbf{E}(\boldsymbol{c}^N) + \frac{\tau}{2}\sum_{n=1}^{N}\left(\frac{\mathbf{d}(\boldsymbol{c}^n,[\boldsymbol{c}^{n-1}]_\delta)}{\tau}\right)^2 \leq \mathbf{E}(\boldsymbol{c}^0) + \frac{K}{2}N\tau. \tag{30}$$

Consequently, for all indices $n\leq N$ and $\underline{n}<\overline{n}\leq N$,

$$\|\nabla f(c_1^n)\|_{L^2}^2 \leq 2\mathbf{E}(\boldsymbol{c}^0) + KN\tau, \qquad \text{for all } n=1,2,\dots,N, \tag{31}$$

$$\mathbf{d}(\boldsymbol{c}^{\overline{n}},\boldsymbol{c}^{\underline{n}}) \leq 2\left(\mathbf{E}(\boldsymbol{c}^0)+KN\tau\right)^{\frac12}\left(\tau(\overline{n}-\underline{n})\right)^{\frac12} \qquad \text{for } 0\leq\underline{n}<\overline{n}\leq N, \tag{32}$$

$$\|\boldsymbol{c}^{\overline{n}}-\boldsymbol{c}^{\underline{n}}\|_{L^2} \leq 2\sqrt[4]{m_1}\left(\mathbf{E}(\boldsymbol{c}^0)+KN\tau\right)^{\frac12}\left(\tau(\overline{n}-\underline{n})\right)^{\frac14}. \tag{33}$$

Proof. By definition of $\boldsymbol{c}^n$ as a minimizer, $\mathbf{E}_{\tau,\delta}(\boldsymbol{c}^n;\boldsymbol{c}^{n-1})\leq \mathbf{E}_{\tau,\delta}(\boldsymbol{c}^{n-1};\boldsymbol{c}^{n-1})$, which amounts to

$$\mathbf{E}(\boldsymbol{c}^n) + \frac{\tau}{2}\left(\frac{\mathbf{d}(\boldsymbol{c}^n;[\boldsymbol{c}^{n-1}]_\delta)}{\tau}\right)^2 \leq \mathbf{E}(\boldsymbol{c}^{n-1}) + \frac{1}{2\tau}\mathbf{d}(\boldsymbol{c}^{n-1},[\boldsymbol{c}^{n-1}]_\delta)^2. \tag{34}$$

The last term is bounded by $K\delta/(2\tau) \leq K\tau/2$ thanks to Lemma 13 from the appendix, and to our assumption $\delta \leq \tau^2$ from (24). Summation of (34) from $n = 1$ to $n = N$ yields (30), and (31) is an immediate consequence from the definition of $\mathbf{E}$. To conclude (32) from here, we use the triangle inequality for $\mathbf{d}$ — which is inherited from $\mathbf{W}$ — and Hölder's inequality for sums,

$$\mathbf{d}(\boldsymbol{c}^{\overline{n}}, \boldsymbol{c}^{\underline{n}}) \leq \sum_{n=\underline{n}+1}^{\overline{n}} \mathbf{d}(\boldsymbol{c}^n, \boldsymbol{c}^{n-1}) \leq \left(\tau \sum_{n=\underline{n}+1}^{\overline{n}} \left(\frac{\mathbf{d}(\boldsymbol{c}^n, \boldsymbol{c}^{n-1})}{\tau} \right)^2 \right)^{\frac{1}{2}} \big(\tau(\overline{n} - \underline{n})\big)^{\frac{1}{2}}.$$

The expression inside the first pair of brackets is now estimated with the help of (30) above, and another application of Lemma 13:

$$\begin{aligned} \tau \sum_{n=\underline{n}+1}^{\overline{n}} \left(\frac{\mathbf{d}(\boldsymbol{c}^n, \boldsymbol{c}^{n-1})}{\tau} \right)^2 &\leq \tau \sum_{n=\underline{n}+1}^{\overline{n}} \left[2 \left(\frac{\mathbf{d}(\boldsymbol{c}^n, [\boldsymbol{c}^{n-1}]_\delta)}{\tau} \right)^2 + \frac{2K\delta}{\tau^2} \right] \\ &\leq 4 \left[\mathbf{E}(\boldsymbol{c}^0) + \frac{KT}{2} \right] + \frac{2K\delta}{\tau} N. \end{aligned}$$

Substitution of this estimate above and recalling (24) produces (32). Estimate (33) emerges as a consequence of (31) and (32) via Lemma 14 from the appendix. □

The bound (30) can be formulated as a weighted H^1-estimate on the Kantorovich potentials.

Corollary 4. *At each $n = 1, 2, \ldots$, we have that*

$$[c_1^{n-1}]_\delta = (\mathrm{id} - \nabla\psi_1^n)\#c_1^n, \quad \textit{and} \quad [c_2^{n-1}]_\delta = (\mathrm{id} - \nabla\psi_2^n)\#c_2^n, \tag{35}$$

and therefore, with the same constant K as in Lemma 3 above, for all $N = 1, 2, \ldots$,

$$\tau \sum_{n=1}^{N} \int_\Omega \left(\frac{c_1^n}{m_1} \left| \frac{\nabla\psi_1^n}{\tau} \right|^2 + \frac{c_2^n}{m_2} \left| \frac{\nabla\psi_2^n}{\tau} \right|^2 \right) \mathrm{d}x \leq 2\mathbf{E}(\boldsymbol{c}^0) + \frac{K\delta N}{\tau}. \tag{36}$$

Proof. The relations (35) express the property of the Kantorovich potential ψ_i^n that $x \mapsto x - \nabla\psi_i^n(x)$ is a transport map from c_i^n to $[c_i^{n-1}]_\delta$. In fact, it is the *optimal* transport map, see Section 2.3, and hence (22) implies that

$$\begin{aligned} \left(\frac{\mathbf{d}\big(\boldsymbol{c}^n, [\boldsymbol{c}^{n-1}]_\delta\big)}{\tau} \right)^2 &= \frac{\mathbf{W}(c_1^n, [c_1^{n-1}]_\delta)^2}{m_1\tau^2} + \frac{\mathbf{W}(c_2^n, [c_2^{n-1}]_\delta)^2}{m_2\tau^2} \\ &= \int_\Omega \left(\frac{c_1^n}{m_1} \left| \frac{\nabla\psi_1^n}{\tau} \right|^2 + \frac{c_2^n}{m_2} \left| \frac{\nabla\psi_2^n}{\tau} \right|^2 \right) \mathrm{d}x. \end{aligned}$$

By non-negativity of $\mathbf{E}$, the desired estimate (36) is now implied by (30). □

The third a priori estimate below is more specific to the system (1), and is also more difficult to prove.

Lemma 5. *There is a constant C, only depending on the parameters of the problem, such that for all $N = 1, 2, \ldots$:*

$$\tau \sum_{n=1}^{N} \int_\Omega \big\| f(c_1^n) \big\|_{H^2}^2 \, \mathrm{d}x \leq C(1 + N\tau). \tag{37}$$

Moreover, c_1^n and $f(c_1^n)$ satisfy homogeneous Neumann boundary conditions at each $n = 1, 2, \ldots$

Remark 2. *If $1/(f')^2$ has a bounded derivative — as is the case for the f from (4) — then one also obtains the analogous estimate as (37) for c_1 itself in place of $f(c_1)$. Indeed, with $c_1 = f^{-1}(f(c_1))$,*

$$\Delta c_1 = \frac{1}{f'(c_1)}\Delta f(c_1) - \frac{f''(c_1)}{f'(c_1)^3}|\nabla f(c_1)|^2,$$

with bounded factors

$$\frac{1}{f'} \quad \text{and} \quad -\frac{f''}{(f')^3} = \frac{1}{2}\left(\frac{1}{(f')^2}\right)'.$$

Combining this with the Gagliardo-Nirenberg inequality

$$\|\nabla f\|_{L^4}^2 \le 3\|f\|_{L^\infty}\|f\|_{H^2},$$

that is easily derived using integration by parts, shows that $\|\Delta c_1\|_{L^2}^2 \le C\|f(c_1)\|_{H^2}^2$, and therefore, see (41) below, also $\|c_1\|_{H^2}^2 \le C\|f(c_1)\|_{H^2}^2$.

We divide the proof of Lemma 5 into two parts: the first part contains the formal calculations — for smooth and positive classical solutions to (1) — that lead to (14), the second part is the fully rigorous justification of (37) as a time-discrete version of (14), using the flow interchange technique from [21].

Formal calculation leading to (14). Assume that a smooth and classical solution $\boldsymbol{c}$ to (1) with $0 < c_1 < 1$ is given. We consider the dissipation of the entropy functional defined in (13). We have, thanks to the no-flux and Neumann boundary conditions (2),

$$\begin{aligned} -\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{H}(\boldsymbol{c}) &= -\int_\Omega \left[\frac{\log c_1}{m_1}\,\partial_t c_1 + \frac{\log c_2}{m_2}\,\partial_t c_2\right]\mathrm{d}x \\ &= \int_\Omega \left[\nabla c_1\cdot\nabla\mu_1 + \nabla c_2\cdot\mu_2\right]\mathrm{d}x \\ &= \int_\Omega \nabla c_1\cdot\nabla[\mu_1-\mu_2]\,\mathrm{d}x \\ &= \int_\Omega f'(c_1)\Delta c_1\Delta f(c_1)\,\mathrm{d}x - \chi\int_\Omega |\nabla c_1|^2\,\mathrm{d}x. \end{aligned} \tag{38}$$

We shall now use various manipulations to obtain a lower bound on

$$J := \int_\Omega f'(c_1)\Delta c_1\Delta f(c_1)\,\mathrm{d}x. \tag{39}$$

On the one hand,

$$\Delta f(c_1) = f'(c_1)\Delta c_1 + f''(c_1)|\nabla c_1|^2. \tag{40}$$

And on the other hand, thanks to the homogeneous Neumann boundary conditions from (2b) — that are inherited from c_1 to $f(c_1)$ thanks to $0 < c_1 < 1$ — and the convexity of Ω, we have that (see e.g., [12, Lemma 5.1])

$$\int_\Omega \big(\Delta f(c_1)\big)^2\,\mathrm{d}x \ge \int_\Omega \|\nabla^2 f(c_1)\|^2\,\mathrm{d}x, \tag{41}$$

where $\|A\| = \sqrt{\mathrm{tr}(A^TA)}$ is the Frobenius norm of the square matrix A. Thus, we obtain

$$J \ge \int_\Omega \left[\|\nabla^2 f(c_1)\|^2 - \frac{f''(c_1)}{f'(c_1)^2}|\nabla f(c_1)|^2\Delta f(c_1)\right]\mathrm{d}x. \tag{42}$$

Now introduce $f, g : (0,1) \to \mathbb{R}$ by

$$g(r) := \frac{f''(r)}{f'(r)^2}, \quad h(r) := \frac{g'(r)}{f'(r)},$$

and notice that

$$\nabla g(c_1) = h(c_1)\,\nabla f(c_1). \tag{43}$$

In the following, we write shortly f, g and h for $f(c_1)$, $g(c_1)$ and $h(c_1)$. Thanks again to the homogeneous Neumann boundary conditions and to (43), the divergence theorem implies that

$$\begin{aligned} 0 &= \frac{d}{d+2}\int_\Omega \operatorname{div}\left(g|\nabla f|^2\nabla f\right)\mathrm{d}x \\ &= \frac{d}{d+2}\int_\Omega \left[g\Delta f|\nabla f|^2 + 2g\nabla f\cdot\nabla^2 f\nabla f + h|\nabla f|^4\right]\mathrm{d}x. \end{aligned}$$

Adding the final integral expression to the right-hand side of (42) produces

$$J \geq \int_\Omega \left[\|\nabla^2 f\|^2 - \frac{2g}{d+2}\Delta f|\nabla f|^2 + \frac{2dg}{d+2}\nabla f\cdot\nabla^2 f\cdot\nabla f + \frac{dh}{d+2}|\nabla f|^4\right]\mathrm{d}x.$$

Next, introduce the matrix-valued function $R : \Omega \to \mathbb{R}^{d\times d}$ by

$$R := \nabla^2 f(c_1) - \frac{\Delta f(c_1)}{d}\mathbf{1}_d.$$

Then, using that $\mathrm{tr}\mathbf{1}_d = d$ and $\mathrm{tr}R = 0$, we obtain that

$$\|\nabla^2 f(c_1)\|^2 = \mathrm{tr}\left[\left(R + \frac{\Delta f(c_1)}{d}\mathbf{1}_d\right)^2\right] = \|R\|^2 + \frac{(\Delta f(c_1))^2}{d},$$

which allows to conclude that

$$J \geq \frac{1}{d}\int_\Omega (\Delta f)^2\,\mathrm{d}x + \int_\Omega \left[\|R\|^2 + \frac{2dg}{d+2}\nabla f\cdot R\cdot\nabla f + \frac{dh}{d+2}|\nabla f|^4\right]\mathrm{d}x.$$

The last step is to verify that the expression inside the final integral is pointwise non-negative:

$$\begin{aligned} &\|R\|^2 + \frac{2dg}{d+2}\nabla f\cdot R\cdot\nabla f + \frac{dh}{d+2}|\nabla f|^4 \\ &\quad = \left\|R + \frac{dg}{d+2}\nabla f\,\nabla f^T\right\|^2 + \left[\frac{dh}{d+2} - \left(\frac{dg}{d+2}\right)^2\right]|\nabla f|^4. \end{aligned}$$

The squared norm is trivially non-negative. For the coefficient of the term $|\nabla f|^4$ to be non-negative, it suffices to have $h \geq g^2$. Since

$$h - g^2 = \frac{1}{f'}\left(\frac{f''}{(f')^2}\right)' - \left(\frac{f''}{(f')^2}\right)^2 = \frac{f'''}{(f')^3} - 3\frac{(f'')^2}{(f')^4} = -\frac{1}{2}\left(\frac{1}{(f')^2}\right)'',$$

the assumed concavity of $1/(f')^2$ is sufficient to guarantee $h \geq g^2$. In summary,

$$J \geq \frac{1}{d}\int_\Omega \Delta f(c_1)^2\,\mathrm{d}x. \tag{44}$$

It remains to estimate the other integral. Recall that f is continuous, and that f' is positive with $1/(f')^2$ concave, so there is a constant $a > 0$ such that $|f| \leq a$ and

$f' \geq a^{-1}$. Since Ω is bounded, and thanks to the Neumann boundary conditions (2b),

(45)
$$\chi \int_\Omega |\nabla c_1|^2 \,\mathrm{d}x \leq a^2 \chi \int_\Omega |\nabla f(c_1)|^2 \,\mathrm{d}x = -a^2 \chi \int_\Omega f(c_1) \Delta f(c_1) \,\mathrm{d}x \\ \leq a^2 \chi \big(a^2 |\Omega|\big)^{\frac{1}{2}} \big(dJ\big)^{\frac{1}{2}} \leq \frac{1}{2} J + \frac{d\chi^2 a^4}{2} |\Omega|.$$

Going back to (38), we arrive at (14), or more specifically:

$$-\frac{\mathrm{d}}{\mathrm{d}t} \mathbf{H}(\boldsymbol{c}) \geq \frac{1}{2d} \int_\Omega (\Delta f)^2 \,\mathrm{d}x - \frac{d\chi^2 a^4}{2} |\Omega|. \tag{46}$$

An integration of this inequality in time provides

$$\int_0^T \int_\Omega (\Delta f)^2 \,\mathrm{d}x \leq 2d \big[\mathbf{H}(\boldsymbol{c}^0) - \mathbf{H}\big(\boldsymbol{c}(T)\big)\big] + d^2 \chi^2 a^4 |\Omega| T. \tag{47}$$

Notice that the value of the entropy $\mathbf{H}(\boldsymbol{c})$ is uniformly bounded from above and below for all $\boldsymbol{c} \in \mathbf{X}_{\mathrm{mass}}$. The estimate (37) under consideration is a time-discrete version of (47), using that the integral over $\Delta f(c_1)$ on the left hand side yields control on the H^2-norm of $f(c_1)$ by means of another application of (41) and interpolation with the trivial $L^\infty(L^2)$-bound on c_1. □

Making the formal calculations rigorous. For each fixed n, we show the following time-step version of (47):

$$\tau \int_\Omega \big(\Delta f(c_1^n)\big)^2 \,\mathrm{d}x \leq 2d \big[\mathbf{H}(\boldsymbol{c}^{n-1}) - \mathbf{H}(\boldsymbol{c}^n)\big] + \tau(d^2 \chi^2 a^4 |\Omega| + K), \tag{48}$$

where K is independent of τ. With (48) at hand, the estimate (37) follows by summation over $n = 1, 2, \ldots, N$.

The starting point for the derivation of (48) is a particular variation of the minimizer $\boldsymbol{c}_\tau^n$ of $\mathbf{E}_{\tau,\delta}(\cdot; \boldsymbol{c}_\tau^{n-1})$: consider the family $\boldsymbol{c}^s = (c_1^s, c_2^s) \in \mathbf{X}_{\mathrm{mass}}$, where c_1^s and c_2^s are the time-s-solutions to the heat flow on Ω for data c_1^n and c_2^n, with homogeneous Neumann boundary conditions:

$$\partial_s c_i^s = \Delta c_i^s \quad \text{for } (s,x) \in \mathbb{R}_{>0} \times \Omega, \tag{49a}$$

$$\mathbf{n} \cdot \nabla c_i^s = 0 \quad \text{on } \mathbb{R}_{>0} \times \partial\Omega, \tag{49b}$$

$$c_i^s{}_{|_{s=0}} = c_i^n \quad \text{in } \Omega. \tag{49c}$$

The pair $\boldsymbol{c}^s = (c_1^s, c_2^s)$ has a variety of nice properties that facilitate the further analysis. Thanks to the smoothing effect of the heat equation, the map $(s,x) \mapsto c_i^s(x)$ is a C^∞-function on $\mathbb{R}_{>0} \times \Omega$, and it satisfies both the equation (49a) and the boundary condition (49b) in the classical sense. Moreover, one has $0 < \inf_x c_i^s(x) \leq \sup_x c_i^s(x) < 1$ for each $s > 0$, which implies that the map $(s;x) \mapsto f(c_i^s(x))$ inherits the C^∞-smoothness as well as the homogeneous Neumann boundary conditions,

$$\mathbf{n} \cdot \nabla f(c_i^s) = 0 \quad \text{on } \mathbb{R}_{>0} \times \partial\Omega. \tag{50}$$

Concerning the attainment of the initial condition (49c): it follows from $\mathbf{E}(\boldsymbol{c}^n) < \infty$ that $f(c_i^n) \in H^1(\Omega)$, and hence also $c_i^n \in H^1(\Omega)$ in view of Assumption 1. This implies

$$c_i^s \to c_i^n \quad \text{in } H^1(\Omega) \text{ as } s \downarrow 0. \tag{51}$$

Note, however, that we cannot conclude $f(c_i^s) \to f(c_i^n)$ in $H^1(\Omega)$ from here because of $f'(r) \to +\infty$ for $r \downarrow 0$ and for $r \uparrow 1$. Finally, the incompressibility constraint is preserved,

$$c_1^s + c_2^s = 1. \tag{52}$$

There are many further possibilities for the perturbation $(\boldsymbol{c}^s)$ that would share the aforementioned properties. Our motivation for the particular choice (49) is that solutions to the heat equation form a so-called EVI_0-flow of the entropy $\tilde{\mathbf{H}}$ in the L^2-Wasserstein metric [2, Theorem 11.1.4]; we emphasize that convexity of Ω is essential here. The EVI_0-property means that $\mathbb{R}_{\geq 0} \ni s \mapsto \mathbf{W}(c_i^s, [c_i^{n-1}]_\delta)^2$ is absolutely continuous — and in particular differentiable at almost every $s > 0$ — and that its derivative satisfies

$$\frac{1}{2} \limsup_{s \downarrow 0} \frac{\mathrm{d}}{\mathrm{d}s} \mathbf{W}(c_i^s, [c_i^{n-1}]_\delta)^2 \leq \tilde{\mathbf{H}}([c_i^{n-1}]_\delta) - \tilde{\mathbf{H}}(c_i^n). \tag{53}$$

We combine (53) with the fact that $\mathbf{E}_{\tau,\delta}(\boldsymbol{c}^s; \boldsymbol{c}^{n-1}) \geq \mathbf{E}_{\tau,\delta}(\boldsymbol{c}^n; \boldsymbol{c}^{n-1})$ by definition of $\boldsymbol{c}^n$ as a minimizer. The latter can be equivalently formulated as

$$\mathbf{E}(\boldsymbol{c}^n) - \mathbf{E}(\boldsymbol{c}^s) \leq \frac{1}{2\tau} \big[\mathbf{d}(\boldsymbol{c}^s, [\boldsymbol{c}^{n-1}]_\delta)^2 - \mathbf{d}(\boldsymbol{c}^n, [\boldsymbol{c}^{n-1}]_\delta)^2 \big].$$

Plugging in the definition of $\mathbf{d}$, dividing by $s > 0$, and passing to the limit $s \downarrow 0$ yields in view of (53):

$$\begin{aligned}
&\limsup_{s \downarrow 0} \frac{\mathbf{E}(\boldsymbol{c}^n) - \mathbf{E}(\boldsymbol{c}^s)}{s} \leq \frac{1}{2\tau} \limsup_{s \downarrow 0} \frac{\mathrm{d}}{\mathrm{d}s} \Big(\mathbf{d}(\boldsymbol{c}^s, [\boldsymbol{c}^{n-1}]_\delta)^2 \Big) \\
&\leq \frac{1}{2m_1\tau} \limsup_{s \downarrow 0} \frac{\mathrm{d}}{\mathrm{d}s} \mathbf{W}(c_1^s; [c_1^{n-1}]_\delta)^2 + \frac{1}{2m_2\tau} \limsup_{s \downarrow 0} \frac{\mathrm{d}}{\mathrm{d}s} \mathbf{W}(c_2^s; [c_2^{n-1}]_\delta)^2 \\
&\leq \frac{\tilde{\mathbf{H}}([c_1^{n-1}]_\delta) - \tilde{\mathbf{H}}(c_1^n)}{m_1\tau} + \frac{\tilde{\mathbf{H}}([c_2^{n-1}]_\delta) - \tilde{\mathbf{H}}(c_2^n)}{m_2\tau} = \frac{\mathbf{H}([\boldsymbol{c}^{n-1}]_\delta) - \mathbf{H}(\boldsymbol{c}^n)}{\tau}.
\end{aligned}$$

For simplification of the left-hand side above, observe that $\mathbf{E}(\boldsymbol{c}^n) - \mathbf{E}(\boldsymbol{c}^s) = \mathbf{E}_1(c_1^n) - \mathbf{E}_1(c_1^s)$ thanks to (52). For further estimation of the right-hand side, we use that $\mathbf{H}$ is a non-negative convex functional, and thus

$$\mathbf{H}([\boldsymbol{c}^{n-1}]_\delta) \leq (1-\delta)\mathbf{H}(\boldsymbol{c}^{n-1}) + \delta \mathbf{H}(\boldsymbol{\rho}) \leq \mathbf{H}(\boldsymbol{c}^{n-1}) + K\delta,$$

where $K = \mathbf{H}(\boldsymbol{\rho})$ depends only on the parameters of the problem. In summary, we have obtained so far that

$$\limsup_{s \downarrow 0} \frac{\mathbf{E}_1(c_1^n) - \mathbf{E}_1(c_1^s)}{s} \leq \frac{\mathbf{H}(\boldsymbol{c}^{n-1}) - \mathbf{H}(\boldsymbol{c}^n)}{\tau} + K\frac{\delta}{\tau}. \tag{54}$$

The remaining step is to derive a lower bound on the expression on the left-hand side in (54) of the same form as the right-hand side in (46). Ideally, we would like to express the left-hand side of (54) by means of the fundamental theorem of calculus as an average of $-\mathrm{d}\mathbf{E}_1(c_1^s)/\mathrm{d}s$. The technical difficulty here is that $\mathbf{E}_1(c_1^s) \to \mathbf{E}_1(c_1^n)$ as $s \downarrow 0$ might fail; note that Assumption 1 guarantees lower — but a priori *not upper* — semi-continuity of $\mathbf{E}_1$ with respect to the H^1-convergence (51). To overcome this, introduce for $\varepsilon \in (0,1)$ the following approximations $f_\varepsilon : [0,1] \to \mathbb{R}$ of f:

$$f_\varepsilon\left(\frac{1}{2} + z\right) = (1-\varepsilon)^{-1} f\left(\frac{1}{2} + (1-\varepsilon)z\right) \quad \text{for } -\frac{1}{2} \leq z \leq \frac{1}{2}.$$

Thanks to Assumption 1, f_ε' is positive, $1/(f_\varepsilon')^2$ is concave, and $f_\varepsilon(1-r) = -f_\varepsilon(r)$. Moreover, since $f'(\frac{1}{2}+z)$ is non-decreasing for $z>0$ and non-increasing for $z<0$ thanks to concavity of $1/(f')^2$ and symmetry of $f'(r)$ about $r=\frac{1}{2}$, it follows with $f_\varepsilon'(\frac{1}{2}+z) = f'(\frac{1}{2}+(1-\varepsilon)z)$ for all $z\in[-\frac{1}{2},\frac{1}{2}]$ that

$$0 < f_\varepsilon'(r) \le f'(r) \quad \text{for all } r\in[0,1]. \tag{55}$$

Observe further that $f_\varepsilon : [0,1]\to\mathbb{R}$ is smooth up to the boundary, and in particular, f_ε' is bounded. Therefore, the desired continuity, i.e., $f_\varepsilon(c_1^s)\to f_\varepsilon(c_1^n)$ in $H^1(\Omega)$ as $s\downarrow 0$, follows directly from (51).

From the smoothness of c_1^s for $s>0$ it follows in particular that $f_\varepsilon(c_1^s)$ is a smooth curve in $H^1(\Omega)$ for $s>0$ with $\partial_s f_\varepsilon(c_1^s) = f_\varepsilon'(c_i^s)\Delta c_1^s$. Observing further that $f_\varepsilon(c_1^s)$ satisfies homogeneous Neumann boundary conditions since c_1^s does, the fundamental theorem of calculus now implies for any $\bar s>0$ that

$$\begin{aligned}\frac{1}{2}\int_\Omega |\nabla f_\varepsilon(c_1^n)|^2\,\mathrm{d}x - \frac{1}{2}\int_\Omega |\nabla f_\varepsilon(c_1^{\bar s})|^2\,\mathrm{d}x &= -\int_0^{\bar s}\int_\Omega \nabla f_\varepsilon(c_1^s)\cdot\nabla\partial_s f_\varepsilon(c_1^s)\,\mathrm{d}x\,\mathrm{d}s\\ &= \int_0^{\bar s}\int_\Omega f_\varepsilon'(c_1^s)\Delta c_1^s \Delta f_\varepsilon(c_1^s)\,\mathrm{d}x\,\mathrm{d}s.\end{aligned}$$

The integrand for the s-integral is of the form J in (39). Since in the derivation of (44), no property of f other than smoothness, positivity of f', and concavity of $1/(f')^2$ was used, the estimate (44) also holds with f_ε in place of f, i.e.,

$$\int_\Omega f_\varepsilon'(c_1^s)\Delta c_1^s\Delta f_\varepsilon(c_1^s)\,\mathrm{d}x \ge \frac{1}{d}\int_\Omega \left[\Delta f_\varepsilon(c_1^s)\right]^2\mathrm{d}x$$

for each $s>0$; the technical hypotheses for the derivation of (44) — smoothness of c_1^s, the bounds $0<c_1^s<1$, and the homogeneous Neumann boundary conditions for $f(c_1^s)$ — are guaranteed by the properties of the heat flow.

Now we pass to the limit $\varepsilon\downarrow 0$. On the one hand, we can directly estimate $\int_\Omega |\nabla f_\varepsilon(c_1^n)|^2\,\mathrm{d}x \le \int_\Omega |\nabla f(c_1^n)|^2\,\mathrm{d}x$ thanks to (55). On the other hand, using that $f_\varepsilon(c_1^s)\to f(c_1^s)$ uniformly as well as the lower semi-continuity of the H^1- and the H^2-semi-norms with respect to convergence in measure, we finally arrive at

$$\frac{1}{2}\int_\Omega |\nabla f(c_1^n)|^2\,\mathrm{d}x - \frac{1}{2}\int_\Omega |\nabla f(c_1^{\bar s})|^2\,\mathrm{d}x \ge \frac{1}{d}\int_0^{\bar s}\int_\Omega \left[\Delta f(c_1^s)\right]^2\mathrm{d}x\,\mathrm{d}s. \tag{56}$$

Another — this time completely straight-forward — application of the fundamental theorem of calculus provides

$$\begin{aligned}&\frac{\chi}{2}\int_\Omega c_1^n(1-c_1^n)\,\mathrm{d}x - \frac{\chi}{2}\int_\Omega c_1^s(1-c_1^{\bar s})\,\mathrm{d}x = -\frac{\chi}{2}\int_0^{\bar s}\int_\Omega (1-2c_1^s)\partial_s c_1^s\,\mathrm{d}x\,\mathrm{d}s\\ &= \chi\int_0^{\bar s}\int_\Omega |\nabla c_1^s|^2\,\mathrm{d}x\,\mathrm{d}s \ge -\int_0^{\bar s}\left(\frac{1}{2d}\int_\Omega\left[\Delta f(c_1^s)\right]^2\mathrm{d}x + \frac{d\chi^2a^4|\Omega|}{2}\right)\mathrm{d}s,\end{aligned} \tag{57}$$

where we have derived the last estimate in analogy to (45), with $a>0$ defined there. Summation of (56) and (57) yields

$$\int_0^{\bar s}\left(\frac{1}{2d}\int_\Omega\left[\Delta f(c_1^n)\right]^2\mathrm{d}x - \frac{d\chi^2a^4|\Omega|}{2}\right)\mathrm{d}s \le \mathbf{E}_1(c_1^n) - \mathbf{E}_1(c_1^{\bar s}). \tag{58}$$

We substitute this estimate into (54) and obtain, using again the lower semi-continuity of the H^2-semi-norm,

$$\frac{1}{2d}\int_\Omega \left[\Delta f(c_1^s)\right]^2 \mathrm{d}x - \frac{d\chi^2 a^2 |\Omega|^4}{2} \le \frac{\mathbf{H}(\boldsymbol{c}^{n-1}) - \mathbf{H}(\boldsymbol{c}^n)}{\tau} + K\frac{\delta}{\tau}.$$

Recalling (24), this is (48).

Concerning the boundary condition: the estimate (56) implies in particular that there is a sequence (s_k) of $s_k > 0$ with $s_k \downarrow 0$ such that $\Delta f(c_1^{s_k})$ is bounded in $L^2(\Omega)$. This implies weak convergence of a further subsequence $f(c_1^{s_k'})$ to $f(c_1^n)$ in $H^2(\Omega)$, and this is sufficient to conclude that the normal trace $\mathbf{n}\cdot\nabla f(c_1^{s_k'})$ converges weakly in $L^2(\partial\Omega)$ to $\mathbf{n}\cdot\nabla f(c_1^n)$. In particular, $f(c_1^{s_k'})$'s homogeneous Neumann boundary condition is inherited by $f(c_1^n)$, and by Assumption 1, also c_1^n itself satisfies homogeneous Neumann conditions. □

Corollary 6. *There is a constant C, only depending on the parameters of the problem, such that, for all $N = 1, 2, \ldots$,*

$$\tau\sum_{n=1}^N \left\|\mathfrak{F}[c_1^n]\right\|_{L^2}^2 \le C(1 + N\tau). \tag{59}$$

Proof. This follows immediately from (37), since

$$\|\mathfrak{F}[c_1^n]\|_{L^2} \le \left\|\Delta f(c_1^n)\right\|_{L^2} + \chi\|\omega\|_{C^0}^2 \left\|c_1^n - \frac{1}{2}\right\|_{L^2} \le \left\|f(c_1^n)\right\|_{H^2} + M,$$

where M only depends on the parameters of the problem. □

5. A priori estimates on the auxiliary potentials

The aim of the current section is to derive — on the basis of the estimates on $\boldsymbol{c}^n$ — a priori estimates on the discrete approximation of the auxiliary functions $\boldsymbol{q}^n$. We start by showing that thanks to our construction of $\boldsymbol{c}^n$ and $\boldsymbol{q}^n$, the constitutive equation (18) holds with $\boldsymbol{c}^n$ in place of the true solution $\boldsymbol{c}$. Recall the definition of $\mathfrak{F}$ given there. Further recall that $\omega : [0,1] \to \mathbb{R}$ has been fixed such that (15) holds.

Proposition 7. *At each $n \ge 1$,*

$$\omega(c_1^n)q_2^n - \omega(c_2^n)q_1^n = \mathfrak{F}[c_1^n]. \tag{60}$$

Proof. Thanks to the continuity of $\boldsymbol{c}^n$ — recall that $H^2(\Omega) \subset C(\overline{\Omega})$ since $d \le 3$ — the set $P = \{x \in \Omega \,|\, 0 < c_1^n(x) < 1\}$ is open. Let $\eta \in C_c^\infty(\Omega)$ with support in P, and of vanishing mean, i.e., $\int_\Omega \eta(x)\,\mathrm{d}x = 0$. Define $\tilde{\boldsymbol{c}}^h = (\tilde{c}_1^h, \tilde{c}_2^h)$ with $\tilde{c}_1^h := c_1^n + h\eta$ and $\tilde{c}_2^h := c_2^n - h\eta$ for all $h > 0$ sufficiently small such that $\tilde{\boldsymbol{c}}^h \in \mathbf{X}_{\mathrm{mass}}$. Then $\mathbf{E}_{\tau,\delta}(\tilde{\boldsymbol{c}}^h; \boldsymbol{c}^{n-1}) \ge \mathbf{E}_{\tau,\delta}(\boldsymbol{c}^n; \boldsymbol{c}^{n-1})$ by definition of $\boldsymbol{c}^n$ as a global minimizer.

Recall that the (φ_i^n, ψ_i^n) are the (uniquely determined since $[c_i^{n-1}]_\delta > 0$) pairs of Kantorovich potentials for the optimal transport from $[c_i^{n-1}]_\delta$ to c_i^n normalized by (28). Analogously, let $(\tilde{\varphi}_i^h, \tilde{\psi}_i^h)$ be the (still uniquely determined) pair of potentials for the optimal transport from $[c_i^{n-1}]_\delta$ to $\tilde{c}_i^h$, normalized such that $\varphi_i^h(\bar{x}) = \varphi_i^n(\bar{x})$ for all $h > 0$ at some arbitrarily chosen $\bar{x} \in \Omega$. By the stability of optimal pairs, see e.g. [25, Theorem 1.52], it follows that $\tilde{\varphi}_i^h \to \varphi_i^n$ and $\tilde{\psi}_i^h \to \psi_i^n$ uniformly on Ω as $h \to 0$.

Using the dual characterization (23) of the Wasserstein distance, we obtain:

$$\begin{aligned}
&\int_\Omega \big(\tilde\psi_1^h c_1^n + \tilde\varphi_1^h[c_1^{n-1}]_\delta + \tilde\psi_2^h c_2^n + \tilde\varphi_2^h[c_2^{n-1}]_\delta\big)\,\mathrm{d}x + \mathbf{E}_1(c_1^n)\\
&\le \int_\Omega \big[\psi_1^n c_1^n + \varphi_1^n[c_1^{n-1}]_\delta + \psi_2^n c_2^n + \varphi_2^n[c_2^{n-1}]_\delta\big]\,\mathrm{d}x + \mathbf{E}_1(c_1^n)\\
&\quad = \mathbf{E}_{\tau,\delta}(\boldsymbol{c}^n;\boldsymbol{c}^{n-1})\\
&\qquad \le \mathbf{E}_{\tau,\delta}(\tilde{\boldsymbol{c}}^h;\boldsymbol{c}^{n-1})\\
&\qquad\quad = \int_\Omega \big(\tilde\psi_1^h \tilde c_1^h + \tilde\varphi_1^h[c_1^{n-1}]_\delta + \tilde\psi_2^h \tilde c_2^h + \tilde\varphi_2^h[c_2^{n-1}]_\delta\big)\,\mathrm{d}x + \mathbf{E}_1(\tilde c_1^h).
\end{aligned}$$

Subtracting the first line from the ultimate one, and dividing by $h>0$ yields:

(61)
$$\begin{aligned}
0 \le& \frac{1}{h}\int_\Omega \big(\tilde\psi_1^h(\tilde c_1^h - c_1^n) + \tilde\psi_2^h(\tilde c_2^h - c_2^n)\big)\,\mathrm{d}x + \frac{\mathbf{E}_1(\tilde c_1^h) - \mathbf{E}_1(c_1^n)}{h}\\
&= \int_\Omega (\tilde\psi_1^h - \tilde\psi_2^h)\eta\,\mathrm{d}x + \int_\Omega \frac{|\nabla f(\tilde c_1^h)|^2 - |\nabla f(c_1^n)|^2}{2h}\,\mathrm{d}x + \chi\int_\Omega \frac{\tilde c_1^h\tilde c_2^h - c_1^n c_2^n}{2h}\,\mathrm{d}x.
\end{aligned}$$

On the one hand, it follows immediately by boundedness of η that

(62)
$$\int_\Omega \frac{\tilde c_1^h\tilde c_2^h - c_1^n c_2^n}{2h}\,\mathrm{d}x = \int_\Omega \frac{h(c_2^n - c_1^n)\eta - h^2\eta^2}{2h}\,\mathrm{d}x \to \frac{1}{2}\int_\Omega (c_2^n - c_1^n)\eta\,\mathrm{d}x \quad \text{as } h\downarrow 0.$$

On the other hand, thanks to the elementary inequality $|a|^2 - |b|^2 \le 2a\cdot(a-b)$ for vectors $a,b\in\mathbb{R}^d$, and by the homogeneous Neumann boundary conditions satisfied by $f(c_1^n)$ and hence also by $f(\tilde c_1^h)$, we have that

$$\begin{aligned}
\int_\Omega \frac{|\nabla f(\tilde c_1^h)|^2 - |\nabla f(c_1^n)|^2}{2h}\,\mathrm{d}x &\le \int_\Omega \nabla f(\tilde c_1^h)\cdot\nabla\left[\frac{f(\tilde c_1^h) - f(c_1^n)}{h}\right]\mathrm{d}x\\
&= -\int_\Omega \Delta f(\tilde c_1^h)\,\frac{f(\tilde c_1^h) - f(c_1^n)}{h}\,\mathrm{d}x.
\end{aligned}$$

On the compact support $K\subset P$ of η, we have $\kappa \le c_1^n \le 1-\kappa$ for a suitable constant $\kappa>0$. We further have $\kappa/2 \le \tilde c_1^h \le 1-\kappa/2$ for all sufficiently small $h>0$. By smoothness of f on $[\kappa/2, 1-\kappa/2]$ thanks to Assumption 1, it follows that

$$\frac{f(\tilde c_1^h) - f(c_1^n)}{h} \to f'(c_1^n)\eta \quad \text{uniformly as } h\downarrow 0. \tag{63}$$

And it further follows that also

$$\Delta f(\tilde c_1^h) \to \Delta f(c_1^n) \quad \text{strongly in } L^2(\Omega) \text{ as } h\downarrow 0 \tag{64}$$

because of the following. We know from Lemma 5 that $f(c_1^n)$ lies in $H^2(\Omega)$, i.e., has square integrable first and second order derivatives. Again thanks to Assumption 1, f has a smooth inverse f^{-1} on $[f(\kappa), f(1-\kappa)]$. By the chain rule for the concatenation of Sobolev functions with smooth maps, it follows that $c_1^n = f^{-1}(f(c_1^n))$ has square integrable first and second order weak derivatives on K. By smoothness of η, the first and second order derivatives of c_1^n are uniformly approximated by the respective ones of $\tilde c_1^h$ on K. Using again the smoothness of f on $[\kappa/2, 1-\kappa/2]$, we conclude uniform approximation of $\Delta f(c_1^n)$ by $\Delta f(\tilde c_1^h)$ as $h\downarrow 0$. Now (64) follows

since $\tilde{c}_1^h = c_1^n$ in $\Omega \setminus K$. Plugging (62), (63) and (64) into (61), we obtain in the limit $h \downarrow 0$ that

$$0 \leq \int_\Omega \big[\psi_1^n - \psi_2^n - f'(c_1^n)\Delta f(c_1^n) - \chi\big(c_1^n - \tfrac{1}{2}\big)\big]\eta \,\mathrm{d}x.$$

The same inequality is true also for $-\eta$ in place of η, and thus is an equality. Since η was an arbitrary test function with support in P of zero average, there is a constant A such that

$$\psi_1^n - \psi_2^n + A = f'(c_1^n)\Delta f(c_1^n) + \chi\big(c_1^n - \tfrac{1}{2}\big)$$

holds a.e. on P. Multiplication by $1/f'(c_1^n) = \omega(c_1^n)\omega(c_2^n)$ leads to

$$\omega(c_1^n)\omega(c_2^n)[\psi_1^n - \psi_2^n + A] = \Delta f(c_1^n) + \chi\big(c_1^n - \tfrac{1}{2}\big)\omega(c_1^n)\omega(c_2^n). \tag{65}$$

On the complement $\Omega \setminus P$, where either $c_1^n = 0$ or $c_2^n = 0$, the left-hand side of (65) above vanishes a.e. because of $\omega(0) = 0$, and for the same reason, the second term on the right-hand side vanishes as well. Also $\Delta f(c_1^n)$ vanishes a.e., because $f(c_1^n) \in H^2(\Omega)$, and so all of its first and second order weak partial derivatives are zero a.e. on the level sets, see e.g. [11, Theorem 4.4]. That is, the validity of (65) extends from P to all of Ω.

Now integrate (65) on Ω to obtain:

$$\int_\Omega \frac{\psi_1^n - \psi_2^n + \chi\big(c_1^n - \frac{1}{2}\big) + A}{f'(c_1^n)} \,\mathrm{d}x = \int_\Omega \Delta f(c_1^n) \,\mathrm{d}x = 0,$$

where we have used that $f(c_1^n)$ satisfies homogeneous Neumann boundary conditions. In view of the normalization (28), it follows that $A = 0$. Finally, recalling the definition (16) of q_1 and q_2, the claim of the lemma now follows from (65). □

With the consitutive relation (60) at hand, we can now make the idea outlined in Section 1.4 of the introduction rigorous and prove τ-uniform integrability of the q_i^n. In the following, let

$$p_d := \frac{d}{d-1} = \begin{cases} 2 & \text{if } d = 2, \\ 3/2 & \text{if } d = 3. \end{cases} \tag{66}$$

Lemma 8. *There is a constant C, only depending on the parameters of the problem, such that, for all $N = 1, 2, \ldots$,*

$$\tau \sum_{n=1}^{N} \big(\|q_1^n\|_{L^{p_d}}^2 + \|q_2^n\|_{L^{p_d}}^2\big) \leq C(1 + N\tau). \tag{67}$$

Proof. We introduce the quantity

$$\bar{\mu}^n := \frac{c_1^n \psi_1^n}{m_1 \tau} + \frac{c_2^n \psi_2^n}{m_2 \tau} = \alpha(c_1^n) q_1^n + \alpha(c_2^n) q_2^n, \tag{68}$$

where the equality follows by definition (16) of the q_i^n, and since $\alpha(r)\omega(r) = r$. We notice further that, by the normalization (28),

$$\int_\Omega \bar{\mu}^n \,\mathrm{d}x = 0. \tag{69}$$

Next, we recall that

$$\mathfrak{F}[c_1^n] = \omega(c_2^n) q_1^n - \omega(c_1^n) q_2^n \tag{70}$$

by Proposition 7. Multiply (68) by $\omega(c_1^n)$ and (70) by $\alpha(c_2^n)$, then the sum amounts to

$$\omega(c_1^n)\bar{\mu}^n + \alpha(c_2^n)\mathfrak{F}[c_1^n] = (c_1^n + c_2^n)q_1^n = q_1^n.$$

Similarly, we obtain for q_2^n:

$$\omega(c_2^n)\bar{\mu}^n - \alpha(c_1^n)\mathfrak{F}[c_1^n] = (c_1^n + c_2^n)q_2^n = q_2^n.$$

Below, we show that

$$\tau \sum_{n=1}^{N} \left\|\bar{\mu}^n\right\|_{L^{pd}}^2 \leq C(1 + N\tau), \tag{71}$$

which in combination with the bound (59) on $\mathfrak{F}[c_1^n]$, and the fact that α and ω are bounded functions, yields (67).

To obtain (71), we estimate the gradient of $\bar{\mu}$ in $L^2(0,T;L^1(\Omega))$. From the definition of $\bar{\mu}^n$ in (68) and the fact that $\nabla c_2^n = -\nabla c_1^n$, it follows that

$$\nabla\bar{\mu}^n = \nabla c_1^n \left(\frac{\psi_1^n}{m_1\tau} - \frac{\psi_2^n}{m_2\tau}\right) + \frac{c_1^n}{m_1}\frac{\nabla\psi_1^n}{\tau} + \frac{c_1^n}{m_2}\frac{\nabla\psi_2^n}{\tau}. \tag{72}$$

We treat the two groups of terms on the right hand side separately. For estimation of the first term, we observe that $\omega(c_1^n)\omega(c_2^n)\nabla f(c_1^n) = \nabla c_1^n$, since $\omega(c_1^n)\omega(c_2^n)f'(c_1^n) = 1$ on the positivity set $P := \{0 < c_1^n < 1\}$, and both sides vanish a.e. on the complement $\Omega \setminus P$. Therefore, also recalling (70) again,

$$\nabla c_1^n \left(\frac{\psi_1^n}{m_1\tau} - \frac{\psi_2^n}{m_2\tau}\right) = \nabla f(c_1^n)\left[\omega(c_2^n)q_1^n - \omega(c_1^n)q_2^n\right] = \nabla f(c_1^n)\,\mathfrak{F}[c_1^n],$$

hence it follows that

$$\int_\Omega \left|\nabla c_1^n \left(\frac{\psi_1^n}{m_1\tau} - \frac{\psi_2^n}{m_2\tau}\right)\right| \mathrm{d}x \leq \|\nabla f(c_1^n)\|_{L^2}\|\mathfrak{F}[c_1^n]\|_{L^2}.$$

The second group of terms on the right hand-side of (72) is estimated by means of Hölder's inequality,

$$\int_\Omega \left|\frac{c_1^n}{m_1}\frac{\nabla\psi_1^n}{\tau} + \frac{c_1^n}{m_2}\frac{\nabla\psi_2^n}{\tau}\right| \mathrm{d}x \leq K\left[\int_\Omega \left(\frac{c_1^n}{m_1}\left|\frac{\nabla\psi_1^n}{\tau}\right|^2 + \frac{c_2^n}{m_2}\left|\frac{\nabla\psi_2^n}{\tau}\right|^2\right) \mathrm{d}x\right]^{1/2},$$

with a K that only depends on the parameters of the problem. Thanks to the normalization (69), it follows by means of the Poincare-Wirtinger inequality that

$$\begin{aligned}
\tau \sum_{n=1}^{N} \left\|\bar{\mu}^n\right\|_{L^{pd}}^2 &\leq C\tau \sum_{n=1}^{N} \left[\int_\Omega |\nabla\bar{\mu}^n| \,\mathrm{d}x\right]^2 \mathrm{d}t \\
&\leq C \sup_n \|\nabla f(c_1^n)\|_{L^2}^2 \tau \sum_{n=1}^{N} \|\mathfrak{F}[c_1]\|_{L^2}^2 \\
&\quad + CK^2\tau \sum_{n=1}^{N} \int_\Omega \left(\frac{c_1^n}{m_1}\left|\frac{\nabla\psi_1^n}{\tau}\right|^2 + \frac{c_2^n}{m_2}\left|\frac{\nabla\psi_2^n}{\tau}\right|^2\right) \mathrm{d}x,
\end{aligned}$$

with a constant C that only depends on the geometry of Ω. And so, recalling the estimates (31) on $\nabla f(c_1^n)$ in L^2, (59) on $\mathfrak{F}[c_1^n]$ in L^2, and (36) on the ψ_i^n in a weighted H^1-norm, we arrive at (71). □

6. Convergence and conclusion of the proof of Theorem 1

In this final section, we show that the time-discrete approximations $(\boldsymbol{c}_\tau^n)$ and $(\boldsymbol{q}_\tau^n)$ converge to a weak solutions of the initial boundary value problem (1)–(3) in the sense of Theorem 1. First, introduce the usual piecewise constant interpolations in time $\bar{\boldsymbol{c}}^\tau = (\bar{c}_1^\tau, \bar{c}_2^\tau)$ and $\bar{\boldsymbol{q}}^\tau = (\bar{q}_1^\tau, \bar{q}_2^\tau)$ with $\bar{c}_i^\tau \in L^\infty(\Omega_T)$ and $\bar{q}_i^\tau \in L^{p_d}(\Omega_T)$ by

$$\bar{c}_i^\tau(t;\cdot) = c_i^n, \quad \bar{q}_i^\tau(t;\cdot) = q_i^n \quad \text{for all } t \text{ with } (n-1)\tau < t \le n\tau.$$

Recall that $d = 2$ or $d = 3$, and the definition (66) of p_d.

Lemma 9. *There are functions $c_1, c_2 \in L^\infty_{loc}(\mathbb{R}_{\ge 0}; H^1(\Omega))$ with $f(c_1), f(c_2) \in L^2_{loc}(\mathbb{R}_{\ge 0}; H^2(\Omega))$, and $q_1, q_2 \in L^{p_d}(\mathbb{R}_{\ge 0} \times \Omega)$ such that, for each $T > 0$, in the limit $\tau \downarrow 0$, at least along a suitable sequence,*

$$\bar{q}_i^\tau \rightharpoonup q_i \quad \textit{weakly in } L^{p_d}(\Omega_T), \tag{73}$$

$$\bar{c}_i^\tau \to c_i \quad \textit{strongly in } L^r(\Omega_T), \textit{ for each } 1 \le r < \infty, \tag{74}$$

$$\nabla f(\bar{c}_i^\tau) \to \nabla f(c_i) \quad \textit{strongly in } L^{24/7}(\Omega_T), \tag{75}$$

$$f(\bar{c}_i^\tau) \rightharpoonup f(c_i) \quad \textit{weakly in } L^2(0,T;H^2(\Omega)). \tag{76}$$

Moreover, the limits c_i are Hölder continuous as curves in $L^2(\Omega)$.

Proof. The statements (73)–(76) are shown separately.

Proof of (73): recall that (67) provides a τ-uniform bound on $\bar{q}_i^\tau$ in $L^{p_d}(\Omega_T)$. Since this space is reflexive, there exist subsequences with respective weak limits.

Proof of (74): from (31) and the fact that $f'(r) \ge f'(1/2) > 0$ thanks to Assumption 1, it follows for $i = 1, 2$, and for any $T > 0$ that

$$\|\bar{c}_i^\tau\|^2_{L^\infty(0,T;H^1(\Omega))}\,\mathrm{d}t \le K \tag{77}$$

with a bound K that might depend on T, but is independent of τ. Moreover, (33) shows that the same sequences satisfy a uniform quasi-Hölder estimate in time,

$$\sup_{0<s<t<T} \big\|\bar{c}_i^\tau(s) - \bar{c}_i^\tau(t)\big\|_{L^2(\Omega)} \le C\big(\tau + |t-s|\big)^{1/4}. \tag{78}$$

We can thus invoke the generalized version of the Aubin-Lions compactness lemma from [24, Theorem 2]. There, we choose $L^2(\Omega)$ as the base space. The role of the coercive integrand is played by the $H^1(\Omega)$-norm — whose sublevels are clearly compact in $L^2(\Omega)$ by Rellich's theorem — so that (77) amounts to the required integral bound. Moreover, almost-continuity in time is guaranteed by (78). We thus conclude strong convergence of the $\bar{c}_i^\tau$ to respective limits c_i in $L^2(\Omega_T)$. And thanks to the uniform bound $0 \le \bar{c}_i^\tau \le 1$, this implies strong convergence in *any* $L^r(\Omega_T)$ with $r < \infty$. Moreover, these limits belong to $L^\infty(0,T;H^1(\Omega))$ by lower semi-continuity of the H^1-norm, and are Hölder continuous curves with respect to $L^2(\Omega)$, again thanks to (77) and (78) above.

Proof of (75): since $f : [0,1] \to \mathbb{R}$ is a continuous function, we conclude that also $f(\bar{c}_i^\tau)$ converges to the respective $f(c_i)$ in any $L^q(\Omega_T)$ with $q < \infty$. Further, observe that (37) implies that

$$\|f(\bar{c}_i^\tau)\|^2_{L^2(0,T;H^2(\Omega))} \le K \tag{79}$$

with a constant K that might depend on T, but not on τ. Thanks to lower semi-continuity of the H^2-norm, it follows that $f(c_i) \in L^2(0,T;H^2(\Omega))$ satisfies the same bound (79). We are now going to show that this implies convergence of $\nabla f(\bar{c}_i^\tau)$ to

$\nabla f(c_i)$ in $L^{24/7}(\Omega_T)$. By the Gagliardo-Nirenberg and Hölder's inequality, we have (independently of the dimension d):

$$\begin{aligned}
&\big\|\nabla\big[f(\bar{c}_i^\tau) - f(c_i)\big]\big\|_{L^{24/7}(\Omega_T)}^{24/7} = \int_0^T \big\|\nabla\big[f(\bar{c}_i^\tau) - f(c_i)\big]\big\|_{L^{24/7}(\Omega)}^{24/7}\,\mathrm{d}t \\
&\le C\int_0^T \big(\|f(\bar{c}_i^\tau)\|_{H^2(\Omega)} + \|f(c_i)\|_{H^2(\Omega)}\big)^{12/7}\|f(\bar{c}_i^\tau) - f(c_i)\|_{L^{12}(\Omega)}^{12/7}\,\mathrm{d}t \\
&\le C\left(\int_0^T \big[\|f(\bar{c}_i^\tau)\|_{H^2(\Omega)}^2 + \|f(c_i)\|_{H^2(\Omega)}^2\big]\,\mathrm{d}t\right)^{6/7}\left(\int_0^T \|f(\bar{c}_i^\tau) - f(c_i)\|_{L^{12}(\Omega)}^{12}\,\mathrm{d}t\right)^{1/7} \\
&\le C(2K)^{6/7}\|f(\bar{c}_i^\tau) - f(c_i)\|_{L^{12}(\Omega_T)}^{12/7},
\end{aligned}$$

where K is the bound from (79). Therefore, convergence of $f(c_i^\tau)$ carries over to convergence of $\nabla f(c_i^\tau)$.

Proof of (76): by (79) and reflexivity of $L^2(0,T;H^2(\Omega))$, we conclude weak convergence of $f(\bar{c}_i^\tau)$ in that space. For identification of the limit, we use (75) above. □

Having proven the existence of limits $\boldsymbol{c}$ and $\boldsymbol{q}$, we shall now verify that these satisfy the equations (21a) and (21c). The proof of (21a) is divided into two steps: in Lemma 10 below, we derive a discrete-in-time version of the continuity equation (21a), and in the subsequent Lemma 11, we pass to the limit $\tau \downarrow 0$.

Lemma 10. *Let $\zeta \in C^\infty(\overline{\Omega})$ satisfy homogeneous Neumann boundary conditions. Then*

(80)
$$\int_\Omega \zeta\frac{c_1^n - c_1^{n-1}}{\tau}\,\mathrm{d}x = -m_1\int_\Omega q_1^n\left[\alpha(c_1^n)\Delta\zeta + \omega(1-c_1^n)\,\nabla f(c_1^n)\cdot\nabla\zeta\right]\mathrm{d}x + \tau\boldsymbol{\epsilon}^n[\zeta],$$

where the error term satisfies

$$|\boldsymbol{\epsilon}^n[\zeta]| \le \frac{1}{2}\|\zeta\|_{C^2}\int_\Omega c_1^n\left|\frac{\nabla\psi_1^n}{\tau}\right|^2\,\mathrm{d}x + \|\zeta\|_{C^0}|\Omega|. \tag{81}$$

Proof. Recalling the representation (35) of c_1^{n-1} as push-foward of c_1^n, we obtain

$$\begin{aligned}
\int_\Omega \zeta\frac{c_1^n - c_1^{n-1}}{\tau}\,\mathrm{d}x &= \int_\Omega \zeta\frac{c_1^n - [c_1^{n-1}]_\delta}{\tau}\,\mathrm{d}x + \int_\Omega \zeta\frac{[c_1^{n-1}]_\delta - c_1^{n-1}}{\tau}\,\mathrm{d}x \\
&= \frac{1}{\tau}\int_\Omega\big[\zeta - \zeta\circ(\mathrm{id} - \nabla\psi_1^n)\big]c_1^n\,\mathrm{d}x + \frac{\delta}{\tau}\int_\Omega\zeta(\rho_1 - c_1^{n-1})\,\mathrm{d}x \\
&= \int_\Omega\left[\nabla\zeta\cdot\left(\frac{\nabla\psi_1^n}{\tau}\right) + \frac{\tau}{2}\left(\frac{\nabla\psi_1^n}{\tau}\right)^T\cdot\widehat{\nabla^2\zeta}\cdot\left(\frac{\nabla\psi_1^n}{\tau}\right)\right]c_1^n\,\mathrm{d}x \\
&\qquad + \frac{\delta}{\tau}\int_\Omega\zeta(\rho_1 - c_1^{n-1})\,\mathrm{d}x \\
&= \int_\Omega\nabla\zeta\cdot\left(\frac{\nabla\psi_1^n}{\tau}\right)c_1^n\,\mathrm{d}x + \tau\boldsymbol{\epsilon}^n[\zeta].
\end{aligned}$$

Above, $\widehat{\nabla^2\zeta}$ is the average of the Hessian $\nabla^2\zeta$ along the straight line segment joining x to $x - \nabla\psi_1^n(x)$. Consequently, also using that $|c_1^{n-1} - \rho_1| \le 1$ and that $\delta \le \tau^2$

by (24), we obtain the estimate (81) on $\boldsymbol{\epsilon}^n[\zeta]$. Now integrate by parts in the final integral above,

$$\int_\Omega \nabla\zeta\cdot\left(\frac{\nabla\psi_1^n}{\tau}\right)c_1^n\,\mathrm{d}x = -\int_\Omega\left[\frac{\psi_1^n}{\tau}c_1^n\Delta\zeta^n+\left(\frac{\psi_1^n}{\tau}\nabla c_1^n\right)\cdot\nabla\zeta\right]\mathrm{d}x. \tag{82}$$

We rewrite the integral on the right-hand side. First, observe that

$$c_1^n\psi_1^n = m_1\tau\alpha(c_1^n)q_1^n, \tag{83}$$

using on $\{c_1^n>0\}$ that $q_1^n=\omega(c_1^n)\psi_1^n/(m_1\tau)$ by definition, and on $\{c_1^n=0\}$ that both sides are zero, thanks to $\alpha(0)=0$. And second, observe that

$$\nabla c_1^n\,\psi_1^n = m_1\tau\omega(c_2^n)\nabla f(c_1^n)\,q_1^n, \tag{84}$$

since $\nabla c_1^n=\omega(c_1^n)\omega(c_2^n)\nabla f(c_1^n)$ on the positivity set $P=\{0<c_1^n<1\}$ by the fact that $f'(r)\omega(r)\omega(1-r)$ for $0<r<1$, and on the complement $\Omega\setminus P$ by the fact that both ∇c_1^n and $\nabla f(c_1^n)$ vanish a.e. Substitution of (83)&(84) in (82) yields (80). □

Lemma 11. *For all test functions $\xi\in C^\infty_{c,n}(\mathbb{R}_{>0}\times\Omega)$,*

$$\int_0^\infty\int_\Omega\left[-\partial_t\xi\,c_1+m_1\left(\Delta\xi\,\alpha(c_1)q_1+\nabla\xi\cdot\nabla f(c_1)\,\omega(1-c_1)q_1\right)\right]\mathrm{d}x\,\mathrm{d}t=0. \tag{85}$$

Proof. Introduce $\zeta^n(x):=\xi(n\tau;x)$ for $n=1,2,\ldots$, and the following piecewise constant and piecewise linear in time approximations ξ^τ and $\hat\xi^\tau$ of ξ, respectively, by:

$$\bar\xi^\tau(t;\cdot)=\zeta^n\quad\text{and}\quad\hat\xi^\tau(t;\cdot)=\frac{t-(n-1)\tau}{\tau}\zeta^{n+1}+\frac{n\tau-t}{\tau}\zeta^n$$

for all $t\in((n-1)\tau,n\tau]$. Use ζ^n for ζ in (80), sum over n:

$$\begin{aligned}\tau\sum_n\boldsymbol{\epsilon}^n[\zeta_n] &= \tau\sum_n\int_\Omega\left[c_1^n\frac{\zeta^n-\zeta^{n+1}}{\tau}+\Delta\zeta^n\alpha(c_1^n)q_1^n+\nabla\zeta^n\cdot\nabla f(c_1^n)\,\omega(1-c_1^n)q_1^n\right]\mathrm{d}x\\ &= \int_0^\infty\int_\Omega\left[\bar c_1^\tau\partial_t\hat\xi^\tau+\Delta\bar\xi^\tau\alpha(\bar c_1^\tau)\bar q_1^\tau+\nabla\bar\xi^\tau\cdot\nabla f(\bar c_1^\tau)\,\omega(1-\bar c_1^\tau)\bar q_1^\tau\right]\mathrm{d}x\,\mathrm{d}t.\end{aligned}$$

We pass to the limit $\tau\downarrow0$ on both sides. On the left-hand side, we have thanks to (81) and (30),

$$\begin{aligned}\tau\sum_{n=1}^N\left|\boldsymbol{\epsilon}^n[\zeta_n]\right| &\le \frac{m_1\|\xi\|_{C^2}}{2}\tau\sum_{n=1}^N\int_\Omega\left|\frac{\nabla\psi_1^n}{\tau}\right|\frac{c_1^n}{m_1}\,\mathrm{d}x+\tau(N\tau)|\Omega|\|\xi\|_{C^0}\\ &\le 2m_1\|\xi\|_{C^2}\mathbf{E}(\boldsymbol{c}^0)\,\tau+\tau|\Omega_T|\big(m_1+\|\xi\|_{C^0}\big),\end{aligned}$$

which converges to zero as $\tau\to0$. On the right-hand side, we use that $\partial_t\hat\xi^\tau\to\partial_t\xi$ as well as $\nabla\bar\xi^\tau\to\nabla\xi$ and $\Delta\bar\xi^\tau\to\Delta\xi$ uniformly. Moreover, by (74), and since $\alpha,\omega:[0,1]\to\mathbb{R}$ are continuous, we have in particular that

$$\alpha(\bar c_1^\tau)\to\alpha(c_1)\quad\text{and}\quad\omega(1-\bar c_1^\tau)\to\omega(1-c_1)$$

in $L^{24}(\Omega_T)$. In view of (73) and (75),

$$\bar q_1^\tau\nabla f(\bar c_1^\tau)\rightharpoonup q_1\nabla f(c_1)\quad\text{in } L^{24/23}(\Omega_T).$$

Therefore, the integral converges. □

The purpose of the next and final lemma is to derive the constitutive equations (21b) and (21c).

Lemma 12. *Let c_i and q_i be as in Lemma 9, then $c_1 + c_2 = 1$ and*

$$\omega(c_1)\, q_2 - \omega(c_2)\, q_1 = \Delta f(c_1) + \chi\big(c_1 - \tfrac{1}{2}\big)\omega(c_1)\omega(c_2). \tag{86}$$

Proof. Because of (29), we have $\bar{c}_1^\tau + \bar{c}_2^\tau = 1$, which clearly yields $c_1 + c_2 = 1$ in the limit, using the strong convergence from (74).

Next, recall that (60) is precisely (86), with $\bar{\boldsymbol{c}}^\tau$ in place of $\boldsymbol{c}$, and with $\bar{\boldsymbol{q}}^\tau$ in place of $\boldsymbol{q}$, i.e.,

$$\omega(\bar{c}_1^\tau)\, \bar{q}_2^\tau - \omega(\bar{c}_2^\tau)\, \bar{q}_1^\tau = \Delta f(\bar{c}_1^\tau) + \chi\big(\bar{c}_1^\tau - \tfrac{1}{2}\big)\omega(\bar{c}_1^\tau)\omega(\bar{c}_2^\tau). \tag{87}$$

By the strong convergence (74) of $\bar{c}_i^\tau$ and thanks to the continuity of ω, it follows that $\omega(\bar{c}_i^\tau)$ converges to $\omega(c_i)$ strongly in, say, $L^3(\Omega_T)$. In combination with the weak convergence (73) of the $\bar{q}_i^\tau$, we obtain weak convergence of the products,

$$\omega(\bar{c}_1^\tau)\, \bar{q}_2^\tau \rightharpoonup \omega(c_1) q_2 \quad \text{and} \quad \omega(\bar{c}_2^\tau)\, \bar{q}_1^\tau \rightharpoonup \omega(c_2) q_1$$

in $L^1(\Omega)$. Trivially, also

$$\big(\bar{c}_1^\tau - \tfrac{1}{2}\big)\omega(\bar{c}_1^\tau)\omega(\bar{c}_2^\tau) \to \big(c_1 - \tfrac{1}{2}\big)\omega(c_1)\omega(c_2)$$

strongly in $L^1(\Omega_T)$. Finally, weak convergence $\Delta f(\bar{c}_1^\tau) \rightharpoonup \Delta f(\bar{c}_1)$ in $L^2(\Omega_T)$ is implied by (76). We thus obtain (86) as limit of (87). □

The proof of Theorem 1 is a conclusion of Lemma 11 and Lemma 12.

Appendix A

Lemma 13. *There is a constant K, expressible in terms of ρ_1/m_1, ρ_2/m_2, and geometric properties of Ω, such that for all $\boldsymbol{c} \in \mathbf{X}_{mass}$:*

$$\mathbf{d}(\boldsymbol{c}, [\boldsymbol{c}]_\delta)^2 \leq K\delta. \tag{88}$$

Consequently, for any $\boldsymbol{c}, \bar{\boldsymbol{c}} \in \mathbf{X}_{mass}$:

$$\mathbf{d}(\boldsymbol{c}, \bar{\boldsymbol{c}})^2 \leq 2\mathbf{d}\big(\boldsymbol{c}, [\bar{\boldsymbol{c}}]_\delta\big)^2 + 2K\delta. \tag{89}$$

Proof. Define a (sub-optimal) transport plan γ from c_i to $[c_i]_\delta = (1-\delta)c_i + \delta\rho_i$ as follows:

$$\gamma = (1-\delta)(\mathrm{id}, \mathrm{id})\#(c_i \mathcal{L}_\Omega) + \frac{\delta}{|\Omega|}(c_i \mathcal{L}_\Omega) \otimes \mathcal{L}_\Omega.$$

The marginals are as desired, i.e., for any $\xi, \eta \in C(\Omega)$, we have that

$$\begin{aligned}
\iint_{\Omega\times\Omega} \xi(x)\, \mathrm{d}\gamma(x,y) &= (1-\delta)\int_\Omega \xi(x) c_i(x)\, \mathrm{d}x + \delta \int_\Omega \xi(x) c_i(x)\, \mathrm{d}x \fint_\Omega \mathrm{d}y \\
&= \int_\Omega \xi(x)\eta(x)\, \mathrm{d}x, \\
\iint_{\Omega\times\Omega} \eta(y)\, \mathrm{d}\gamma(x,y) &= (1-\delta)\int_\Omega \eta(y) c_i(y)\, \mathrm{d}x + \delta \fint_\Omega c_i(x)\, \mathrm{d}x \int_\Omega \eta(y)\, \mathrm{d}y \\
&= \int_\Omega \eta(y)\big[(1-\delta)c_i(y) + \delta\rho_i\big]\, \mathrm{d}y.
\end{aligned}$$

And the corresponding costs amount to

$$\begin{aligned}\iint_{\Omega\times\Omega}|x-y|^2\,\mathrm{d}\gamma(x,y) &= \frac{\delta}{|\Omega|}\iint_{\Omega\times\Omega}|x-y|^2 c_i(x)\,\mathrm{d}x\,\mathrm{d}y\\ &\le \frac{\delta\ \mathrm{diam}(\Omega)^2}{|\Omega|}\int_\Omega c_i(x)\,\mathrm{d}x\int_\Omega \mathrm{d}y = \delta\ \mathrm{diam}(\Omega)^2|\Omega|\rho_i.\end{aligned}$$

In summary,

$$\mathbf{d}(\boldsymbol{c},[\boldsymbol{c}]_\delta)^2 = \frac{\mathbf{W}(c_1,[c_1]_\delta)^2}{m_1}+\frac{\mathbf{W}(c_2,[c_2]_\delta)^2}{m_2} \le \delta\ \mathrm{diam}(\Omega)^2\left(\frac{|\Omega|\rho_1}{m_1}+\frac{|\Omega|\rho_2}{m_2}\right).$$

The inequality (89) now follows from the triangle inequality, that is inherited from $\mathbf{W}$ to $\mathbf{d}$,

$$\mathbf{d}(\boldsymbol{c},\bar{\boldsymbol{c}})^2 \le 2\mathbf{d}\big(\boldsymbol{c},[\bar{\boldsymbol{c}}]_\delta\big)^2 + 2\mathbf{d}\big(\bar{\boldsymbol{c}},[\bar{\boldsymbol{c}}]_\delta\big)^2,$$

in combination with (88). □

Lemma 14. *For all $\boldsymbol{c},\boldsymbol{c}'\in\mathbf{X}_{mass}$ with $c_i,c_i'\in H^1(\Omega)$ and $c_1+c_2\equiv 1\equiv c_1'+c_2'$,*

$$\|\boldsymbol{c}'-\boldsymbol{c}\|_{L^2}^2 \le 2\sqrt{m_1}\big(\|\nabla c_1\|_{L^2}+\|\nabla c_1'\|_{L^2}\big)\mathbf{d}(\boldsymbol{c}',\boldsymbol{c}). \tag{90}$$

Proof. Let (φ_1,ψ_1) be a pair of Kantorovich potentials for the optimal transport from c_1 to c_1'. For each $s\in[0,1]$, define $T_s:\Omega\to\Omega$ by $T_s(x)=x-s\nabla\varphi_1(x)$. For any test function $\zeta\in C^1(\overline{\Omega})$,

$$\begin{aligned}\int_\Omega [c_1'-c_1]\zeta\,\mathrm{d}x &= \int_\Omega \big[\zeta\circ T_1-\zeta\big]c_1\,\mathrm{d}x\\ &= \int_\Omega\left[\int_0^1 \nabla\zeta\circ T_s\cdot\nabla\varphi\,\mathrm{d}s\right]c_1\,\mathrm{d}x\\ &\le \int_0^1\left(\int_\Omega |\nabla\zeta|^2\circ T_s\,c_1\,\mathrm{d}x\right)^{1/2}\left(\int_\Omega|\nabla\varphi_1|^2c_1\,\mathrm{d}x\right)^{1/2}\mathrm{d}s\\ &= \int_0^1\left(\int_\Omega|\nabla\zeta|^2 T_s\#c_1\,\mathrm{d}x\right)^{1/2}\mathrm{d}s\,\mathbf{W}(c_1,c_1').\end{aligned}$$

Using the fact that

$$\sup_\Omega T_s\#c_1 \le \max\left(\sup_\Omega c_1,\sup_\Omega c_1'\right)=1,$$

it follows that

$$\int_\Omega\big|[c_1'-c_1]\zeta\big|\,\mathrm{d}x \le \|\nabla\zeta\|_{L^2}\mathbf{W}(c_1,c_1'),$$

and consequently — using for ζ approximations of $c_1'-c_1$ in C^1 —

$$\|c_1'-c_1\|_{L^2}^2 \le \|\nabla(c_1'-c_1)\|_{L^2}\mathbf{W}(c_1,c_1') \le \big(\|\nabla c_1'\|_{L^2}+\|\nabla c_1\|_{L^2}\big)\mathbf{W}(c_1,c_1').$$

By hypothesis, $c_1-c_1'=c_2'-c_2$. Thus, recalling the definition of $\mathbf{d}$, we obtain

$$\begin{aligned}\|\boldsymbol{c}'-\boldsymbol{c}\|_{L^2}^2 &= 2\|c_1'-c_1\|_{L^2}^2\\ &\le 2\sqrt{m_1}\big(\|\nabla c_1\|_{L^2}+\|\nabla c_1'\|_{L^2}\big)^2\left(\frac{\mathbf{W}(c_1',c_1)^2}{m_1}\right)^{1/2}\\ &\le 2\sqrt{m_1}\big(\|\nabla c_1\|_{L^2}+\|\nabla c_1'\|_{L^2}\big)\mathbf{d}(\boldsymbol{c}',\boldsymbol{c}).\end{aligned}$$

□

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