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On the unique solvability of a nonlocal phase separation problem for multicomponent systems

Jens André Griepentrog[1]

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[1] Weierstrass Institut
for Applied Analysis and Stochastics
Mohrenstrasse 39
10117 Berlin
Germany
E-Mail: griepent@wias-berlin.de

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Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

A nonlocal model of phase separation in multicomponent systems is presented. It is derived from conservation principles and minimization of free energy containing a nonlocal part due to particle interaction. In contrast to the classical Cahn–Hilliard theory with higher order terms this leads to an evolution system of second order parabolic equations for the particle densities, coupled by nonlinear and nonlocal drift terms, and state equations which involve both chemical and interaction potential differences. Applying fixed-point arguments and comparison principles we prove the existence of variational solutions in standard Hilbert spaces for evolution systems. Moreover, using some regularity theory for parabolic boundary value problems in Hölder spaces we get the unique solvability of our problem. We conclude our considerations with the presentation of simulation results for a ternary system.

1 Introduction

We consider a closed multicomponent system with particles of type $k \in \{0, 1, \ldots, n\}$ occupying a spatial domain. In our model we assume, that the particles jump around on a given microscopically scaled lattice following a stochastic exchange process (see [8], [16], [17]). On each lattice site sits exactly one particle (exclusion principle). Two particles of type k and ℓ change their sites x and y with probability $p_{k\ell}(x, y)$ due to diffusion and nonlocal interaction. The hydrodynamical limit leads to a system of conservation laws for $k \in \{0, 1, \ldots, n\}$,

$$u_k' + \nabla \cdot j_k = 0 \text{ in } (0,T) \times U\,, \quad \nu \cdot j_k = 0 \text{ on } (0,T) \times \partial U\,, \quad u_k(0) = g_k \text{ in } U\,,$$

for (scaled) *particle densities* $u_0, u_1, \ldots, u_n$, their *initial values* $g_0, g_1, \ldots, g_n$ and *current densities* $j_0, j_1, \ldots, j_n$. Here, $(0, T)$ denotes a time interval and ν is the outer unit normal on the boundary ∂U of the spatial domain $U \subset \mathbb{R}^m$.

Due to the exclusion principle of the stochastic process we can assume $\sum_{k=0}^n u_k = 1$, $\sum_{k=0}^n g_k = 1$ and $\sum_{k=0}^n j_k = 0$, that means, only n of the above $n+1$ equations are independent of each other. Hence, we can drop out one redundant equation, say the equation for the zero component, and describe the state of the system by the vectors $u = (u_1, \ldots, u_n)$ and $g = (g_1, \ldots, g_n)$. Nevertheless, it is not only comfortable but also necessary to work with the densities of the zero component. Thus, for given u we will always use the notation

$$u_0 \overset{\text{def}}{=} 1 - \sum_{k=1}^{n} u_k \,. \tag{1}$$

To establish thermodynamical relations between current densities, particle densities and their conjugated variables we minimize the free energy functional of the closed system.

In the field of phase separation models the classical Cahn–Hilliard theory deals with sharp interface models. They consider local free energy densities containing squared gradients of the particle densities to describe surface tension and interface movement. The minimization process leads to fourth order Cahn–Hilliard equations (see [1]) where no comparison principle is available. There occur difficulties to ensure the physical requirement $0 \le u_0, u_1, \dots, u_n \le 1$ for the solutions and to prove their uniqueness (see [5]).

In contrast to that it seems to be reasonable and even more adequate to consider diffuse interface models and free energy functionals with nonlocal expressions. As a straightforward generalization of the nonlocal phase separation model for binary systems (see [3], [6], [7], [10]) we will choose $F = F_1 + F_2$ with

$$F_1(u) = \int_U f(u(x))\,dx\,, \quad F_2(u) = \frac{1}{2}\sum_{k=0}^{n}\int_U (Ku)_k(x)\,u_k(x)\,dx\,, \tag{2}$$

$$f(u) = \sum_{k=0}^{n} u_k \log(u_k)\,, \quad (Ku)_k(x) = \sum_{\ell=0}^{n}\int_U \kappa_{k\ell}(x,y)\,u_\ell(y)\,dy\,. \tag{3}$$

The convex function f and the symmetric $(n+1)\times(n+1)$-matrix kernel κ define the chemical part F_1 and the nonlocal interaction part F_2 of the functional F, respectively. Minimizing F under the constraint of particle number conservation we identify the conjugated variables of the densities as *grand chemical potential differences*

$$v_k = \frac{\partial F}{\partial u_k} = \mu_k + w_k\,, \quad k \in \{1,\dots,n\}\,,$$

where μ_k and w_k are *chemical* and *interaction potential differences*, respectively,

$$\mu_k = \frac{\partial F_1}{\partial u_k} = \log(u_k) - \log(u_0)\,, \quad w_k = \frac{\partial F_2}{\partial u_k} = (Ku)_k - (Ku)_0\,, \quad k \in \{1,\dots,n\}\,.$$

The hydrodynamical limit process (see [8], [16], [17]) yields current densities

$$j_k = -\sum_{\ell=1}^{n} a_{k\ell}(u)\nabla v_\ell\,, \quad k \in \{1,\dots,n\}\,,$$

where the *mobility* has the form $a(u) = d(u)(D^2 f(u))^{-1}$ and $d(u)$ denotes the *diffusivity*. Hence, we can interpret the above nonlocal phase separation model as a system of drift-diffusion equations with semilinear diffusion and nonlinear nonlocal drift terms, if we rewrite the currents as

$$j_k = -\sum_{\ell=1}^{n} d_{k\ell}(u)\nabla u_\ell - \sum_{\ell=1}^{n} a_{k\ell}(u)\nabla w_\ell\,, \quad k \in \{1,\dots,n\}\,.$$

For the sake of simplicity we consider only the special case $d_{k\ell} = \delta_{k\ell}$. An elementary computation of the inverse Hessian matrix $(D^2 f(u))^{-1}$ yields the following expressions for the mobility coefficients

$$a_{k\ell}(u) = \delta_{k\ell}\, u_k - u_\ell u_k\,, \quad k,\ell \in \{1,\dots,n\}\,.$$

In Section 2 we formulate the problem and general assumptions. Applying fixed-point arguments and comparison principles in Section 3 we prove the existence of variational solutions in standard Hilbert spaces for evolution systems. Section 4 is dedicated to the regularity theory for parabolic boundary value problems with nonsmooth data in Sobolev–Morrey and Hölder spaces (see [11]) which is the main tool for our proof of the unique solvability given in Section 5. In Section 6 we conclude our considerations with the presentation of simulation results for a ternary system.

2 General assumptions and formulation of the problem

The following general assumptions are valid for the whole work. Let $(0,T)$ be a time interval of finite length and $U \subset \mathbb{R}^m$ a bounded Lipschitz domain. For $\delta > 0$ and $x \in \mathbb{R}^m$ we define the open ball $B(x,\delta) \overset{\text{def}}{=} \{y \in \mathbb{R}^m : |x-y| < \delta\}$. Furthermore, let $D_1 f, \dots, D_m f$ denote the partial derivatives, ∇f the gradient, and f' the time derivative of a function f, respectively.

For the functional analytic formulation of our problem we will use standard Lebesgue and Sobolev spaces

$$H \overset{\text{def}}{=} L^2(U;\mathbb{R}^n)\,, \quad V \overset{\text{def}}{=} H^1(U;\mathbb{R}^n)\,, \quad L^\infty \overset{\text{def}}{=} L^\infty(U;\mathbb{R}^n)\,,$$

respectively, and their generalizations suitable for evolution systems,

$$\mathcal{H}(T) \overset{\text{def}}{=} L^2((0,T);H)\,, \quad \mathcal{V}(T) \overset{\text{def}}{=} L^2((0,T);V)\,, \quad \mathcal{L}^\infty(T) \overset{\text{def}}{=} L^\infty((0,T);L^\infty)\,.$$

Having in mind the notation (1), we define *simplices* $S \subset L^\infty$ and $\mathcal{S}(T) \subset \mathcal{L}^\infty(T)$ by

$$S \overset{\text{def}}{=} \{g \in L^\infty :\ 0 \le g_0, g_1, \dots, g_n \le 1\}\,, \quad \mathcal{S}(T) \overset{\text{def}}{=} \{u \in \mathcal{L}^\infty(T) :\ 0 \le u_0, u_1, \dots, u_n \le 1\}\,.$$

We refer to [9], [15], [18] for the theory of the space

$$\mathcal{W}(T) \overset{\text{def}}{=} \{u \in \mathcal{V}(T) : u' \in \mathcal{V}(T)^*\}\,.$$

Definition 1 We define the linear *diffusion operator* $\mathcal{L} : \mathcal{V}(T) \longrightarrow \mathcal{V}(T)^*$ by

$$\langle \mathcal{L}u, \varphi \rangle \stackrel{\text{def}}{=} \sum_{k=1}^{n} \int_0^T \int_U \nabla u_k \cdot \nabla \varphi_k \, dx \, ds \,, \quad u, \varphi \in \mathcal{V}(T) \,, \tag{4}$$

and the nonlinear *drift operator* $\mathcal{A} : \mathcal{L}^\infty(T) \times \mathcal{V}(T) \longrightarrow \mathcal{V}(T)^*$ by

$$\langle \mathcal{A}(u, w), \varphi \rangle \stackrel{\text{def}}{=} \sum_{k=1}^{n} \sum_{\ell=1}^{n} \int_0^T \int_U a_{k\ell}(u) \nabla w_\ell \cdot \nabla \varphi_k \, dx \, ds \,, \tag{5}$$

for $(u, w) \in \mathcal{L}^\infty(T) \times \mathcal{V}(T)$, $\varphi \in \mathcal{V}(T)$, with coefficients

$$a_{k\ell}(u) \stackrel{\text{def}}{=} \delta_{k\ell} \, u_k - u_\ell u_k \,, \quad k, \ell \in \{1, \ldots, n\} \,. \tag{6}$$

We assume, that the interaction between particles can be described by means of a (possibly nonlinear and nonlocal) Lipschitz continuous *interaction operator* $\mathcal{P} : \mathcal{H}(T) \longrightarrow \mathcal{V}(T)$ which has a Lipschitz constant $L > 0$, that means,

$$\|\mathcal{P}u - \mathcal{P}\hat{u}\|_{\mathcal{V}(T)} \leq L \, \|u - \hat{u}\|_{\mathcal{H}(T)} \quad \text{for all } \; u, \hat{u} \in \mathcal{H}(T) \,. \tag{7}$$

Now, we can rigorously formulate the concept of a solution of our problem.

Definition 2 (Solution) For a given initial value $g \in S$ we are looking for a *solution* $(u, w) \in [\mathcal{W}(T) \cap \mathcal{S}(T)] \times \mathcal{V}(T)$ *of the evolution system*

$$u' + \mathcal{L}u + \mathcal{A}(u, w) = 0 \,, \quad w = \mathcal{P}u \,, \quad u(0) = g \,. \tag{P}$$

3 Existence of solutions

At first we will solve a *regularized* problem with truncated nonlinearities. To do so, for $c \in \mathbb{R}$ we define the truncations

$$c^\bullet \stackrel{\text{def}}{=} -\min\{c, 0\} \,, \quad c^\diamond \stackrel{\text{def}}{=} \min\{\max\{c, 0\}, 1\} \,,$$

and we carry over this setting in the usual way to the concept of truncated functions.

Definition 3 We define a *regularized drift operator* $\mathcal{R} : \mathcal{H}(T) \times \mathcal{V}(T) \longrightarrow \mathcal{V}(T)^*$ by

$$\langle \mathcal{R}(u, w), \varphi \rangle \stackrel{\text{def}}{=} \sum_{k=1}^{n} \sum_{\ell=1}^{n} \int_0^T \int_U r_{k\ell}(u) \nabla w_\ell \cdot \nabla \varphi_k \, dx \, ds \,, \tag{8}$$

for $(u, w) \in \mathcal{H}(T) \times \mathcal{V}(T)$, $\varphi \in \mathcal{V}(T)$, and suitably truncated coefficients

$$r_{k\ell}(u) \stackrel{\text{def}}{=} \sum_{h=0}^{n} \delta_{k\ell} \, u_k^\diamond u_h^\diamond - u_\ell^\diamond u_k^\diamond \,, \quad k, \ell \in \{1, \ldots, n\} \,, \tag{9}$$

and, a *regularized interaction operator* $\mathcal{Q} : \mathcal{H}(T) \longrightarrow \mathcal{V}(T)$ by $\mathcal{Q}u \stackrel{\text{def}}{=} \mathcal{P}u^\diamond$ for $u \in \mathcal{H}(T)$.

Lemma 1 (Solvablity of a regularized problem) *For every $g \in S$ there exists a solution $(u,w) \in \mathcal{W}(T) \times \mathcal{V}(T)$ of the regularized problem*

$$u' + \mathcal{L}u + \mathcal{R}(u,w) = 0\,, \quad w = \mathcal{Q}u\,, \quad u(0) = g\,. \tag{R}$$

Proof 1. Our proof is based on the application of Schauder's fixed-point principle. Let $L > 0$ be a Lipschitz constant of $\mathcal{P} : \mathcal{H}(T) \longrightarrow \mathcal{V}(T)$ (see (7)) and $g \in S$ be a fixed initial value. For every $u \in \mathcal{H}(T)$ we have $\mathcal{Q}u \in \mathcal{V}(T)$ and $\mathcal{R}(u, \mathcal{Q}u) \in \mathcal{V}(T)^*$. Hence, there exists a uniquely determined solution $\mathcal{T}u \in \mathcal{W}(T) \subset C([0,T];H)$ (see [9], [15]) of the evolution problem

$$(\mathcal{T}u)' + \mathcal{L}\mathcal{T}u = -\mathcal{R}(u, \mathcal{Q}u)\,, \quad (\mathcal{T}u)(0) = g\,. \tag{10}$$

In other words, we have properly defined a fixed-point operator $\mathcal{T} : \mathcal{H}(T) \longrightarrow \mathcal{H}(T)$. We can apply Schauder's theorem, if we are able to prove, that $\mathcal{T} : \mathcal{H}(T) \longrightarrow \mathcal{H}(T)$ is completely continuous and $\mathcal{T}[\mathcal{B}] \subset \mathcal{B}$ holds true for a closed ball $\mathcal{B} \subset \mathcal{H}(T)$ with a radius depending only on the data of the problem.

2. Let $u \in \mathcal{H}(T)$ and $\mathcal{T}u \in \mathcal{W}(T)$ be the solution of problem (10). Applying the test function $\varphi = \mathcal{T}u \in \mathcal{W}(T)$ to (10) and Young's inequality to (8) we get the estimate

$$\begin{aligned}
&\sum_{k=1}^{n} \int_0^t \langle (\mathcal{T}u)_k'(s), (\mathcal{T}u)_k(s) \rangle\, ds + \sum_{k=1}^{n} \int_0^t \int_U \nabla(\mathcal{T}u)_k \cdot \nabla(\mathcal{T}u)_k \, dx\, ds \\
&\leq \frac{1}{4} \sum_{k=1}^{n} \sum_{\ell=1}^{n} \int_0^t \int_U |r_{k\ell}(u) \nabla(\mathcal{Q}u)_\ell|^2 \, dx\, ds + \sum_{k=1}^{n} \int_0^t \int_U |\nabla(\mathcal{T}u)_k|^2 \, dx\, ds\,,
\end{aligned}$$

for all $t \in [0,T]$. Using the fact, that by (9) we have $|r_{k\ell}| \leq n$ for $k, \ell \in \{1, \ldots, n\}$, the formula of partial integration yields

$$\frac{1}{2} \sum_{k=1}^{n} \int_U |(\mathcal{T}u)_k(t)|^2 \, dx - \frac{1}{2} \sum_{k=1}^{n} \int_U |g_k|^2 \, dx \leq \frac{n^3}{4} \sum_{\ell=1}^{n} \int_0^T \int_U |\nabla(\mathcal{Q}u)_\ell|^2 \, dx\, ds\,,$$

for all $t \in [0,T]$. Integrating both sides of the inequality over $t \in (0,T)$ we can use the Lipschitz continuity of $\mathcal{P} : \mathcal{H}(T) \longrightarrow \mathcal{V}(T)$ (see (7)) to get

$$\begin{aligned}
\|\mathcal{T}u\|^2_{\mathcal{H}(T)} &\leq T\, \|g\|^2_H + \tfrac{n^3 T}{2}\, \|\mathcal{Q}u\|^2_{\mathcal{V}(T)} \\
&\leq T\, \|g\|^2_H + n^3 T \left\{ \|\mathcal{P}0\|^2_{\mathcal{V}(T)} + \|\mathcal{P}u^\diamond - \mathcal{P}0\|^2_{\mathcal{V}(T)} \right\} \\
&\leq T\, \|g\|^2_H + n^3 T \left\{ \|\mathcal{P}0\|^2_{\mathcal{V}(T)} + L\, \|u^\diamond\|^2_{\mathcal{H}(T)} \right\},
\end{aligned}$$

that means, we have $\|\mathcal{T}u\|^2_{\mathcal{H}(T)} \leq \delta^2$ for all $u \in \mathcal{H}(T)$, if we fix the radius $\delta > 0$ by

$$\delta^2 \stackrel{\text{def}}{=} T\, \|g\|^2_H + n^3 T \left\{ \|\mathcal{P}0\|^2_{\mathcal{V}(T)} + nLT\lambda^m(U) \right\}.$$

Hence, we get $\mathcal{T}[\mathcal{B}] \subset \mathcal{B}$ for the closed ball $\mathcal{B} \stackrel{\text{def}}{=} \{u \in \mathcal{H}(T) : \|u\|_{\mathcal{H}(T)} \leq \delta\}$.

3. Additionally, let $\{u_i\}_{i\in\mathbb{N}} \subset \mathcal{H}(T)$ be a sequence such that $\lim_{i\to\infty} \|u_i - u\|_{\mathcal{H}(T)} = 0$. For every $i \in \mathbb{N}$ there exists a uniquely determined solution $\mathcal{T}u_i \in \mathcal{W}(T)$ of the problem

$$(\mathcal{T}u_i)' + \mathcal{L}\mathcal{T}u_i = -\mathcal{R}(u_i, \mathcal{Q}u_i)\,, \quad (\mathcal{T}u_i)(0) = g\,.$$

Because $\mathcal{T}u \in \mathcal{W}(T)$ is the solution of problem (10), for every $i \in \mathbb{N}$ it follows

$$(\mathcal{T}u_i - \mathcal{T}u)' + \mathcal{L}(\mathcal{T}u_i - \mathcal{T}u) = \mathcal{R}(u, \mathcal{Q}u) - \mathcal{R}(u_i, \mathcal{Q}u_i)\,, \quad (\mathcal{T}u_i - \mathcal{T}u)(0) = 0\,. \tag{11}$$

Applying the test function $\varphi = \mathcal{T}u_i - \mathcal{T}u \in \mathcal{W}(T)$ to (11) Young's inequality yields the following estimate

$$\begin{aligned}
&\sum_{k=1}^{n} \int_0^t \langle (\mathcal{T}u_i - \mathcal{T}u)_k'(s), (\mathcal{T}u_i - \mathcal{T}u)_k(s)\rangle\, ds + \sum_{k=1}^{n} \int_0^t \int_U |\nabla(\mathcal{T}u_i - \mathcal{T}u)_k|^2\, dx\, ds \\
&\le \frac{1}{2} \sum_{k=1}^{n} \sum_{\ell=1}^{n} \int_0^t \int_U |(r_{k\ell}(u) - r_{k\ell}(u_i))\nabla(\mathcal{Q}u)_\ell|^2\, dx\, ds + \frac{1}{2} \sum_{k=1}^{n} \int_0^t \int_U |\nabla(\mathcal{T}u_i - \mathcal{T}u)_k|^2\, dx\, ds \\
&+ \frac{1}{2} \sum_{k=1}^{n} \sum_{\ell=1}^{n} \int_0^t \int_U |r_{k\ell}(u_i)\nabla(\mathcal{Q}u_i - \mathcal{Q}u)_\ell|^2\, dx\, ds + \frac{1}{2} \sum_{k=1}^{n} \int_0^t \int_U |\nabla(\mathcal{T}u_i - \mathcal{T}u)_k|^2\, dx\, ds\,,
\end{aligned}$$

for all $t \in [0, T]$, $i \in \mathbb{N}$. Having in mind, that $|r_{k\ell}| \le n$ for $k, \ell \in \{1, \ldots, n\}$, and applying the formula of partial integration for all $t \in [0, T]$ we get

$$\begin{aligned}
\sum_{k=1}^{n} \int_U |(\mathcal{T}u_i - \mathcal{T}u)_k(t)|^2\, ds &\le \sum_{k=1}^{n} \sum_{\ell=1}^{n} \int_0^T \int_U |(r_{k\ell}(u) - r_{k\ell}(u_i))\nabla(\mathcal{Q}u)_\ell|^2\, dx\, ds \\
&\quad + n^3 \sum_{\ell=1}^{n} \int_0^T \int_U |\nabla(\mathcal{Q}u_i - \mathcal{Q}u)_\ell|^2\, dx\, ds\,.
\end{aligned}$$

The integrands of the first part of the right hand side are majorized by $4n^2|\nabla(\mathcal{Q}u)_\ell|^2$ and in the limit process $i \to \infty$ they tend pointwise to zero, because of the Lipschitz continuity of $u \longmapsto r_{k\ell}(u)$ and the convergence $\lim_{i\to\infty} \|u_i - u\|_{\mathcal{H}(T)} = 0$. Hence, applying Lebesgue's theorem, the first part tends to zero. On the other hand, we have

$$\lim_{i\to\infty} \|\mathcal{Q}u_i - \mathcal{Q}u\|_{\mathcal{V}(T)} = \lim_{i\to\infty} \|\mathcal{P}u_i^\diamond - \mathcal{P}u^\diamond\|_{\mathcal{V}(T)} \le L \lim_{i\to\infty} \|u_i^\diamond - u^\diamond\|_{\mathcal{H}(T)} = 0\,,$$

that means, the second part of the right hand side tends to zero, too. Taking the supremum over all $t \in [0, T]$ on the left hand side we arrive at $\lim_{i\to\infty} \|\mathcal{T}u_i - \mathcal{T}u\|_{\mathcal{H}(T)} = 0$, in other words, $\mathcal{T} : \mathcal{H}(T) \longrightarrow \mathcal{H}(T)$ is continuous.

4. Because of $\mathcal{T}[\mathcal{H}(T)] \subset \mathcal{W}(T)$ and the completely continuous embedding of $\mathcal{W}(T)$ into $\mathcal{H}(T)$ (see [15], [18]), the fixed-point map $\mathcal{T} : \mathcal{H}(T) \longrightarrow \mathcal{H}(T)$ is completely continuous. Having in mind the second step of the proof, Schauder's fixed-point theorem yields a solution $u \in \mathcal{W}(T) \cap \mathcal{B}$ of the equation $\mathcal{T}u = u$. Setting $w = \mathcal{Q}u \in \mathcal{V}(T)$, we have found a solution $(u, w) \in \mathcal{W}(T) \times \mathcal{V}(T)$ of the regularized problem (R). $\square$

Theorem 2 (Solvability of the original problem) *For every $g \in S$ there exists a solution $(u, w) \in [\mathcal{W}(T) \cap \mathcal{S}(T)] \times \mathcal{V}(T)$ of the evolution system* (P).

Proof 1. Let $g \in S$ and $(u, w) \in \mathcal{W}(T) \times \mathcal{V}(T)$ be a solution of the regularized problem (R), which exists by Lemma 1.

2. If we choose the test function $\varphi = (-u_1^\bullet, \ldots, -u_n^\bullet) \in \mathcal{W}(T)$, then from (9) it follows

$$\sum_{k=1}^n \sum_{\ell=1}^n r_{k\ell}(u) \nabla w_\ell \cdot \nabla \varphi_k = -\sum_{k=1}^n \sum_{h=0}^n u_k^\diamond u_h^\diamond \nabla w_k \cdot \nabla u_k^\bullet + \sum_{k=1}^n \sum_{\ell=1}^n u_\ell^\diamond u_k^\diamond \nabla w_\ell \cdot \nabla u_k^\bullet = 0\,,$$

since for all $k \in \{1, \ldots, n\}$ by definition we have $u_k^\diamond \nabla u_k^\bullet = 0$. Hence, applying the above test function φ to (R), and having in mind $g_1, \ldots, g_n \geq 0$, for all $t \in [0, T]$ the formula of partial integration yields

$$\begin{aligned} 0 &= \sum_{k=1}^n \int_0^t \langle u_k'(s), \varphi_k(s) \rangle \, ds + \sum_{k=1}^n \int_0^t \int_U \nabla u_k(s) \cdot \nabla \varphi_k(s) \, dx \, ds \\ &= \sum_{k=1}^n \int_0^t \langle (u_k^\bullet)'(s), u_k^\bullet(s) \rangle \, ds + \sum_{k=1}^n \int_0^t \int_U |\nabla u_k^\bullet(s)|^2 \, dx \, ds \geq \frac{1}{2} \sum_{k=1}^n \int_U |u_k^\bullet(t)|^2 \, dx\,, \end{aligned}$$

that means, we arrive at $u_1, \ldots, u_n \geq 0$.

3. Now, we consider $\varphi = (-u_0^\bullet, \ldots, -u_0^\bullet) \in \mathcal{W}(T)$. From (9) and $u_0^\diamond \nabla u_0^\bullet = 0$ we deduce

$$\begin{aligned} \sum_{k=1}^n \sum_{\ell=1}^n r_{k\ell}(u) \nabla w_\ell \cdot \nabla \varphi_k &= -\sum_{\ell=1}^n \sum_{h=0}^n u_\ell^\diamond u_h^\diamond \nabla w_\ell \cdot \nabla u_0^\bullet + \sum_{k=1}^n \sum_{\ell=1}^n u_\ell^\diamond u_k^\diamond \nabla w_\ell \cdot \nabla u_0^\bullet \\ &= -\sum_{\ell=1}^n u_\ell^\diamond u_0^\diamond \nabla w_\ell \cdot \nabla u_0^\bullet = 0\,. \end{aligned}$$

Thus, applying the test function φ to (R), and remembering the facts $u_0 = 1 - \sum_{k=1}^n u_k$ and $g_0 \geq 0$, for all $t \in [0, T]$ again the formula of partial integration yields

$$\begin{aligned} 0 &= -\sum_{k=1}^n \int_0^t \langle u_k'(s), \varphi_k(s) \rangle \, ds - \sum_{k=1}^n \int_0^t \int_U \nabla u_k(s) \cdot \nabla \varphi_k(s) \, dx \, ds \\ &= \int_0^t \langle (u_0^\bullet)'(s), u_0^\bullet(s) \rangle \, ds + \int_0^t \int_U |\nabla u_0^\bullet(s)|^2 \, dx \, ds \geq \frac{1}{2} \int_U |u_0^\bullet(t)|^2 \, dx\,, \end{aligned}$$

in other words, we get the relation $u_0 \geq 0$, too.

4. It follows from the second and third step of the proof, that for every solution $(u, w) \in \mathcal{W}(T) \times \mathcal{V}(T)$ of the regularized problem (R) in fact $u \in \mathcal{S}(T)$ holds true. Hence, by the definition of truncation we have both $\mathcal{P}u = \mathcal{Q}u$ and $\mathcal{A}(u, w) = \mathcal{R}(u, w)$, that means $(u, w) \in [\mathcal{W}(T) \cap \mathcal{S}(T)] \times \mathcal{V}(T)$ is a solution of the original problem (P), too. □

Remark 1 If $(u, w) \in [\mathcal{W}(T) \cap \mathcal{S}(T)] \times \mathcal{V}(T)$ is a solution of the evolution system (P), then we can apply $\varphi = (1, \ldots, 1) \in \mathcal{W}(T)$ to (P) which yields the particle number conservation for every component,

$$\int_U u_k(t)\, dx = \int_U g_k\, dx \quad \text{for all} \;\; t \in [0, T]\,, \;\; k \in \{0, 1, \ldots, n\}\,.$$

4 Regularity theory in Sobolev–Morrey and Hölder spaces

The proof of the uniqueness result presented in this work is based on the Hölder continuity of the difference of two solutions. Hence, we will assume some natural regularity property of the interaction operator $\mathcal{P} : \mathcal{H}(T) \longrightarrow \mathcal{V}(T)$, which enables us to apply our regularity theory for initial boundary value problems in Sobolev–Morrey and Hölder spaces. For the theory of the above function spaces we refer to [2], [4], [11], [14].

Definition 4 Let $t > 0$, $\sigma \in [0, m+2]$ and $\alpha \in (0, 1]$. A function $u \in \mathcal{H}(t)$ belongs to the *Morrey space* $\mathcal{L}^{2,\sigma}(t)$ iff the sum

$$[u]^2_{\mathcal{L}^{2,\sigma}(t)} \stackrel{\text{def}}{=} \sum_{k=1}^{n} \sup_{(\tau,x)\in(0,t)\times U,\, \delta>0} \left\{ \delta^{-\sigma} \int_{(0,t)\cap(\tau-\delta^2,\tau)} \int_{U\cap B(x,\delta)} |u_k|^2\, dy\, ds \right\},$$

has a finite value. We define the norm of $u \in \mathcal{L}^{2,\sigma}(t)$ by

$$\|u\|^2_{\mathcal{L}^{2,\sigma}(t)} \stackrel{\text{def}}{=} \|u\|^2_{\mathcal{H}(t)} + [u]^2_{\mathcal{L}^{2,\sigma}(t)}\,.$$

Moreover, let $\mathcal{X}^\sigma(t) \subset \mathcal{V}(t)$ be the *Sobolev–Morrey space*

$$\mathcal{X}^\sigma(t) \stackrel{\text{def}}{=} \big\{ u \in \mathcal{H}(t) : D_1 u\,, \ldots, D_m u \in \mathcal{L}^{2,\sigma}(t) \big\}\,,$$

equipped with the norm

$$\|u\|^2_{\mathcal{X}^\sigma(t)} \stackrel{\text{def}}{=} \|u\|^2_{\mathcal{H}(t)} + \sum_{i=1}^{m} \|D_i u\|^2_{\mathcal{L}^{2,\sigma}(t)}\,, \quad u \in \mathcal{X}^\sigma(t)\,.$$

Finally, we introduce $C \stackrel{\text{def}}{=} C\big(\overline{U}; \mathbb{R}^n\big)$ and the *Hölder space* $\mathcal{C}^\alpha(t) \stackrel{\text{def}}{=} C^\alpha([0,t]; C)$ equipped with the norm

$$\|u\|_{\mathcal{C}^\alpha(t)} \stackrel{\text{def}}{=} \sup_{s\in[0,t]} \|u(s)\|_C + \sup_{s,\tau\in[0,t]} \frac{\|u(s) - u(\tau)\|_C}{|s-\tau|^\alpha}\,, \quad u \in \mathcal{C}^\alpha(t)\,.$$

Definition 5 Let $t > 0$ and $\sigma \in [0, m+2]$. A functional $f \in \mathcal{V}(t)^*$ belongs to the *Sobolev–Morrey space* $\mathcal{Z}^\sigma(t) \subset \mathcal{V}(t)^*$ iff there exist functions $z_1, \ldots, z_m \in \mathcal{L}^{2,\sigma}(t)$ and $\zeta \in \mathcal{L}^{2,\sigma-2}(t)$ such that f has a representation

$$\langle f, \varphi \rangle = \sum_{k=1}^{n} \sum_{j=1}^{m} \int_0^t \int_U z_{jk}\, D_j \varphi_k\, dx\, ds + \sum_{k=1}^{n} \int_0^t \int_U \zeta_k\, \varphi_k\, dx\, ds\,, \tag{12}$$

for $\varphi \in \mathcal{V}(t)$. We define the norm of $f \in \mathcal{Z}^\sigma(t)$ by the infimum

$$\|f\|^2_{\mathcal{Z}^\sigma(t)} \stackrel{\text{def}}{=} \inf \left\{ \sum_{j=1}^m \|z_j\|^2_{\mathcal{L}^{2,\sigma}(t)} + \|\zeta\|^2_{\mathcal{L}^{2,\sigma-2}(t)} \right\},$$

where the infimum is taken over all $z_1, \dots, z_m \in \mathcal{L}^{2,\sigma}(t)$ and $\zeta \in \mathcal{L}^{2,\sigma-2}(t)$ such that f can be represented as in (12). Moreover, let $\mathcal{W}^\sigma(t) \subset \mathcal{W}(t)$ be the *Sobolev–Morrey space*

$$\mathcal{W}^\sigma(t) \stackrel{\text{def}}{=} \{u \in \mathcal{X}^\sigma(t) : u' \in \mathcal{Z}^\sigma(t)\},$$

equipped with the norm

$$\|u\|^2_{\mathcal{W}^\sigma(t)} \stackrel{\text{def}}{=} \|u\|^2_{\mathcal{X}^\sigma(t)} + \|u'\|^2_{\mathcal{Z}^\sigma(t)}, \quad u \in \mathcal{W}^\sigma(t).$$

The main tool for our uniqueness proof is the following regularity result for initial boundary value problems with nonsmooth data (see [11]).

Theorem 3 (Regularity) *Let $T > 0$. There exists an $\omega \in (m, m+2)$ such that for all $\sigma \in (m, \omega)$ we can find constants $c_1, c_2 > 0$ such that for all $f \in \mathcal{Z}^\sigma(T)$ the solution $u \in \mathcal{W}(T)$ of the evolution problem*

$$u' + \mathcal{L}u = f, \quad u(0) = 0,$$

belongs to $\mathcal{W}^\sigma(T) \subset \mathcal{C}^\alpha(T)$ for $\alpha = \frac{\sigma - m}{4}$ and the following estimates hold true

$$\|u\|_{\mathcal{C}^\alpha(t)} \le c_1 \|u\|_{\mathcal{W}^\sigma(t)} \le c_2 \|f\|_{\mathcal{Z}^\sigma(t)} \quad \text{for all } t \in (0, T].$$

5 Uniqueness of the solution

Until now we have assumed that the interaction operator $\mathcal{P} : \mathcal{H}(T) \longrightarrow \mathcal{V}(T)$ is Lipschitz continuous with Lipschitz constant $L > 0$ (see (7)). To prove the unique solvability of problem (P) from now on we will additionally assume, that $\mathcal{P} : \mathcal{H}(T) \longrightarrow \mathcal{V}(T)$ has the Volterra property and that the restriction of $\mathcal{P}$ to $\mathcal{L}^\infty(T)$ is a Lipschitz continuous operator from $\mathcal{L}^\infty(T)$ to $\mathcal{X}^\sigma(T)$ for some $\sigma \in (m, \omega)$ (see Theorem 3), that means, there exists a Lipschitz constant $M > 0$, such that

$$\|\mathcal{P}u - \mathcal{P}\hat{u}\|_{\mathcal{X}^\sigma(t)} \le M \|u - \hat{u}\|_{\mathcal{L}^\infty(t)} \quad \text{for all } u, \hat{u} \in \mathcal{L}^\infty(T), \ t \in (0, T]. \tag{13}$$

Theorem 4 (Uniqueness) *For every $g \in S$ the solution $(u, w) \in [\mathcal{W}(T) \cap \mathcal{S}(T)] \times \mathcal{V}(T)$ of the evolution system* (P) *is uniquely determined.*

Proof 1. Let $g \in S$ be a given initial value and $(u, w), (\hat{u}, \hat{w}) \in [\mathcal{W}(T) \cap \mathcal{S}(T)] \times \mathcal{V}(T)$ be solutions of (P). Then, the difference $u - \hat{u} \in \mathcal{W}(T)$ solves the problem

$$(u - \hat{u})' + \mathcal{L}(u - \hat{u}) = \mathcal{A}(\hat{u}, \mathcal{P}\hat{u}) - \mathcal{A}(u, \mathcal{P}u), \quad (u - \hat{u})(0) = 0. \tag{14}$$

2. We estimate the right hand side of (14) in the norm of the space $\mathcal{Z}^\sigma(t)$ for $t \in (0,T]$. Using the boundedness and the Lipschitz continuity of $u \longmapsto a_{k\ell}(u)$ and the fact that $\mathcal{L}^\infty(t)$ is a space of multipliers for $\mathcal{L}^{2,\sigma}(t)$ we can find a constant $c_0 > 0$ such that

$$\begin{aligned}\|\mathcal{A}(\hat{u},\mathcal{P}\hat{u}) - \mathcal{A}(u,\mathcal{P}\hat{u})\|_{\mathcal{Z}^\sigma(t)} &\le \sum_{j=1}^m c_0\,\|u-\hat{u}\|^2_{\mathcal{L}^\infty(t)}\,\|D_j\mathcal{P}\hat{u}\|^2_{\mathcal{L}^{2,\sigma}(t)} \\ &\le 2c_0\,\|u-\hat{u}\|^2_{\mathcal{L}^\infty(t)}\left\{\|\mathcal{P}0\|^2_{\mathcal{X}^\sigma(t)} + \|\mathcal{P}\hat{u} - \mathcal{P}0\|^2_{\mathcal{X}^\sigma(t)}\right\},\end{aligned}$$

and in the same manner,

$$\|\mathcal{A}(u,\mathcal{P}\hat{u}) - \mathcal{A}(u,\mathcal{P}u)\|_{\mathcal{Z}^\sigma(t)} \le \sum_{j=1}^m c_0\,\|D_j\mathcal{P}\hat{u} - D_j\mathcal{P}u\|^2_{\mathcal{L}^{2,\sigma}(t)} \le c_0\,\|\mathcal{P}\hat{u} - \mathcal{P}u\|^2_{\mathcal{X}^\sigma(t)}\,.$$

Hence, the Lipschitz continuity of $\mathcal{P} : \mathcal{L}^\infty(t) \longrightarrow \mathcal{X}^\sigma(t)$ (see (13)) yields a constant $c_1 > 0$ such that

$$\|\mathcal{A}(\hat{u},\mathcal{P}\hat{u}) - \mathcal{A}(u,\mathcal{P}u)\|_{\mathcal{Z}^\sigma(t)} \le c_1\,\|u-\hat{u}\|_{\mathcal{L}^\infty(t)} \quad \text{for all } t \in (0,T]\,. \tag{15}$$

3. Since $(u-\hat{u})(0) = 0$, by Theorem 3 we can find a constant $c_2 > 0$ such that

$$\|u-\hat{u}\|_{\mathcal{C}^\alpha(t)} \le c_2\,\|\mathcal{A}(\hat{u},\mathcal{P}\hat{u}) - \mathcal{A}(u,\mathcal{P}u)\|_{\mathcal{Z}^\sigma(t)} \quad \text{for all } t \in (0,T]\,. \tag{16}$$

4. We choose $\alpha = \frac{\sigma-m}{4} > 0$ and $N \in \mathbb{N}$ large enough such that $2c_1c_2\,T^\alpha \le N^\alpha$. We define points $t_i = i\frac{T}{N}$ of the interval $[0,T]$ for $i \in \{0,\dots,N\}$. Remembering the definition of the Hölder norm, from $(u-\hat{u})(0) = 0$, (15) and (16) for all $s \in \left[0, \frac{T}{N}\right]$ it follows

$$\|(u-\hat{u})(s)\|_{L^\infty} \le s^\alpha\,\|u-\hat{u}\|_{\mathcal{C}^\alpha(t_1)} \le c_1c_2\left(\tfrac{T}{N}\right)^\alpha\|u-\hat{u}\|_{\mathcal{L}^\infty(t_1)} \le \tfrac{1}{2}\,\|u-\hat{u}\|_{\mathcal{L}^\infty(t_1)}\,,$$

that means, $\|u-\hat{u}\|_{\mathcal{C}^\alpha(t_1)} = 0$, and hence, $u\left(\frac{T}{N}\right) - \hat{u}\left(\frac{T}{N}\right) = 0$. Using again (15) and (16) for all $s \in \left[\frac{T}{N}, \frac{2T}{N}\right]$ we get

$$\|(u-\hat{u})(s)\|_{L^\infty} \le \left(s - \tfrac{T}{N}\right)^\alpha\|u-\hat{u}\|_{\mathcal{C}^\alpha(t_2)} \le c_1c_2\left(\tfrac{T}{N}\right)^\alpha\|u-\hat{u}\|_{\mathcal{L}^\infty(t_2)} \le \tfrac{1}{2}\,\|u-\hat{u}\|_{\mathcal{L}^\infty(t_2)}\,,$$

which implies $\|u-\hat{u}\|_{\mathcal{C}^\alpha(t_2)} = 0$. Repeating our arguments after a finite number of steps we arrive at $i = N$ and $\|u-\hat{u}\|_{\mathcal{C}^\alpha(T)} = 0$, in other words, the solution of problem (P) is uniquely determined. □

6 Simulation results for a ternary system

To emphasize the relevance of our nonlocal phase separation model we present an instructive example accompanied by simulation results for a ternary system. Here, we consider the special case, where the nonlocal interaction operator $\mathcal{P} : \mathcal{H}(T) \longrightarrow \mathcal{V}(T)$ can be described by means of the inverse of a second order elliptic operator having appropriate regularity properties.

Definition 6 Let $\mu \in [0, m]$. A function $u \in H$ belongs to the *Morrey space* $L^{2,\mu}$ iff

$$\|u\|^2_{L^{2,\mu}} \stackrel{\text{def}}{=} \|u\|^2_H + \sum_{k=1}^n \sup_{x \in U,\, \delta > 0} \left\{ \delta^{-\mu} \int_{U \cap B(x,\delta)} |u_k|^2 \, dy \right\},$$

has a finite value. Moreover, let $X^\mu \subset V$ be the *Sobolev–Morrey space*

$$X^\mu \stackrel{\text{def}}{=} \left\{ u \in H : D_1 u\,, \ldots, D_m u \in L^{2,\mu} \right\},$$

equipped with the norm $\|u\|^2_{X^\mu} \stackrel{\text{def}}{=} \|u\|^2_H + \sum_{j=1}^m \|D_j u\|^2_{L^{2,\mu}}$ for $u \in X^\mu$.

Let $E : H^1(U) \longrightarrow H^1(U)^*$ be the following elliptic operator

$$\langle Eh, \psi \rangle \stackrel{\text{def}}{=} \frac{1}{\varkappa} \int_U \left\{ \delta^2 \nabla h \cdot \nabla \psi + h \psi \right\} dx\,, \quad h,\, \psi \in H^1(U)\,,$$

where $\delta,\, \varkappa > 0$ are constants representing the *effective range* and *strength* of interaction forces, respectively. If we apply the regularity theory for elliptic boundary value problems in Sobolev–Morrey spaces (see [11], [12], [13]), we can find constants $\sigma \in (m, \omega)$ and $c > 0$ such that the following estimate holds true

$$\|(E^{-1}u_1, E^{-1}u_2)\|_{X^{\sigma-2}} \le c\, \|u\|_{L^\infty} \quad \text{for all } u \in L^\infty\,. \tag{17}$$

Let $\kappa : U \times U \longrightarrow \mathbb{R}$ be Green's function corresponding to $E : H^1(U) \longrightarrow H^1(U)^*$. Specifying the symmetric (3×3)-matrix kernel we define

$$(Ku)(x) = \begin{pmatrix} (Ku)_0(x) \\ (Ku)_1(x) \\ (Ku)_2(x) \end{pmatrix} \stackrel{\text{def}}{=} \int_U \begin{pmatrix} -\kappa(x,y) & +\kappa(x,y) & +\kappa(x,y) \\ +\kappa(x,y) & -\kappa(x,y) & +\kappa(x,y) \\ +\kappa(x,y) & +\kappa(x,y) & -\kappa(x,y) \end{pmatrix} \begin{pmatrix} u_0(y) \\ u_1(y) \\ u_2(y) \end{pmatrix} dy\,,$$

for $u \in H$, $x \in U$, and the free interaction energy (see (2) and (3)) of the state $u \in H$ by

$$F_2(u) \stackrel{\text{def}}{=} \frac{1}{2} \sum_{k=0}^2 \int_U (Ku)_k(x)\, u_k(x)\, dx\,.$$

To define the interaction operator $P : H \longrightarrow V$ we calculate the derivatives of F_2,

$$(Pu)_1 \stackrel{\text{def}}{=} (Ku)_1 - (Ku)_0 = E^{-1}(2 - 4u_1 - 2u_2)\,,$$
$$(Pg)_2 \stackrel{\text{def}}{=} (Ku)_2 - (Ku)_0 = E^{-1}(2 - 2u_1 - 4u_2)\,.$$

Hence, we get a Lipschitz continuous Volterra operator $\mathcal{P} : \mathcal{H}(T) \longrightarrow \mathcal{V}(T)$ by setting $(\mathcal{P}u)(s) \stackrel{\text{def}}{=} Pu(s)$ for $s \in (0,T)$ and $u \in \mathcal{H}(T)$. Because of the continuous embedding of $L^\infty((0,t); X^{\sigma-2})$ into $\mathcal{X}^\sigma(t)$ the above mentioned elliptic regularity theory (see (17)) yields a constant $M > 0$ such that

$$\|\mathcal{P}u - \mathcal{P}\hat{u}\|_{\mathcal{X}^\sigma(t)} \le M\, \|u - \hat{u}\|_{\mathcal{L}^\infty(t)} \quad \text{for all } u, \hat{u} \in \mathcal{L}^\infty(T)\,,\ \ t \in (0,T]\,.$$

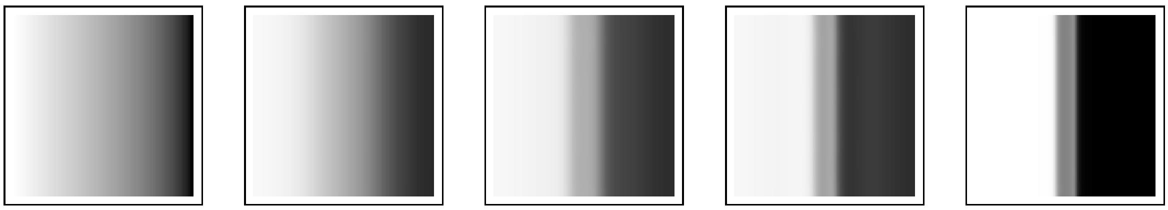

Figure 1: Phase separation process for an initial value which is constant in the vertical direction. The stripe pattern is preserved during the whole evolution.

Figure 2: Phase separation process for a mirror-symmetric initial value. There occur metastable states. Finally, the phases are separated by a straight line and circular arcs.

Applying Theorem 4, for every $g \in S$ there exists a uniquely determined solution $(u, w) \in [\mathcal{W}(T) \cap \mathcal{S}(T)] \times \mathcal{V}(T)$ of the evolution system (P).

In our example, from the structure of the symmetric matrix kernel it follows, that particles of the same type attract and particles of different type repel each other with the same range and strength of interaction. Figures 1 and 2 show simulation results of phase separation processes for the case of a unit square $U \subset \mathbb{R}^2$. Notice, that both initial configurations contain equal numbers of black, white and medium gray particles, respectively.

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