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Parameter Identification in Cahn-Hilliard Systems

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To my parents.
Thank you.
For all.

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Abstract

The Cahn-Hilliard equation is a mathematical model used to study phase separation processes within physics, chemistry or biology. Due to its phenomenological flavour, the model parameters are not known in real-world applications, and a calibration is needed to derive a quantitative agreement with data obtained from experiments. In this thesis, we address the problem of identifying three model parameters within the Cahn-Hilliard equation, i.e. the interface parameter, the double well potential function, and the mobility function from spatially resolved measurements of the phase fraction. We derive identifiability results and establish a linear and a non-linear approach to solve the parameter identification problems numerically.

In the first part of this work, we identify an inherent non-uniqueness of the inverse problem, leading to the exclusion of the interface parameter in the following considerations. We establish the identifiability of the mobility and the potential up to certain scaling invariances under realistic observability conditions. In the second part, we consider an equation error approach to solve the identification problems. Therefore, measurements are directly inserted into the Cahn-Hilliard equation, leading to linear operator equations in Hilbert spaces with perturbed operators. We use Tikhonov regularisation to derive stable approximations for the solutions of the ill-posed problems and show that this approach is well-posed. Numerical experiments demonstrate the feasibility of the method.

The equation error method requires high assumptions on the regularity of the data. We address this issue in the third part of our investigations by considering an output least squares approach. This leads to non-linear inverse problems in Hilbert spaces. Again, Tikhonov regularisation is employed to derive stable approximations for the solution. We show the well-posedness and continuity properties of the non-linear forward operator and establish the existence of solutions to the Tikhonov minimisation problem. A Gauss-Newton iteration is applied to solve the resulting minimisation problem. We show the differentiability of the forward operator and derive a representation for the adjoint operator of the derivative. The results regarding the output least squares approach are established by considering auxiliary variational problems. The existence of unique solutions to those problems is derived by Galerkin approximation and energy estimates. Afterwards, we discuss the discretisation of this approach using a Petrov-Galerkin method and present numerical results.

In the final part of this work, we consider more complex models and present numerical tests, which indicate that the output least squares approach can also be applied to those problems.

Zusammenfassung

Die Cahn-Hilliard Gleichung ist ein mathematisches Modell zur Untersuchung von Phasentrennungsprozessen in der Physik, Chemie oder Biologie. Aufgrund des phänomenologisches Charakters, sind die Modellparameter in realen Anwendungen nicht bekannt, und eine Kalibrierung ist erforderlich, um eine quantitative Übereinstimmung mit experimentell ermittelten Daten zu erzielen. In dieser Arbeit behandeln wir das Problem der Identifikation der drei Modellparameter innerhalb der Cahn-Hilliard Gleichung, diese sind der Grenzflächenparameter, die double-well Potentialfunktion und die Mobilitätsfunktion, aus räumlich verteilten Messungen des Phasenanteils. Wir zeigen Identifizierbarkeitsresultate und präsentieren einen linearen und einen nichtlinearen Zugang zur numerischen Lösung der Parameteridentifikationsprobleme.

Im ersten Teil dieser Arbeit wird eine inhärente Skalierungsinvarianz identifiziert, die dazu führt, dass der Grenzflächenparameter in den folgenden Überlegungen nicht berücksichtigt wird. Wir werden die Identifizierbarkeit der Mobilitätsfunktion und der Potenzialfunktion unter bestimmten Skalierungsinvarianzen unter realistischen Beobachtungsbedingungen zeigen. Im zweiten Teil wird der Equation-Error Ansatz zur Lösung der Identifikationsprobleme betrachtet. Dabei werden Messungen direkt in die Cahn-Hilliard Gleichung eingesetzt und führen zu linearen Operatorgleichungen in Hilberträumen mit gestörten Operatoren. Wir wenden die Tikhonov Regularisierung zur Stabilisierung der schlecht gestellten Probleme an und zeigen, dass dieser Ansatz wohlgestellt ist. Numerische Experimente werden die Durchführbarkeit der Methode zeigen.

Die Equation-Error Methode erfordert hohe Annahmen bezüglich der Regularität der Daten. Wir adressieren dieses Problem im dritten Teil, indem wir einen Output-Least-Squares Ansatz betrachten. Dies führt zu nichtlinearen inversen Problemen in Hilbert Räumen, und wir verwenden wieder Tikhonov Regularisierung, um stabil Approximationen an die Lösung zu bestimmen. Wir zeigen die Wohlgestelltheit und Stetigkeitseigenschaften des nichtlinearen Vorwärtsoperators und die Existenz von Lösungen des Tikhonov Minimierungsproblems. Eine Gauss-Newton Iteration wird angewendet, um das resultierende Minimierungsproblem zu lösen. Wir zeigen die Differenzierbarkeit des Vorwärtsoperators und leiten eine Darstellung des adjungierten Operators der Ableitung her. Diese Resultate zum Output-Least-Squares Ansatz werden wir durch Betrachtungen zu Hilfsvariationsproblemen beweisen. Wir verwenden Galerkin-Approximation und Energieabschätzungen, um Existenzresultate für diese Hilfsprobleme zu zeigen. Anschließend diskutieren wir die Diskretisierung dieses Ansatzes unter Verwendung einer Petrov-Galerkin Methode und präsentieren numerische Ergebnisse.

Im letzten Teil dieser Arbeit werden wir komplexere Modelle betrachten und präsentieren numerische Tests, die darauf hinweisen, dass der Output-Least-Squares Ansatz auch auf diese Probleme angewendet werden kann.

Contents

1. Introduction

Phase-field models are of special interest in a wide range of applications within the fields of physics, chemistry or biology, aiming to effectively model and simulate phase transformation processes. One of the most widely used mathematical models is the Cahn-Hilliard equation, which was initially introduced by Cahn and Hilliard to study phase separation in binary alloys [**23, 24**]. Since then, the Cahn-Hilliard model has been applied in many other applications, e.g. the spinodal decomposition of fluid mixtures [**14**], the modelling of tumour growth [**53**] or phase-field modelling in material science [**20**].

The Cahn-Hilliard equation

We consider the Cahn-Hilliard system described by the equations

$$\partial_t \phi = \operatorname{div}\left(b(\phi)\nabla\mu\right), \tag{1.1}$$

$$\mu = -\gamma\Delta\phi + f(\phi). \tag{1.2}$$

Here, ϕ is the phase fraction of one of two components, μ is a chemical potential, $b(\phi)$ a phase dependent mobility, γ an interface parameter, and $f(\phi)$ is the derivative of a non-convex potential function. The system is complemented with initial conditions and suitable boundary conditions.

The Cahn-Hilliard system (1.1)–(1.2) models a relaxation process governed by decay of an associated free-energy, thus in accordance with the second law of thermodynamics [**23**]. The existence of weak solutions was then shown by Galerkin approximation, relying on energy estimates and using compactness arguments, see e.g. [**43**]. From this starting point, further properties like the regularity of weak solutions or the qualitative behaviour of the evolution have been studied extensively for many different assumptions on the parameters. A detailed review will be presented in Chapter 2. These techniques have also been used to establish suitable numerical approximations; an overview is given in Chapter 5.

Energy stable approximation of gradient systems

In joint work with colleagues within the Collaborative Research Centre TRR 146 *Multiscale Simulation Methods for Soft Matter Systems* and the SPP 2256 *Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials*, we made some new contributions. In [**36**], we proposed a general framework for the numerical approximation of evolution problems that preserves an underlying dissipative gradient structure exactly. The Cahn-Hilliard equation fits into this structure, and we employed this approximation procedure, using relative energy estimates, to conduct a stability and discretisation error analysis, which led to a discretisation with optimal order error estimates, see [**19**]. This approximation approach will be used later on.

Parameter identification

The Cahn-Hilliard equation describes the macroscopic behaviour of physical processes happening on the microscale. It thus has to be understood as a phenomenological model. The model parameters are unknown in real-world applications and must be calibrated to obtain a quantitative agreement with more detailed microscopic descriptions or experimental data [**31, 61**]. Finding the model parameters in (1.1)–(1.2) from measurement data leads to parameter identification problems in non-linear systems of partial differential equations, see e.g. [**6, 63**] for an introduction and references. In the context of the Cahn-Hilliard equation, we are in the field of parameter identification problems in non-linear parabolic equations. Such problems and their stable solution have been studied intensively in the literature; we will give a more detailed review later.

Outline of this thesis

We will study the identification of the model parameters γ, $f(\cdot)$ and $b(\cdot)$ from measurements of the phase fraction ϕ. This problem of identifying the solution-dependent parameters in the Cahn-Hilliard equation has not been investigated before. We will provide a thorough discussion, i.e. establish a complete analysis and present suitable discretisation methods for solving the inverse problems. The results can be summarised into three main contributions. First, we establish identifiability; second, we provide a linear identification approach; and third, we discuss a non-linear identification method. Identifiability and the linear identification method have already been published in [**16**], while the non-linear approach is a new contribution.

Forward problem and identifiability

In Chapter 2, we introduce the setting of this work and recall the existence of solutions of the Cahn-Hilliard equation from the literature and our work [**19**]. The identifiability of the parameter γ, $b(\cdot)$ and $f(\cdot)$ is then investigated, and we first identify an underlying scaling invariance which leads to the exclusion of γ in the following considerations. We will establish identifiability results in three cases: the identification of either $b(\cdot)$ or $f(\cdot)$, and the simultaneous identification of $b(\cdot)$ and $f(\cdot)$.

Equation error approach

In Chapter 3, we employ an equation error method to solve the parameter identification problems. To do this, measurements ϕ^δ will replace ϕ in the system (1.1)–(1.2) and lead to linear operator equations with perturbed operators to identify the parameter functions. Those problems are ill-posed, and Tikhonov regularisation is employed to derive stable reconstructions. The theory of linear inverse problems between Hilbert spaces is well understood and has been successfully applied to other problems in the literature. Here, our main challenges arise from the perturbation of the operator, and a slight extension of the existing analysis on Tikhonov regularisation will be established to cover our problem structure. We will then show that the regularised parameter identification problems of

$b(\cdot)$ and $f(\cdot)$ are well-posed and demonstrate the feasibility of the method in numerical tests.

Output least squares approach

A known drawback of the equation error approach is its dependence on the smoothness of the measurements. Therefore, in Chapter 4, we will consider the output least squares approach, which is now a non-linear problem but can be applied using less regular data and higher noise levels. Non-linear inverse problems are well investigated in the literature, and we apply Tikhonov regularisation to our ill-posed inverse problems. To apply standard theory, we will establish the well-posedness and continuity of the forward operator. This leads to the existence of solutions to the Tikhonov minimisation problem, which we will use to derive stable approximations to the solution of the inverse problems. To solve the resulting optimisation problem, we will propose a Gauss-Newton method. For the realisation of this iterative approach, we will then establish the differentiability of the forward operator and derive a representation of the adjoint operator of the derivative. As we apply standard theory, our main challenge is to derive the required properties of the non-linear operator. This will be achieved via energy estimates and by proving the existence of solutions to auxiliary variational systems, for which Galerkin approximation and, again, energy estimates are employed.

In Chapter 5, we will consider the numerical approximation of the Tikhonov regularisation approach, to which we employ the Petrov-Galerkin method from our work [**19**].

Extensions to more complex models

Within the Collaborative Research Centre TRR 146 and the SPP 2256, further investigations have been made into more complex models, incorporating the Cahn-Hilliard equation. In [**20**], a Cahn-Hilliard/Allen-Cahn model was studied, and, using the techniques of [**19**], a structure-preserving discretisation of this model in [**17**] was derived. We will demonstrate that the output least squares approach can also be applied to these more complex models. Without proof, we will demonstrate the numerical feasibility of the identification method. A direction of future research would also be an analysis of the other models investigated within the research collaboration, i.e. a viscoelastic phase field model [**15, 88, 21**] or a Cahn-Hilliard-Navier-Stokes model [**18**].

List of publications

The following publications were produced as part of the doctorate and collaboration on the projects:

1. H. Egger, O. Habrich, and V. Shashkov. On the energy stable approximation of Hamiltonian and gradient systems. *Comput. Methods Appl. Math.*, 21(2):335–349, 2021.

2. D. Spiller, A. Brunk, O. Habrich, H. Egger, M. Lukáčová-Medviďová, and B. Dünweg. Systematic derivation of hydrodynamic equations for viscoelastic phase separation. *Journal of Physics: Condensed Matter*, 33(36):364001, jul 2021.

3. A. Brunk, B. Dünweg, H. Egger, O. Habrich, M. Lukáčová-Medviďová, and D. Spiller. Analysis of a viscoelastic phase separation model. *Journal of Physics: Condensed Matter*, 33(23):234002, 2021.

4. A. Brunk, H. Egger, and O. Habrich. On uniqueness and stable estimation of multiple parameters in the Cahn-Hilliard equation. *Inverse Problems*, 39(6):Paper No. 065002, 19, 2023.

5. A. Brunk, H. Egger, and O. Habrich. A second-order structure-preserving discretization for the Cahn-Hilliard/Allen-Cahn system with cross-kinetic coupling. *arXiv:2308.01638*, 2023.

6. A. Brunk, H. Egger, O. Habrich, and M. Lukáčová-Medviďová. A second-order fully-balanced structure-preserving variational discretization scheme for the Cahn–Hilliard–Navier–Stokes system. *Math. Models Methods Appl. Sci.*, 33(12):2587–2627, 2023.

7. A. Brunk, H. Egger, O. Habrich, and M. Lukáčová-Medviďová. Stability and discretization error analysis for the Cahn–Hilliard system *via* relative energy estimates. *ESAIM Math. Model. Numer. Anal.*, 57(3):1297–1322, 2023.

In the context of this work, we primarily use work (4) which covers identifiability and the equation error approach. Moreover, the methods developed in the works (1) and (3) are frequently used. The results from Chapter 4 and 5 covering the output least squares approach are not published yet. For the extension of this new approach we use the results from work (5).

2. Analytical results

We start by introducing the setup of the Cahn-Hilliard equation and recalling well-known results regarding the existence of solutions and their properties. After that, we will turn to the parameter identification problems and investigate questions on identifiability from observations of the phase fraction ϕ.

2.1. Introduction

As already mentioned in the introduction, the Cahn-Hilliard system

$$\partial_t \phi = \operatorname{div}\left(b(\phi)\nabla\mu\right), \tag{2.1}$$

$$\mu = -\gamma\Delta\phi + f(\phi), \tag{2.2}$$

has been extensively studied in the literature, and in particular, the existence and regularity of weak solutions have been established under various assumptions on the parameter functions. To simplify the following presentation, we will consider the Cahn-Hilliard equation (2.1)–(2.2) on a d-dimensional cube complemented with periodic boundary conditions, i.e.

(A0) $\Omega \simeq \mathbb{T}^d$, is the d-dimensional torus; functions defined on Ω are assumed to be periodic.

The subsequent analysis of the parameter identification problems is based on the following assumptions on the model parameters γ, $b(\cdot)$ and $f(\cdot)$.

Assumptions 2.1.1. The domain satisfies (A0). Moreover,

(A1) $\gamma > 0$ is a positive constant;

(A2) $b : \mathbb{R} \to \mathbb{R}_+$ satisfies $b \in C^2(\mathbb{R})$ with $0 < c_b \leq b(s) \leq C_b$ for all $s \in \mathbb{R}$ and $\|b'\|_\infty \leq C_{b'}$, $\|b''\|_\infty \leq C_{b''}$;

(A3) $f(s) = \lambda'(s)$ with $\lambda \in C^4(\mathbb{R})$ such that $\lambda(s), \lambda''(s) \geq -c_{\lambda_1}$, for some $c_{\lambda_1} \geq 0$. Furthermore, λ and its derivatives are bounded by $|\lambda^{(k)}(s)| \leq C^{(k)}_{\lambda_2} + C^{(k)}_{\lambda_3}|s|^{4-k}$ for $0 \leq k \leq 4$ with constants $C^{(k)}_{\lambda_2}, C^{(k)}_{\lambda_3} \geq 0$.

The assumptions (A1)–(A3) are standard, enabling us to establish the existence, uniqueness, and regularity of smooth solutions to the Cahn-Hilliard system (2.1)–(2.2), see Subsection 2.2.

Existence of solutions and properties

Let us start with an overview of the literature regarding solutions to the Cahn-Hilliard equation. The Cahn-Hilliard model possesses a gradient flow structure that results in energy decay during the evolution. Based on the model's thermodynamic consistency, weak solutions have been established using Galerkin approximation, energy estimates, and compactness arguments. For the case of constant mobility and a polynomial potential function, the existence and regularity of weak solutions have been established in [**41**], where a fourth-order system has been analysed after elimination of the chemical potential by inserting it into the first equation. In [**40**], an existence result has been established for the mixed formulation (2.1)–(2.2) of the Cahn-Hilliard equation. The analysis was extended to logarithmic potentials, see [**30**], and (non-)degenerate concentration dependent mobility functions, see [**8, 9, 43**]. Let us also mention further results concerning extensions to multi-component Cahn-Hilliard systems, see [**7, 11**], and multi-physical systems, e.g. incompressible Cahn-Hilliard-Navier-Stokes systems [**13, 49**]. In recent works, viscoelastic phase separation models have also been considered; see our work [**15**] in project C3 of the TRR 146, and further [**14**].

Besides the existence of weak solutions, the qualitative behaviour of solutions has also been investigated. The thin interface limit $\gamma \to 0$ has been considered in [**50, 51**]. The long-term behaviour was investigated, and convergence of solutions to an equilibrium state was established in [**83, 95**]. Further insights into the qualitative behaviour of solutions have been established by using the technique of formal asymptotic expansions; see [**10**] and references therein. For further extensions and properties of the Cahn-Hilliard equation and its solutions, we refer to [**28**] and references therein.

In Section 2.2, we will introduce our notation and recall the precise results regarding the existence, uniqueness and regularity of solutions we require. Therein, we will highlight the regularities of the solutions, which will be relevant for our later analysis.

Parameter identification

The identification of the model parameters γ, $b(\cdot)$ and $f(\cdot)$ in the Cahn-Hilliard equation has not been studied before. We first note that from the two system variables (ϕ, μ) in the Cahn-Hilliard equation, only observations of the phase fraction ϕ are typically available from simulations of microscopic models or experimental investigations [**61**]. The chemical potential μ is realistically not directly measurable in experiments. Thus, we will study the identification of the model parameters from observations of the phase fraction ϕ only. Our inverse problem then reads: Given spatially distributed measurements of the phase fraction ϕ, identify the model parameters γ, $b(\cdot)$ and $f(\cdot)$. First of all, this leads to the question of identifiability of the parameters from the given data ϕ.

Parameter identification problems in nonlinear parabolic equations have been covered extensively, and, in particular, questions on identifiability, also denoted as the uniqueness of the inverse problem, have been addressed. A structurally similar problem to our identification of the mobility $b(\cdot)$ is the identification of the nonlinear conductivity function $a(u)$ in $\partial_t u = \operatorname{div}(a(u)\nabla u)$, in the context of heat transfer and porous medium flow. This problem has been studied in [**25, 27, 35**], wherein uniqueness results have also been derived.

For a uniqueness result concerning a related linear elliptic problem, we refer to [**4**] and references provided therein. The identifiability of multiple parameters has also been analysed. We refer to [**12, 22, 34, 37, 48, 80**] for results in the direction of nonlinear elliptic and parabolic problems and to [**77**] for results in context of a population model. Further, there are identifiability results in the context of chemotaxis problems, see [**38, 52**], which are closest to our following analysis regarding the applied proof techniques.

In Section 2.3, we will identify scaling invariances characterising an inherent non-uniqueness of the parameter identification problem. Therefore, the identification of the interface parameter γ will be excluded in our subsequent investigation. As a result, we will only consider the identification of the mobility $b(\cdot)$ and the potential derivative $f(\cdot)$, and address the following questions:

(i) Is it possible to uniquely identify the parameter $f(\cdot)$ from observations of ϕ?

(ii) Is it possible to uniquely identify the parameter $b(\cdot)$ from observations of ϕ?

Both questions will be answered positively under reasonable observability conditions while γ and the other parameter function are known. Subsequently, we extend the question on identifiability. The parameters $b(\cdot)$, $f(\cdot)$ are one-dimensional functions. At the same time, the observations ϕ are typically available in space and time. Hence, we expect the inverse problems to be overdetermined, which raises a third question:

(iii) Is it possible to uniquely identify both parameters $b(\cdot), f(\cdot)$ simultaneously from observations of ϕ?

Again, the answer will be positive, now under abstract observability conditions, which can, in principle, be checked based on the available data. The questions (i)–(iii) are formally discussed in Section 2.4, and we will establish uniqueness results for each of the three cases.

Our main contributions in this chapter are the identifiability results for the identification problems and the identification of the underlying non-uniqueness, formalised as a scaling invariance. These results have also been published in [**16**].

2.2. Existence, uniqueness and regularity of solutions

Before we consider solutions and their properties, let us introduce our notation.

Notation

By $L^p(\Omega), W^{k,p}(\Omega)$ we denote the standard Lebesgue and Sobolev spaces and by $\|\cdot\|_{0,p}$, $\|\cdot\|_{k,p}$ the corresponding norms. In the Hilbert space case $p = 2$, we write $H^k(\Omega) = W^{k,2}(\Omega)$ and abbreviate $\|\cdot\|_k = \|\cdot\|_{k,2}$. We will, when it is clear, omit the symbol Ω and briefly write L^p for $L^p(\Omega)$. The corresponding dual spaces are denoted by $H^{-s}(\Omega) = H^s(\Omega)'$. Note that for $s = 0$, we have $H^s(\Omega) = H^{-s}(\Omega) = L^2(\Omega)$ where we identified $L^2(\Omega)$ with its dual. The norm of the dual spaces is given by

$$\|r\|_{H^{-s}} = \sup_{v\in H^s(\Omega)} \frac{\langle r, v\rangle_{H^s}}{\|v\|_{H^s}},$$

where $\langle \cdot, \cdot \rangle_{H^s}$ denotes the duality product on $H^{-s}(\Omega) \times H^s(\Omega)$ for any $s \geq 0$. Note that for functions $u, v \in H^0(\Omega) = L^2(\Omega)$ we have $\langle u, v \rangle = \int_\Omega u\, v\, dx$, i.e. for sufficiently regular functions the duality product can be identified with the scalar product of $L^2(\Omega)$. By $L^p(a, b; X), W^{k,p}(a, b; X)$ and $H^k(a, b; X)$, we denote the Bochner spaces of appropriate integrable or differentiable functions in time with values in some space X. If $(a, b) = (0, T)$ we also abbreviate $L^p(X)$ or $W^{k,p}(X)$. The spaces are equipped with their standard norms, see [**46**]. The inner product of a space X, if it exists, is denoted by $(\cdot, \cdot)_X$. Generic constants are denoted by C and may differ from line to line. Further we will abbreviate $\int_0^t \int_\Omega$ by $\int_{\Omega_t}$.

Solutions of the Cahn-Hilliard equation

Let us now establish the existence of solutions and their properties. By a periodic **weak solution** of (2.1)–(2.2) on the interval $(0, T)$, we mean a pair of functions

$$\begin{aligned} &\phi \in L^2(0, T; H^3(\Omega)) \cap H^1(0, T; H^1(\Omega)'), \\ &\mu \in L^2(0, T; H^1(\Omega)), \end{aligned}$$

satisfying the variational identities

$$(\partial_t \phi(t), v) + (b(\phi(t))\nabla\mu(t), \nabla v) = 0, \tag{2.3}$$

$$(\mu(t), w) - (\gamma\nabla\phi(t), \nabla w) - (f(\phi(t)), w) = 0, \tag{2.4}$$

for all test functions $v, w \in H^1(\Omega)$ and a.a. $0 < t < T$. The pair (ϕ, μ) is a **smooth solution** of (2.1)–(2.2) when it satisfies

$$\begin{aligned} &\phi \in L^\infty(0, T; H^3(\Omega)) \cap L^2(0, T; H^5(\Omega)) \cap H^1(0, T; H^1(\Omega)), \\ &\mu \in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^3(\Omega)). \end{aligned}$$

Under the Assumptions 2.1.1 on the model parameters, the existence of weak solutions and their regularity properties can be deduced from classical results.

Lemma 2.2.1 ([**19, Lem. 2**]). *Let Assumptions 2.1.1 hold. Then for any $\phi_0 \in H^1(\Omega)$, there exists at least one periodic weak solution (ϕ, μ) of problem (2.1)–(2.2) with initial value $\phi(0) = \phi_0$. If $\phi_0 \in H^k(\Omega)$,$1 \leq k \leq 3$ then*

$$\|\phi\|_{L^\infty(H^k)} + \|\phi\|_{L^2(H^{k+2})} + \|\partial_t\phi\|_{L^2(H^{k-2})} + \|\mu\|_{L^2(H^k)} + \|\mu\|_{L^\infty(H^{k-2})} \leq C_T(\|\phi_0\|_k)$$

with $C_T(\|\phi_0\|_k)$ depending only on the bounds for the coefficients, the domain Ω, the time horizon T, and the bounds for the initial value. In dimension $d = 3$, the estimates $k > 1$ are only valid for sufficiently small T. Moreover, if $\phi_0 \in H^k(\Omega)$, $k \geq 2$, then the weak solution is unique.

Proof. For $k = 1$ and dimensions $d = 2, 3$, the existence of weak solutions and a-priori bounds for any time $T > 0$ are classical results obtained by Galerkin approximation, energy estimates, and compactness arguments, see e.g. [**43**] for details. For $k > 1$, the improved regularity and the bounds are achieved through a bootstrapping argument and elliptic regularity arguments, utilising regularity results of the Poisson problem, see [**13, 19**] and references therein for details. In the case $k \geq 2$, the uniqueness of the solution is demonstrated in [**13**] using classical methods. □

Note, our definition of smooth solutions corresponds to the case $k = 3$ in Lemma 2.2.1. In particular, a smooth solution is unique and also a strong solution (in the sense of [**54**]). Smooth solutions and their properties are a necessary precondition in the upcoming analysis of identifiability in Section 2.4 and the identification methods in Chapters 3 and 4. Let us gather some regularities and bounds of smooth solutions in the following remark.

Remark 2.2.2 (Regularity of smooth solutions)**.** Based on the estimates in Lemma 2.2.1 and embedding theorems for Bochner spaces, see [**92, Ch. 25**], we can conclude that smooth solutions (ϕ, μ) are continuous functions in time, i.e. we have that

$$(\phi, \mu) \in C([0, T]; H^3(\Omega) \times H^1(\Omega)),$$

and consequently, ϕ is uniformly bounded on $\Omega \times [0, T]$. Especially, we have that ϕ and $\nabla\phi$ are bounded in $L^\infty(0, T; L^\infty(\Omega))$. This boundedness will be necessary to analyse the nonlinear identification method in Chapter 4. In particular, when combined with the bounds on the parameter functions, it allows to uniformly bound terms like $f(\phi)$. For later reference, let us explicitly state the important uniform bounds:

$$\|\phi\|_{C([0,T];H^3(\Omega))} + \|\nabla\phi\|_{L^\infty(0,T;L^\infty(\Omega))} + \max_{0\leq i\leq 2}\|f^{(i)}(\phi)\|_{C(\Omega_T)} \leq C(\|\phi_0\|_{H^3(\Omega)}).$$

Remark 2.2.3 (Degenerate parameters)**.** Our analysis considers the non-degenerate case, where the double-well potential $\lambda(\cdot)$ and its derivatives are polynomially bounded, and the mobility function $b(\cdot)$ is strictly positive. For more general model parameter functions, such as logarithmic potentials or degenerate mobilities, smooth solutions are expected to stay away from the pure states. Therefore, the parameter functions can be regularised outside the range of the solutions, ensuring the validity of the previous assumptions. The approach of regularising the model functions is also employed in the proof of the existence of solutions in the degenerate case, see [**10, 43**]. However, incorporating a complete discussion of this case would complicate analysing the parameter identification problems in the subsequent chapters. Thus, we will not discuss this case in further detail.

In summary, for any choice of model parameters satisfying Assumptions 2.1.1, we have existence of a unique smooth solution with the discussed properties, which are required in the following analysis.

2.3. Scaling invariances

We will later study in detail the question, if observations of the phase fraction ϕ uniquely determine the model parameters γ, $b(\cdot)$, and $f(\cdot)$. As we have already indicated, this is not the case due to the assumption that the chemical potential μ is unknown. In the following lemma, we present the canonical scaling invariance that characterises the inherent non-uniqueness of the parameter identification problem.

Lemma 2.3.1 ([**16, Lem. 3**])**.** *Let (ϕ, μ) be a periodic solution of* (2.1)–(2.2) *for the parameters (γ, b, f). Then for any $c \in \mathbb{R}$ and $d > 0$, the tuple $(\hat{\phi}, \hat{\mu}) = (\phi, \mu/d + c)$ is a solution of* (2.1)–(2.2) *for the parameters*

$$\hat{\gamma} = \gamma/d, \qquad \hat{b}(s) = d \cdot b(s), \qquad \textit{and} \qquad \hat{f}(s) = f(s)/d + c.$$

Proof. Firstly, as (ϕ, μ) is a solution to (2.1)–(2.2), it satisfies the variational identities (2.3)–(2.4) for the parameters (γ, b, f). A constant rescaling of $b \to b \cdot d$ and $\mu \to \mu/d$ in (2.3) maintains the validity of the identity with rescaled parameter $\hat{b} = b \cdot d$ and chemical potential $\hat{\mu} = \mu/d$. Additionally, another rescaling of $\gamma \to \gamma/d, f \to f/d$ restores the validity of (2.4), which establishes the claim of the lemma for $c = 0$. Secondly, a constant shift $\mu \to \mu + c$ and $f \to f + c$ leaves the identity (2.4) valid, which establishes the claim of the lemma for $d = 1$. When combined with the first rescaling, we obtain the desired result. □

Remark 2.3.2. We immediately infer from Lemma 2.3.1 that when utilising distributed observations of the phase fraction ϕ only, the parameters $\gamma, b(\cdot)$ and $f(\cdot)$ can be identified at most up to the previous invariant scaling, i.e. solutions to the inverse problem are not unique. However, it is easily seen that when γ is known, the rescaling with the parameter d is not feasible. Thus, we assume $\gamma > 0$ to be known in the following and the remainder of the thesis. The invariance with respect to the constant c is not removable. Hence, our analysis investigates the identification of $b(\cdot)$, and $f(\cdot)$ up to a constant. If γ is unknown, one must choose an artificial value, e.g. $\gamma = 1$. By the previous invariances, one then identifies rescaled parameter functions $\hat{b}(s)$ and $\hat{f}(s)$.

2.4. Identifiability results

We will now investigate the identification of

(i) the potential derivative $f(\cdot)$ in Subsection 2.4.1,

(ii) the mobility function $b(\cdot)$ in Subsection 2.4.2,

(iii) the simultaneous identification of both parameter functions in Subsection 2.4.3.

As noted in Remark 2.3.2, we assume that the interface parameter $\gamma > 0$ is known. Under this assumption and in view of Lemma 2.3.1, we can at most expect to be able to identify the mobility $b(\cdot)$ uniquely from spatially distributed measurements of ϕ. In contrast, the potential derivative $f(\cdot)$ can be at most determined up to a constant shift. Moreover, it is clear that both parameter functions can only be identified on the range of the available data ϕ, denoted by $\operatorname{ran}(\phi)$.

2.4.1. Identification of $f(\cdot)$

We first study the identification of the parameter function $f(\cdot)$ from distributed measurements ϕ. The other parameters γ and $b(\cdot)$ are assumed to be known.

First, we eliminate the chemical potential μ by inserting its equation (2.2) into (2.1), which results in the fourth-order formulation of the Cahn-Hilliard equation. Afterwards, we obtain the weak form of this equation by multiplying it by a periodic test function $v \in H^1(\Omega)$ and integrating it over the domain Ω. After integration-by-parts and using the periodicity of ϕ and v, we arrive at the variational identity

$$\int_\Omega b(\phi) f'(\phi) \nabla\phi \cdot \nabla v \, dx = \int_\Omega b(\phi)\gamma \nabla\Delta\phi \cdot \nabla v \, dx - \int_\Omega \partial_t \phi \, v \, dx. \tag{2.5}$$

For the subsequent arguments, we will further transform the identity. To do so, we introduce the primitive function

$$v : \Omega \to \mathbb{R}, \qquad v(x) := \int_0^{\phi(x)} w(s)/b(s)\, ds$$

for any smooth test function $w : \operatorname{ran}(\phi) \to \mathbb{R}$. Since we have assumed $b(\cdot)$ to be strictly positive, the primitive is well-defined. Upon inserting the primitive v as a test function into the previous variational identity, we obtain

$$\int_\Omega f'(\phi) w(\phi) |\nabla\phi|^2 \, dx = \int_\Omega w(\phi)\gamma\nabla\Delta\phi \cdot \nabla\phi \, dx - \int_\Omega \int_0^{\phi(x)} w(s)/b(s)\, ds\, \partial_t\phi \, dx. \tag{2.6}$$

Based on this identity, we can deduce the following result concerning the identifiability of the potential derivative $f(\cdot)$.

Theorem 2.4.1 ([**16, Thm. 5**]). *Let Assumptions 2.1.1 hold and ϕ be a smooth solution of (2.1)–(2.2) on $\Omega \times [0, T]$. Further, assume that $\gamma > 0$ and $b(\cdot)$ are known. Then $f'(\cdot)$ is uniquely determined on $R_t := \{s = \phi(x, t) : x \in \Omega\}$ from observations of $\phi(\cdot, t)$ and $\partial_t\phi(\cdot, t)$ on Ω for $0 \le t \le T$.*

Proof. Throughout the following discussion, we always consider ϕ at a specific time point $t \in [0, T]$, i.e. $\phi(x) = \phi(x, t)$ for a fixed t. Let us assume $f_1(\cdot)$, $f_2(\cdot)$ to be two functions leading to the same solution ϕ. By inserting the functions $f_1(\cdot)$ and $f_2(\cdot)$ into equation (2.6) and subtracting the resulting identities, we obtain

$$\int_\Omega (f_1'(\phi) - f_2'(\phi))\, w(\phi)\, |\nabla\phi|^2 \, dx = 0. \tag{2.7}$$

Further we define $W(s) := f_1(s) - f_2(s)$ for $s \in \mathbb{R}$, and $w(s) = W'(s)$, and observe that $\nabla W(\phi) = w(\phi)\nabla\phi$. Under the Assumptions 2.1.1 we are now allowed to insert $w(\cdot)$ in the previous variational identity (2.7), and derive

$$\int_\Omega |\nabla W(\phi)|^2 \, dx = \int_\Omega |\nabla(f_1(\phi) - f_2(\phi))|^2 \, dx = \int_\Omega |f_1'(\phi) - f_2'(\phi)|^2 |\nabla\phi|^2 \, dx = 0.$$

Consequently $f_1(\phi) - f_2(\phi)$ is constant on Ω, which implies that $f_1(x) = f_2(x)$ for all $x \in R_t$, i.e. $f'(\cdot)$ can be uniquely determined on R_t. □

Remark 2.4.2. In the proof, we considered measurements of a single time point only. However, if we have measurements of ϕ on a space-time cylinder $\Omega \times [t_1, t_2]$ with $t_1 < t_2$, then the time derivative $\partial_t\phi$ is also known on this set. By using measurements from multiple points in time, we then can determine $f'(\cdot)$ on the set $R_{[t_1,t_2]} = \bigcup_{t_1 \le t \le t_2} R_t$.

In the previous proof, the knowledge of the mobility function is implicitly utilised, as the last term of the identity (2.6) depends on $b(\cdot)$. Thus, assuming that the mobility function is known is indeed necessary. However, upon considering the last term of identity (2.6), we observe that the term vanishes if we assume $\partial_t\phi = 0$ on Ω. The remaining terms then correspond to an equilibrium distribution. In this particular equilibrium case, the potential derivative $f(\cdot)$ can be determined without knowledge of the mobility. This is analysed in the following result.

Theorem 2.4.3 ([**16, Thm. 7**])**.** *Let Assumptions 2.1.1 hold and* $(\phi_\infty, \mu_\infty)$ *be an equilibrium for* (2.1)–(2.2)*, i.e.* $(\phi_\infty, \mu_\infty)$ *satisfy*

$$0 = \operatorname{div}(b(\phi_\infty)\nabla\mu_\infty), \tag{2.8}$$

$$\mu_\infty = -\gamma\Delta\phi_\infty + f(\phi_\infty). \tag{2.9}$$

Further, assume that $\gamma > 0$ *to be known. Then the function* $f'(\cdot)$ *is determined uniquely on* $R_\infty = \{s = \phi_\infty(x) : x \in \Omega\}$ *from knowledge of* ϕ_∞*.*

Proof. In principle, the assertion can be directly inferred from the previous theorem. Nevertheless, we provide a different, more direct, proof here. By multiplying equation (2.8) with μ_∞ and integrating over the domain Ω, we obtain after using integration-by-parts and the periodic boundary conditions that

$$0 = \int_\Omega \operatorname{div}(b(\phi_\infty)\nabla\mu_\infty)\mu_\infty \, dx = -\int_\Omega b(\phi_\infty)|\nabla\mu_\infty|^2 dx.$$

As the mobility $b(\cdot)$ was assumed to be strictly positive, this implies that μ_∞ must be constant. Substituting $\mu_\infty = C$ into equation (2.9) yields

$$f(\phi_\infty) = \gamma\Delta\phi_\infty + C.$$

From this, we directly deduce that $f(\cdot)$ is determined up to a constant on R_∞. Let us mention that knowledge of the mobility function $b(\cdot)$ was not required for this deduction. $\square$

In fact, the constant $\mu_\infty = C$ is then known, as it can be computed by testing equation (2.9) with the constant function $v \equiv 1$.

Remark 2.4.4 (Stationary states)**.** The convergence of the phase fraction ϕ to an equilibrium distribution ϕ_∞ was investigated and shown in the literature. We refer to [**83, 95**] for details and proofs.

In conclusion, we established that the potential derivative $f(x)$ can be identified up to a constant, provided that the value x has been attained from the measurements of ϕ, an expected and natural identifiability condition.

2.4.2. Identification of $b(\cdot)$

Next, we address the identification of the mobility function $b(\cdot)$ while assuming that the other parameters γ and $f(\cdot)$ are known. At first, we observe that the chemical potential $\mu = -\gamma\Delta\phi + f(\phi)$ is determined from observations of ϕ, as γ and $f(\cdot)$ are known. Hence, we are left with the first equation (2.1) of the Cahn-Hilliard system, i.e.

$$\operatorname{div}(b(\phi)\nabla\mu) = \partial_t\phi \qquad \text{on } \Omega \times (0, T). \tag{2.10}$$

In the following theorem, we present a conditional identifiability result utilising equation (2.10). The subsequent proof then employs similar arguments as those used in [**38**].

Theorem 2.4.5 ([**16, Thm. 8**]). *Let Assumptions 2.1.1 hold and (ϕ, μ) be a smooth solution of* (2.1)–(2.2) *on $\Omega \times [0, T]$. Further, assume that $\gamma > 0$ and $f(\cdot)$ are known. Then $b(\cdot)$ can be determined uniquely from observations of $\phi(\cdot, t)$ and $\partial_t \phi(\cdot, t)$ on the set*

$$\widetilde{R}_t = \{s = \phi(x, t) : x \in \Omega \text{ and } \nabla\mu(x, t) \neq 0\} \subset R_t.$$

Proof. We consider ϕ at a fixed time point $t \in [0, T]$, without explicitly making reference to the time point t, i.e. $\phi(x) = \phi(x, t)$. Let us assume $b_1(\cdot)$ and $b_2(\cdot)$ to be two distinct mobility functions, both yielding the same solution ϕ of the Cahn-Hilliard system (2.1)–(2.2), while using the same γ and $f(\cdot)$. We define the auxiliary function $B_+(s) = \max(b_1(s) - b_2(s), 0)$, and will argue subsequently that

$$\operatorname{div}(B_+(\phi)\nabla\mu) = 0 \qquad \text{on } \Omega. \tag{2.11}$$

To this end, we initially observe that the function $B_+(\phi)\nabla\mu$ is weakly differentiable, and proceed by considering the equation on subdomains of Ω. First, we consider the set

$$\Omega_+(t) := \{x \in \Omega : B_+(\phi(x, t)) > 0\} = \{x \in \Omega : b_1(\phi(x, t)) > b_2(\phi(x, t))\}.$$

By inserting $b = b_1$ and $b = b_2$ into equation (2.10), followed by subtracting the resulting equations, we derive the validity of equation (2.11) on the set $\Omega_+(t)$. Second, we consider the set $\Omega \setminus \Omega_+$ and readily conclude the validity of equation (2.11), as $B_+(\phi)\nabla\mu \equiv 0$ on this set. Therefore, we can multiply equation (2.11) by μ and integrate over the domain Ω. By employing integration-by-parts and periodic boundary conditions, we obtain

$$0 = \int_\Omega \operatorname{div}(B_+(\phi)\nabla\mu)\mu \, dx = -\int_\Omega B_+(\phi)|\nabla\mu|^2 \, dx.$$

Consequently, we deduce that $B_+(\phi) \equiv 0$ on the set $\{s = \phi(x, t) \in \widetilde{R}_t : x \in \Omega_+\}$. By employing the same arguments, we verify that $B_-(\phi) = \min(b_1(\phi) - b_2(\phi), 0)$ is constant zero on the set $\{s = \phi(x, t) \in \widetilde{R}_t : x \in \Omega_-\}$, where we used the analogously defined set $\Omega_-(t) := \{x \in \Omega : b_1(\phi(x, t)) < b_2(\phi(x, t))\}$. By combining the assertions on the subsets Ω_+ and Ω_-, we deduce that $b_1(s) = b_2(s)$ on $\widetilde{R}_t$. □

Remark 2.4.6. Similar to the identification of $f(\cdot)$, if we have access to data $\phi(x, t)$ not only from a single time point but from a space-time cylinder $\Omega \times [t_1, t_2]$ for $t_1 < t_2$, then $\partial_t \phi$ is also known on this set. Consequently, we can determine the mobility $b(\cdot)$ on $\widetilde{R}_{[t_1,t_2]} = \bigcup_{t_1 \le t \le t_2} \widetilde{R}_t$. Therein we can take the closure of the sets, given that the function $b(\cdot)$ was assumed to be smooth; see Assumptions 2.1.1. Additionally, let us comment on the non-zero condition of $\nabla\mu$ contained in the definition of the sets $\widetilde{R}_t$ and $\widetilde{R}_{[t_1,t_2]}$. We observe that if $\nabla\mu \equiv 0$ on a set $\{(x, t) : \phi(x, t) \in (s_1, s_2)\}$, hence $(s_1, s_2) \notin \widetilde{R}_{[t_1,t_2]}$, then $b(s)$ for $s_1 < s < s_2$ does not influence the evolution of ϕ. Consequently, the mobility cannot be identified on this set from observations of ϕ. Hence, the condition on $\nabla\mu$ can be understood as an observability condition; see also [**4, 81**].

In conclusion, we established that the mobility function $b(\cdot)$ can be uniquely determined under an inherent observability condition on the chemical potential μ, which is determined from the knowledge of ϕ, γ and $f(\cdot)$.

2.4.3. Simultaneous identification of $f(\cdot)$ and $b(\cdot)$

Next, we consider the simultaneous identification of both parameter functions $b(\cdot)$ and $f(\cdot)$, while $\gamma > 0$ is assumed to be known. We will establish an identifiability result, assuming a suitable observability condition. For similar arguments, we refer to [**4, 82**].

To begin, let ϕ be a smooth periodic solution of the Cahn-Hilliard system (2.1)–(2.2), and let us define the auxiliary function $c(s) := b(s)f'(s)$. Note that since $b(\cdot)$ is strictly positive, it is possible to deduce the function $f'(\cdot)$ through the knowledge of $c(\cdot)$. By inserting $c(\cdot)$ into the variational identity (2.5) and rearranging terms, we obtain

$$\int_\Omega -b(\phi)\gamma\nabla\Delta\phi\nabla v\,dx + \int_\Omega c(\phi)\nabla\phi\nabla v\,dx = \int_\Omega \partial_t\phi\, v\,dx, \tag{2.12}$$

for all periodic test functions $v \in H^1(\Omega)$ and all time points t under consideration. To proceed, we now introduce the Heaviside function $H(s)$ and its regularised piecewise linear approximations $H_\varepsilon(s)$, i.e.

$$H(s) = \begin{cases} 0, & s \leq 0, \\ 1, & s > 0, \end{cases} \qquad \text{and} \qquad H_\varepsilon(s) = \begin{cases} s/\varepsilon, & 0 < s < \varepsilon, \\ H(s), & \text{else,} \end{cases}$$

for some $\varepsilon > 0$. We test the identity (2.12) with $v = H_\varepsilon(\phi - s)$. For ease of presentation, we only consider the term involving $c(\phi)$ and obtain

$$\begin{aligned} \int_\Omega c(\phi)\nabla\phi\nabla H_\varepsilon(\phi)\,dx &= \frac{1}{\varepsilon}\int_{0<\phi<\varepsilon} c(\phi)|\nabla\phi|^2\,dx \\ &= \frac{1}{\varepsilon}\int_{\phi>\varepsilon} c(\phi)|\nabla\phi|^2\,dx - \frac{1}{\varepsilon}\int_{\phi>0} c(\phi)|\nabla\phi|^2\,dx. \end{aligned}$$

Then by applying the co-area formula, see [**47, Sec. 3.4**], we derive

$$\begin{aligned} &\frac{1}{\varepsilon}\int_\varepsilon^\infty \int_{\phi=s} c(s)|\nabla\phi|\,d\mathcal{H}^{d-1}\,ds - \frac{1}{\varepsilon}\int_0^\infty \int_{\phi=s} c(s)|\nabla\phi|\,d\mathcal{H}^{d-1}\,ds. \\ &\qquad = \frac{1}{\varepsilon}\int_0^\varepsilon \int_{\phi=s} c(s)|\nabla\phi|\,d\mathcal{H}^{d-1}\,ds, \end{aligned}$$

where $d\mathcal{H}^{d-1}$ denotes the $(d-1)$-dimensional Hausdorff measure. By taking the limit $\varepsilon \to 0$, also considering the remaining terms of identity (2.12), we derive

$$-b(s)\int_{\{\phi=s\}} \gamma\nabla\Delta\phi\frac{\nabla\phi}{|\nabla\phi|}d\mathcal{H}^{d-1} + c(s)\int_{\{\phi=s\}} |\nabla\phi|\,d\mathcal{H}^{d-1} = \int_\Omega \partial_t\phi\, H(\phi - s)\,dx. \tag{2.13}$$

As the integrals on the left-hand side are the same as those appearing in the co-area formula, they are well-defined for almost every value of s; see again [**47, Sec. 3.4**] for details. Also consider [**72**] for an application in a similar context. For every $t \in [0, T]$, (2.13) is a linear equation for the two scalar values $b(s)$ and $c(s)$. From this, we deduce the following result.

Theorem 2.4.7 (**[16, Thm. 10]**). *Let Assumptions 2.1.1 hold, ϕ be a smooth solution of* (2.1)–(2.2) *and $\gamma > 0$ known. Define*

$$A_b(s,t) := -\int_{\{\phi(\cdot,t)=s\}} \gamma \nabla\Delta\phi(x,t)\frac{\nabla\phi(x,t)}{|\nabla\phi(x,t)|}\,dx, \quad A_c(s,t) := \int_{\{\phi(\cdot,t)=s\}} |\nabla\phi(x,t)|\,dx,$$
$$A(s,t) := \int_\Omega \partial_t\phi(x,t)H(\phi(x,t)-s)\,dx,$$

and assume that $\{(A_b(s,t_i), A_c(s,t_i)) : i = 1,2\}$ are linearly independent. Then $b(s)$, $c(s)$, and $f'(s) = c(s)/b(s)$ are uniquely determined.

Proof. From equation (2.13) and considering the definition of A_b, A_c and A, we obtain

$$\begin{aligned} A_b(s,t_1)\,b(s) + A_c(s,t_1)\,c(s) &= A(s,t_1),\\ A_b(s,t_2)\,b(s) + A_c(s,t_2)\,c(s) &= A(s,t_2), \end{aligned}$$

which comprises of two linear equations for determining the two scalar values $b(s)$, $c(s)$. By assumption, the two equations are linearly independent, and thus, the system possesses a unique solution, yielding the claim of the theorem. □

Remark 2.4.8. In contrast to the previous identifiability results, Theorem 2.4.7 yields a conditional identifiability result. In principle, the required linear independence of the coefficients A_b, A_c can be verified explicitly by utilising the data ϕ, prior to any computation of the values $b(s), c(s)$. If this observability condition holds true, the unique identification of the two scalar values $b(s)$, $f'(s)$ can be achieved by solving the linear system (2.13). Moreover, the reconstructions depend stable on the data ϕ and $\partial_t\phi$.

Conclusion

In this chapter, we investigated the identifiability of the parameter functions $\gamma, b(\cdot)$ and $f(\cdot)$ using observations of the phase fraction ϕ and established identifiability results considering the scaling invariance. In summary, we note that

(i) the interface parameter γ should be fixed,

(ii) the potential derivative $f(\cdot)$ can only be identified up to a constant,

(iii) both parameters $b(\cdot)$ and $f(\cdot)$ can only be identified on the range of the available data ϕ.

Hence, in the following chapters, we establish methods to identify the parameter functions $b(\cdot)$ and $f(\cdot)$ considering the conditions (i)–(iii).

3. Regularised inversion by equation error methods

In the previous Chapter 2, we established the unique identifiability of $b(\cdot)$ and $f(\cdot)$, the latter up to a constant, separately and simultaneously. In this chapter, we present a linear approach for the stable identification of the parameter functions $b(\cdot)$ and $f(\cdot)$ from observations of the phase fraction ϕ. We will study the identification method theoretically and then turn to its practical realisation.

3.1. Introduction

We consider the Cahn-Hilliard system

$$\partial_t \phi = \operatorname{div}\left(b(\phi)\nabla\mu\right), \tag{3.1}$$

$$\mu = -\gamma\Delta\phi + f(\phi), \tag{3.2}$$

complemented with periodic boundary conditions and appropriate assumptions on the parameter functions. For convenience of the reader, we repeat them here.

Assumptions 3.1.1. We impose the following assumptions on the model parameters:

(A1) $\gamma > 0$ is a positive constant;

(A2) $b : \mathbb{R} \to \mathbb{R}_+$ satisfies $b \in C^2(\mathbb{R})$ with $0 < c_b \leq b(s) \leq C_b$ for all $s \in \mathbb{R}$ and $\|b'\|_\infty \leq C_{b'}$, $\|b''\|_\infty \leq C_{b''}$;

(A3) $f(s) = \lambda'(s)$ with $\lambda \in C^4(\mathbb{R})$ such that $\lambda(s), \lambda''(s) \geq -c_{\lambda_1}$, for some $c_{\lambda_1} \geq 0$. Furthermore, λ and its derivatives are bounded by $|\lambda^{(k)}(s)| \leq C^{(k)}_{\lambda_2} + C^{(k)}_{\lambda_3}|s|^{4-k}$ for $0 \leq k \leq 4$ with constants $C^{(k)}_{\lambda_2}, C^{(k)}_{\lambda_3} \geq 0$.

Equation error approach

As our initial approach to address the parameter identification of $b(\cdot)$ and $f(\cdot)$, we consider an equation error approach in the spirit of [**6, 57**]. To this end, we insert equation (3.2) of the chemical potential μ into equation (3.1), and replace ϕ by measurements ϕ^δ in the resulting partial differential equation, yielding

$$\partial_t \phi^\delta = -\gamma \operatorname{div}(b(\phi^\delta)\nabla\Delta\phi^\delta) + \operatorname{div}(b(\phi^\delta)f'(\phi^\delta)\nabla\phi^\delta). \tag{3.3}$$

By defining $c(\cdot) = b(\cdot)f'(\cdot)$, $y^\delta = \partial_t \phi^\delta$ and an operator $T^\delta(b,c) = r$, where r is the right-hand side of equation (3.3), we derive a linear operator equation of the form

$$T^\delta(b,c) = y^\delta, \tag{3.4}$$

with perturbed operators T^δ and data y^δ. This inverse problem is ill-posed, and a regularisation method is required to derive stable approximations for the solution. We will employ the well-known Tikhonov regularisation; see [**45**] for a comprehensive analysis of the method considering non-perturbed operators.

Related results

Equation error methods have been proposed and analysed in [**26, 57**] to compute stable approximations for the identification problem of the nonlinear function $a(u)$ in $\partial_t u = \operatorname{div}(a(u)\nabla u)$. Initially, these approaches have been developed for related linear elliptic problems, for instance in [**2, 4, 69, 71**], see also [**3, 68, 91**]. Moreover, the simultaneous identification of multiple parameters in nonlinear elliptic and parabolic problems has also been investigated, see e.g. [**12, 22, 37, 48, 80**]. Further, relevant research can also be found in the context of chemotaxis, as demonstrated in [**38, 52**]. For analysis and examples involving equations of the form (3.4), we refer to [**26, 38, 57, 90**].

The standard approach to identity parameter functions in nonlinear parabolic equations is the output least squares method, which results in a minimisation problem constrained by the nonlinear system (3.1)–(3.2). The computation of a solution then requires subroutines to compute the forward operator, its derivative, and potentially the adjoint derivative if a Newton-type method is employed. Consequently, this method tends to be computationally expensive. Equation error methods present a computationally cheaper approach if appropriate data is available. Nevertheless, we will investigate the output least squares method in Chapter 4.

Let us point out that the main advantage of the equation error approach is that it linearises the inverse problem compared to the nonlinear output least squares method. Hence, the linear method is less involved concerning the required analysis and routines and has cheaper computational costs. However, the quality of reconstructions is only as good as the available data. We will comment on this at the end of the chapter.

Outline of this chapter

We will employ an equation error approach of the form (3.3). This approach reduces the parameter identification problems of $b(\cdot)$ and $f(\cdot)$ to linear ill-posed operator equations with perturbed operators as in equation (3.4). The stable solution to these equations is then achieved using standard regularisation methods. In Section 3.2, we will consider abstract linear ill-posed operator equations with perturbed operators in Hilbert spaces. We employ Tikhonov regularisation to derive stable approximations for the solution and recall the existing theory documented in the literature. The results will provide the theoretical support for the following analysis in Section 3.3, where we consider the regularised approach of equation (3.4) for deriving stable reconstructions of the parameter functions $b(\cdot)$ and $f(\cdot)$. Therein, we show that the abstract result from Section 3.2 applies to our problems, provided the data satisfies reasonable smoothness assumptions. In Section 3.4, we present the numerical realisation of the developed approach to verify its feasibility and conclude with a discussion of its advantages and limitations.

Our main contributions in this chapter are the developed linear approaches to identify the parameters $b(\cdot)$ and $f(\cdot)$ in the Cahn-Hilliard system, which we study from a theoretical and numerical point of view. These results have also been published in [**16**].

3.2. Equation error approach

We consider linear operator equations of the general form

$$T^\delta x = y^\delta, \tag{3.5}$$

with perturbed operators $T^\delta : X \to Y$ and data y^δ, where X, Y are Hilbert spaces. Here, the unknown parameter functions are denoted by x. Recall that the equation error approach described by equation (3.3) leads to such linear operator equations. Hence, equation (3.5) represents our parameter identification problems in an abstract form. Inverse problems of the form (3.5) are in most cases ill-posed. Hence, in the specific cases considered in the following, we use Tikhonov regularisation to derive stable approximations of the parameters x, i.e. we define regularised solutions x_α^δ by

$$\|T^\delta x - y^\delta\|_Y^2 + \alpha \|x\|_X^2 \to \min_{x\in X}. \tag{3.6}$$

Let us now consider the subsequent abstract result provided in [**26, 38**] and also investigated in [**90**]. This result will serve as theoretical support for using (3.6) before we proceed with the specific parameter identification problems of $f(\cdot)$ and $b(\cdot)$ in the Cahn-Hilliard system (3.1)–(3.2). To this end, we denote by $R(T)$ the range of the operator T. Moreover, we call $x \in X$ a least-squares solution of the unperturbed problem $Tx = y$ if

$$\|Tx - y\|_Y = \inf\{\|T\tilde{x} - y\|_Y \,:\, \tilde{x} \in X\},$$

and we call $x^\dagger \in X$ a minimum-norm solution of $Tx = y$ if $x^\dagger$ is a least squares solution of $Tx = y$ and

$$\|x^\dagger\|_X = \inf\{\|\tilde{x}\|_X \,:\, \tilde{x} \text{ is a least squares solution of } Tx = y\}.$$

Theorem 3.2.1 ([**16, Thm. 12**]). *Let $T, T^\delta : X \to Y$ be bounded linear operators between Hilbert spaces X and Y. Further let $y \in R(T)$, $y^\delta \in Y$, and assume that*

$$\|T - T^\delta\|_{X\to Y} \le C\delta \qquad \text{and} \qquad \|y - y^\delta\| \le C'\delta. \tag{3.7}$$

Then for $\alpha = \delta^{2\gamma}$ with $0 < \gamma < 1$, the regularised solutions x_α^δ, determined by

$$\|T^\delta x - y^\delta\|_Y^2 + \alpha \|x\|_X^2 \to \min_{x\in X}, \tag{3.8}$$

converge to the minimum-norm solution $x^\dagger$ of $Tx = y$ with $\delta \to 0$. If $x^\dagger = (T^*T)^\mu w$ for some $w \in X$ and $0 \le \mu \le 1$, then furthermore

$$\|x^\dagger - x_\alpha^\delta\|_X \le C'' \delta^{\min(1-\gamma, 2\mu\gamma)}. \tag{3.9}$$

For $\gamma = 1/(2\mu + 1)$, one thus obtains the order optimal rate $\|x_\alpha^\delta - x^\dagger\|_X \le C''\delta^{\frac{2\mu}{2\mu+1}}$.

Proof. The results follow from a modification of the arguments given in [**45, Ch. 4,5**], and we only present the detailed steps for the second claim, i.e. we show (3.9). By using the triangle inequality, we can split the error into two components

$$\|x_\alpha^\delta - x^\dagger\|_X \leq \|x_\alpha^\delta - \tilde{x}_\alpha\|_X + \|\tilde{x}_\alpha - x^\dagger\|_X,$$

where we inserted $\tilde{x}_\alpha = (T^{\delta,*}T^\delta + \alpha I)^{-1}T^{\delta,*}\tilde{y}$ and $\tilde{y} = T^\delta x^\dagger$. Recall that by definition $x_\alpha^\delta = (T^{\delta,*}T^\delta + \alpha I)^{-1}T^{\delta,*}y^\delta$, and similar for $x^\dagger$. Inserting the definitions, using spectral estimates and the assumptions of the theorem, then yields

$$\|x_\alpha^\delta - \tilde{x}_\alpha\|_X \leq \alpha^{-1/2}\left(\|y^\delta - y\|_Y + \|Tx^\dagger - T^\delta x^\dagger\|_Y\right) \leq \alpha^{-1/2}\delta(C + C').$$

As a preliminary step for the second error component, we use the condition (3.7) on the operator perturbation and interpolation estimates to deduce that

$$x^\dagger = (T^*T)^\mu w = (T^{\delta,*}T^\delta)^\mu w + \eta \qquad \text{with} \qquad \|\eta\|_X \leq c\delta^{\min(2\mu,1)};$$

see e.g. [**90**] for details. Using this, we then estimate for the second error component

$$\begin{aligned}\|\tilde{x}_\alpha - x^\dagger\|_X &\leq \|(T^{\delta,*}T^\delta + \alpha I)^{-1}T^{\delta,*}T^\delta x^\dagger - x^\dagger\|_Y \\ &= \|r_\alpha(T^{\delta,*}T^\delta)((T^{\delta,*}T^\delta)^\mu w + \eta)\|_Y \leq \alpha^\mu\|w\|_X + c\delta^{\min(2\mu,1)},\end{aligned}$$

where we used the abbreviation $r_\alpha(\lambda) = (\lambda+\alpha)^{-1}\lambda - 1 = -\alpha/(\lambda+\alpha)$ and applied spectral estimates for the residual functional in the second and third step; see [**45, Ch. 4,5**]. Combining the two bounds of the error components and choosing $\alpha = \delta^{2\gamma}$ yields

$$\begin{aligned}\|x_\alpha^\delta - x^\dagger\|_X &\leq c'(\alpha^{-1/2}\delta + \alpha^\mu + \delta^{\min(2\mu,1)}) \\ &\leq c'(\delta^{1-\gamma} + \delta^{2\gamma\mu} + \delta^{\min(2\mu,1)}).\end{aligned}$$

The error bound (3.9) then follows by comparing the three terms. □

Remark 3.2.2. The previous theorem provides estimates that establish convergence rates for Tikhonov regularisation of linear inverse problems with perturbed operators, subject to the usual source conditions. These conditions are sufficient but also necessary for the predicted convergence rates; see [**45, Sec. 4.2**]. Moreover, the previous theorem shows that convergence rates can be guaranteed for Tikhonov regularisation without knowing the precise smoothness of the solution $x^\dagger$. However, these rates may not be of optimal order. In [**90**], the author also established convergence rates for parameter choice according to the discrepancy principle under the conditions on the operator perturbations stated in our theorem.

In the following section, we will transform the parameter identification problems of $b(\cdot)$ and $f(\cdot)$, outlined in Section 2.4, into linear operator equations of the form (3.5). Using reasonable assumptions on observations ϕ^δ, we will show that the conditions (3.7) of the previous abstract theorem are satisfied. The abstract result will then guarantee the convergence of the regularised solutions.

3.3. Parameter identification problems

We will now apply the equation error approach to the parameter identification problems of $b(\cdot)$ and $f(\cdot)$ in the Cahn-Hilliard system (3.1)–(3.2), which is complemented with periodic boundary conditions. Let us start with the following assumptions on the available data.

Assumptions 3.3.1. Let ϕ^δ be spatially resolved measurements of ϕ for particular time steps $t \in [0,T]$, and assume that

$$\|\phi(\cdot,t) - \phi^\delta(\cdot,t)\|_{H^3(\Omega)} \leq \delta, \qquad \|\partial_t\phi(\cdot,t) - \partial_t\phi^\delta(\cdot,t)\|_{H^{-1}(\Omega)} \leq \delta, \tag{3.10}$$

with known noise level $\delta > 0$, and we assume that $\phi^\delta \in (-1,1)$.

Considering the regularity results for the true solution, stated in Lemma 2.2.1, the validity of Assumption 3.3.1 is realistic at least after appropriate pre-smoothing of the data, see [**68, 69**] for considerations in this direction. Further, the assumption $\phi^\delta \in (-1,1)$ simplifies the presentation and is realistic as phase fraction measurements outside this interval are not physically reasonable and would be discarded.

By inserting the data ϕ^δ into (3.1)–(3.2), we transform the parameter identification problems of $f(\cdot)$ and $b(\cdot)$ into ill-posed linear operator equations of the form $T^\delta x = y^\delta$. Using the Assumption 3.3.1 on the observations ϕ^δ, we then show that the conditions (3.7) of Theorem 3.2.1 are satisfied.

3.3.1. Identification of $f(\cdot)$

We assume that $\gamma > 0$ and $b(\cdot)$ are known and study the identification of the potential derivative $f(\cdot)$ in the Cahn-Hilliard system (3.1)–(3.2) given measurements ϕ^δ. Similar to Subsection 2.4.1, we eliminate the chemical potential μ by inserting (3.2) into (3.1). Moreover, we define the auxiliary function $c(s) := b(s)f'(s)$. This results in

$$\operatorname{div}(c(\phi)\nabla\phi) = \gamma \operatorname{div}(b(\phi)\nabla\Delta\phi) + \partial_t\phi. \tag{3.11}$$

Note again that since the mobility function $b(\cdot)$ is strictly positive, it allows us to uniquely and stably determine $f'(\cdot)$ from knowledge of the auxiliary function $c(\cdot)$. Throughout the following discussion, we consider ϕ from a single time point $t \in (0,T)$, and we write ϕ for $\phi(\cdot,t)$. Recalling Theorem 2.4.1 on identifiability of $f(\cdot)$, the parameter function $f'(\cdot)$ can be uniquely determined on the range R_t, which corresponds to the values attained by the data ϕ. As discussed in Subsection 2.4.1, a similar statement holds if we use observations from a whole time interval.

Equation error approach

By replacing the true solution ϕ in (3.11) with the measurements ϕ^δ, we derive

$$\operatorname{div}(c(\phi^\delta)\nabla\phi^\delta) = \gamma \operatorname{div}(b(\phi^\delta)\nabla\Delta\phi^\delta) + \partial_t\phi^\delta.$$

We then define the perturbed operator

$$T^\delta : H^2(-1,1) \to H^{-1}(\Omega), \quad c(\cdot) \to \operatorname{div}(c(\phi^\delta)\nabla\phi^\delta), \tag{3.12}$$

and the corresponding perturbed right-hand side by $y^\delta := \partial_t \phi^\delta + \gamma \operatorname{div}(b(\phi^\delta)\nabla\Delta\phi^\delta)$. Recall that we assumed $\phi^\delta \in (-1,1)$ allowing us to define the domain of T^δ as $H^2(-1,1)$. Hence, we transformed the inverse problem of $f(\cdot)$ into a linear operator equation of the form (3.5), i.e. $T^\delta(c) = y^\delta$. To derive stable reconstructions, we then apply Tikhonov regularisation and aim to solve

$$\|T^\delta c - y^\delta\|^2_{H^{-1}(\Omega)} + \alpha\|c\|^2_{H^2(-1,1)} \to \min_{c\in H^2(-1,1)}, \tag{3.13}$$

which yields a reconstruction $c^\delta_\alpha(\cdot)$ of the parameter function $c(\cdot)$, which is then used to determine $f^\delta_\alpha(\cdot)$.

Analysis of the linear operator equation

We now show that the conditions (3.7) of Theorem 3.2.1 are satisfied, which will verify that the outlined approach is well-posed. Verifying the linearity of the operator T^δ is straightforward. By using integration-by-parts and Assumptions 3.1.1 on the parameter functions, we estimate

$$\begin{aligned}\|T^\delta c\|_{H^{-1}(\Omega)} &= \sup_{v\in H^1(\Omega)} \frac{(c(\phi^\delta)\nabla\phi^\delta, \nabla v)_{L^2(\Omega)}}{\|v\|_{H^1(\Omega)}} \\ &\le \|c(\phi^\delta)\nabla\phi^\delta\|_{L^2(\Omega)} \le \|c\|_{L^\infty(-1,1)}\|\phi^\delta\|_{H^1(\Omega)}.\end{aligned}$$

From the Assumptions 3.3.1 on the perturbed data, we know that the last term is bounded. Further, using the continuous embedding of $H^1(-1,1)$ in $L^\infty(-1,1)$, we derive $\|T^\delta c\|_{H^{-1}(\Omega)} \le C\|c\|_{H^2(-1,1)}$, which shows that T^δ is a bounded operator. By employing a similar estimate, one can further show that $\|y^\delta\|_{H^{-1}(\Omega)} \le C'$.

In the next step, we will confirm the validity of the two conditions in Theorem 3.2.1. We estimate the dual norm as before and use the triangle inequality to obtain

$$\begin{aligned}\|T^\delta c - Tc\|_{H^{-1}(\Omega)} &= \|\operatorname{div}(c(\phi^\delta)\nabla\phi^\delta) - \operatorname{div}(c(\phi)\nabla\phi)\|_{H^{-1}(\Omega)} \\ &\le \|c(\phi^\delta)\nabla\phi^\delta - c(\phi)\nabla\phi\|_{L^2(\Omega)} \\ &\le \|c(\phi^\delta)\nabla(\phi^\delta - \phi)\|_{L^2(\Omega)} + \|(c(\phi) - c(\phi^\delta))\nabla\phi\|_{L^2(\Omega)}.\end{aligned}$$

By employing the mean value theorem and using the uniform bounds of the parameter functions, see Assumptions 3.1.1, we deduce

$$\begin{aligned}\|T^\delta c - Tc\|_{H^{-1}(\Omega)} &\le \|c\|_{L^\infty(-1,1)}\|\nabla(\phi^\delta - \phi)\|_{L^2(\Omega)} + \|c'\|_{L^\infty(-1,1)}\|\phi - \phi^\delta\|_{L^\infty(\Omega)}\|\nabla\phi\|_{L^2(\Omega)} \\ &\le C\|\phi - \phi^\delta\|_{H^1(\Omega)}\|c\|_{H^2(-1,1)}.\end{aligned}$$

In the last estimate, we again used the continuous embedding of $H^1(-1,1)$ in $L^\infty(-1,1)$. Hence, from the Assumptions 3.3.1 on the data, we infer that the first condition of Theorem 3.2.1 is valid, i.e.

$$\|T^\delta c - Tc\|_{H^{-1}(\Omega)} \le C\,\delta\,\|c\|_{H^2(-1,1)}.$$

By employing similar arguments, we can estimate the perturbations in the data to derive the validity of the second condition, i.e.

$$\begin{aligned}\|y^\delta - y\|_{H^{-1}(\Omega)} &\leq \|\gamma \operatorname{div}(b(\phi^\delta)\nabla\Delta\phi^\delta) - \gamma \operatorname{div}(b(\phi)\nabla\Delta\phi)\|_{H^{-1}(\Omega)} + \|\partial_t\phi^\delta - \partial_t\phi\|_{H^{-1}(\Omega)} \\ &\leq C'\delta.\end{aligned}$$

Note, for this estimate, we used the assumption on the data that the perturbations are bounded in the space $H^3(\Omega)$.

Summary

We verified in the previous analysis that the conditions of Theorem 3.2.1 are satisfied. Hence, from Theorem 3.2.1, we deduce that our approach to derive reconstructions by minimising the Tikhonov functional (3.13) is well-posed in the following sense. The computation of the regularised approximations $c_\alpha^\delta(\cdot)$ is stable and the approximations $c_\alpha^\delta(\cdot)$ converge to the minimum norm solution $c^\dagger(\cdot)$ of the unperturbed problem $T(c) = y$; provided $\delta \to 0$ and appropriate chosen regularisation parameter α. We conclude that the parameter function $f(\cdot)$ can be reconstructed by the proposed approach up to a constant.

Remark 3.3.2 (Observations from a time interval)**.** If we have observations ϕ^δ available on a whole time interval (t_1, t_2), then it is sufficient to assume $\phi \in L^\infty(t_1, t_2; H^3(\Omega))$ and further that

$$\|\phi - \phi^\delta\|_{L^2(t_1,t_2;H^3(\Omega))} \leq \delta, \qquad \|\partial_t\phi - \partial_t\phi^\delta\|_{L^2(t_1,t_2;H^{-1}(\Omega))} \leq \delta, \tag{3.14}$$

which is slightly weaker than Assumption 3.3.1. By using interpolation inequalities, we also deduce that $\|\phi - \phi^\delta\|_{L^\infty(t_1,t_2;H^1(\Omega))} \leq C\delta$. We then define $Y = L^2(t_1, t_2; H^{-1}(\Omega))$ as the image space of the operator T^δ, which is defined as in (3.12), and define the Tikhonov minimisation problem as in (3.13) inserting the corresponding spaces X, Y. By employing similar arguments as before and using the Assumptions (3.14), one can show that T^δ is a bounded linear operator. Moreover, one can also show that the two conditions of Theorem 3.2.1 are valid, i.e.

$$\|T^\delta c - Tc\|_{L^2(t_1,t_2;H^{-1}(\Omega))} \leq C\,\delta\,\|c\|_{H^2(-1,1)} \qquad \text{and} \qquad \|y^\delta - y\|_{L^2(t_1,t_2;H^{-1}(\Omega))} \leq C'\delta.$$

Consequently, Theorem 3.2.1 again guarantees the convergence of the regularised solutions $c_\alpha^\delta(\cdot)$ to the minimum-norm solution $c^\dagger(\cdot)$ of the operator problem $T(c) = y$. Hence, the proposed approach is also applicable if observations from a whole time interval are available.

3.3.2. Identification of $b(\cdot)$

As a next step in our analysis, we address the identification of the mobility function $b(\cdot)$ while assuming that $\gamma > 0$ and $f(\cdot)$ are known. To do this, we consider equation (3.1) and obtain upon rearranging terms

$$\operatorname{div}\left(b(\phi)\nabla\mu\right) = \partial_t\phi. \tag{3.15}$$

Throughout the following discussion, we consider ϕ at a single time point $t \in (0, T)$, and we write ϕ for $\phi(\cdot, t)$. Recalling Theorem 2.4.5 on identifiability of $b(\cdot)$, the parameter function can be determined uniquely on the range $\widetilde{R}_t$, i.e. values attained by the data ϕ where the non-zero condition on $\nabla \mu$ holds.

Equation error approach

We observe that the chemical potential μ can be approximated from the data $\phi^\delta = \phi^\delta(\cdot, t)$ at $t \in (0, T)$. By inserting the data ϕ^δ, we obtain from equation (3.2) an approximation μ^δ of the chemical potential

$$\mu^\delta = -\gamma \Delta \phi^\delta + f(\phi^\delta).$$

We then replace ϕ and μ in equation (3.15) by ϕ^δ and μ^δ and derive

$$\operatorname{div}\left(b(\phi^\delta)\nabla \mu^\delta\right) = \partial_t \phi^\delta.$$

Next, we define the perturbed operator

$$T^\delta : H^2(-1,1) \to H^{-1}(\Omega), \qquad b(\cdot) \mapsto \operatorname{div}(b(\phi^\delta)\nabla \mu^\delta), \tag{3.16}$$

and the perturbed right-hand side $y^\delta = \partial_t \phi^\delta$. Hence, we transformed the inverse problem of $b(\cdot)$ into a linear operator equation of the form $T^\delta(b) = y^\delta$. Like before, recall that the perturbed data satisfies $\phi^\delta(x,t) \in (-1,1)$, allowing to define the domain of T^δ as $H^2(-1,1)$. We again use Tikhonov regularisation to stabilise the inverse problem, i.e. we aim to solve

$$\|T^\delta b - y^\delta\|^2_{H^{-1}(\Omega)} + \alpha \|b\|^2_{H^2(-1,1)} \to \min_{b \in H^2(-1,1)}, \tag{3.17}$$

which yields the regularised reconstruction $b^\delta_\alpha(\cdot)$ of the parameter function $b(\cdot)$.

Analysis of the linear operator equation

We continue to show that the conditions of Theorem 3.2.1 are satisfied, which will verify that the approach (3.17) is well-posed to identify the mobility $b(\cdot)$. By using similar arguments as in Subsection 2.4.1, we can show that T^δ is linear and bounded, and further, by Assumption 3.3.1, we know that $y^\delta = \partial_t \phi^\delta$ is in $Y = H^{-1}(\Omega)$.

Let us next turn to verify the two conditions (3.7) in Theorem 3.2.1. As a preliminary step, we estimate the perturbation in the chemical potential. By similar arguments as in Subsection 3.3.1, that are the triangle inequality, the mean value theorem and the uniform bounds on the parameter functions from Assumptions 3.1.1, we obtain

$$\begin{aligned} \|\mu^\delta - \mu\|_{H^1(\Omega)} &\leq \|-\gamma \Delta(\phi^\delta - \phi) + f(\phi^\delta) - f(\phi)\|_{H^1(\Omega)} \\ &\leq \gamma \|\phi^\delta - \phi\|_{H^3(\Omega)} + \|f'\|_{L^\infty(-1,1)} \|\phi^\delta - \phi\|_{H^1(\Omega)} \leq C\delta. \end{aligned}$$

For the last estimate, we also employed Assumption 3.3.1 on the data noise. Now we verify the first condition of (3.7). Using the perturbation estimate of the chemical potential, we can estimate the perturbation of the operator T^δ and obtain by similar arguments as before

$$\begin{aligned}\|T^\delta b - Tb\|_{H^{-1}(\Omega)} &\leq \|b(\phi^\delta)\nabla\mu^\delta - b(\phi)\nabla\mu\|_{H^{-1}(\Omega)} \\ &\leq \|b\|_{L^\infty(-1,1)}\|\nabla(\mu^\delta - \mu)\|_{L^2(\Omega)} + \|b'\|_{L^\infty(-1,1)}\|\nabla\mu\|_{L^2(\Omega)}\|\phi - \phi^\delta\|_{L^\infty(\Omega)} \\ &\leq C\,\delta\,\|b\|_{H^2(-1,1)}.\end{aligned}$$

Once more, we used Sobolev embeddings and the uniform bounds for the parameter $b(\cdot) \in H^2(-1,1)$ from the Assumptions 3.1.1. This estimate verifies the first condition of Theorem 3.2.1. The second condition follows directly from the Assumptions 3.3.1 on the data noise, i.e. $\|y - y^\delta\|_{H^{-1}(\Omega)} = \|\partial_t\phi - \partial_t\phi^\delta\|_{H^{-1}(\Omega)} \leq \delta$.

Summary

We conclude that the conditions of Theorem 3.2.1 are satisfied. Hence, we deduce that the approach (3.17) is well-posed in the same sense as before, i.e. we derive stable reconstructions $b_\alpha^\delta(\cdot)$ and the approximations converge to the minimum norm solution $b^\dagger(\cdot)$ of the unperturbed problem $T(b) = y$, if $\delta \to 0$ and $\alpha(\delta)$ chosen appropriately. We summarise that the parameter function $b(\cdot)$ can be reconstructed by the proposed approach (3.17).

Remark 3.3.3 (Observations from a time interval)**.** Similar to the previous considerations in Subsection 3.3.1, if we have measurements ϕ^δ for a whole time interval (t_1, t_2), we use $Y = L^2(t_1, t_2; H^{-1}(\Omega))$ as image space in the definition of the operator T^δ, and further use the bounds (3.14) for the assumptions on the data noise. Similar arguments as before then lead to the conclusion that T^δ is linear, bounded and satisfies the two conditions of the abstract Theorem 3.2.1, i.e.

$$\|T^\delta b - Tb\|_{L^2(H^{-1}(\Omega))} \leq C\,\delta\,\|b\|_{H^2(-1,1)} \qquad \text{and} \qquad \|y - y^\delta\|_{L^2(H^{-1}(\Omega))} \leq \delta.$$

Consequently, the abstract results of Theorem 3.2.1 can again be applied to deduce stability and convergence of the approximations $b_\alpha^\delta(\cdot)$. Hence, the proposed approach is also applicable if observations from a time interval are available.

3.3.3. Simultaneous identification of $f(\cdot)$ and $b(\cdot)$

We assume $\gamma > 0$ to be known and consider the simultaneous identification of the parameter functions $b(\cdot)$ and $f(\cdot)$. Analogue to Subsection 2.4.1, we eliminate the chemical potential μ by inserting (3.2) into (3.1). Rearranging the resulting terms yields

$$-\gamma\,\mathrm{div}(b(\phi)\nabla\Delta\phi) + \mathrm{div}(c(\phi)\nabla\phi) = \partial_t\phi, \tag{3.18}$$

where we introduced the auxiliary function $c(s) = f'(s)b(s)$, as before. Recall that the function $f'(\cdot)$ can be reconstructed through the knowledge of $b(\cdot)$ and $c(\cdot)$, since $b(\cdot)$ is strictly positive. We recall from Theorem 2.4.7 that the parameters $b(\cdot)$ and $c(\cdot)$ can be identified uniquely if an abstract observability condition holds.

Equation error approach

Similar to before, we replace the true solution ϕ in (3.18) with data $\phi^\delta = \phi^\delta(\cdot, t)$ for a single time instance, we derive

$$-\gamma \operatorname{div}(b(\phi^\delta)\nabla\Delta\phi^\delta) + \operatorname{div}(c(\phi^\delta)\nabla\phi^\delta) = \partial_t\phi^\delta.$$

We define the perturbed forward operator

$$\begin{aligned} T^\delta : H^2(-1,1)^2 &\mapsto H^{-1}(\Omega), \\ (b,c) &\mapsto -\gamma \operatorname{div}(b(\phi^\delta)\nabla\Delta\phi^\delta) + \operatorname{div}(c(\phi^\delta)\nabla\phi^\delta) \end{aligned} \tag{3.19}$$

and the corresponding right-hand side by $y^\delta = \partial_t\phi^\delta$. Hence, we transformed the inverse problem of $b(\cdot)$ and $f(\cdot)$ into a linear operator equation of the form (3.5), i.e. $T^\delta(b,c) = y^\delta$. For the stable solution of the parameter identification problem, we propose Tikhonov regularisation and aim to solve

$$\|T^\delta(b,c) - y^\delta\|^2_{H^{-1}(\Omega)} + \alpha\|(b,c)\|^2_{H^2(-1,1)} \to \min_{(b,c)\in H^2(-1,1)^2}, \tag{3.20}$$

which yields reconstructions $b^\delta_\alpha(\cdot)$ and $c^\delta_\alpha(\cdot)$, which are used to determine $f^\delta_\alpha = c^\delta_\alpha(\cdot)/b^\delta_\alpha(\cdot)$.

Analysis of the linear operator equation

In order to verify that the outlined approach is well-posed, we consider the conditions of Theorem 3.2.1. By employing the same arguments used in the previous two subsections, one verifies that T^δ is linear and bounded. Moreover, the conditions (3.7) of Theorem 3.2.1 are satisfied, i.e. one verifies that

$$\|T^\delta(b,c) - T(b,c)\|_{H^{-1}(\Omega)} \leq C\,\delta\,\|(b,c)\|_{H^2(-1,1)}$$

by similar arguments as before, while $\|y - y^\delta\|_{H^{-1}(\Omega)} \leq \delta$ holds by the Assumptions 3.3.1 on the data perturbation.

Summary

As the conditions of Theorem 3.2.1 are satisfied, we deduce that our approach (3.20) is well-posed in the sense that we derive stable reconstructions $(b^\delta_\alpha(\cdot), c^\delta_\alpha(\cdot))$ and the approximations converge to the minimum norm solution $(b^\dagger(\cdot), c^\dagger(\cdot))$ as described for the previous cases. We summarise that the parameter functions $b(\cdot)$ and $f(\cdot)$ can be reconstructed by the proposed approach (3.20).

Remark 3.3.4 (Observations from a time interval)**.** As before, if we have observations ϕ^δ available on a whole time interval (t_1, t_2), we define $Y = L^2(t_1, t_2; H^{-1}(\Omega))$ as image space in the definition of the operator T^δ. Using (3.14) as assumptions on the data noise, one establishes the two conditions (3.7) of Theorem 3.2.1. This yields the convergence of approximate solutions and serves as a theoretical backup of the proposed regularisation approach, i.e. to identify the parameters from data satisfying the abstract observability conditions from Theorem 2.4.7.

3.4. Numerical illustration

Let us briefly recap the main results obtained in the previous sections. We considered an equation error approach to solve the parameter identification problems. To this end, we inserted distributed observations ϕ^δ into the Cahn-Hilliard equation (3.1)–(3.2) and interpreted the resulting equations as linear operator equations $T^\delta x = y^\delta$, where x denotes the parameter functions. By defining the linear operators on suitable spaces and using Tikhonov regularisation, we established that we can derive approximations of the parameter functions by minimising the corresponding Tikhonov functional.

To illustrate our theoretical results, let us now briefly report on the actual performance of the proposed regularisation strategies for model problems in dimension $d = 1, 2$. First, we discuss a one-dimensional test case in Subsection 3.4.1–3.4.4, which allows for a simple depiction of the observability conditions. The actual implementation is then discussed in detail. Second, we present results obtained from a test in two dimensions in Subsection 3.4.5. The implementation details carry over almost verbatim from the one-dimensional test case.

3.4.1. Forward problem

Let us describe the setup of our model problem in dimension $d = 1$. As computational domain, we choose $\Omega = (0, 1)$ and (3.1)–(3.2) are supplemented by periodic boundary conditions. We select as potential derivative the function

$$f(s) = 2(s + 0.99)^3(s - 0.99)(3s - 0.99),$$

which is the derivative of the polynomial double-well potential $\lambda(s) = (s-0.99)^2(s+0.99)^4$ and recall that only $f(s)$ appears in equation (3.2). The mobility function for our model problem is chosen as

$$b(\phi) = (1 - \phi)^4(1 + \phi)^2 + 0.2,$$

and we set $\gamma = 0.003$ for the interface parameter. As the initial value for the phase fraction, we choose

$$\phi_0(x) = 0.1 \sin(2\pi x) - 0.1 \sin(4\pi x) + 0.1 \sin(12\pi x) + 0.1.$$

We then deduce from Lemma 2.2.1 that the solution ϕ is uniformly bounded on $\Omega \times [0, T]$, see also Remark 2.2.2. Hence, the functions $\lambda(\cdot)$ and $b(\cdot)$ could be modified outside of the range of ϕ. Up to such modification, which does not affect our analysis, we deduce that the chosen model parameters satisfy the Assumptions 3.1.1.

3.4.2. Data generation

To generate appropriate data for the inverse problem, we first compute an approximate solution $\phi_{h,\tau}$ utilising the structure-preserving variational discretisation method described in [**19, 36**]. The method employs quadratic finite elements in space and a Petrov-Galerkin time-discretisation with piecewise linear ansatz functions. Details on the implementation can be found in Section 5.1. The resulting solution of this simulation is a function $\phi_{h,\tau}$, which is continuous, piecewise linear in time and piecewise quadratic in space. For the discretisation parameters, we choose uniform grids in space and time with mesh size $h = 5 \cdot 10^{-3}$ and time step $\tau = 2 \cdot 10^{-5}$. The simulation is computed up to the final time $T = 0.02$. Let us note that the following results do not depend on the choice of the method employed to produce the data. Any other appropriate method to solve the Cahn-Hilliard equation could be used as well.

In order to avoid inverse crimes, we employ a different discretisation strategy for the inverse problem. We use cubic splines in space, choose a piecewise linear approximation in time and a backward difference quotient for the discrete time derivative. For the grids, we use uniform spatial and temporal grids with mesh size $\tilde{h}$ and $\tilde{\tau}$, different from those used to generate the data. Therefore, we first compute an approximation $\tilde{\phi}_{\tilde{h},\tilde{\tau}}$, which is piecewise linear in time and a cubic spline in space, by interpolating the data $\phi_{h,\tau}$ on the grid with $\tilde{h}$, $\tilde{\tau}$. This approximation $\tilde{\phi}_{\tilde{h},\tilde{\tau}}$ plays the role of the perturbed data ϕ^δ in our theoretical findings in Section 3.3. Let us note that the perturbations here stem from discretisation and interpolation errors, and we do not add any additional artificial noise. Moreover, we compute a cubic spline approximation $\tilde{\mu}_{\tilde{h},\tilde{\tau}}$ of the chemical potential utilising the identity (3.2). We tested different choices for $\tilde{h}$ and $\tilde{\tau}$, resulting in comparable outcomes. To simplify the presentation, we present the results for $\tilde{h} = 2h$ and $\tilde{\tau} = 2\tau$ in the subsequent discussion.

In Figure 3.1, we depict contour plots of the interpolated functions $\tilde{\phi}_{2h,2\tau}$ and $\partial_x \tilde{\mu}_{2h,2\tau}$. From these depictions, we can derive information about the identification intervals $R_t = \{s = \phi^\delta(x,t) : x \in \Omega\}$ and $\tilde{R}_t = \{s = \phi(x,t) : x \in \Omega,\ \partial_x \mu(x,t) \neq 0\}$, where the parameter functions $f'(\cdot)$ and $b(\cdot)$ can be uniquely identified.

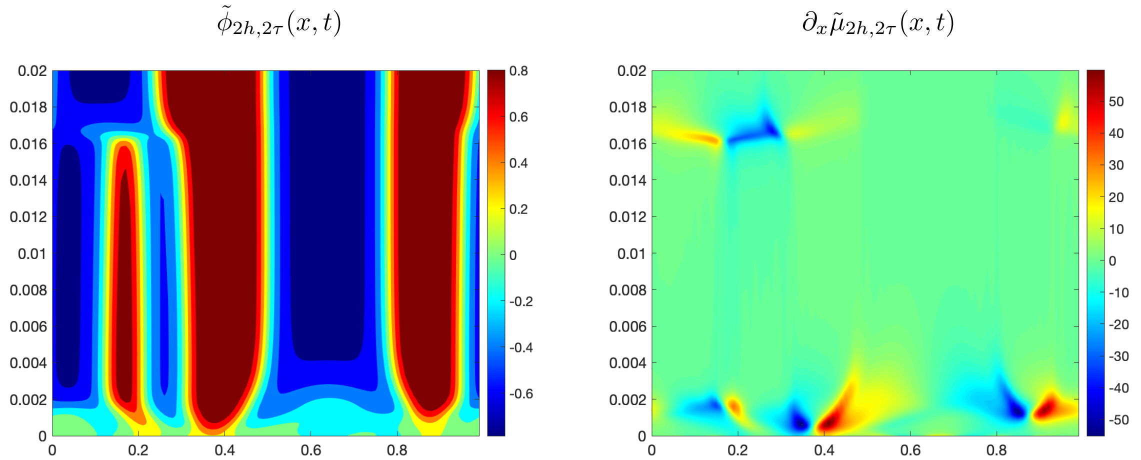

Figure 3.1.: Contour plots of $\tilde{\phi}_{2h,2\tau}(x,t)$ (left) and $\partial_x \tilde{\mu}_{2h,2\tau}(x,t)$ (right) with $x \in (0,1)$ on the x-axis and $t \in [0, 0.02]$ on the y-axis. The colour bar for the left plot shows the range $R = \{\phi^\delta(x,t) : x \in \Omega,\ t \in (0,T)\}$ of data that are attained. The right plot reveals areas where information about the mobility function $b(\cdot)$ can be inferred from the data, i.e. areas where $\partial_x \mu$ is nonzero.

3.4.3. Numerical solution to the inverse problem

We now consider the implementation of the equation error methods introduced in Subsection 3.3. Therefore, we use the following discretisation strategy. The functions ϕ^δ, μ^δ used to define the perturbed operators T^δ in Subsection 3.3 are approximated by the cubic splines $\tilde{\phi}_{2h,2\tau}$ and $\tilde{\mu}_{2h,2\tau}$. The time derivatives are approximated by utilising backward difference quotients. Lastly, the parameter functions $f(\cdot)$ and $b(\cdot)$ are discretised using natural cubic splines on a uniform grid of the interval $[-1, 1]$ with a grid size $\sigma = 0.01$.

Let us discuss some details on the implementation of the perturbed version of the operator equation (3.11), i.e.

$$\operatorname{div}(c(\phi^\delta)\nabla\phi^\delta) = \gamma \operatorname{div}(b(\phi^\delta)\nabla\Delta\phi^\delta) + \partial_t\phi^\delta,$$

which is used to identify the potential derivative $f(\cdot)$. A similar strategy is used to discretise the other two inverse problems.

Numerical realisation of identifying $f(\cdot)$

We approximate the right-hand side y^δ by a vector $\mathtt{y}$, whose ith entry is computed by

$$\mathtt{y}_i = (d_\tau\tilde{\phi}_{2h}, \tilde{\psi}_i)_{L^2(\Omega)} - \gamma(b(\tilde{\phi}_{2h})\nabla\Delta\tilde{\phi}_{2h}, \nabla\tilde{\psi}_i)_{L^2(\Omega)},$$

where $\tilde{\psi}_i$ denotes the ith periodic cubic spline basis function, $\tilde{\phi}_{2h} = \tilde{\phi}_{2h,\tau}(\cdot, t)$ is the evaluation of the data at time t, and $d_\tau\tilde{\phi}_{2h} = \frac{1}{2\tau}(\tilde{\phi}_{2h,2\tau}(\cdot, t) - \tilde{\phi}_{2h,2\tau}(\cdot, t - 2\tau))$ is the approximation for the time derivative by the backward difference quotient. For the left-hand side, we assemble the matrix representation of the operator $T^\delta : c \mapsto \operatorname{div}(c(\tilde{\phi}_{2h})\nabla\tilde{\phi}_{2h})$ by

$$\mathtt{T}_{ij} = -(\theta_j(\tilde{\phi}_{2h})\nabla\tilde{\phi}_{2h}, \tilde{\psi}_i)_{L^2(\Omega)}$$

where θ_j is the jth natural cubic spline basis function for the parameter function $c(s) = \sum_j c_j\theta_j(s)$. Moreover, we define the matrices $\mathtt{M}_{ij} = (\tilde{\psi}_j, \tilde{\psi}_i)_{H^1(\Omega)}$ and $\mathtt{R}_{ij} = (\theta_j, \theta_i)_{H^2(-1,1)}$, which represent the scalar products on $H^1(\Omega)$ and $H^2(-1, 1)$. The discretisation of the Tikhonov functional (3.13) for the inverse problem (3.11) is then given by

$$(\mathtt{Tc} - \mathtt{y})^\top\mathtt{M}^{-1}(\mathtt{Tc} - \mathtt{y}) + \alpha\mathtt{c}^\top\mathtt{Rc},$$

where $\mathtt{c} = (c_1, \ldots, c_N)^\top$ denotes the coefficient vector of the parameter function $c(\cdot)$. The minimisation of the Tikhonov functional is then derived by solving the corresponding normal equations, for which we employ the conjugate gradient algorithm.

Problem dimension and computational costs

By utilising data for a single time step, the discretisation of the operator T^δ results in a matrix $\mathtt{T}$ of size 100×201. This implies that our discrete problem is underdetermined for the given discretisation parameters. If we use data for multiple timesteps, we obtain a matrix of size $100nt \times 201$ by padding the blocks for the individual time steps. However, the resulting normal equations have the size 201×201. Therefore, the computational costs of the method stem primarily from the matrix assembly computations.

3.4.4. Numerical results

We will now present numerical results obtained for the three parameter identification problems discussed in Section 2.4 utilising the regularised equation error methods discussed in Section 3.3. The regularisation parameter α is chosen heuristically, i.e. we use the L-curve-criterium as parameter choice rule; see [**45, 58**]. Here, we consider the one-dimensional model problem and refer to Section 3.4.5 for the two dimensional tests.

Identification of $f(\cdot)$

We assume that γ and $b(\cdot)$ are known, defined as in Subsection 3.4.1 and consider the identification of the potential derivative $f(\cdot)$. As stated in Lemma 2.3.1, we can determine $f(\cdot)$ only up to a constant. Thus, we will identify and depict only the derivative $f'(\cdot)$ in the following. Recall that the function $f'(\cdot)$ can only be uniquely determined on the range of data R_t; see Theorem 2.4.1. In Figure 3.2, we depict the true value $f'(\cdot)$ and the

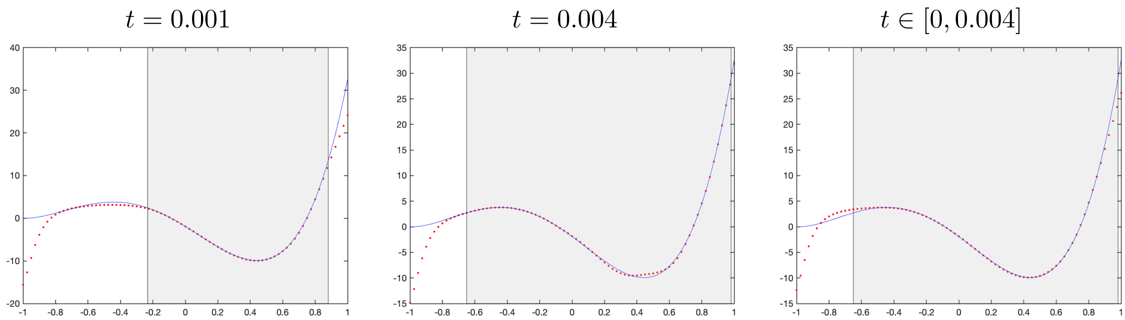

Figure 3.2.: Reconstruction of $f'(\cdot)$ using interpolated data $\tilde{\phi}_{2h,2\tau}(\cdot, t)$, for t as specified in the title of the plots. The range of the data R_t is shaded in grey. The solid blue line depicts the true function $f'(\cdot)$, while the dotted red line is the reconstruction $(f_\alpha^\delta)'(\cdot)$ computed by the regularised equation error method of Section 3.3.1. The regularisation parameter was determined as $\alpha = 10^{-6}, 10^{-8}, 10^{-5}$ in the three tests, respectively.

corresponding reconstruction $(f_\alpha^\delta)'(\cdot)$, determined by our approach. The equation error method yields stable and accurate reconstructions in all three cases, where we varied the utilised data. As expected from Theorem 2.4.1, the function $f'(\cdot)$ can only be reliably reconstructed within the range of available data R_t. The regularisation enforces stability but also introduces a certain bias in regions without available data.

Identification of $b(\cdot)$

We assume that γ and the potential derivative $f(\cdot)$ are known, defined as in Subsection 3.4.1 and consider the identification of the mobility $b(\cdot)$. Recall that the mobility $b(\cdot)$ can only be determined uniquely on the range $\tilde{R}_t = \{s = \phi(x,t) : x \in \Omega,\ \partial_x \mu(x,t) \neq 0\}$ of the available data, where the gradient of the chemical potential μ does not vanish, see Theorem 2.4.5. Note that $\tilde{R}_t$ can be determined prior to the reconstruction, and we used Figure 3.1 to choose t appropriately. In Figure 3.3, we depict the reconstructions obtained

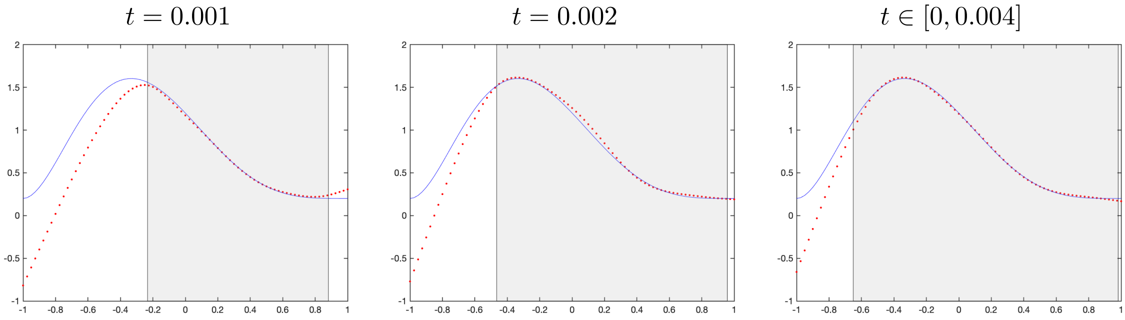

Figure 3.3.: Reconstructions of the mobility function $b(\cdot)$ derived from interpolated data $\tilde{\phi}_{2h,2\tau}(\cdot, t)$ for time points t specified in the title of the plots. The range of the data R_t is shaded in grey. The solid blue line is the true parameter, while the dotted red line depicts the reconstructions. The regularisation parameter was set to $\alpha = 10^{-5}$ for all tests.

from distributed phase fraction data, where we consider three cases varying the utilised data. The reconstructed mobility aligns well with the true parameter $b(\cdot)$ on the range of attained data, while the regularisation introduces a certain bias outside of this range.

Simultaneous identification of $f(\cdot)$ and $b(\cdot)$

We assume that γ is known and consider the identification of both parameter functions $b(\cdot)$ and $f(\cdot)$. From Theorem 2.4.7, we know that the simultaneous identification of both parameters $f(\cdot)$ and $b(\cdot)$ requires observations at multiple time steps. Therefore, in

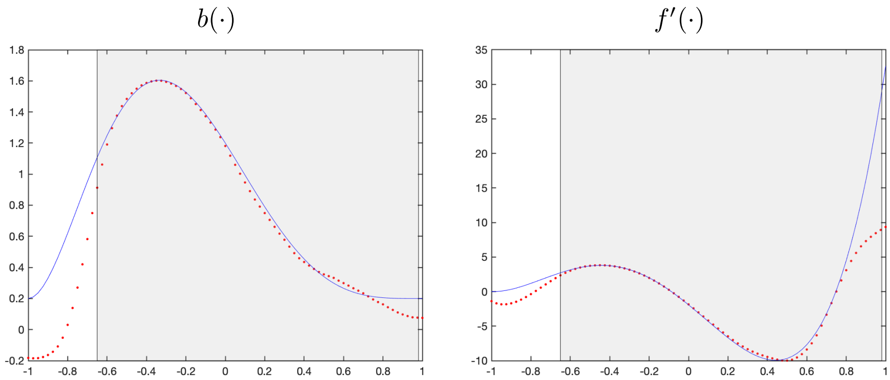

Figure 3.4.: Simultaneous reconstructions of $b(\cdot)$ and $f'(\cdot)$ from interpolated data $\tilde{\phi}_{2h,2\tau}(\cdot, t)$ with $t \in [0, 0.004]$. The range of the attained data R_t is depicted in grey. The solid blue line denotes the true parameter functions, while the corresponding reconstructions are depicted by dotted red lines. The regularisation parameter was set to $\alpha = 10^{-8}$.

Figure 3.4, we only consider reconstructions obtained for data on a whole time interval. Again, the regularised equation error method yields stable and accurate reconstructions of the parameter functions on the range of available data. Besides, we also verified the validity of the observability condition derived in Theorem 2.4.7 by numerically computing the integrals $A_b(s,t_i)$, $A_c(s,t_i)$ for different values of s and t_i. In most cases, we observed the required linear independence.

3.4.5. Numerical results in two dimensions

Let us now consider a model problem in dimension $d = 2$. The implementation is, in principle, similar to the model problem in dimension $d = 1$, and we only highlight the differences. We use a similar setup as in Section 3.4.1 for our model problem in dimension $d = 2$. As the computational domain, we choose the unit square $\Omega = (0,1)^2$. Further, the Cahn-Hilliard system (3.1)–(3.2) is complemented by periodic boundary conditions. We select, similar to the 1-d experiment, the following parameter functions

$$f(s) = 0.3(2(s+0.99)^3(s-0.99)(3s-0.99)), \qquad b(s) = (1-s)^4(1+s)^2 + 0.1,$$

where f is the derivative of the double well potential $\lambda(s) = 0.3(s-0.99)^2(s+0.99)^4$, and we set $\gamma = 0.003$ for the interface parameter. As the initial value for the phase fraction, we choose

$$\phi_0(x,y) = -0.1\cos(4\pi x)\sin(2\pi y) + 0.05\sin(2\pi x)\sin(4\pi y).$$

As before, we deduce from Lemma 2.2.1 that the solution ϕ is uniformly bounded on $\Omega \times [0,T]$, see also Remark 2.2.2. Here, the chosen model parameters satisfy the Assumptions 3.1.1, up to modifications which do not affect the analysis.

Data generation

We choose the same discretisation strategy as in Section 3.4.2 to produce data $\phi_{h,\tau}$ for the inverse problem, that is, the structure-preserving variational discretisation method described in [**36, 19**]; see also Section 5.1. For the discretisation, we use a uniform triangulation in space with mesh size $h = 1/128$ and a uniform grid in time with time step size $\tau = 2.5 \cdot 10^{-4}$. The simulation is computed up to the final time $T = 0.15$.

Again, we employ a different discretisation strategy for the inverse problem to avoid inverse crimes. Here, we proceed as in Section 3.4.2. By interpolating the data $\phi_{h,\tau}$ on the grid with $\tilde{h}$, $\tilde{\tau}$, we compute an approximation $\tilde{\phi}_{\tilde{h},\tilde{\tau}}$ which is piecewise linear in time, and, in extension for dimension $d = 1$, we use a tensor product structure for the cubic spline approximation in space. The approximation $\tilde{\phi}_{\tilde{h},\tilde{\tau}}$ plays the role of the perturbed data ϕ^δ. The discretisation parameters are set to $\tilde{h} = 2h = 1/64$ and $\tilde{\tau} = 2\tau = 5 \cdot 10^{-4}$. In Figure 3.5, we depict the evolution of the interpolated data and provide a plot of the corresponding energy.

Numerical realisation

The numerical solution of the inverse problem is realised in the same way as in Section 3.4.3. The observability conditions can again be checked prior to computation. Here, we used the plot of the energy evolution, see Figure 3.5, to identify regions where the mobility $b(\cdot)$ can be identified. Hence, we chose points in time where the energy is dissipated substantially.

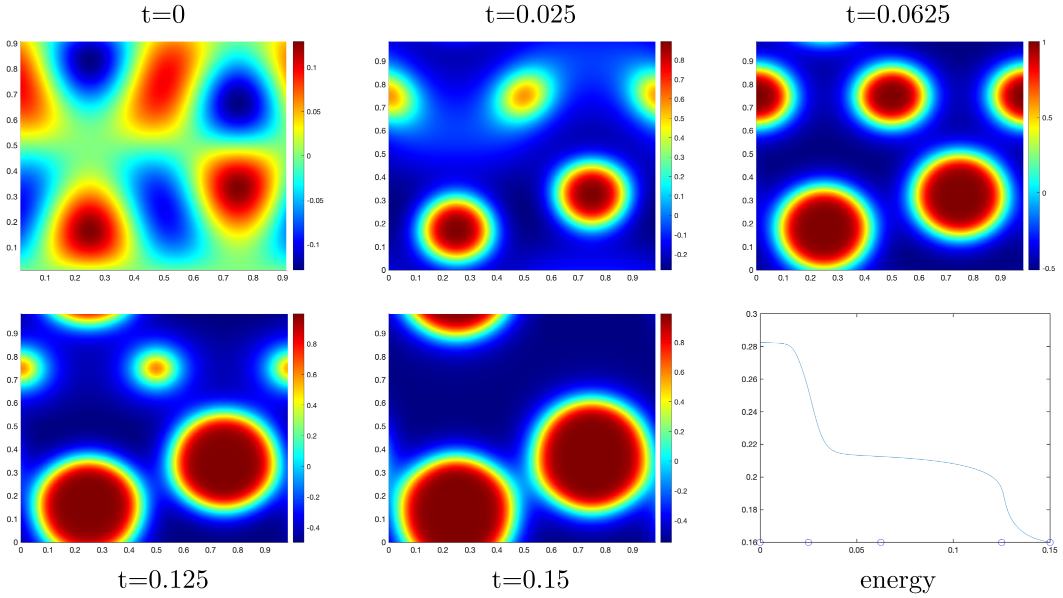

Figure 3.5.: Snapshots of the phase fraction $\tilde{\phi}_{\tilde{h},\tilde{\tau}}$ for time points t specified in the title of the plots. The colour bar on the right of each plot shows the range $R = \{\phi^\delta(x,t) : x \in \Omega, t \in (0,T)\}$ of data that are attained. The evolution of the energy $\mathcal{E}(\phi) = \int_\Omega \frac{\gamma}{2}|\nabla\phi|^2 + \lambda(\phi)\,dx$, $(f(s) = \lambda'(s))$, is depicted with additional markers on the x-axis which correspond to the time points of the snapshots. The Cahn-Hilliard equation satisfies an energy-dissipation relation, i.e. it holds $\partial_t\mathcal{E}(\phi) = -\int_\Omega b(\phi)|\nabla\mu|\,dx$. Hence, we use the depiction of the energy to quickly identify regions where we expect $\nabla\mu$ to be non-constant such that $b(\cdot)$ can be identified.

Numerical results

The computed approximations for the identification problem of either $f(\cdot)$ or $b(\cdot)$ are depicted in Figures 3.6 and 3.7, respectively. We observe that the reconstructions again are in good agreement with the true parameter functions on the range of attained data. Outside of this interval, the regularisation leads to a certain bias, as expected.

In Figure 3.8, we depict the result of the simultaneous identification of both parameter functions. The results also show a good agreement with the true parameters.

Final remarks

In our presentation of numerical results, we only considered data whose perturbation stems from discretisation and interpolation errors. In principle, one can use data perturbed by additional artificial noise. Then one has to include a presmoothing of the data, as considered in [**69**] to satisfy Assumptions 3.3.1. We performed some tests using a smoothing step, which shows the feasibility of this approach. However, this approach is heuristically and roughly spoken, the equation error method yields good results as long as the smoothed data yields an appropriate approximation of the third derivative of ϕ. In summary, the equation error methods yield reconstructions, which show good alignment

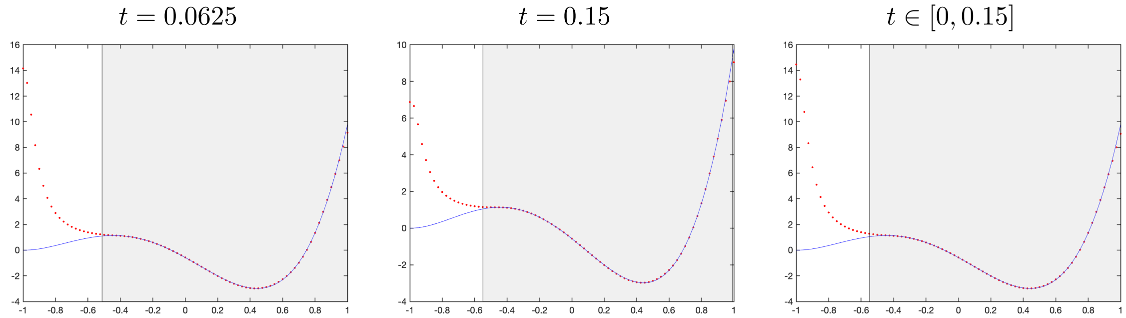

Figure 3.6.: Reconstruction of $f'(\cdot)$ using interpolated data $\tilde{\phi}_{2h,2\tau}(\cdot, t)$, for t as specified in the title of the plots. The range of the data R_t is shaded in grey. The solid blue line depicts the true function $f'(\cdot)$, while the dotted red line is the reconstruction $(f^{\delta}_{\alpha})'(\cdot)$ computed by the regularised equation error method of Section 3.3.1. The L-curve criterium determined the regularisation parameter as $\alpha = 10^{-4}$ in all three tests.

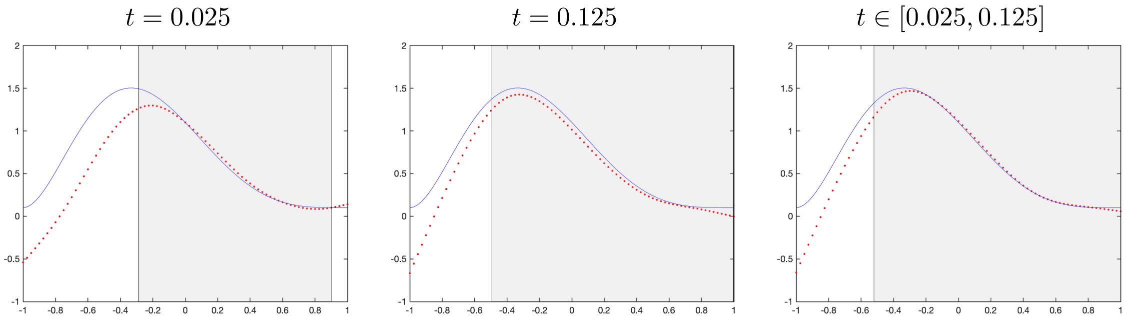

Figure 3.7.: Reconstructions of the mobility function $b(\cdot)$ derived from perturbed data $\tilde{\phi}_{2h,2\tau}(\cdot, t)$ for time points t specified in the title of the plots. The range of attained data R_t is depicted in grey. The solid blue line is the true parameter, while the dotted red line depicts the reconstructions. The regularisation parameter was set to $\alpha = 10^{-4}$ for all tests.

with the true parameters if the quality of the data or smoothed data is appropriate.

3.4.6. Discussion

In this chapter, we studied the stable identification of the parameter functions $b(\cdot)$ and $f(\cdot)$. We established the identification via a regularised equation error approach, which led to linear operator equations with perturbed operators, and we demonstrated the feasibility of the approach in the presence of discretisation errors.

The main disadvantage of the equation error method is its dependence on appropriate data, leading to limitations in its application. With increasing noise level δ, potentially by adding artificial noise, the quality of the reconstructions reduces. This problem can be circumvented to some extent by pre-smoothing the data. Alternatively, it becomes necessary to consider a different method, such as the output least squares method, which

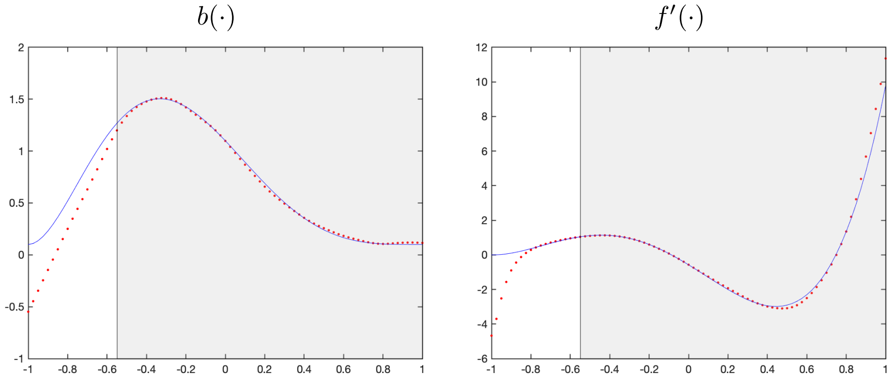

Figure 3.8.: Simultaneous reconstructions of $b(\cdot)$ and $f'(\cdot)$ from perturbed data $\tilde{\phi}_{2h,2\tau}(\cdot, t)$ with $t \in [0, 0.15]$. The range of the attained data is again depicted in grey. The solid blue line denotes the true parameter functions, while dotted red lines depict the corresponding reconstructions. The regularisation parameter was set as $\alpha = 10^{-8}$.

we discuss in the next chapter.

We close this chapter by mentioning some directions for future research. The methods developed to establish the uniqueness of the parameter identification problems might serve as a starting point to derive abstract source conditions or stability estimates; see [**63**] and [**72**] and further references therein. Another direction is the generalisation of the results to more realistic models for phase separation processes; consider the references [**1, 20, 62**] or [**78**] for some examples. With increasing complexity of the model, more parameters or parameter functions are introduced, which increases the difficulty of deriving suitable linear operator equations.

4. Regularised inversion by an output least squares method

In the previous Chapter 3, we studied the parameter identification problem of $b(\cdot)$ and $f(\cdot)$ in the Cahn-Hilliard equation

$$\partial_t \phi = \operatorname{div}\left(b(\phi)\nabla\mu\right), \tag{4.1}$$

$$\mu = -\gamma\Delta\phi + f(\phi), \tag{4.2}$$

by an equation error approach. To this end, we inserted the data ϕ^δ for ϕ in (4.1)–(4.2), which led to linear inverse problems with perturbed operators. In principle, this is a feasible method. However, we required high regularity on the data ϕ^δ, which must be distributed, and we can only identify the parameters where measurements are available. Moreover, in some sense, the method is fine-tuned to the Cahn-Hilliard equation and is not straightforwardly applicable to more complex models. To overcome these issues, we will consider a non-linear approach, namely the output least squares method.

Output least squares approach

We introduce the parameter-to-measurement mapping

$$F : \mathcal{D}(F) \subset X \to Y, \quad (b(\cdot), f(\cdot)) \mapsto \phi,$$

which is usually referred to as the *forward operator*, where ϕ is the first component of the solution (ϕ,μ) to the Cahn-Hilliard system (4.1)–(4.2), with $(b(\cdot), f(\cdot))$ inserted as parameter functions. Note, the operator F is nonlinear. We then consider the following inverse problem:

Given measurements ϕ^δ, find parameter functions $(b(\cdot), f(\cdot))$ such that

$$F(b, f) = \phi^\delta.$$

This parameter identification problem has the abstract form of a nonlinear inverse problem $F(x) = y^\delta$ in Hilbert spaces, where y^δ denotes measurements of exact data y. Such problems are in many cases inherently ill-posed, especially in infinite dimensional spaces, and applying regularisation techniques is necessary. In order to solve the inverse problem $F(x) = y^\delta$, we will apply Tikhonov regularisation. Hence, stable approximations to the true parameter $x^\dagger$, which fulfils $F(x^\dagger) = y$, are derived by minimising the Tikhonov functional

$$\min_{x\in\mathcal{D}(F)} J_\alpha^\delta(x) := \frac{1}{2}\|F(x) - y^\delta\|_Y^2 + \frac{\alpha}{2}\|x - x^*\|_X^2\ , \tag{4.3}$$

where $\alpha > 0$ is a regularisation parameter and x^* is an initial guess for the parameter.

Related results

The analysis of nonlinear inverse problems is considerably more involved in comparison to linear inverse problems, which had to be solved by applying the equation error approach. Nevertheless, such problems have been studied in the literature. For instance, a comprehensive discussion on the regularisation of nonlinear problems can be found in [**45**]. For an overview of parameter estimation problems in nonlinear systems of partial differential equations, consider [**6, 63**].

Identification problems based on spatial measurements have been addressed across a diverse range of applications, see e.g [**38**], where a chemotaxis model is considered, or [**77**] where a population model is considered. Further, the nonlinear identification of a solution-dependent heat conduction coefficient, approached as a control problem, has been analysed in [**27**]. For an identification problem for an elliptic equation of two variables, consider [**4**]. In recent work, [**65**] considers Bayesian parameter identification in a phase-field model for tumour growth. Most relevant to our analysis, there are control problems discussed in [**29, 64**], which consider linear control variables in tumour and diffuse interface models, both involving the Cahn-Hilliard equation as a part of their models. The analysis of those problems goes back to ideas of [**74**]. To our knowledge, the identification of the phase fraction dependent parameter functions $b(\cdot)$ and $f(\cdot)$ has not been covered before.

Outline of this chapter

We will consider the stable identification of the parameter functions (f, b) in the Cahn-Hilliard system (4.1)–(4.2) phrased as nonlinear inverse problem

$$F(b, f) = \phi^\delta. \tag{4.4}$$

To obtain stable approximations to the true parameter functions $(b^\dagger, c^\dagger)$, which fulfils $F(b^\dagger, c^\dagger) = \phi$, by minimising the Tikhonov functional

$$\min_{(b,f)\in\mathcal{D}(F)} J_\alpha^\delta(b, f) := \frac{1}{2}\|F(b, f) - \phi^\delta\|_Y^2 + \frac{\alpha}{2}\|(b, f) - (b^*, f^*)\|_X^2 \ , \tag{4.5}$$

where $\alpha > 0$ is a regularisation parameter, (b^*, f^*) is an initial guess for the parameter functions, and X, Y are Hilbert spaces. To be able to apply standard theory, the operator $F(\cdot)$ must fulfil some properties, e.g. well-posedness, continuity and weak-continuity. In our problem the forward operator has the special structure $F(\cdot) = L(S(\cdot))$, where $L(\cdot)$ is a linear operator, and $S(\cdot)$ is the solution operator mapping parameters (b, f) to the corresponding solution of the Cahn-Hilliard system (4.1)–(4.2). In short,

$$\begin{aligned} S : \mathcal{D}(S) \subset X \to Z, &\quad (b, f) \mapsto (\phi, \mu) \\ L : Z \to Y, &\quad (\phi, \mu) \mapsto (\phi). \end{aligned}$$

As $L(\cdot)$ is a linear operator, the problem of showing certain properties of the forward operator $F(\cdot) = L(S(\cdot))$ reduces to the properties of the solution operator $S(\cdot)$. Hence, we will proceed as follows. In Section 4.1, we will show that the solution operator is well-defined, continuous and weakly continuous. This allows us to establish the existence of a minimum of the Tikhonov functional (4.5) in Section 4.2. For the numerical realisation of the Tikhonov regularisation, we will propose a projected Gauss-Newton iteration; also in Section 4.2. Therefore, we need to establish the differentiability of the operator $F(\cdot)$, which again will be reduced to a corresponding study of the solution operator $S(\cdot)$. This is presented in Section 4.3. Moreover, for the iterative procedure, we need to calculate the outcome of an application of $F'(x)^*$. For this we derive a representation of $F'(x)^*$ in Section 4.4.

Challenges and related results

Let us discuss some challenges of the upcoming analysis. The following discussion and proofs essentially rely on defining auxiliary variational problems for which we derive energy estimates and the existence of solutions by standard Galerkin approximation.

In the work [**64**], the authors discussed an optimal control problem in a Cahn-Hilliard-chemotaxis system. The main analytical novelty was considering a phase fraction dependent mobility for the Cahn-Hilliard equation. While well-posedness and continuity of the solution operator presented no problems, they encountered difficulties in establishing Fréchet differentiability of the solution operator. Those problems have been overcome by establishing continuity estimates in higher norms. We encounter similar difficulties for our identification problems of $b(\cdot)$ and $f(\cdot)$. Hence, we will also derive continuity estimates in higher norms, which will be necessary to establish Fréchet differentiability of $S(\cdot)$. Namely our proof requires, among others, that $\nabla\phi \in L^\infty(0,T;L^\infty(\Omega))$ and $\mu \in L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^3(\Omega))$. The basis of these estimates is the high regularity of smooth solutions, as stated in Section 2.2.

Hence, our main contribution in this chapter is the complete analysis of the Tikhonov regularisation approach. We will adjust the proof ideas of the existing analysis, which did not cover identifying the identification of phase fraction dependent parameter functions in the Cahn-Hilliard equation. Regarding the three parameter identification problems discussed in Section 3.3, our analysis will be formulated for the case of simultaneous identification. The separate identification of a single parameter function, either $b(\cdot)$ or $f(\cdot)$, is then deduced by directly reducing the obtained results.

4.1. The solution operator $S(\cdot)$

In this section, we will first establish the well-posedness of the solution operator $S(\cdot)$, which maps parameters (b, f) to the corresponding solution of the Cahn-Hilliard system (4.1)–(4.2). After that, we derive energy estimates for the operator $S(\cdot)$, leading to continuity and weak continuity of the solution operator $S(\cdot)$. We already note here that the energy estimates are in higher norms than required for the continuity properties. However, they will be required later on.

4.1.1. Set-up and well-posedness

Let us start by presenting a recap of the solvability of the Cahn-Hilliard equation. Afterwards, we define the set-up for the solution operator $S(\cdot)$ and deduce its well-posedness.

Recap: solutions of the Cahn-Hilliard equation

As before, we consider the Cahn-Hilliard system (4.1)–(4.2) on a periodic domain Ω and complement the equations with periodic boundary conditions. For convenience of the reader, let us recall the main assumptions already used in the previous chapters.

Assumptions 4.1.1. We impose the following assumptions on the domain and the parameters:

(A0) $\Omega \simeq \mathbb{T}^d$, is the d-dimensional torus; functions defined on Ω are assumed to be periodic.

(A1) $\gamma > 0$ is a positive constant;

(A2) $b : \mathbb{R} \to \mathbb{R}_+$ satisfies $b \in C^2(\mathbb{R})$ with $0 < c_b \leq b(s) \leq C_b$ for all $s \in \mathbb{R}$ and $\|b'\|_\infty \leq C_{b'}$, $\|b''\|_\infty \leq C_{b''}$;

(A3) $f(s) = \lambda'(s)$ with $\lambda \in C^4(\mathbb{R})$ such that $\lambda(s), \lambda''(s) \geq -c_{\lambda_1}$, for some $c_{\lambda_1} \geq 0$. Furthermore, λ and its derivatives are bounded by $|\lambda^{(k)}(s)| \leq C_{\lambda_2}^{(k)} + C_{\lambda_3}^{(k)}|s|^{4-k}$ for $0 \leq k \leq 4$ with constants $C_{\lambda_2}^{(k)}, C_{\lambda_3}^{(k)} \geq 0$.

In addition, we assume $\phi_0 \in H^3(\Omega)$.

Under these conditions, we established in Lemma 2.2.1 the existence of solutions and their regularities. In particular, for $\phi_0 \in H^3(\Omega)$, we have a unique solution (ϕ, μ), denoted as smooth solution, satisfying the regularities

$$
\begin{aligned}
&\phi \in L^\infty(0,T; H^3(\Omega)) \cap L^2(0,T; H^5(\Omega)) \cap H^1(0,T; H^1(\Omega)),\\
&\mu \in L^\infty(0,T; H^1(\Omega)) \cap L^2(0,T; H^3(\Omega)).
\end{aligned} \tag{4.6}
$$

As noted in Remark 2.2.2, the smooth solution (ϕ, μ) is a continuous function in time

$$
(\phi, \mu) \in C([0,T]; H^3(\Omega) \times H^1(\Omega)),
$$

such that we have the following uniform bounds

$$
\|\phi\|_{C([0,T];H^3(\Omega))} + \|\nabla\phi\|_{L^\infty(0,T;L^\infty(\Omega))} + \max_{0\leq i\leq 2} \|f^{(i)}(\phi)\|_{C(\Omega_T)} \leq C(\|\phi_0\|_{H^3(\Omega)}). \tag{4.7}
$$

Throughout this chapter, we maintain the assumption that the interface parameter $\gamma > 0$ is known. Furthermore, we restrict the analysis to dimension $d = 2$. In this case, the a-priori bounds of solutions to the Cahn-Hilliard equation are global; see Lemma 2.2.1. This is not true in dimension $d = 3$, where the bounds are only valid up to a particular time T, which is usually very small. Moreover, this simplifies the analysis in the following, as we can use interpolation inequalities in two dimensions.

Parameter-to-solution operator $S(\cdot)$

Let us introduce the parameter-to-solution operator, in the following denoted solution operator. To begin, we define the domain of the operator $S(\cdot)$, denoted by $\mathcal{D}(S)$, as follows

$$\mathcal{D}(S) := \{(b, f) \in (H^2(I))^2 : \text{ Assumptions 4.1.1 hold}\},$$

where $I := [a_1, a_2]$ is an interval chosen large enough, such that it holds $\phi(x,t) \in I$ for all $x \in \Omega$ and $t \in [0,T]$. Note that such an interval exists at least until a time T, as smooth solutions are uniformly bounded by the initial distribution ϕ_0. The domain $\mathcal{D}(S)$ is non-empty and convex, as one can easily deduce by choosing convex combinations and the observation that they still satisfy the bounds in Assumption 4.1.1. Moreover, together the two properties imply that $\mathcal{D}(S)$ is weakly closed. Then we define the solution operator

$$S : \mathcal{D}(S) \subset (H^2(I))^2 \to (L^2(0,T; L^2(\Omega)))^2, \quad S(b,f) \mapsto (\phi, \mu),$$

where (ϕ, μ) is the solution of (4.1)–(4.2) with initial conditions $\phi(0) = \phi_0$. If initial data $\phi_0 \in H^3(\Omega)$ is provided, the Cahn-Hilliard system (4.1)–(4.2) has a unique smooth solution. Consequently, it follows that the solution operator $S : (b,f) \mapsto (\phi, \mu)$ is well defined on $\mathcal{D}(S)$.

Remark 4.1.2 (Separate identification)**.** For the identification problems involving only one of the parameter functions $b(\cdot)$ or $f(\cdot)$ (while the other one is known), the definitions of the domain as well as the solution operator are analogous. The subsequent analysis can then readily be reduced to separate parameter identification problems.

In the following, we will derive continuity properties of the solution operator $S(\cdot)$. These properties are then used to deduce properties of the forward operator $F(\cdot)$.

4.1.2. Continuity estimates for $S(\cdot)$

The following theorem establishes estimates for the difference of two smooth solutions of the Cahn-Hilliard equation (4.1)–(4.2), i.e. $(\phi_1, \mu_1) - (\phi_2, \mu_2)$, which yield continuity and Lipschitz continuity of the solution operator $S(b,f)$. Moreover, we derive estimates in higher norms, which will be necessary to analyse the differentiability of $S(b,f)$ later.

Theorem 4.1.3. *Let Assumptions 4.1.1 and $d = 1,2$. Further let $\{(\phi_i, \mu_i)\}_{i=1,2}$ denote two smooth solutions of* (4.1)–(4.2) *corresponding to parameters $\{b_i, f_i\}_{i=1,2}$ and the same initial data $\phi_0 \in H^3(\Omega)$. Then there exists a constant C depending on the uniform bounds of the parameter functions, the domain Ω and the a-priori bounds of the solutions, such that*

$$\begin{aligned}\|\phi_1 - \phi_2\|_{L^\infty(H^2)\cap L^2(H^4)} + \|\partial_t(\phi_1 - \phi_2)\|_{L^2(L^2)} + \|\mu_1 - \mu_2\|_{L^2(H^2)\cap L^\infty(L^2)} \\ \leq C\left(\|b_1 - b_2\|_{H^2} + \|f_1 - f_2\|_{H^2}\right).\end{aligned} \tag{4.8}$$

Before we start with the proof, let us make some remarks. As noted in Section 4.1.1, we restrict our analysis to dimension $d = 1,2$, which simplifies the analysis. We expect the following considerations can be extended to dimension $d = 3$ under additional assumptions on ϕ_0. The basis of the estimates of the theorem is the high regularity of smooth solutions (4.6) and, notably, the proof requires that $\nabla\phi \in L^\infty(0,T;L^\infty(\Omega))$. The following proof is inspired by [**64**] and is divided into four steps. At first, we establish a variational system that is fulfilled by the differences of two solutions. Subsequently, by testing the system, we derive energy estimates and use Gronwall arguments to derive a first estimate of the form (4.8). The subsequent steps will establish such estimates in stronger norms, using elliptic regularity and a Gronwall argument.

Throughout the analysis, we will often estimate the difference of parameter functions, for instance, $b_1(\phi) - b_2(\phi)$, integrated over the space-time domain. For those terms, we initially estimate

$$\int_{\Omega_t} |b_1(\phi) - b_2(\phi)|\, dx\, ds = \int_{\Omega_t} |(b_1 - b_2)(\phi)|\, dx\, ds \le C(t,\Omega)\|b_1 - b_2\|^2_{L^\infty(I)},$$

where we used that $b_i(\cdot)$ and ϕ are uniformly bounded by Assumptions 4.1.1 and the a-priori bounds (4.7). Again by the uniform bounds of ϕ, and the embedding of $H^1(I)$ into $L^\infty(I)$, we derive the estimate

$$\int_{\Omega_t} |b_1(\phi) - b_2(\phi)|\, dx\, ds \le C\|b_1 - b_2\|^2_{L^\infty(I)} \le C\|b_1 - b_2\|^2_{H^2(I)}.$$

These details will be omitted in the following.

Proof. Let $\{(\phi_i, \mu_i)\}_{i=1,2}$ be smooth solutions of (4.1)–(4.2) corresponding to parameters $\{b_i, f_i\}_{i=1,2}$ with initial data $\phi_0 \in H^3(\Omega)$. Further, we define $\hat\phi := \phi_1 - \phi_2$, and analogously introduce $\hat\mu$. Additionally we define $\hat b(\cdot) := b_1(\cdot) - b_2(\cdot)$ and similarly $\hat f(\cdot)$.

We substitute the solutions $\{(\phi_i, \mu_i)\}_{i=1,2}$, as well as the respective parameter functions, into (4.1)–(4.2), and subtract the resulting equations. With the additional insertion of a zero, that is $b_2(\phi_2)\nabla\mu_1$, we find the following system satisfied by $\hat\phi, \hat\mu$ almost everywhere in $\Omega_T := \Omega \times [0,T]$:

$$\partial_t\hat\phi = \operatorname{div}\left((b_1(\phi_1) - b_2(\phi_2))\nabla\mu_1\right) + \operatorname{div}\left(b_2(\phi_2)\nabla\hat\mu\right), \tag{4.9}$$

$$\hat\mu = -\gamma\Delta\hat\phi + f_1(\phi_1) - f_2(\phi_2). \tag{4.10}$$

First step: In the usual manner, we multiply the system with test functions and use integration by parts. Here, we select $v = \gamma\hat\phi$ as test function for equation (4.9), and for (4.10) we select $w = b_2(\phi_2)\hat\mu$ as well as $w = -\varepsilon\phi$, where $\varepsilon > 0$ is a constant to be determined later. The resulting equations are the following

$$\begin{aligned}
\gamma(\partial_t\hat\phi, \hat\phi) &= -\gamma((b_1(\phi_1) - b_2(\phi_2))\nabla\mu_1, \nabla\hat\phi) - \gamma(b_2(\phi_2)\nabla\hat\mu, \nabla\hat\phi), \\
(\hat\mu, b_2(\phi_2)\hat\mu) &= \gamma(\nabla\hat\phi, b_2(\phi_2)\nabla\hat\mu) + \gamma(\nabla\hat\phi, \hat\mu\, b_2'(\phi_2)\nabla\phi_2) + (f_1(\phi_1) - f_2(\phi_2), b_2(\phi_2)\hat\mu), \\
-\varepsilon(\hat\mu, \hat\phi) &= -\gamma\varepsilon(\nabla\hat\phi, \nabla\hat\phi) - \varepsilon(f_1(\phi_1) - f_2(\phi_2), \hat\phi).
\end{aligned}$$

Upon adding the three equations, the term $\gamma(b_2(\phi_2)\nabla\hat\mu, \nabla\hat\phi)$ cancels out, and using the lower bound on the parameter function $b(\cdot)$, see Assumptions 4.1.1, we obtain

$$\begin{aligned}\frac{\gamma}{2}\frac{d}{dt}\|\hat{\phi}\|_{L^2}^2+c_b\|\hat{\mu}\|_{L^2}^2 + \varepsilon\gamma\|\nabla\hat{\phi}\|_{L^2}^2 &\leq \varepsilon\int_\Omega |\hat{\mu}||\hat{\phi}|\,dx \\ &+\varepsilon\int_\Omega |f_1(\phi_1)-f_2(\phi_2)||\hat{\phi}|\,dx + C_b\int_\Omega |f_1(\phi_1)-f_2(\phi_2)||\hat{\mu}|\,dx \\ &+\int_\Omega |b_2'(\phi_2)||\nabla\phi_2||\hat{\mu}||\nabla\hat{\phi}|\,dx + \gamma\int_\Omega |b_1(\phi_1)-b_2(\phi_2)||\nabla\mu_1||\nabla\hat{\phi}|\,dx \\ &=: (i)+(ii)+(iii)+(iv)+(v).\end{aligned} \tag{4.11}$$

The terms (i)–(v) on the right-hand side are now estimated separately. By employing Hölder's inequality and Young's inequality, using appropriate factors, we obtain

$$(i) = \varepsilon\int_\Omega |\hat{\mu}||\hat{\phi}|\,dx \leq \varepsilon\|\hat{\mu}\|_{L^2}\|\hat{\phi}\|_{L^2} \leq \frac{c_b}{4}\|\hat{\mu}\|_{L^2}^2 + C_\varepsilon\|\hat{\phi}\|_{L^2}^2.$$

To estimate the second term, we utilise the triangle inequality and the mean value theorem to estimate

$$\begin{aligned}(ii) &= \varepsilon\int_\Omega |f_1(\phi_1)-f_2(\phi_2)||\hat{\phi}|\,dx \\ &\leq \varepsilon\int_\Omega |f_1(\phi_1)-f_1(\phi_2)||\hat{\phi}| + |f_1(\phi_2)-f_2(\phi_2)||\hat{\phi}|\,dx \\ &\leq \varepsilon\int_\Omega |f_1'(\zeta)(\phi_1-\phi_2)||\hat{\phi}| + |f_1(\phi_2)-f_2(\phi_2)||\hat{\phi}|\,dx,\end{aligned}$$

with $\zeta(x,t)\in[\min\{\phi_1(x,t)-\phi_2(x,t)\},\max\{\phi_1(x,t)-\phi_2(x,t)\}]$. Using the uniform bound $\|f'(\phi_i)\|_{C(\Omega_T)} \leq C(\|\phi_0\|_{H^3(\Omega)})$, see (4.7), and applying Young's inequality, we derive

$$\begin{aligned}(ii) &\leq C\|f_1'\|_{L^\infty}\int_\Omega |\hat{\phi}|^2\,dx + C(\|f_1(\phi_2)-f_2(\phi_2)\|_{L^2}^2 + \|\hat{\phi}\|_{L^2}^2) \\ &\leq C(\|\hat{\phi}\|_{L^2}^2 + \|\hat{f}\|_{H^2}^2),\end{aligned} \tag{4.12}$$

where C depends on the domain Ω, the constant ε and the uniform bound of $f'(\cdot)$. Using similar arguments as before, we bound the third term in the following manner

$$\begin{aligned}(iii) &= C_b\int_\Omega |f_1(\phi_1)-f_2(\phi_2)||\hat{\mu}|\,dx \\ &\leq C_b\|f_1'\|_{L^\infty}\|\hat{\phi}\|_{L^2}\|\hat{\mu}\|_{L^2} + C_b\|f_1(\phi_2)-f_2(\phi_2)\|_{L^2}\|\hat{\mu}\|_{L^2} \\ &\leq C(\|\hat{\phi}\|_{L^2}^2 + \|\hat{f}\|_{H^2}^2) + \frac{c_b}{4}\|\hat{\mu}\|_{L^2}^2,\end{aligned}$$

where the constant C depends on the bounds of the parameter functions $b(\cdot), f'(\cdot)$ and a constant derived from Young's inequality. Additionally, we applied the continuous embedding of $H^1(I)$ into $L^\infty(I)$, which will be utilised on various occasions in the subsequent estimates but will not be explicitly mentioned all the time. To estimate the fourth term, we use the uniform a-priori bounds (4.7), i.e. $\nabla\phi$ is a-priori bounded in $L^\infty(0,T;L^\infty(\Omega))$, which consequently establish the boundedness of $\|b_2'(\phi_2)\nabla\phi_2\|_{L^\infty(L^\infty)}$, and obtain

$$\begin{aligned}(iv) &= \int_\Omega |b_2'(\phi_2)||\nabla\phi_2||\hat{\mu}||\nabla\hat{\phi}|\,dx \le \|b_2'(\phi_2)\nabla\phi_2\|_{L^\infty}\int_\Omega |\hat{\mu}||\nabla\hat{\phi}|\,dx\\ &\le \frac{1}{c_b}\|b_2'(\phi_2)\nabla\phi_2\|_{L^\infty}^2\|\nabla\hat{\phi}\|_{L^2}^2 + \frac{c_b}{4}\|\hat{\mu}\|_{L^2}^2\\ &\le \overline{C}\|\nabla\hat{\phi}\|_{L^2}^2 + \frac{c_b}{4}\|\hat{\mu}\|_{L^2}^2,\end{aligned}$$

where $\overline{C}$ is a uniform constant. For the fifth term, we again apply Hölder's inequality

$$(v) = \gamma\int_\Omega |b_1(\phi_1)-b_2(\phi_2)||\nabla\mu_1||\nabla\hat{\phi}|\,dx \le \gamma\|(b_1(\phi_1)-b_2(\phi_2))\nabla\mu_1\|_{L^2}\|\nabla\hat{\phi}\|_{L^2}. \tag{4.13}$$

Let us consider the first term on the right hand side and recall that $\nabla\mu_1 \in L^4(0,T;L^4(\Omega))$, $b \in C^2(\mathbb{R})$, and $\{\phi_i\}_{i=1,2}$ are uniformly bounded to deduce that

$$\begin{aligned}\|(b_1(\phi_1)-b_2(\phi_2))\nabla\mu_1\|_{L^2}^2 &\le \|\nabla\mu_1\|_{L^4}^2\left(\|b_1(\phi_1)-b_1(\phi_2)\|_{L^4}^2 + \|b_1(\phi_2)-b_2(\phi_2)\|_{L^4}^2\right)\\ &\le \|\nabla\mu_1\|_{L^4}^2\left(C_{b'}\|\hat{\phi}\|_{L^4}^2 + C\|\hat{b}\|_{H^1}^2\right).\end{aligned}$$

Next, we employ an interpolation inequality, which holds in dimension $d=2$, i.e for $\phi \in H^1(\Omega)$ it holds

$$\|\phi\|_{L^4(\Omega)} \le C(\Omega)\left(\|\phi\|_{L^2(\Omega)}^{\frac{1}{2}}\|\nabla\phi\|_{L^2(\Omega)}^{\frac{1}{2}} + \|\phi\|_{L^2(\Omega)}\right),$$

details can be found in the appendix. Using this, along with Young's inequality, we further estimate

$$\begin{aligned}\|(b_1(\phi_1)-b_2(\phi_2))\nabla\mu_1\|_{L^2}^2 &\le \|\nabla\mu_1\|_{L^4}^2\left(C_{b'}\left(\|\hat{\phi}\|_{L^2}^{\frac{1}{2}}\|\nabla\hat{\phi}\|_{L^2}^{\frac{1}{2}} + \|\hat{\phi}\|_{L^2}\right)^2 + C\|\hat{b}\|_{H^1}^2\right)\\ &\le \|\nabla\mu_1\|_{L^4}^2\left(C_{b'}(\|\hat{\phi}\|_{L^2}\|\nabla\hat{\phi}\|_{L^2} + \|\hat{\phi}\|_{L^2}^2) + C\|\hat{b}\|_{H^1}^2\right)\\ &\le \|\nabla\hat{\phi}\|_{L^2}^2 + C\left((\|\nabla\mu_1\|_{L^4}^4 + \|\nabla\mu_1\|_{L^4}^2)\|\hat{\phi}\|_{L^2}^2 + \|\nabla\mu_1\|_{L^4}^2\|\hat{b}\|_{H^1}^2\right)\\ &\le \|\nabla\hat{\phi}\|_{L^2}^2 + C\|\hat{b}\|_{H^2}^2 + C(1+\|\nabla\mu_1\|_{L^4}^4)\|\hat{\phi}\|_{L^2}^2.\end{aligned}$$

Utilising this assertion, we deduce that (4.13) can be estimated further to derive a bound of the fifth term

$$\begin{aligned}(v) &\le C\|(b_1(\phi_1)-b_2(\phi_2))\nabla\mu_1\|_{L^2}^2 + \|\nabla\hat{\phi}\|_{L^2}^2\\ &\le C\|\hat{b}\|_{H^2}^2 + 2\|\nabla\hat{\phi}\|_{L^2}^2 + C(1+\|\nabla\mu_1\|_{L^4}^4)\|\hat{\phi}\|_{L^2}^2.\end{aligned}$$

Gathering the estimates for (i)–(v), we establish the differential inequality

$$\begin{aligned}&\frac{\gamma}{2}\frac{d}{dt}\|\hat{\phi}\|_{L^2}^2 + \frac{c_b}{4}\|\hat{\mu}\|_{L^2}^2 + \left(\varepsilon\gamma - 2 - \overline{C}\right)\|\nabla\hat{\phi}\|_{L^2}^2\\ &\qquad\le C\left(1+\|\nabla\mu_1\|_{L^4}^4\right)\left(\|\hat{\phi}\|_{L^2}^2 + \|\hat{f}\|_{H^2}^2 + \|\hat{b}\|_{H^2}^2\right),\end{aligned}$$

where C depends only on the domain Ω, the constant ε and the uniform bounds on the parameter functions $b(\cdot)$,$f(\cdot)$, see Assumptions 4.1.1. Choosing a sufficiently large value for ε results in a positive coefficient in front of $\|\nabla\hat{\phi}\|_{L^2}^2$. Additionally, by interpolation, see [**73**], it holds that $\nabla\mu_1 \in L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega)) \subset L^4(0,T;L^4(\Omega))$ for dimension $d = 2$. Hence, the preceding inequality remains valid upon integration over the time interval $(0,T)$, such that an application of the Gronwall inequality, see Lemma A.2.1, using that $\nabla\mu_1 \in L^4(0,T;L^4(\Omega))$, yields

$$\sup_{t\in(0,T)} \|\hat{\phi}(t)\|_{L^2}^2 + \|\hat{\mu}\|_{L^2(L^2)}^2 + \|\nabla\hat{\phi}\|_{L^2(L^2)}^2 \le C(\|\hat{f}\|_{H^2}^2 + \|\hat{b}\|_{H^2}^2) =: C(*).$$

Hence we conclude that we established as first estimate

$$\|\hat{\phi}\|_{L^\infty(L^2)\cap L^2(H^1)} + \|\hat{\mu}\|_{L^2(L^2)} \le C(\|\hat{f}\|_{H^2}^2 + \|\hat{b}\|_{H^2}^2) = C(*). \tag{4.14}$$

In the following, we will use the notation $C(*)$ to represent bounds that depend on the difference of the parameter functions as defined.

Second step: To show higher regularity of $\hat{\phi}$, we first establish an additional bound for the terms in (4.10). By using the bounds given in (4.14) and the Assumptions 4.1.1 for $f(\cdot)$, we estimate in a similar manner as in (4.12) that

$$\|f_1(\phi_1) - f_2(\phi_2)\|_{L^2(L^2)}^2 \le C\left(\|\phi_1 - \phi_2\|_{L^2(L^2)}^2 + \|\hat{f}\|_{H^2}^2\right) \le C(*).$$

Now, we consider equation (4.10) from the perspective of an elliptic equation for $\hat{\phi}$. By virtue of elliptic regularity [**46**], we infer

$$\|\Delta\hat{\phi}\|_{L^2(L^2)} \le C(\|\hat{\mu}\|_{L^2(L^2)} + \|f_1(\phi_1) - f_2(\phi_2)\|_{L^2(L^2)}^2).$$

Consequently, given that the domain Ω is periodic, we derive the estimate

$$\|\hat{\phi}\|_{L^2(H^2(\Omega))} \le C(\|\hat{\phi}\|_{L^2(L^2(\Omega))} + \|\Delta\hat{\phi}\|_{L^2(L^2(\Omega))}) \le C(*).$$

Third step: We will test the system (4.9)–(4.10) with suitable functions and use the previously established estimate (4.14) to derive energy estimates, which will lead to bounds of $\hat{\phi}$ and $\hat{\mu}$ with respect to $\hat{b}$ and $\hat{f}$ in higher norms. For this purpose, we test (4.9) with $v = \hat{\mu}$ and (4.10) with $w = \partial_t\hat{\phi}$, that is

$$\begin{aligned}
(\partial_t\hat{\phi}, \hat{\mu}) &= -((b_1(\phi_1) - b_2(\phi_2))\nabla\mu_1, \nabla\hat{\mu}) - (b_2(\phi_2)\nabla\hat{\mu}, \nabla\hat{\mu}),\\
(\hat{\mu}, \partial_t\hat{\phi}) &= \gamma(\nabla\hat{\phi}, \nabla\partial_t\hat{\phi}) + (f_1(\phi_1) - f_2(\phi_2), \partial_t\hat{\phi}).
\end{aligned}$$

By subtracting both equations and integrating over $(0,t)$, we obtain

$$\begin{aligned}
&\frac{\gamma}{2}\|\nabla\hat{\phi}(t)\|_{L^2}^2 + \int_{\Omega_t} b_2(\phi_2)|\nabla\hat{\mu}|^2\,dx\,ds\\
&\le \int_{\Omega_t} |b_1(\phi_1) - b_2(\phi_2)||\nabla\mu_1||\nabla\hat{\mu}|\,dx\,ds + \int_0^T (f_1(\phi_1) - f_2(\phi_2), \partial_t\hat{\phi})\,ds\\
&=: (i) + (ii).
\end{aligned} \tag{4.15}$$

To estimate the first term, we employ Hölder's inequality and similar reasoning as for the bounds of the terms in (4.13), and derive

$$\begin{aligned}(i) &\leq \|b_1(\phi_1) - b_2(\phi_2)\|_{L^4(L^4)}\|\nabla\mu_1\|_{L^4(L^4)}\|\nabla\hat{\mu}\|_{L^2(L^2)} \\ &\leq C\left(C_b\|\hat{\phi}\|_{L^4(L^4)} + \|\hat{b}\|_{H^2}\right)\|\nabla\mu_1\|_{L^4(L^4)}\|\nabla\hat{\mu}\|_{L^2(L^2)}.\end{aligned}$$

Once more, we utilised the boundedness of $\nabla\mu_1$ in $L^4(0,T;L^4(\Omega))$ by interpolation. With the bounds given in (4.14) and Young's inequality, we can now derive the following estimate for the term (i) of (4.15):

$$(i) \leq C(*)^{\frac{1}{2}}\|\nabla\mu_1\|_{L^4(L^4)}\|\nabla\hat{\mu}\|_{L^2(L^2)} \leq C(*) + \frac{c_b}{4}\|\nabla\hat{\mu}\|^2_{L^2(L^2)}.$$

The second term of (4.15) is estimated to

$$(ii) \leq \|f_1(\phi_1) - f_2(\phi_2)\|_{L^2(H^1)}\|\partial_t\hat{\phi}\|_{L^2(H^{-1})}. \tag{4.16}$$

We continue to derive estimates for the two terms separately. First, by employing integration by parts, we establish a bound for $\partial_t\hat{\phi}$, that is

$$\begin{aligned}\|\partial_t\hat{\phi}\|_{L^2(H^{-1})} &= \sup_{v\in L^2(H^1)}\frac{(-(b_1(\phi_1)-b_2(\phi_2))\nabla\mu_1 - b_2(\phi_2)\nabla\hat{\mu}, \nabla v)_{L^2(L^2)}}{\|v\|_{L^2(H^1)}}, \\ &\leq \|(b_1(\phi_1)-b_2(\phi_2))\nabla\mu_1\|_{L^2(L^2)} + C_b\|\nabla\hat{\mu}\|_{L^2(L^2)} \\ &\leq \|b_1(\phi_1)-b_2(\phi_2)\|_{L^4(L^4)}\|\nabla\mu_1\|_{L^4(L^4)} + C_b\|\nabla\hat{\mu}\|_{L^2(L^2)}.\end{aligned}$$

Subsequently, with the boundedness of $\nabla\mu_1$ in $L^4(0,T;L^4(\Omega))$, the stated assumptions on $b(\cdot)$, and the established bounds (4.14), we deduce

$$\|\partial_t\hat{\phi}\|_{L^2(H^{-1})} \leq C(\|\hat{\phi}\|_{L^4(L^4)} + \|\hat{b}\|_{H^2}) + C_b\|\nabla\hat{\mu}\|_{L^2(L^2)} \leq C(*)^{\frac{1}{2}} + C_b\|\nabla\hat{\mu}\|_{L^2(L^2)}, \tag{4.17}$$

as first estimate of the terms in (4.16). Here we used that by interpolation [**73**] it holds

$$\|\hat{\phi}\|_{L^4(L^4)} \leq C(\|\hat{\phi}\|_{L^2(W^{1,2})} + \|\hat{\phi}\|_{L^\infty(L^2)}).$$

Next, we establish an estimate of the difference of the functions $f_1(\cdot), f_2(\cdot)$ in (4.16) in $L^2(0,T;W^{1,2}(\Omega))$. By differentiation and application of the triangle inequality, we get

$$\begin{aligned}&\|\nabla(f_1(\phi_1) - f_2(\phi_2))\|_{L^2(L^2)} \\ &\qquad \leq \|f_1'(\phi_1)\nabla\phi_1 - f_1'(\phi_2)\nabla\phi_2\|_{L^2(L^2)} + \|(f_1'(\phi_2) - f_2'(\phi_2))\nabla\phi_2\|_{L^2(L^2)} \\ &\qquad \leq \|(f_1'(\phi_1) - f_1'(\phi_2))\nabla\phi_1\|_{L^2(L^2)} + \|f_1'(\phi_2)(\nabla\phi_1 - \nabla\phi_2)\|_{L^2(L^2)} \\ &\qquad\quad + \|(f_1'(\phi_2) - f_2'(\phi_2))\nabla\phi_2\|_{L^2(L^2)}.\end{aligned}$$

By employing the mean value theorem, utilising the bounds of $f_i(\cdot)$, and applying Hölder's inequality, we further estimate this to

$$C(f_1'')\|\hat{\phi}\|_{L^4(L^4)}\|\nabla\phi_1\|_{L^4(L^4)} + C(f_1')\|\nabla\hat{\phi}\|_{L^2(L^2)} + \|\hat{f}\|_{H^2}\|\nabla\phi_2\|_{L^2(L^2)}.$$

Hence, together with the established bounds (4.14), we derive

$$\|\nabla(f_1(\phi_1) - f_2(\phi_2))\|_{L^2(L^2)} \leq C(\|\hat{\phi}\|_{L^2(H^1)} + \|\hat{f}\|_{H^2}) \leq C(*)^{\frac{1}{2}}, \tag{4.18}$$

as second estimate of the terms in (4.16). Combining the previous estimates (4.18) and (4.17), we can further bound (4.16) by

$$(ii) \leq \|f_1(\phi_1) - f_2(\phi_2)\|_{L^2(H^1)}\|\partial_t\hat{\phi}\|_{L^2(H^{-1})} \leq \frac{c_b}{4}\|\nabla\hat{\mu}\|^2_{L^2(L^2)} + C(*).$$

By combination of the inequality (4.15) and the bounds on (i)–(ii), we deduce that

$$\|\hat{\phi}\|^2_{L^\infty(H^1)} + \|\nabla\hat{\mu}\|^2_{L^2(L^2)} + \|\partial_t\hat{\phi}\|^2_{L^2(H^{-1})} \leq C(*).$$

Further, combining this inequality with the bound (4.18), we obtain by elliptic regularity that

$$\|\hat{\phi}\|_{L^2(H^3)} \leq C(*)$$

and conclude the third step.

Fourth step: In order to derive our final estimates, we will test (4.9) with $v = \Delta^2\hat{\phi}$, derive energy estimates and employ a Gronwall argument at the end. We initially derive a bound for the difference of the functions $f_i(\cdot)$ in $L^2(0,T;W^{2,2}(\Omega))$. By differentiation, we compute

$$\begin{aligned}&\|\Delta(f_1(\phi_1) - f_2(\phi_2))\|^2_{L^2}\\ &\qquad \leq \int_\Omega |f_1''(\phi_1)|\nabla\phi_1|^2 + f_1'(\phi_1)\Delta\phi_1 - f_2''(\phi_2)|\nabla\phi_2|^2 - f_2'(\phi_2)\Delta\phi_2|^2\,dx,\end{aligned}$$

and by introducing appropriate zero terms, we can further estimate

$$\begin{aligned}C\int_\Omega &|(f_1''(\phi_1) - f_1''(\phi_2))|\nabla\phi_1|^2 + f_1''(\phi_2)(\nabla\hat{\phi}\nabla\phi_1 + \nabla\phi_2\nabla\hat{\phi}) + (f_1'' - f_2'')(\phi_2)|\nabla\phi_2|^2|^2\\ &|(f_1'(\phi_1) - f_1'(\phi_2))\Delta\phi_1 + f_1'(\phi_2)\Delta(\phi_1 - \phi_2) + (f_1' - f_2')(\phi_2)\Delta\phi_2|^2\,dx =: (i) + (ii).\end{aligned}$$

To estimate the terms of (i), we employ the mean value theorem, along with the uniform bounds for $f''(\cdot)$ and $f'''(\cdot)$ from Assumptions 4.1.1, and the uniform bounds of the solutions $\phi_i, \nabla\phi_i \in L^\infty(0,T;L^\infty(\Omega))$ to obtain

$$\begin{aligned}(i) &\leq C(\|f_1'''(\zeta)\hat{\phi}|\nabla\phi_1|^2\|^2_{L^2} + \|\nabla\hat{\phi}\|^2_{L^2} + \|(f_1'' - f_2'')(\phi_2)|\nabla\phi_2|^2\|^2_{L^2})\\ &\leq C(\|\hat{\phi}\|^2_{L^2} + \|\nabla\hat{\phi}\|^2_{L^2} + \|\hat{f}''\|^2_{L^2}).\end{aligned}$$

Considering $\Delta\phi_i \in L^2(0,T;H^2)$, we proceed to estimate the terms of (ii) and derive

$$\begin{aligned}(ii) &\leq C(\|f_1''(\zeta)\hat{\phi}\Delta\phi_1\|^2_{L^2} + \|f_1'(\phi_2)\Delta\hat{\phi}\|^2_{L^2} + \|(f_1' - f_2')(\phi_2)\Delta\phi_2\|^2_{L^2})\\ &\leq C(\|\hat{\phi}\|^2_{L^4}\|\Delta\phi_1\|^2_{L^4} + \|\Delta\hat{\phi}\|^2_{L^2} + \|\hat{f}'\|^2_{L^\infty})\\ &\leq C(\|\hat{\phi}\|^2_{H^1} + \|\Delta\hat{\phi}\|^2_{L^2} + \|\hat{f}'\|^2_{H^1}).\end{aligned}$$

By combining the estimates of (i) and (ii), we obtain the bound

$$\|\Delta(f_1(\phi_1) - f_2(\phi_2))\|_{L^2}^2 \le C(\|\hat{\phi}\|_{L^2}^2 + \|\nabla\hat{\phi}\|_{L^2}^2 + \|\Delta\hat{\phi}\|_{L^2}^2 + \|\hat{f}\|_{H^2}^2). \tag{4.19}$$

Now, we continue with testing the first system equation (4.9) by $v = \Delta^2\hat{\phi}$, i.e.

$$\frac{1}{2}\frac{d}{dt}\|\Delta\hat{\phi}\|_{L^2}^2 = (\mathrm{div}((b_1(\phi_1) - b_2(\phi_2))\nabla\mu_1), \Delta^2\hat{\phi}) + (\mathrm{div}(b_2(\phi_2)\nabla\hat{\mu}), \Delta^2\hat{\phi}) := (i) + (ii).$$

Applying Young's inequality, we can estimate (i) as follows

$$(i) \le C\|\mathrm{div}((b_1(\phi_1) - b_2(\phi_2))\nabla\mu_1)\|_{L^2}^2 + \frac{\gamma c_b}{4}\|\Delta^2\hat{\phi}\|_{L^2}^2.$$

We recall that $\mu_1 \in L^2(0,T;H^3(\Omega))$ and proceed to calculate the application of the divergence operator. This yields after another application of Hölder's inequality

$$\begin{aligned}(i) \le\, & C(\|b_1'(\phi_1)\nabla\phi_1 - b_2'(\phi_2)\nabla\phi_2\|_{L^2}^2\|\nabla\mu_1\|_{L^\infty}^2 + \|b_1(\phi_1) - b_2(\phi_2)\|_{L^6}^2\|\Delta\mu_1\|_{L^3}^2) \\ & + \frac{\gamma c_b}{4}\|\Delta^2\hat{\phi}\|_{L^2}^2.\end{aligned}$$

Using similar arguments as in the derivation of bound (4.19), we then estimate the differences involving the mobility functions $b_i(\cdot)$ and obtain

$$(i) \le C(\|\hat{\phi}\|_{H^1}^2 + \|\hat{b}\|_{H^2}^2)(\|\nabla\mu_1\|_{L^\infty}^2 + \|\Delta\mu_1\|_{L^3}^2) + \frac{\gamma c_b}{4}\|\Delta^2\hat{\phi}\|_{L^2}^2.$$

For the terms of (ii), we apply the divergence operator, along with Hölder's and Young's inequality, while considering the regularity of ϕ_i, to estimate

$$\begin{aligned}(ii) &= (b_2'(\phi_2)\nabla\phi_2\nabla\hat{\mu}, \Delta^2\hat{\phi}) + (b_2(\phi_2)\Delta\hat{\mu}, \Delta^2\hat{\phi}) \\ &\le C\|\nabla\hat{\mu}\|_{L^2}^2\|\nabla\phi_2\|_{L^\infty}^2 + \frac{\gamma c_b}{4}\|\Delta^2\hat{\phi}\|_{L^2}^2 + (b_2(\phi_2)\Delta\hat{\mu}, \Delta^2\hat{\phi}).\end{aligned}$$

We consider the last term and insert $\hat{\mu} = -\gamma\Delta\hat{\phi} + f_1(\phi_1) - f_2(\phi_2)$, i.e. the definition of $\hat{\mu}$ in (4.10). This is then estimated in a similar fashion as before, while also utilising the estimate (4.19) on the difference of $f_i(\cdot)$ and the uniform boundedness of $b_2(\phi_2)$, such that

$$\begin{aligned}(b_2(\phi_2)\Delta\hat{\mu}, \Delta^2\hat{\phi}) &= (b_2(\phi_2)\Delta(-\gamma\Delta\hat{\phi} + f_1(\phi_1) - f_2(\phi_2)), \Delta^2\hat{\phi}) \\ &\le -\gamma(b_2(\phi_2)\Delta^2\hat{\phi}, \Delta^2\hat{\phi}) + \frac{\gamma c_b}{4}\|\Delta^2\hat{\phi}\|_{L^2}^2 \\ &\quad + C(\|\hat{\phi}\|_{H^1}^2 + \|\Delta\hat{\phi}\|_{L^2}^2 + \|\hat{f}\|_{H^2}^2).\end{aligned}$$

From this calculation, we then deduce

$$(ii) \le -\frac{\gamma c_b}{2}\|\Delta^2\hat{\phi}\|_{L^2}^2 + C(\|\nabla\phi_2\|_{L^\infty}^2\|\nabla\hat{\mu}\|_{L^2}^2 + \|\hat{\phi}\|_{H^1}^2 + \|\Delta\hat{\phi}\|_{L^2}^2 + \|\hat{f}\|_{H^2}^2).$$

By gathering the estimates of (i)–(ii), we obtain the following differential inequality

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|\Delta\hat{\phi}\|_{L^2}^2 + \frac{\gamma c_b}{4}\|\Delta^2\hat{\phi}\|_{L^2}^2 \le\, & C(\|\nabla\mu_1\|_{L^\infty}^2 + \|\Delta\mu_1\|_{L^3}^2)(\|\hat{\phi}\|_{H^1}^2 + \|\hat{b}\|_{H^2}^2) \\ & + C(\|\nabla\phi_2\|_{L^\infty}^2\|\nabla\hat{\mu}\|_{L^2}^2 + \|\hat{\phi}\|_{H^1}^2 + \|\Delta\hat{\phi}\|_{L^2}^2 + \|\hat{f}\|_{H^2}^2).\end{aligned}$$

Recall that $\mu_i \in L^2(0,T;H^3(\Omega)) \cap L^\infty(0,T;H^1(\Omega))$ and $\nabla\phi_i \in L^\infty(0,T;L^\infty(\Omega))$, such that $\nabla\mu_i \in L^2(0,T;L^\infty(\Omega))$ and $\Delta\mu_i \in L^2(0,T;H^1(\Omega))$. Now by integrating over the time interval $(0,t)$, we derive

$$\begin{aligned}
&\|\Delta\hat{\phi}(t)\|_{L^2}^2 + \frac{\gamma c_b}{4}\|\Delta^2\hat{\phi}\|_{L^2(L^2)}^2 \\
&\qquad \le C(\|\nabla\mu_1\|_{L^2(L^\infty)}^2 + \|\Delta\mu_1\|_{L^2(L^3)}^2)(\|\hat{\phi}\|_{L^\infty(H^1)}^2 + \|\hat{b}\|_{H^2}^2) \\
&\qquad\quad + C(\|\nabla\phi_2\|_{L^\infty(L^\infty)}^2\|\nabla\hat{\mu}\|_{L^2(L^2)}^2 + \|\hat{\phi}\|_{L^2(H^1)}^2 + \|\Delta\hat{\phi}\|_{L^2(L^2)}^2 + \|\hat{f}\|_{H^2}^2) \\
&\qquad \le C(*) + C\int_0^t \|\Delta\hat{\phi}\|_{L^2}^2\, ds.
\end{aligned}$$

By employing a Gronwall argument, see Lemma A.2.1, and utilising elliptic regularity [**46, 89**], we deduce

$$\|\hat{\phi}\|_{L^\infty(H^2)\cap L^2(H^4)} \le C(*).$$

which is the final estimate for $\hat{\phi}$. Additionally, since we estimated $\hat{\phi}$ in $L^\infty(0,T;H^2(\Omega))$ and $(f_1 - f_2)(\cdot)$ in $L^\infty(0,T;L^2(\Omega))$ to $C(*)$, we deduce from the second system equation (4.10) that

$$\|\hat{\mu}\|_{L^\infty(L^2)} \le C(*).$$

Lastly, we take the Laplacian of equation (4.10). By considering that we already estimated $\hat{\phi}$ in $L^2(0,T;H^4(\Omega))$ and $\Delta(f(\phi_1) - f(\phi_2)$ in $L^2(0,T;L^2(\Omega)))$ to $C(*)$, we observe finally that

$$\|\hat{\mu}\|_{L^\infty(L^2)\cap L^2(H^2)} \le C(*).$$

which completes the proof. □

By an inspection of the first step in the proof, we deduce the following result.

Corollary 4.1.4. *Under the assumptions of Theorem 4.1.3, one has the estimate*

$$\|(\phi_1,\mu_1) - (\phi_2,\mu_2)\|_{L^2(L^2)} \le C\|(b_1,f_1) - (b_2,f_2)\|_{H^1}$$

4.1.3. Properties of $S(\cdot)$

Let us now establish some further important properties of the solution operator. Recall, that

$$S : \mathcal{D}(S) \subset (H^2(I))^2 \to (L^2(0,T;L^2(\Omega)))^2, \quad S(b,f) \mapsto (\phi,\mu),$$

is well-defined, where

$$\mathcal{D}(S) := \{(b,f) \in (H^2(I))^2 : \text{ Assumptions 4.1.1 hold}\}.$$

Now, we interpret the solution operator as a composition $S(\cdot) = \tilde{S}(E(\cdot))$ of the two operators

$$\begin{aligned}
&\tilde{S} : (H^1(I))^2 \to (L^2(0,T;L^2(\Omega)))^2, && x \mapsto (\phi,\mu),\\
&E : (H^2(I))^2 \to (H^1(I))^2, && x \mapsto x.
\end{aligned}$$

From Corollary 4.1.4, we know that $\tilde{S}$ is a Lipschitz continuous operator, it holds

$$\|\tilde{S}(b_1, f_1) - \tilde{S}(b_2, f_2)\|_{L^2(L^2)} \leq C\|(b_1, f_1) - (b_2, f_2)\|_{H^1}. \tag{4.20}$$

Further, as the embedding $H^2(I)$ into $H^1(I)$ is compact, we know that E is a compact linear operator. Hence, we derive the following lemma.

Lemma 4.1.5. *Let Assumptions 4.1.1 hold. The solution operator $S(\cdot)$ is well-defined and Lipschitz continuous. Further, $S(\cdot)$ maps sequences in $\mathcal{D}(S)$ weakly convergent in $(H^2(I))^2$ to strongly convergent sequences in $(L^2(0,T;L^2(\Omega)))^2$, i.e. $S(\cdot)$ is completely (weak-to-strong) continuous.*

Proof. Well-definedness is clear. Lipschitz continuity follows from the observation that $\tilde{S}(\cdot)$ and $E(\cdot)$, as a linear operator, are already Lipschitz continuous operators. Hence, it is left so show that $S(\cdot)$ is weak-to-strong continuous. This assertion follows from the Lipschitz estimate (4.20) for $\tilde{S}(\cdot)$ and the fact that $E(\cdot)$ is a compact linear operator. □

In particular, as $S(\cdot)$ is weak-to-strong-continuous, $S(\cdot)$ is also weakly continuous.

4.2. Tikhonov regularisation

Let us now consider the Tikhonov regularisation of the inverse problem

$$F(b, f) = \phi^\delta. \tag{4.21}$$

In our problem the forward operator has the special structure $F(\cdot) = L(S(\cdot))$, where $S(\cdot)$ is the solution operator to the Cahn-Hilliard system (4.1)–(4.2) as before and

$$L : (L^2(0,T;L^2(\Omega)))^2 \to L^2(0,T;L^2(\Omega)), \quad (x_1, x_2) \mapsto x_1.$$

One immediately sees that $L(\cdot)$ is a linear and continuous operator. This leads us to the definition of the forward operator

$$F(b, f) : \mathcal{D}(F) \subset (H^2(I))^2 \to L^2(0,T;L^2(\Omega)), \quad (b, f) \mapsto L(S(b, f)) = \phi,$$

where $\mathcal{D}(F) := \mathcal{D}(S) = \{(b, f) \in (H^2(I))^2 :\ \text{Assumptions 4.1.1 hold}\}$. We assume that the measurements ϕ^δ satisfy the following condition

$$\|\phi - \phi^\delta\|_{L^2(0,T;L^2(\Omega))} \leq \delta$$

with a known noise level $\delta > 0$. Our aim is to obtain stable approximations to the true parameter functions satisfying $F(b^\dagger, c^\dagger) = \phi$, by minimising the Tikhonov functional

$$\min_{(b,f)\in\mathcal{D}(F)} J_\alpha^\delta(b, f) := \frac{1}{2}\|F(b, f) - \phi^\delta\|^2_{L^2(L^2)} + \frac{\alpha}{2}\|(b, f) - (b^*, f^*)\|^2_{H^2(I)}\ , \tag{4.22}$$

where $\alpha > 0$ is a regularisation parameter and (b^*, f^*) is an initial guess of the parameter functions, which, as f can only be identified up to constant, determines the constant C.

4.2.1. Existence of minimisers

Using the previously established properties of the solution operator $S(\cdot)$, we can now establish the following theorem.

Theorem 4.2.1. *Let Assumptions 4.1.1 hold. Then for any $\alpha > 0$ and any $\phi^\delta \in L^2(0,T;L^2(\Omega))$, the Tikhonov problem (4.22) has a minimiser $(b_\alpha^\delta, f_\alpha^\delta) \in \mathcal{D}(F)$.*

Proof. The domain $\mathcal{D}(F)$ is closed and convex, hence it is weakly closed. Further, the solution operator $S(\cdot)$ is continuous and weak-to-strong continuous. As $L(\cdot)$ is a continuous linear operator, we deduce that $F(\cdot) = L(S(\cdot))$ is also continuous and weak-to-strong continuous. In particular $F(\cdot)$ is weakly continuous. Now existence of a solution follows from standard theory, see Theorem A.1.1. □

Remark 4.2.2. $L(\cdot)$ can be interpreted as a measurement operator which here amounts to taking full observations of the phase fraction ϕ. Other measurement setups, including partial or boundary observations of ϕ, could be considered similarly.

4.2.2. Realisation of Tikhonov regularisation

Using $x = (b, f)$, $y^\delta = \phi^\delta$ and $X = (H^2(I))^2$, $Y = L^2(0,T;L^2(\Omega))$, we can rewrite (4.22) in compact form

$$\min_{x\in\mathcal{D}(F)} J_\alpha^\delta(b,f) := \frac{1}{2}\|F(x) - y^\delta\|_Y^2 + \frac{\alpha}{2}\|x - x^*\|_X^2 \ . \tag{4.23}$$

Motivation

Let us assume for a moment that $\mathcal{D}(F) = X$, i.e. we consider an unconstrained version of the minimisation problem (4.23). Assuming that $F(\cdot)$ is Fréchet differentiable, we formally calculate the derivative $J'(x)$ of the Tikhonov functional (4.23) in the direction of $h \in X$

$$\begin{aligned} J'(x)h &= \big(F(x) - y^\delta, F'(x)h\big)_Y + \alpha\,(x - x^*, h)_X \\ &= \big(F'(x)^*(F(x) - y^\delta) + \alpha(x - x^*), h\big)_X , \end{aligned}$$

where $F'(x)$ denotes the Fréchet derivative of $F(x)$, and $F'(x)^*$ it's adjoint operator, which is defined by $(F'(x)^*y, h)_X := (y, F'(x)h)_Y$ for all $h \in X$ and $y \in Y$. This leads to the necessary first-order optimality condition

$$0 \overset{!}{\equiv} \big(F'(x)^*(F(x) - y^\delta) + \alpha(x - x^*), h\big)_X , \tag{4.24}$$

for all $h \in X$. In order to solve equation (4.24), one can employ a Gauss-Newton approach. In essence, the approach involves adapting Newton's method while neglecting the terms involving second-order derivatives of $F(\cdot)$. This results in the Gauss-Newton iteration

$$\begin{aligned} (F'(x^k)^*\,F'(x^k) + \alpha^k I)\Delta x^k &= F'(x^k)^*(y^\delta - F(x^k)) - \alpha^k(x^k - x^*), \\ x^{k+1} &= x^k + \Delta x^k, \end{aligned}$$

where $\alpha^k = 1/2^k$. This approach is referred to as the Levenberg-Marquardt method. It was initially formulated as a trust region approach involving the solution of a linearised Tikhonov problem on a domain around the current iterate. However, this iteration scheme has several other possible interpretations and derivations, e.g. as a preconditioned version of the Landweber iteration. We refer to [**45, Ch.11**] and [**67**] for more comprehensive details towards the iterative regularisation of nonlinear problems, including discussions on the convergence of the Gauss-Newton method, which we do not address here.

Projected Gauss-Newton iteration

Now, we consider the minimisation problem (4.23) including $\mathcal{D}(F)$ as defined in Section 4.1.1. The Gauss-Newton iteration, as described, has to be adapted to be applied. In order to solve the minimisation problem, we use a projected Gauss-Newton iteration

$$\begin{aligned}(F'(x^k)^* F'(x^k) + \alpha^k I)\Delta x^k &= F'(x^k)^*(y^\delta - F(x^k)) - \alpha^k(x^k - x^*),\\ x^{k+1} &= P_{\mathcal{D}(F)}(x^k + \omega\Delta x^k),\end{aligned}$$

where $0 < \omega < 1$ is a stepsize, $\alpha^k = 1/2^k$, and $P_{\mathcal{D}(F)}$ denotes the projection to $\mathcal{D}(F)$ in order to incorporate the constraints on the parameter functions, especially the positivity constraint of $b(\cdot)$. We stop the iteration according to the discrepancy principle, which is a parameter choice rule for the regularisation parameter α; see [**45**]. It reads as follows: choose $\overline{\alpha} = \alpha(\delta, y^\delta)$ such that

$$\overline{\alpha} = \sup\{\alpha > 0 : \|F(x^\delta_\alpha) - y^\delta\|_Y \leq \tau\delta\} \text{ for some } \tau > 1.$$

Since the Gauss-Newton matrix is positive definite, Δx^k is a decent direction. The projected Gauss-Newton method combined with a suitable step size rule can therefore be understood as a descent method for (4.23), see [**60**]. The projected Gauss-Newton iteration in combination with the discrepancy principle has been analysed in [**5, 66**]. Moreover, for applications of this method to solve minimisation problem of the structure (4.23), we refer to [**39, 77**].

Summary and further outline

Let us briefly summarise. We have shown that the non-linear identification problem has a solution and proposed a Gauss-Newton method to compute the minimiser. Now, in order to apply the iterative solution method, we require the Fréchet derivative $F'(x)$. As the forward operator is defined as $F(\cdot) = L(S(\cdot))$, we only need to study the Fréchet derivative $S'(x)$ of the solution operator, which will be presented in the following Section 4.3. Further, to facilitate the iterative solution method, we will establish a representation of the adjoint operator $F'(x)^*$. This is presented in Section 4.4.

4.3. Fréchet derivative of the solution operator $S(\cdot)$

We recall that the goal of this section is to establish the differentiability of the solution operator $S(\cdot)$, which will lead to differentiability of the forward operator $F(\cdot)$.

Let Assumptions 4.1.1 hold and consider a fixed pair of parameter functions $(b, f) \in \mathcal{D}(S)$ with corresponding smooth solution (ϕ, μ) of the Cahn-Hilliard system (4.1)–(4.2). Moreover assume that we have functions $(\hat{b}, \hat{f}) \in (H^2(I))^2$, such that the pair of functions $(b + \hat{b}, f + \hat{f})$ remains in $\mathcal{D}(S)$, hence also satisfying Assumptions 4.1.1. In this setting, we analyse the following linearised state equations for the variables (ψ, ξ):

$$\partial_t \psi - \operatorname{div}(b'(\phi)\psi\nabla\mu) - \operatorname{div}(b(\phi)\nabla\xi) = \operatorname{div}(\hat{b}(\phi)\nabla\mu) \qquad \text{in } \Omega \times (0, T), \tag{4.25}$$

$$\xi + \gamma\Delta\psi - f'(\phi)\psi = \hat{f}(\phi) \qquad \text{in } \Omega \times (0, T), \tag{4.26}$$

with initial condition $\psi(0, x) = 0$ and complemented with periodic boundary conditions.

In the following two subsections, we show that the system (4.25)–(4.26) possesses a unique solution (ψ, ξ) for any admissible $(\hat{b}, \hat{f})$. Afterwards, we prove that using the solution (ψ, ξ), the Fréchet derivative of the solution operator $S(\cdot)$ is defined by $S'(b, f)(\hat{b}, \hat{f}) = (\psi, \xi)$.

4.3.1. Existence of solutions to the linearised problem

Let us start with stating the following result regarding the existence of solutions to the linearised system (4.25)–(4.26).

Theorem 4.3.1. *Let Assumptions 4.1.1 hold. For any admissible $(\hat{b}, \hat{f}) \in (H^2(I))^2$, the system (4.25)–(4.26) has a unique solution (ψ, ξ) with the regularity*

$$\begin{aligned} &\psi \in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^3(\Omega)) \cap H^1(0, T; (H^1(\Omega))') := Z_\psi, \\ &\xi \in L^2(0, T; H^1(\Omega)), \end{aligned} \tag{4.27}$$

satisfying $\psi(0, x) = 0$ in $L^2(\Omega)$, and equation (4.26), i.e.

$$\xi + \gamma\Delta\psi - f'(\phi)\psi = \hat{f}(\phi),$$

a.e. in $\Omega \times (0, T)$, and it holds

$$\langle \partial_t \psi, v\rangle_{H^1} + \int_\Omega (b'(\phi)\psi\nabla\mu + b(\phi)\nabla\xi) \cdot \nabla v \, dx = -\int_\Omega \hat{b}(\phi)\nabla\mu \cdot \nabla v \, dx \tag{4.28}$$

for a.e. $t \in (0, T)$ and for all test functions $v \in H^1(\Omega)$. Moreover, there exists a positive constant C, not depending on $(\psi, \xi), (\hat{b}, \hat{f})$, such that

$$\|\psi\|_{Z_\psi} + \|\xi\|_{L^2(H^1)} \leq C(\|\hat{b}\|_{H^2} + \|\hat{f}\|_{H^2}). \tag{4.29}$$

Before we go into the details of the proof, let us briefly highlight the main arguments. The theorem is established by Galerkin approximation, which involves introducing a finite-dimensional approximation, deriving a-priori estimates, and then employing compactness arguments to go to the limit. Since many steps align with standard arguments for a linear system, we will not consider every single step in detail. Instead, we will present the derivation of the a-priori-estimates.

The approach for this proof is inspired by [**64**] and divided into five steps. In the first step, we derive energy estimates and use a Gronwall argument to derive the first estimates of the solution (ψ, ξ). The following three steps will establish estimates of the solution in norms as stated in the theorem. Lastly, we derive uniqueness by considering the difference between two solutions and following the same testing strategy as before.

Proof of Theorem 4.3.1. We multiply the system (4.25)–(4.26) with test functions v, w, integrate over the domain Ω and use integration-by-parts to obtain the following weak formulation

$$\langle \partial_t \psi, v\rangle_{H^1} + (b'(\phi)\psi\nabla\mu, \nabla v) + (b(\phi)\nabla\xi, \nabla v) = -(\hat{b}(\phi)\nabla\mu, \nabla v), \tag{4.30}$$

$$(\xi, w) - (\gamma\nabla\psi, \nabla w) - (f'(\phi)\psi, w) = (\hat{f}(\phi), w), \tag{4.31}$$

for all test functions $v, w \in H^1(\Omega)$ and a.a. $0 < t < T$ and $\psi(0, x) = 0$.

As initial consideration, we observe that by testing (4.30) with $v \equiv 1$, we deduce $\langle \partial_t\psi(t), 1\rangle = 0$. After integrating over the time domain $[0, t]$ and considering that $\psi(0, x) = 0$, it follows that $\int_\Omega \psi(t, x)\, dx = \int_\Omega \psi(0, x)\, dx = 0$, i.e. the mean value is constant zero in time.

First step: We test (4.30) with $v = \xi$ and (4.31) with $w = -\partial_t\psi$, and add the resulting identities. Upon integration over the interval $(0, t)$, taking into account that $\psi(0, x) = 0$ and using the lower bound of $b(\cdot)$, see Assumptions 4.1.1, we arrive at

$$\begin{aligned}
&\frac{\gamma}{2}\|\nabla\psi(t)\|^2_{L^2} + c_b\int_0^t \|\nabla\xi\|^2_{L^2}\, ds \\
&\le \int_{\Omega_t} -\hat{b}(\phi)\nabla\mu\nabla\xi - \hat{f}(\phi)\partial_t\psi - f'(\phi)\psi\partial_t\psi - b'(\phi)\psi\nabla\mu\nabla\xi\, dx\, ds \\
&=: (i) + (ii) + (iii) + (iv).
\end{aligned} \tag{4.32}$$

The terms (i)–(iv) are now individually estimated. For the first term, we apply Hölder and Young inequalities to derive

$$\begin{aligned}
|(i)| &\le \int_0^t \|\hat{b}(\phi)\nabla\mu\|_{L^2}\|\nabla\xi\|_{L^2}\, ds \\
&\le \int_0^t C\|\hat{b}(\phi)\nabla\mu\|^2_{L^2} + \frac{c_b}{4}\|\nabla\xi\|^2_{L^2}\, ds \\
&\le C(\|\nabla\mu\|^2_{L^2(L^2)})\|\hat{b}(\phi)\|^2_{L^\infty(\Omega_t)} + \frac{c_b}{4}\int_0^t \|\nabla\xi\|^2_{L^2}\, ds.
\end{aligned}$$

For the second term, we employ integration-by-parts in the time direction, and once again apply Hölder and Young estimates to deduce

$$\begin{aligned}
|(ii)| &\le \left|\int_\Omega \hat{f}(\phi(t))\psi(t)\, dx\right| + \left|\int_0^t\int_\Omega \hat{f}'(\phi)\partial_t\phi\psi\, dx\, ds\right| \\
&\le \|\hat{f}(\phi(t))\|_{L^2}\|\psi(t)\|_{L^2} + \int_0^t \|\psi\|_{L^6}\|\hat{f}'(\phi)\|_{L^2(\Omega)}\|\partial_t\phi\|_{L^3}\, ds \\
&\le C(\|\hat{f}(\phi)\|^2_{L^\infty(\Omega_T)}) + \frac{\gamma}{4}\|\psi(t)\|^2_{L^2} + \int_0^t \|\psi\|^2_{H^1} + C\|\hat{f}'(\phi)\|^2_{L^\infty(\Omega)}\|\partial_t\phi\|^2_{H^1}\, ds.
\end{aligned}$$

We have also made use of the embedding of $H^1(\Omega)$ into $L^p(\Omega)$ for $1 \le p \le 6$ in dimension $d = 2$. For the third term, we once more apply integration-by-parts in the time direction and compute

$$
\begin{aligned}
|(iii)| &= \left| \int_0^t \int_\Omega f'(\phi) \frac{\partial_t |\psi|^2}{2} \, dx \, ds \right| \\
&\leq \left| \frac{1}{2} \int_\Omega f'(\phi(t)) |\psi(t)|^2 \, dx \right| + \left| \frac{1}{2} \int_0^t \int_\Omega f''(\phi) \partial_t \phi \, \psi^2 \, dx \, ds \right| .
\end{aligned}
$$

By the uniform boundedness of ϕ, see (4.7), and the bounds for $f(\cdot)$ and its derivatives provided by Assumptions 4.1.1, we deduce

$$
|(iii)| \leq \|f'(\phi)\|_{L^\infty(\Omega_t)} \|\psi(t)\|_{L^2}^2 + \|f''(\phi)\|_{L^\infty(\Omega_t)} \left| \int_0^t \int_\Omega \partial_t \phi \, \psi^2 \, dx \, ds \right| .
$$

By applying Hölder and Young inequalities, along with standard Sobolev embeddings, we derive the following estimate

$$
\begin{aligned}
|(iii)| &\leq \|f'(\phi)\|_{L^\infty(\Omega_t)} \|\psi(t)\|_{L^2}^2 + \|f''(\phi)\|_{L^\infty(\Omega_t)} \int_0^t \|\partial_t \phi\|_{L^6} \|\psi\|_{L^3} \|\psi\|_{L^2} \, ds \\
&\leq \|f'(\phi)\|_{L^\infty(\Omega_t)} \|\psi(t)\|_{L^2}^2 + \|f''(\phi)\|_{L^\infty(\Omega_t)} \int_0^t \|\psi\|_{H^1}^2 + \|\partial_t \phi\|_{H^1}^2 \|\psi\|_{L^2}^2 \, ds.
\end{aligned}
$$

Moving on to the last term (iv), we begin by using the bounds on $b(\cdot)$, the uniform boundedness of ϕ, and Hölder's inequality to estimate

$$
\begin{aligned}
|(iv)| &\leq C(b', \phi) \int_0^t \int_\Omega |\psi \nabla \mu \nabla \xi| \, dx \, ds \leq C(b', \phi) \int_0^t \|\psi \nabla \mu\|_{L^2} \|\nabla \xi\|_{L^2} \, ds \\
&\leq C(b', \phi) \int_0^t \|\psi\|_{L^4} \|\nabla \mu\|_{L^4} \|\nabla \xi\|_{L^2} \, ds.
\end{aligned}
$$

Subsequently, utilising the interpolation inequality (A.3), i.e.

$$
\|\psi\|_{L^4(\Omega)} \leq C(\Omega) \left(\|\psi\|_{L^2(\Omega)}^{\frac{1}{2}} \|\nabla \psi\|_{L^2(\Omega)}^{\frac{1}{2}} + \|\psi\|_{L^2(\Omega)} \right),
$$

and Young's inequality, we obtain

$$
\begin{aligned}
|(iv)| &\leq C(b', \phi) \int_0^t \|\nabla \mu\|_{L^4} \|\nabla \xi\|_{L^2} \left(\|\psi\|_{L^2}^{\frac{1}{2}} \|\nabla \psi\|_{L^2}^{\frac{1}{2}} + \|\psi\|_{L^2} \right) \, ds \\
&\leq \frac{c_b}{4} \int_0^t \|\nabla \xi\|_{L^2}^2 \, ds + C(b', \phi) \int_0^t \|\nabla \mu\|_{L^4}^2 \|\psi\|_{L^2} \left(\|\nabla \psi\|_{L^2} + \|\psi\|_{L^2} \right) \, ds \\
&\leq \frac{c_b}{4} \int_0^t \|\nabla \xi\|_{L^2}^2 \, ds + C(b', \phi) \int_0^t (1 + \|\nabla \mu\|_{L^4}^4) \|\psi\|_{L^2}^2 + \|\nabla \psi\|_{L^2}^2 \, ds.
\end{aligned}
$$

To summarise, considering the estimates of the terms (i)–(iv) on the right-hand side of inequality (4.32), using the boundedness of the parameter functions and also of the solutions (ϕ, μ), we obtain the integral inequality

$$
\begin{aligned}
&\frac{\gamma}{4} \|\nabla \psi(t)\|_{L^2}^2 + \frac{c_b}{2} \int_0^t \|\nabla \xi\|_{L^2}^2 \, ds \\
&\leq C \int_0^t (1 + \|\nabla \mu\|_{L^4}^4 + \|\partial_t \phi\|_{H^1}^2) \|\psi\|_{L^2}^2 + \|\nabla \psi\|_{L^2}^2 \, ds + C(\|\hat{b}\|_{H^2}^2 + \|\hat{f}\|_{H^2}^2),
\end{aligned}
$$

where C denotes a constant independent of (ψ, ξ) but relies on the bounds of the parameter functions and a-priori estimates of (ϕ, μ). Now, by using Poincaré's inequality, we simplify the integral inequality to

$$
\begin{aligned}
&\frac{\gamma}{4}\|\nabla\psi(t)\|_{L^2}^2 + \frac{c_b}{2}\int_0^t \|\nabla\xi\|_{L^2}^2\, ds \\
\leq & C\int_0^t (1 + \|\nabla\mu\|_{L^4}^4 + \|\partial_t\phi\|_{H^1}^2)\|\nabla\psi\|_{L^2}^2\, ds + C(\|\hat{b}\|_{H^2}^2 + \|\hat{f}\|_{H^2}^2).
\end{aligned}
$$

Note that the mapping $s \to \|\partial_t\phi(s)\|_{H^1}^2$ is indeed in $L^1(0,t)$, a consequence of the regularity of smooth solutions, see (4.6). We recall from (4.6) that $\partial_t\phi \in L^2(0,T;H^1(\Omega))$ and by interpolation, see [**73**], it holds that $\mu \in L^4(0,T;L^4(\Omega))$, which allows us to apply the Gronwall Lemma A.2.1. Consequently, we obtain the a-priori bounds

$$
\|\psi\|_{L^\infty(H^1)} + \|\nabla\xi\|_{L^2(L^2)} \leq C(\|\hat{b}\|_{H^2}^2 + \|\hat{f}\|_{H^2}^2).
$$

Now, an estimate for $\xi \in L^2(0,T;L^2(\Omega))$ is left in this first step. By testing (4.31) with $w \equiv 1$ and making use of the fact that $f'(\phi) \in L^\infty(0,T;L^\infty(\Omega))$, we estimate the mean value $M(t)$ of $\xi(t)$ and compute

$$
M(t) := \int_\Omega \xi(t)\, dx = \int_\Omega f'(\phi)\psi + \hat{f}(\phi)\, dx \leq C(f',\phi)\|\psi(t)\|_{L^2(\Omega)} + C(\hat{f},\phi).
$$

Hence, by Poincaré's inequality we obtain

$$
\|\xi(t)\|_{L^2} \leq C\|\nabla\xi(t)\|_{L^2} + CM(t)^2
$$

and since $\psi \in L^2(0,T;L^2(\Omega))$ we can bound the mean value $M(t)$ in $L^2(0,T;L^2(\Omega))$, i.e. we deduce $\xi \in L^2(0,T;H^1(\Omega))$.

Second step: We aim to improve the regularity of ψ and proceed by testing the second system equation (4.31) with $w = \Delta\psi$. In fact, this test function is feasible because one selects an appropriate Galerkin approximation space that is stable due to construction. By applying integration-by-parts, we derive the estimate

$$
\gamma\int_\Omega |\Delta\psi|^2\, dx \leq \int_\Omega |\nabla\xi\nabla\psi + f'(\phi)\psi\Delta\psi + \hat{f}(\phi)\Delta\psi|\, dx.
$$

We estimate the terms on the right-hand side employing Hölder and Young inequalities, and utilise the bounds on the parameter functions $f(\cdot)$, $\hat{f}(\cdot)$, as well as the uniform bounds of ϕ. This results in

$$
\frac{\gamma}{2}\int_\Omega |\Delta\psi|^2\, dx \leq C(1 + \|\nabla\xi\|_{L^2}^2 + \|\psi\|_{H^1}^2).
$$

Through integration over the interval $[0,t]$ and recognising that ξ and ψ are already in $L^2(0,T;H^1(\Omega))$, we conclude that $\Delta\psi$ is bounded in $L^2(0,T;L^2(\Omega))$. Hence, we deduce that $\psi \in L^2(0,T;H^2(\Omega))$.

Third step: To derive a bound of ψ in $L^2(0,T;H^3(\Omega))$, we make use of elliptic regularity theory [**46**]. To achieve this, we consider the second equation of the linear system (4.26) as an elliptic problem for ψ. Note that beside ψ all the terms in (4.26) are already bounded in $L^2(0,T;H^1(\Omega))$ due to the previous estimates, the uniform bounds on ϕ and the parameter functions. The estimate for ψ is then readily obtained through the application of elliptic regularity, resulting in

$$\|\psi\|_{L^2(H^3)} \leq C(\|\hat{b}\|_{H^2}^2 + \|\hat{f}\|_{H^2}^2).$$

Fourth step: It remains to establish $\partial_t\psi$ in $L^2(0,T;(H^1(\Omega))')$, alongside the verification of equation (4.28). To address this, we recall the definition of the dual norm

$$\|\partial_t\psi(t)\|_{(H^1)'} = \sup_{v\in H^1} \frac{\langle \partial_t\psi(t), v\rangle_{H^1}}{\|v\|_{H^1}}.$$

Initially, we consider the duality product in the numerator by inserting the variational equation (4.30) and proceeding to estimate it using the Cauchy-Schwarz inequality. This results in

$$\begin{aligned}\langle \partial_t\psi, v\rangle_{H^1} &= -(b'(\phi)\psi\nabla\mu, \nabla v) - (b(\phi)\nabla\xi, \nabla v) - (\hat{b}(\phi)\nabla\mu, \nabla v)\\ &\leq (\|b'(\phi)\psi\nabla\mu\|_{L^2} + \|b(\phi)\nabla\xi\|_{L^2} + \|\hat{b}(\phi)\nabla\mu\|_{L^2})\|\nabla v\|_{L^2}.\end{aligned}$$

Consequently, we deduce that the dual norm is bounded by

$$\|\partial_t\psi(t)\|_{(H^1)'} \leq \|b'(\phi)\psi\nabla\mu\|_{L^2} + \|b(\phi)\nabla\xi\|_{L^2} + \|\hat{b}(\phi)\nabla\mu\|_{L^2}.$$

Through integration over the time interval $[0,T]$, while utilising the bounds of $b(\cdot)$ and ϕ, we compute for an arbitrary test function $v \in L^2(0,T;H^1(\Omega))$ the estimate

$$\begin{aligned}\|\partial_t\psi\|_{L^2((H^1)')}^2 &= \int_0^T \|\partial_t\psi\|_{(H^1)'}^2\,ds\\ &\leq \int_0^T \|b'(\phi)\psi\nabla\mu\|_{L^2}^2 + \|b(\phi)\nabla\xi\|_{L^2}^2 + \|\hat{b}(\phi)\nabla\mu\|_{L^2}^2\,ds\\ &\leq \int_0^T \|b'(\phi)\|_{L^\infty(\Omega)}^2\|\psi\|_{L^\infty}^2\|\nabla\mu\|_{L^2}^2 + \|b(\phi)\|_{L^\infty(\Omega)}^2\|\nabla\xi\|_{L^2}^2 + \|\hat{b}(\phi)\|_{L^\infty(\Omega)}^2\|\nabla\mu\|_{L^2}^2\,ds\\ &\leq C(b')\|\nabla\mu\|_{L^\infty(L^2)}\|\psi\|_{L^2(L^\infty)}^2 + C(b)\|\nabla\xi\|_{L^2(L^2)}^2 + \|\nabla\mu\|_{L^2(L^2)}^2\|\hat{b}\|_{H^2}^2.\end{aligned}$$

Thus, we deduce, using the previously established estimates of ψ and ξ, that $\psi \in H^1(0,T;(H^1(\Omega))')$ and one has

$$\|\partial_t\psi\|_{L^2((H^1)')} \leq C(\|\hat{b}\|_{H^2}^2 + \|\hat{f}\|_{H^2}^2).$$

Uniqueness: The system (4.30)–(4.31) is linear with respect to the variables ψ and ξ. Hence we consider the system (4.30)–(4.31) for two solutions $\{(\psi_i,\xi_i)\}_{i=1,2}$, and subsequently subtract the equations. Then, the differences $\hat{\psi} := \psi_1 - \psi_2$ and $\hat{\xi} := \xi_1 - \xi_2$ also fulfil the system (4.30)–(4.31) with $\hat{b}(\cdot)$ and $\hat{f}(\cdot)$ constant zero. Given the regularity of the solutions $\{(\psi_i,\xi_i)\}_{i=1,2}$, we are able to repeat the same testing procedure employed previously and derive bounds with respect to $\hat{b}(\cdot)$ and $\hat{f}(\cdot)$. However, as $\hat{b}(\cdot)$ and $\hat{f}(\cdot)$ are zero, it follows that the differences $\hat{\psi}, \hat{\xi}$ are zero almost everywhere on $\Omega \times [0,T]$. Hence, the uniqueness of the solution is established. □

4.3.2. Fréchet differentiability of the solution operator $S(\cdot)$

We have previously established the existence of unique solutions (ψ, ξ) for the linearised problem. In this section, we show that these solutions define the Fréchet derivative of the solution operator $S(\cdot)$. Afterwards, we will deduce differentiability of the forward operator $F(\cdot)$.

Theorem 4.3.2. *Let Assumptions 4.1.1 hold, $(b_1, f_1) \in \mathcal{D}(S)$, and let (ψ, ξ) be the unique solution to the linearised system* (4.25)–(4.26)*. Then for any $(\hat{b}, \hat{f}) \in (H^2(I))^2$, such that $b_2 := b_1 + \hat{b}, f_2 := f_1 + \hat{f} \in \mathcal{D}(S)$, there exists a positive constant C, not depending on $(\hat{b}, \hat{f})$, such that*

$$\|(\bar{\phi}, \bar{\mu})\|_{Z_{S'}} \leq C\|(b_2, f_2) - (b_1, f_1)\|^2_{H^2} = C\|(\hat{b}, \hat{f})\|^2_{H^2},$$

where $\bar{\phi} := \phi_2 - \phi_1 - \psi$, $\bar{\mu} := \mu_2 - \mu_1 - \xi$ with $(\phi_i, \mu_i) := S(b_i, f_i)$ for $i = 1, 2$, and $Z_{S'}$ denotes the product space

$$Z_{S'} := \big(L^2(0,T; H^2(\Omega)) \cap L^\infty(0,T; L^2(\Omega)) \cap H^1(0,T; (H^2(\Omega))')\big) \times L^2(0,T; L^2(\Omega)).$$

Then, for any $(b, f) \in \mathcal{D}(S)$ the Fréchet derivative $S'(b, f) \in \mathcal{L}((H^2(I))^2, Z_{S'})$, is defined as follows: For any $(\hat{b}, \hat{f}) \in (H^2(I))^2$, we have $S'(b, f)(\hat{b}, \hat{f}) = (\psi, \xi)$, where (ψ, ξ) is the unique solution of the linearised problem (4.25)–(4.26) *corresponding to $(\hat{b}, \hat{f})$.*

Before going into the details, let us again briefly sketch the main arguments. The subsequent proof is inspired by ideas presented in [**29, 64**]. We start by deriving a problem that is solved by the variables $(\bar{\phi}, \bar{\mu})$. Then, we establish energy estimates and employ a Gronwall argument to obtain a first estimate with respect to $(\hat{b}, \hat{f})$. Finally, we show this estimate in a higher norm.

Let us point out that higher regularity of smooth solutions (ϕ, μ), see (4.6), along with the estimates derived in Theorem 4.1.3, i.e. the estimates of $(\hat{\phi}, \hat{\mu})$ to $(\hat{b}, \hat{f})$ in higher norms, are necessary for the upcoming proof.

Proof of Theorem 4.3.2. Let us begin by observing that for any (b_1, f_1) in the interior of $\mathcal{D}(S)$, there exits a neighbourhood around (b_1, f_1) where, for sufficiently small $(\hat{b}, \hat{f})$, we have $(b_2, f_2) \in \mathcal{D}(S)$. Subsequently, both (ϕ_2, μ_2) and the linearised solution (ψ, ξ) corresponding to $(\hat{b}, \hat{f})$ are well defined. From Theorem 4.3.1, we know that the mapping $S'(b_1, f_1) : (\hat{b}, \hat{f}) \to (\psi, \xi)$ is both linear and continuous as a mapping from $(H^2(I))^2$ to $Z_{S'}$. Therefore, we consider the mapping

$$\begin{aligned} r : (H^2(I))^2 &\to Z_{S'}, \\ (\hat{b}, \hat{f}) &\mapsto r(\hat{b}, \hat{f}) := (\bar{\phi}, \bar{\mu}) = S(b_2, f_2) - S(b_1, f_1) - S'(b_1, f_1)(\hat{b}, \hat{f}). \end{aligned}$$

To establish Fréchet differentiability [**60**], we aim to show that $r \in o(\|(\hat{b}, \hat{f})\|_{H^2})$, more precisely, we will prove that

$$\|r(\hat{b}, \hat{f})\|_{Z_{S'}} = \|(\bar{\phi}, \bar{\mu})\|_{Z_{S'}} \leq C\|(\hat{b}, \hat{f})\|^2_{H^2}.$$

From the regularities of smooth solutions, see (4.6) and Theorem 4.3.1, we infer that the residuals $(\bar{\phi}, \bar{\mu})$ satisfy the regularities

$$\begin{aligned}&\bar{\phi} \in L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^3(\Omega)) \cap H^1(0,T;(H^1(\Omega))'),\\ &\bar{\mu} \in L^2(0,T;H^1(\Omega))\end{aligned}$$

with $\bar{\phi}(0,x) = 0$.

First step: Now, we derive a system of equations that will be fulfilled by $(\bar{\phi}, \bar{\mu})$. Let (ϕ_1, μ_1) and (ϕ_2, μ_2) correspond to the solution of the Cahn-Hilliard system (4.1)–(4.2), with (b_1, f_1) and $(b_2, f_2) = (b_1 + \hat{b}, f_1 + \hat{f})$ being substituted for the parameter functions. Moreover, let (ψ, ξ) be the unique solution of the linearised system (4.25)–(4.26), and let $(\bar{\phi}, \bar{\mu})$ as defined before.

By combining the Cahn-Hilliard system (4.1)–(4.2) with the linearised system (4.25)–(4.26), we obtain the following equations satisfied by $(\bar{\phi}, \bar{\mu})$

$$\begin{aligned}\partial_t \bar{\phi} + \operatorname{div}(-b_2(\phi_2)\nabla\mu_2 + b_1(\phi_1)\nabla\mu_1 + b_1'(\phi_1)\psi\nabla\mu_1 + b_1(\phi_1)\nabla\xi) &= -\operatorname{div}(\hat{b}(\phi_1)\nabla\mu_1),\\ \bar{\mu} + \gamma\Delta\bar{\phi} - (f_2(\phi_2) - f_1(\phi_1) - f_1'(\phi_1)\psi) &= -\hat{f}(\phi_1).\end{aligned}$$

We will now use Taylor's theorem to rewrite the system, which will then be used to derive the energy estimates. By considering the definitions of $\bar{\phi}, \phi^\delta$ and ψ, and using Taylor's theorem, we obtain the identity

$$\begin{aligned}f_2(\phi_2) - f_1(\phi_1) - f_1'(\phi_1)\psi &= f_1(\phi_2) - f_1(\phi_1) - f_1'(\phi_1)(\phi_2 - \phi_1) + f_1'(\phi_1)\bar{\phi} + \hat{f}(\phi_2)\\ &= (\phi_2 - \phi_1)^2 \frac{f_1''(\zeta)}{2} + f_1'(\phi_1)\bar{\phi} + \hat{f}(\phi_2)\end{aligned}$$

with $\zeta(x,t) \in [\min\{\phi_2(x,t) - \phi_1(x,t)\}, \max\{\phi_2(x,t) - \phi_1(x,t)\}]$. Recall that the smooth solutions ϕ_1, ϕ_2 are uniformly bounded, see (4.7). Consequently, using the Assumptions 4.1.1 on $f(\cdot)$, it follows that the function $f''(\zeta)$ is bounded in the space $L^\infty(\Omega_T)$ by a uniform constant C.

Again, through the application of Taylor's theorem, we derive a similar identity with respect to terms involving $b(\cdot)$

$$\begin{aligned}&b_2(\phi_2)\nabla\mu_2 - b_1(\phi_1)\nabla\mu_1 - b_1'(\phi_1)\psi\nabla\mu_1 - b_1(\phi_1)\nabla\xi\\ &\qquad = (b_1(\phi_2) - b_1(\phi_1))\nabla(\mu_2 - \mu_1) + (b_1'(\phi_1)\bar{\phi} + (\phi_2 - \phi_1)^2\frac{b_1''(\zeta)}{2})\nabla\mu_1\\ &\qquad\quad + b_1(\phi_1)\nabla\bar{\mu} + \hat{b}(\phi_2)\nabla\mu_2\\ &\qquad =: g_b + b_1(\phi_1)\nabla\bar{\mu} + \hat{b}(\phi_2)\nabla\mu_2.\end{aligned}$$

Let us come back to the previous system for $(\bar{\phi}, \bar{\mu})$. By incorporating the previously derived identities and considering the regularities of $(\bar{\phi}, \bar{\mu})$, we deduce that $(\bar{\phi}, \bar{\mu})$ satisfy

$$\langle \partial_t \bar{\phi}, v\rangle_{H^1} + \int_\Omega (g_b + b_1(\phi_1)\nabla\bar{\mu})\nabla v\, dx = \int_\Omega (\hat{b}(\phi_1)\nabla\mu_1 - \hat{b}(\phi_2)\nabla\mu_2)\nabla v\, dx \tag{4.33}$$

for all $v \in H^1(\Omega)$ and a.e. $t \in (0,T)$, and

$$\bar{\mu} + \gamma\Delta\bar{\phi} - (\phi_2 - \phi_1)^2 \frac{f_1''(\zeta)}{2} + f_1'(\phi_1)\bar{\phi} = -\hat{f}(\phi_1) + \hat{f}(\phi_2) \tag{4.34}$$

a.e. in $\Omega \times [0,T]$.

Second step: Now, we turn to the derivation of energy estimates required to apply the Gronwall argument. To do this, we will employ a similar testing procedure as in Theorem 4.1.3, i.e. we will test (4.33) with $v = \bar{\phi}$, and (4.34) with $w = \varepsilon\bar{\phi}$ and $w = b_1(\phi_1)\bar{\mu}$.

Before we start to test the first equation (4.33), we will establish a bound for g_b in $L^2(0,t;L^2(\Omega))$. At first, we estimate

$$\begin{aligned}\|g_b\|^2_{L^2(L^2)} \leq &\int_0^t \int_\Omega |b_1(\phi_2) - b_1(\phi_1)|^2 |\nabla(\mu_2 - \mu_1)|^2 \,dx\,ds \\ &+ \int_0^t \int_\Omega |b_1'(\phi_1)\bar{\phi} - (\phi_2 - \phi_1)^2 \frac{b_1''(\zeta)}{2}|^2 |\nabla\mu_1|^2 \,dx\,ds := (i) + (ii).\end{aligned}$$

For the term (i), we employ Hölder's inequality along with the mean value theorem, and use the bounds on $b_1(\cdot), b_2(\cdot)$, the regularity of $\phi_2 - \phi_1$, $\nabla(\mu_2 - \mu_1)$, and the bounds on the differences established in Theorem 4.1.3. This leads us to the estimate

$$\begin{aligned}(i) &\leq \int_0^t \|b_1(\phi_2) - b_1(\phi_1)\|^2_{L^3} \|\nabla(\mu_2 - \mu_1)\|^2_{L^6} \,ds \\ &\leq \int_0^t \|b_1'(\zeta)(\phi_2 - \phi_1)\|^2_{L^3} \|\nabla(\mu_2 - \mu_1)\|^2_{L^6} \,ds \\ &\leq C\|\phi_2 - \phi_1\|^2_{L^\infty(L^3)} \|\nabla(\mu_2 - \mu_1)\|^2_{L^2(L^6)} \\ &\leq C(\|(\hat{b},\hat{f})\|^4_{H^2}).\end{aligned}$$

Regarding the second term (ii), we use similar bounds while additionally incorporating the regularity of smooth solutions, in particular $\nabla\mu_1 \in L^2(0,T;H^2(\Omega)) \cap L^\infty(0,T;L^2(\Omega))$, see (4.6). This leads us to the following

$$\begin{aligned}(ii) &\leq \int_0^t \int_\Omega |b_1'(\phi_1)\bar{\phi}|^2 |\nabla\mu_1|^2 \,dx\,ds + \int_0^t \int_\Omega |(\phi_2 - \phi_1)^2 \frac{b_1''(\zeta)}{2}|^2 |\nabla\mu_1|^2 \,dx\,ds \\ &\leq C\int_0^t \|\bar{\phi}\|^2_{L^2} \|\nabla\mu_1\|^2_{L^\infty} \,ds + C\int_0^t \int_\Omega |\phi_2 - \phi_1|^4 |\nabla\mu_1|^2 \,dx\,ds \\ &\leq C\int_0^t \|\bar{\phi}\|^2_{L^2} \|\nabla\mu_1\|^2_{L^\infty} \,ds + C\|\phi_2 - \phi_1\|^2_{L^\infty(L^\infty)} \|\phi_2 - \phi_1\|^2_{L^2(L^\infty)} \|\nabla\mu_1\|^2_{L^\infty(L^2)} \\ &\leq C(\int_0^t \|\bar{\phi}\|^2_{L^2} \|\nabla\mu_1\|^2_{L^\infty} \,ds + \|(\hat{b},\hat{f})\|^4_{H^2}).\end{aligned}$$

Let us point out that the estimates of $\hat{\phi}$ and $\hat{\mu}$ to $(\hat{b},\hat{f})$ in higher norms, see Theorem 4.1.3, are necessary for the estimates of (i)–(ii), especially $\phi \in L^\infty(0,T;L^\infty(\Omega))$

and $\mu \in L^2(0,T;W^{1,6}(\Omega))$. By combining the estimates of (*i*)–(*ii*) and utilising Sobolev embeddings, we derive

$$\|g_b\|^2_{L^2(L^2)} \leq C(\|(\hat{b},\hat{f})\|^4_{H^2} + \int_0^t \|\mu_1\|^2_{H^3}\|\bar{\phi}\|^2_{L^2}\,ds).$$

Moreover, utilising this bound and applying another Young inequality allows us to deduce

$$\begin{aligned}\left|\int_0^t\int_\Omega g_b\nabla\bar{\phi}\,dx\,ds\right| &\leq \|g_b\|_{L^2(L^2)}\|\nabla\bar{\phi}\|_{L^2(L^2)}\\ &\leq C(\|(\hat{b},\hat{f})\|^4_{H^2} + \int_0^t \|\mu_1\|^2_{H^3}\|\bar{\phi}\|^2_{L^2}\,ds) + \|\nabla\bar{\phi}\|^2_{L^2(L^2)},\end{aligned}$$

which we will employ in a moment.

We now proceed to test the equations (4.33)–(4.34). We begin by testing equation (4.33) with $v=\bar{\phi}$, integrating over $[0,t]$ and using the previous estimate, which results in

$$\begin{aligned}\frac{1}{2}\|\bar{\phi}(t)\|^2_{L^2} =& \int_0^t\int_\Omega(-g_b - b_1(\phi_1)\nabla\bar{\mu} + \hat{b}(\phi_1)\nabla\mu_1 - \hat{b}(\phi_2)\nabla\mu_2)\nabla\bar{\phi}\,dx\,ds\\ \leq& C\left(\|(\hat{b},\hat{f})\|^4_{(H^2)^2} + \int_0^t \|\mu_1\|^2_{H^3}\|\bar{\phi}\|^2_{L^2}\,ds\right) + \|\nabla\bar{\phi}\|^2_{L^2(L^2)} + \int_0^t\int_\Omega -b_1(\phi_1)\nabla\bar{\mu}\nabla\bar{\phi}\,dx\,ds\\ &+\int_0^t\int_\Omega(\hat{b}(\phi_1)\nabla\mu - \hat{b}(\phi_2)\nabla\mu_2)\nabla\bar{\phi}\,dx\,ds \quad =: (i)+(ii)+(iii)+(iv). \qquad (4.35)\end{aligned}$$

As we will see later, the third integral (*iii*) will cancel out and we continue to establish an estimate for the last integral, denoted by (*iv*). We initially observe that employing the mean value theorem yields the identity

$$\begin{aligned}\hat{b}(\phi_2)\nabla\mu_2 - \hat{b}(\phi_1)\nabla\mu_1 &= (\hat{b}(\phi_2) - \hat{b}(\phi_1))\nabla\mu_1 + \hat{b}(\phi_2)\nabla(\mu_2-\mu_1)\\ &= \hat{b}'(\zeta)(\phi_2-\phi_1)\nabla\mu_1 + \hat{b}(\phi_2)\nabla(\mu_2-\mu_1).\end{aligned}$$

We substitute the obtained identity into the integrand of (*iv*) and apply Hölder's inequality. By using the bounds on the parameter functions from Assumptions 4.1.1, along with the Sobolev embedding $H^2(I)$ in $W^{1,\infty}(I)$ to bound $\hat{b}(\cdot)$, we derive the estimate

$$\begin{aligned}(iv) &\leq \int_0^t\int_\Omega(\hat{b}'(\zeta)(\phi_2-\phi_1)\nabla\mu_1 + \hat{b}(\phi_2)\nabla(\mu_2-\mu_1))\nabla\bar{\phi}\,dx\,ds\\ &\leq \int_0^t \|\hat{b}\|_{H^2}\|(\phi_2-\phi_1)\nabla\mu_1\|_{L^2}\|\nabla\bar{\phi}\|_{L^2} + \|\hat{b}\|_{H^2}\|\nabla(\mu_2-\mu_1)\|_{L^2}\|\nabla\bar{\phi}\|_{L^2}\,ds.\end{aligned}$$

This term is further estimated by using the corresponding regularity of the involved differences and of μ_1, resulting in

$$\begin{aligned}(iv) \leq& C\int_0^t \|\hat{b}\|^2_{H^2}\|\nabla\mu_1\|^2_{L^2}\|\phi_2-\phi_1\|^2_{L^\infty} + \|\nabla\bar{\phi}\|^2_{L^2} + \|\hat{b}\|^2_{H^2}\|\nabla(\mu_2-\mu_1)\|^2_{L^2}\,ds\\ \leq& \|\nabla\bar{\phi}\|^2_{L^2(L^2)} + C\|\hat{b}\|^2_{H^2}(\|\nabla\mu_1\|^2_{L^\infty(L^2)}\|\phi_2-\phi_1\|^2_{L^2(L^\infty)} + \|\nabla(\mu_2-\mu_1)\|^2_{L^2(L^2)})\\ \leq& \|\nabla\bar{\phi}\|^2_{L^2(L^2)} + C(\|(\hat{b},\hat{f})\|^4_{H^2}).\end{aligned}$$

Hence, we have established all needed bounds of inequality (4.35), which yields

$$\begin{aligned}\frac{1}{2}\|\bar\phi(t)\|_{L^2}^2 \leq & C\left(\|(\hat b,\hat f)\|_{H^2}^4 + \int_0^t \|\mu_1\|_{H^3}^2\|\bar\phi\|_{L^2}^2\,ds\right) + \|\nabla\bar\phi\|_{L^2(L^2)}^2 \\ & + \int_0^t\int_\Omega -b_1(\phi_1)\nabla\bar\mu\nabla\bar\phi\,dx\,ds \end{aligned} \tag{4.36}$$

We proceed by testing equation (4.34) with $w=\varepsilon\bar\phi$, applying integration-by-parts, and using the periodic boundary conditions. Upon integrating over $(0,t)$, this leads to the following identity

$$\varepsilon\gamma\|\nabla\bar\phi\|_{L^2(L^2)}^2 = \varepsilon\int_0^t -((\phi_2-\phi_1)^2\frac{f_1''(\zeta)}{2} + f_1'(\phi_1)\bar\phi,\bar\phi) + (\bar\mu,\bar\phi) + (\hat f(\phi_1),\bar\phi) - (\hat f(\phi_2),\bar\phi)\,ds,$$

where ε is a positive constant, which is specified later. An application of the mean value theorem and Young's inequality with constant $c_b/4\gamma$ yields the following estimate for the right-hand side

$$\begin{aligned}\varepsilon\gamma\|\nabla\bar\phi\|_{L^2(L^2)}^2 \leq & \int_0^t -\varepsilon\left((\phi_2-\phi_1)^2\frac{f_1''(\zeta)}{2} + f_1'(\phi_1)\bar\phi,\bar\phi\right) + \frac{c_b}{8\gamma}\|\bar\mu\|_{L^2}^2 \\ & + \left(\frac{2\gamma\varepsilon^2}{c_b}+1\right)\|\bar\phi\|_{L^2}^2 + \frac{\varepsilon^2}{2}\|\hat f\|_{H^2}^2\|\phi_2-\phi_1\|_{L^2}^2\,ds.\end{aligned}$$

We denote the terms by $(i)-(iv)$. The term (iv) is bounded by the estimates of Theorem 4.1.3, i.e. (iv) is bounded by $C(\|(\hat b,\hat f)\|_{H^2}^4)$.The terms (ii) and (iii) remain unchanged. As preliminary estimate for the term (i), we first utilise an interpolation inequality, and again the bounds provided in Theorem 4.1.3, to derive

$$\begin{aligned}\int_0^t \|(\phi_2-\phi_1)^2\frac{f_1''(\zeta)}{2}\|_{L^2}^2\,ds \leq & C\|\phi_2-\phi_1\|_{L^4(L^4)}^4 \\ & \leq C(\|\phi_2-\phi_1\|_{L^\infty(L^2)} + \|\phi_2-\phi_1\|_{L^2(W^{1,2})})^4 \leq C(\|(\hat b,\hat f)\|_{H^2}^4).\end{aligned}$$

For the term (i), we now apply Hölder and Young inequalities, along with the previous estimate, and the uniform bounds on $f_1(\cdot)$ and ϕ_1, yielding the following

$$\begin{aligned}\varepsilon\int_0^t & -((\phi_2-\phi_1)^2\frac{f_1''(\zeta)}{2} + f_1'(\phi_1)\bar\phi,\bar\phi)\,ds \\ & \leq C\int_0^t \|(\phi_2-\phi_1)^2\frac{f_1''(\zeta)}{2}\|_{L^2}^2 + \|f_1'(\phi_1)\bar\phi\|_{L^2}^2 + \|\bar\phi\|_{L^2}^2\,ds \\ & \leq C(\|(\hat b,\hat f)\|_{H^2}^4) + C\int_0^t \|\bar\phi\|_{L^2}^2\,ds.\end{aligned}$$

Combining the estimates for (i)–(iv) results in the inequality

$$\varepsilon\gamma\|\nabla\bar\phi\|_{L^2(L^2)}^2 \leq C\int_0^t\|\bar\phi\|_{L^2}^2\,ds + \frac{c_b}{8\gamma}\|\bar\mu\|_{L^2(L^2)}^2 + C(\|(\hat b,\hat f)\|_{H^2}^4).$$

Moreover, in addition with the inequality (4.36), we derive as intermediate inequality

$$\begin{aligned}\frac{1}{2}\|\bar{\phi}(t)\|_{L^2}^2 + (\varepsilon\gamma - 2)\|\nabla\bar{\phi}\|_{L^2(L^2)}^2 \leq & C\int_0^t (1 + \|\mu_1\|_{H^3}^2)\|\bar{\phi}\|_{L^2}^2\,ds + \frac{c_b}{8\gamma}\|\bar{\mu}\|_{L^2(L^2)}^2 \\ & + C(\|(\hat{b},\hat{f})\|_{H^2}^4) + \int_0^t\int_\Omega -b_1(\phi_1)\nabla\bar{\mu}\cdot\nabla\bar{\phi}\,dx\,ds.\end{aligned} \tag{4.37}$$

We once more test the second system equation (4.34), this time using $w = b_1(\phi_1)\bar{\mu}$, which is feasible due to the sufficient regularity of $b_1(\phi_1)$. By using integration-by-parts in space, followed by integrating over the time domain and reordering of the terms, we arrive at a similar inequality as before

$$\begin{aligned} c_b\|\bar{\mu}\|_{L^2(L^2)}^2 &\leq \int_0^t (\bar{\mu}, b_1(\phi_1)\bar{\mu})\,ds \\ &= \int_0^t ((\phi_2-\phi_1)^2\frac{f_1''(\zeta)}{2} + f_1'(\phi_1)\bar{\phi}, b_1(\phi_1)\bar{\mu}) + \gamma(\nabla\bar{\phi},\nabla(b_1(\phi_1)\bar{\mu})) \\ &\qquad - (\hat{f}'(\phi_1)+\hat{f}'(\phi_2), b_1(\phi_1)\bar{\mu})\,ds.\end{aligned}$$

We denote the terms by (i)–(iii), and estimate the terms individually employing similar arguments as before

$$\begin{aligned}(iii) &\leq \int_0^t C\|\hat{f}\|_{H^2}^2\|\phi_2-\phi_1\|_{L^2}^2\,ds + \frac{c_b}{8}\|\bar{\mu}\|_{L^2(L^2)}^2 \leq C(\|(\hat{b},\hat{f})\|_{H^2}^4) + \frac{c_b}{8}\|\bar{\mu}\|_{L^2(L^2)}^2, \\ (i) &\leq C(\|(\hat{b},\hat{f})\|_{H^2}^4) + \int_0^t C\|\bar{\phi}\|_{L^2}^2 + \frac{c_b}{8}\|\bar{\mu}\|_{L^2}^2\,ds.\end{aligned}$$

For the term (ii), we differentiate using the product rule

$$(ii) = \int_0^t \gamma(\nabla\bar{\phi},\nabla(b_1(\phi_1)\bar{\mu}))\,ds = \int_0^t \gamma(\nabla\bar{\phi}, b_1(\phi_1)\nabla\bar{\mu}) + \gamma(\nabla\bar{\phi},\bar{\mu}\ b_1'(\phi_1)\nabla\phi_1)\,ds,$$

and then proceed to estimate the latter term as follows

$$\begin{aligned}\gamma\int_0^t (\nabla\bar{\phi},\bar{\mu}\ b_1'(\phi_1)\nabla\phi_1)\,ds &\leq \gamma\int_0^t \|b_1'(\phi_1)\nabla\phi_1\|_{L^\infty}\|\nabla\bar{\phi}\|_{L^2}\|\bar{\mu}\|_{L^2}\,ds \\ &\leq \frac{2\gamma^2}{c_b}\|b_1'(\phi_1)\nabla\phi_1\|_{L^\infty(L^\infty)}^2\|\nabla\bar{\phi}\|_{L^2(L^2)}^2 + \frac{c_b}{8}\|\bar{\mu}\|_{L^2(L^2)}^2 \\ &\leq \overline{C}\|\nabla\bar{\phi}\|_{L^2(L^2)}^2 + \frac{c_b}{8}\|\bar{\mu}\|_{L^2(L^2)}^2,\end{aligned}$$

where $\overline{C}$ is a uniform constant. By combining the estimates of (i)–(iii), we get

$$\begin{aligned} & c_b\|\bar{\mu}\|_{L^2(L^2)}^2 - \overline{C}\|\nabla\bar{\phi}\|_{L^2(L^2)}^2 \\ &\quad \leq C(\|(\hat{b},\hat{f})\|_{H^2}^4) + \int_0^t C\|\bar{\phi}\|_{L^2}^2 + \frac{3c_b}{8}\|\bar{\mu}\|_{L^2}^2\,ds + \int_0^t \gamma(\nabla\bar{\phi}, b_1(\phi_1)\nabla\bar{\mu})\,ds.\end{aligned} \tag{4.38}$$

We multiply (4.38) by $1/\gamma$ and then add the previous inequality (4.37) to derive

$$\begin{aligned}\frac{1}{2}\|\bar{\phi}(t)\|_{L^2}^2 + (\varepsilon\gamma - 2 - \overline{C})\|\nabla\bar{\phi}\|_{L^2(L^2)}^2 + \frac{c_b}{2\gamma}\|\bar{\mu}\|_{L^2(L^2)}^2& \\ \leq C\int_0^t (1+\|\mu\|_{H^3}^2)\|\bar{\phi}\|_{L^2}^2\,ds + C(\|(\hat{b},\hat{f})\|_{H^2}^4).&\end{aligned}$$

Now, by choosing ε to be sufficiently large such that the prefactor on the left is positive, the inequality simplifies to

$$\|\bar{\phi}(t)\|_{L^2}^2 + \|\nabla\bar{\phi}\|_{L^2(L^2)}^2 + \|\bar{\mu}\|_{L^2(L^2)}^2 \leq C\int_0^t (1+\|\mu_1\|_{H^3}^2)\|\bar{\phi}\|_{L^2}^2\,ds + C(\|(\hat{b},\hat{f})\|_{H^2}^4)$$

for any $t \in (0,T]$. Through the application of a Gronwall argument, see Lemma A.2.1, we consequently deduce the estimate

$$\|\bar{\phi}\|_{L^\infty(L^2)\cap L^2(H^1)} + \|\bar{\mu}\|_{L^2} \leq C(\|(\hat{b},\hat{f})\|_{H^2}^2).$$

Third step: We will now show the estimate in two other norms. First, we consider (4.34) as an elliptic problem for $\bar{\psi}$. Therefore, by utilising the previously established estimates of $\bar{\phi}, \bar{\mu}$, we deduce from elliptic regularity theory that

$$\begin{aligned}\|\bar{\phi}\|_{L^2(H^2)} &\leq C(\|(\phi_2-\phi_1)^2\frac{f_1''(\zeta)}{2} + f_1'(\phi_1)\bar{\phi}\|_{L^2(L^2)} + \|\bar{\mu}\|_{L^2(L^2)} + \|\hat{f}(\phi_1)+\hat{f}(\phi_2)\|_{L^2(L^2)})\\ &\leq C(\|(\hat{b},\hat{f})\|_{H^2}^2).\end{aligned}$$

Second, it remains to show that $\bar{\phi} \in H^1(0,T;(H^2(\Omega))')$. By testing equation (4.33) with $v \in L^2(0,T;H^2(\Omega))$, using integration by parts, and utilising the previously established estimate of $\bar{\mu}$, we obtain the following estimate

$$\begin{aligned}&\left|\int_0^T \langle\partial_t\bar{\phi}, v\rangle_{H^2(\Omega)}\,ds\right|\\ &\leq \int_0^T\int_\Omega |g_b\nabla v + b_1(\phi_1)\bar{\mu}\Delta v + \bar{\mu}\,b_1'(\phi_1)\nabla\phi_1\nabla v + (\hat{b}(\phi_1)\nabla\mu_1 - \hat{b}(\phi_2)\nabla\mu_2)\nabla v|\,dx\,ds\\ &\leq \Big(C(\|(\hat{b},\hat{f})\|_{H^2}^2) + C\|\bar{\mu}\|_{L^2(L^2)} + C(\|b_1'(\phi_1)\nabla\phi_1\|_{L^\infty(L^\infty)})\|\bar{\mu}\|_{L^2(L^2)}\Big)\|v\|_{L^2(H^2)}\\ &\leq C(\|(\hat{b},\hat{f})\|_{H^2}^2)\|v\|_{L^2(H^2)},\end{aligned}$$

which concludes the proof. □

From differentiability of the solution operator $S(\cdot)$, we directly deduce the differentiability of the forward operator $F(\cdot) = L(S(\cdot))$, defined in Section 4.2, by employing the chain rule. Recall that $L(\cdot)$ is the linear continuous measurement operator.

Corollary 4.3.3. *Let Assumptions 4.1.1 hold. Then the forward operator $F(\cdot) = L(S(\cdot))$ is Fréchet differentiable and defined by $F'(b,f)(\hat{b},\hat{f}) := \psi$.*

4.4. Adjoint operator $F'(x)^*$

The proposed iterative method for minimising the Tikhonov functional requires the application of the adjoint operator $F'(x)^*$. Hence, we will derive a representation of the adjoint operator $F'(x)^*$ that can be used for the implementation later on. In optimal control theory, the adjoint equations are derived from differentiation of the Lagrangian function, see for instance [**60**]. Here, we only briefly present the involved steps and start by defining the Lagrangian

$$\begin{aligned}\mathscr{L}\left((b,f),(\phi,\mu),(p,q)\right) := &\int_{\Omega_T} \frac{1}{2}|\phi-\phi^\delta|^2\,dx\,ds + \int_0^T (\partial_t\phi,p) + (b(\phi)\nabla\mu,\nabla p)\,ds\\ &+ \int_0^T (\mu,q) - \gamma(\nabla\phi,\nabla q) - (f(\phi),q)\,ds,\end{aligned}$$

where, with respect to optimal control theory, the first integral is the cost functional, and the other ones are the state equations (4.1)–(4.2) tested with adjoint variables (p,q). The adjoint equations are then derived from differentiating the Lagrangian by the state variables (ϕ,μ). We denote the direction of the derivative by $\tilde{\phi}$ and $\tilde{\mu}$, and derive the following derivatives

$$\begin{aligned}\partial_\phi\mathscr{L}' &= \int_0^T (\phi-\phi^\delta,\tilde{\phi})\,ds + \int_0^T (\partial_t\tilde{\phi},p) + (b'(\phi)\tilde{\phi}\nabla\mu,\nabla p) - \gamma(\nabla\tilde{\phi},\nabla q) - (f'(\phi)\tilde{\phi},q)\,ds,\\ \partial_\mu\mathscr{L}' &= \int_0^T (b(\phi)\nabla\tilde{\mu},\nabla p) + (\tilde{\mu},q)\,ds,\end{aligned}$$

which yields the so-called adjoint problem, i.e. find adjoint variables (p,q) such that $\partial_\phi\mathscr{L}'(\tilde{\phi}) + \partial_\mu\mathscr{L}'(\tilde{\mu}) = 0$ for all directions $\tilde{\phi},\tilde{\mu}$. From these preliminary considerations, and by using integration by parts in time and imposing an additional boundary condition $p(T,x)=0$ for all $x\in\Omega$, we deduce the subsequent problem for the adjoint states.

Let Assumptions 4.1.1 hold, and let (b,f) be a fixed pair of parameter functions with corresponding smooth solution (ϕ,μ). We will analyse the subsequent system for the adjoint states (p,q):

$$-\partial_t p + b'(\phi)\nabla\mu\nabla p + \gamma\,\mathrm{div}(\nabla q) - f'(\phi)q = -r^\delta \qquad \text{in } \Omega\times(0,T) \tag{4.39}$$

$$q = \mathrm{div}(b(\phi)\nabla p) \qquad \text{in } \Omega\times(0,T) \tag{4.40}$$

with $p(T,x)=0$ in Ω, periodic boundary conditions and data $r^\delta\in L^2(0,T;L^2(\Omega))$. Later on the data r^δ takes the form $\phi-\phi^\delta$, wherein ϕ^δ corresponds to observations of ϕ.

In the following Subsection 4.4.1, we establish the existence of unique solutions (p,q) for the adjoint problem. Afterwards, we will derive a representation of the adjoint operator $F'(x)^*$, which will implicitly define the application as the solution of a Laplace problem. This will be presented in Subsection 4.4.2.

4.4.1. Existence of solutions to the adjoint problem

The following theorem establishes the existence of a unique solution (p,q) of the adjoint problem (4.39)–(4.40).

Theorem 4.4.1. *Let Assumptions 4.1.1 hold and $r^\delta \in L^2(0,T;L^2(\Omega))$. Then for any $(b,f) \in \mathcal{D}(S)$, there exists a unique pair (p,q), associated to the smooth solution $S(b,f) = (\phi,\mu)$, with regularity*

$$p \in L^2(0,T;H^2(\Omega)) \cap H^1(0,T;(H^2(\Omega))') \cap L^\infty(0,T;L^2(\Omega)),$$
$$q \in L^2(0,T;L^2(\Omega)),$$

which satisfies $p(T,x) = 0$ in $L^2(\Omega)$; and (4.40), i.e.

$$q = \operatorname{div}(b(\phi)\nabla p),$$

holds a.e. Furthermore, it holds

$$0 = \langle -\partial_t p, v\rangle_{H^2} + \int_\Omega (b'(\phi)\nabla\mu\nabla p - f'(\phi)q + r^\delta)v + \gamma q \Delta v \, dx \tag{4.41}$$

for a.e. $t \in (0,T)$ and for all $v \in H^2(\Omega)$.

The proof is inspired by [**29, 64**]. We will test (4.39)–(4.40) to derive energy estimates and employ a Gronwall argument. Afterwards, we improve the regularity of (p,q) and show the uniqueness of the solution.

Proof. We omit the comprehensive discussion of the Galerkin approximation and proceed by establishing the required a-priori estimates.

First step: Similar to the proofs of Theorem 4.1.3 and Theorem 4.3.2, we test the first equation (4.39) with $v = b(\phi)p$ and the second equation (4.40) with $w = \gamma q$ and $w = \varepsilon p$.

Let us start by considering the following identity

$$\frac{1}{2}\frac{d}{dt}\left(\int_\Omega b(\phi)|p|^2 \, dx\right) = (\partial_t p, b(\phi)p) + \frac{1}{2}\int_\Omega |p|^2 b'(\phi)\partial_t\phi \, dx. \tag{4.42}$$

We test the first system equation (4.39) with the function $v = b(\phi)p$. By utilising the previous identity and computing the derivative $\nabla(b(\phi)p)$, we obtain the following identity by rearranging the terms

$$\begin{aligned} -\frac{1}{2}\frac{d}{dt}\int_\Omega b(\phi)|p|^2 &= -\frac{1}{2}\int_\Omega b'(\phi)\partial_t\phi|p|^2 - b(\phi)b'(\phi)p\nabla\mu\nabla p + \gamma b(\phi)\nabla q\nabla p \\ &\quad + \gamma p\, b'(\phi)\nabla q\nabla\phi + f'(\phi)b(\phi)qp - b(\phi)r^\delta p \, dx. \end{aligned}$$

Moreover, we test the system equation (4.40), using two different test functions $w = \gamma q$ and $w = \varepsilon p$, where ε is a positive constant that will be specified later. Adding these equations to the previously derived one results in

$$\begin{aligned} -\frac{1}{2}\frac{d}{dt}\int_\Omega b(\phi)|p|^2 \, dx + \gamma\|q\|_{L^2}^2 + \varepsilon\|b^{\frac{1}{2}}(\phi)\nabla p\|_{L^2}^2 & \\ = -\frac{1}{2}\int_\Omega b'(\phi)\partial_t\phi|p|^2 - b(\phi)b'(\phi)p\nabla\mu\nabla p + \gamma p b'(\phi)\nabla q\nabla\phi & \\ - \varepsilon qp + f'(\phi)b(\phi)qp - b(\phi)r^\delta p \, dx. & \end{aligned}$$

We label the terms on the right-hand side as (i)–(vi). By employing Hölder's and Young's inequality and using the uniform boundedness of $b(\phi), f(\phi)$ and its derivatives, see Assumptions 4.1.1 and (4.7), we estimate the terms (iv)–(vi) as follows

$$
\begin{aligned}
(iv)+(v)+(vi) &\leq \varepsilon\|q\|_{L^2}\|p\|_{L^2} + C(f',b)\|q\|_{L^2}\|p\|_{L^2} + C(b)\|r^\delta\|_{L^2}\|p\|_{L^2} \\
&\leq C(1+\varepsilon^2)(\|p\|_{L^2}^2 + \|r^\delta\|_{L^2}^2) + \frac{\gamma}{4}\|q\|_{L^2}^2.
\end{aligned} \tag{4.43}
$$

We will now estimate the terms (i)–(iii) separately, using the regularity of the smooth solution (ϕ,μ). Let us briefly remind ourselves that

$$
\begin{aligned}
\phi &\in W^{1,2}(0,T;L^2(\Omega)) \cap L^\infty(0,T;W^{1,\infty}(\Omega)) \cap L^2(0,T;H^4(\Omega)), \\
\nabla\mu &\in L^2(0,T;H^2(\Omega)).
\end{aligned}
$$

To estimate the term (i), we apply Hölder and Young inequalities, along with the interpolation inequality $\|f\|_{L^4} \leq C(\|f\|_{L^2}^{\frac{1}{2}}\|\nabla f\|_{L^2}^{\frac{1}{2}} + \|f\|_{L^2})$ [**73**], resulting in

$$
\begin{aligned}
(i) &\leq C(b')\|\partial_t\phi\|_{L^2}\|p\|_{L^4}^2 \\
&\leq C(b')\|\partial_t\phi\|_{L^2}\|p\|_{L^2}(\|\nabla p\|_{L^2} + \|p\|_{L^2}) \\
&\leq C(1+\|\partial_t\phi\|_{L^2}^2)\|p\|_{L^2}^2 + \|\nabla p\|_{L^2}^2.
\end{aligned} \tag{4.44}
$$

Similarly, we derive an estimate for the term (ii)

$$
(ii) \leq C(b)\|\nabla\mu\|_{L^\infty}|\int_\Omega p\nabla p\,dx| \leq C(b,\|\nabla\mu\|_{L^\infty}^2)\|p\|_{L^2}^2 + \|\nabla p\|_{L^2}^2. \tag{4.45}
$$

To address the third term, we use integration-by-parts to see that

$$
\int_\Omega pb'(\phi)\nabla q\nabla\phi\,dx = \int_\Omega q\left(b''(\phi)p|\nabla\phi|^2 + b'(\phi)\nabla p\nabla\phi + b'(\phi)p\Delta\phi\right)\,dx.
$$

This identity is substituted for the term (iii), and then estimated by Hölder and Young inequalities to obtain

$$
\begin{aligned}
(iii) &= \gamma\int_\Omega q\,p(b''(\phi)|\nabla\phi|^2 + b'(\phi)\Delta\phi) + q(b'(\phi)\nabla p\nabla\phi)\,dx \\
&\leq C(1+\|\Delta\phi\|_{L^\infty})\|p\|_{L^2}\|q\|_{L^2} + \|b'(\phi)\nabla\phi\|_{L^\infty}\|q\|_{L^2}\|\nabla p\|_{L^2} \\
&\leq C(1+\|\Delta\phi\|_{L^\infty}^2)\|p\|_{L^2}^2 + \frac{2}{\gamma}\|b'(\phi)\nabla\phi\|_{L^\infty}^2\|\nabla p\|_{L^2}^2 + \frac{\gamma}{4}\|q\|_{L^2}^2.
\end{aligned} \tag{4.46}
$$

By combining the estimates for the terms (i)–(vi) and integrating over the interval $[t,T]$, with $t\in[0,T)$, taking into account $p(T,x)=0$, and rearranging terms, we arrive at

$$
\begin{aligned}
&\frac{c_b}{2}\|p(t)\|_{L^2}^2 + \frac{\gamma}{2}\|q\|_{L^2(t,T;L^2)}^2 + (\varepsilon c_b - 2 - \frac{2}{\gamma}\|b'(\phi)\nabla\phi\|_{L^\infty(L^\infty)}^2)\|\nabla p\|_{L^2(t,T;L^2)}^2 \\
&\quad\leq \int_t^T C(\varepsilon^2 + \|\Delta\phi\|_{L^\infty}^2 + \|\nabla\mu\|_{L^\infty}^2 + \|\partial_t\phi\|_{L^2}^2)\|p\|_{L^2}^2\,ds + C\|r^\delta\|_{L^2(s,T;L^2)}^2.
\end{aligned}
$$

Now, by choosing a sufficiently large ε, the inequality simplifies to

$$\begin{aligned}&\|p(t)\|_{L^2}^2 + \|q\|_{L^2(t,T;L^2)}^2 + \|\nabla p\|_{L^2(t,T;L^2)}^2 \\ &\leq C\int_t^T (1 + \|\Delta\phi\|_{L^\infty}^2 + \|\nabla\mu\|_{L^\infty}^2 + \|\partial_t\phi\|_{L^2}^2)\|p\|_{L^2}^2\,ds + C\|r^\delta\|_{L^2(t,T;L^2)}^2.\end{aligned}$$

By applying a Gronwall argument backwards in time, we obtain the bounds

$$\|p\|_{L^\infty(L^2)\cap L^2(H^1)} + \|q\|_{L^2(L^2)} \leq C.$$

Second step: We will now derive bounds of p in further norms. First, we employ an elliptic regularity argument to improve the regularity of p. Therefore, we consider the second equation (4.40) as an elliptic problem for p. Given that $q \in L^2(0,T;L^2(\Omega))$, and that $b(\phi)$ strictly positive and uniformly bounded, see (4.7), we deduce from elliptic regularity theory, see [**46**], that

$$\|p\|_{L^2(H^2)} \leq C.$$

Second, we will establish $\partial_t p \in L^2(0,T;(H^2(\Omega))')$. To achieve this, let us consider v to be an arbitrary function in $L^2(0,T;H^2(\Omega))$ and use it to test the first system equation (4.39). Using integration-by-parts and previously derived bounds on (p,q), we derive

$$\begin{aligned}\left|\int_0^T \langle\partial_t p, v\rangle_{H^2}\,ds\right| &\leq \left|\int_0^T\int_\Omega \gamma q\Delta v + f'(\phi)qv + r^\delta v + b'(\phi)\nabla\mu\nabla p\, v\,dx\,ds\right| \\ &\leq C(f')\|q\|_{L^2(L^2)}(\|\Delta v\|_{L^2(L^2)} + \|v\|_{L^2(L^2)}) + \|r^\delta\|_{L^2(L^2)}\|v\|_{L^2(L^2)} \\ &\quad + C(b')\|\nabla\mu\|_{L^\infty(L^2)}\|\nabla p\|_{L^2(L^2)}\|v\|_{L^2(L^\infty)} \\ &\leq C\|v\|_{L^2(H^2)}.\end{aligned}$$

Therefore we have established that $p \in H^1(0,T;(H^2(\Omega))')$, concluding the derivation of regularities for p and q.

Third step: Next, we address the uniqueness of solutions. Let $(p_1,q_1),(p_2,q_2)$ denote two solutions, and let us define the differences as $\hat{p} := p_1 - p_2, \hat{q} := q_1 - q_2$, with initial data $\hat{p}(T,x) = 0$. The differences, $\hat{p}$ and $\hat{q}$, have the following regularities

$$\begin{aligned}&\hat{p} \in L^2(0,T;H^2(\Omega)) \cap L^\infty(0,T;L^2(\Omega)) \cap H^1(0,T;(H^2(\Omega))'), \\ &\hat{q} \in L^2(0,T;L^2(\Omega)),\end{aligned}$$

and $\hat{p}(T) = 0$ in $L^2(\Omega)$. Further, equation (4.40) holds a.e. and we also have

$$0 = \langle -\partial_t\hat{p}, v\rangle_{H^2} + \int_\Omega b'(\phi)\nabla\mu\nabla\hat{p}v + \gamma\hat{q}\Delta v - f'(\phi)\hat{q}v\,dx \tag{4.47}$$

for a.e. $t \in (0,T)$ and for all $v \in H^2(\Omega)$. The following approach involves applying the same testing procedure as before and then utilising a Gronwall argument to establish the uniqueness of solutions. For this, we first have to show that $v = b(\phi)\hat{p}$ is an admissible test function, i.e. we show v is an element of $L^2(0,T;H^2(\Omega))$. Therefore, as a preliminary step, we compute

$$\Delta(b(\phi)\hat{p}) = b(\phi)\Delta\hat{p} + b'(\phi)\nabla\phi\nabla\hat{p} + b''(\phi)|\nabla\phi|^2\nabla\hat{p} + b'(\phi)\Delta\phi\hat{p} + b'(\phi)\nabla\phi\nabla\hat{p}.$$

By using the uniform boundedness of ϕ and $\nabla\phi$, see (4.7), as well as the fact that $\partial_i\partial_j\phi \in L^2(0,T;H^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega))$ and $\hat{p} \in L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^2(\Omega))$, we deduce that all terms can be estimated such that consequently

$$\|b(\phi)\hat{p}\|_{L^2(H^2)} \leq C.$$

Now, we proceed with the testing procedure and derive the a-priori-estimates. Inserting $v = b(\phi)\hat{p}$ as test function into (4.47), and making use of the previously established identity (4.42), yields the following

$$\begin{aligned} 0 = &-\frac{1}{2}\frac{d}{dt}\int_\Omega b(\phi)|\hat{p}|^2\,dx + \frac{1}{2}\int_\Omega |\hat{p}|^2 b'(\phi)\partial_t\phi\,dx \\ &+ \int_\Omega b(\phi)b'(\phi)\hat{p}\nabla\mu\nabla\hat{p} - f'(\phi)b(\phi)\hat{q}\hat{p} + \gamma\hat{q}\Delta(b(\phi)\hat{p})\,dx. \end{aligned} \tag{4.48}$$

Moreover, the following identity is derived through differentiation,

$$\int_\Omega \hat{q}\Delta(b(\phi)\hat{p})\,dx = \int_\Omega \hat{q}(\operatorname{div}(b(\phi)\nabla\hat{p}) + b''(\phi)|\nabla\phi|^2\hat{p} + b'(\phi)\hat{p}\Delta\phi + b'(\phi)\nabla\phi\nabla\hat{p}\,dx.$$

Using this, and also inserting the second system equation (4.40) into (4.48), we obtain

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\int_\Omega b(\phi)|\hat{p}|^2\,dx = &\frac{1}{2}\int_\Omega |\hat{p}|^2 b'(\phi)\partial_t\phi\,dx + \int_\Omega b(\phi)b'(\phi)\hat{p}\nabla\mu\nabla\hat{p} - f'(\phi)b(\phi)\hat{q}\hat{p}\,dx \\ &+ \int_\Omega \gamma|\hat{q}|^2 + \gamma\hat{q}(b''(\phi)|\nabla\phi|^2\hat{p} + b'(\phi)\hat{p}\Delta\phi + b'(\phi)\nabla\phi\nabla\hat{p})\,dx. \end{aligned}$$

We label the terms as (i)–$(viii)$. These can be estimated similarly to the first step of this proof. To be precise: we estimate (i) from below using the lower bound of $b(\cdot)$, (ii) is estimated as in (4.44), (iii) as in (4.45), (iv) as in (4.43), and $(vi), (vii), (viii)$ as in (4.46). Moreover, by testing the second system equation (4.40) with $w = \varepsilon\hat{p}$ in order to derive control on $\nabla\hat{p}$, we will obtain a similar inequality as before, just without the data term involving r^δ, that is

$$\begin{aligned} &\|\hat{p}(t)\|_{L^2}^2 + \|\hat{q}\|_{L^2(t,T;L^2)}^2 + \|\nabla\hat{p}\|_{L^2(t,T;L^2)}^2 \\ &\qquad \leq C\int_t^T (1 + \|\Delta\phi\|_{L^\infty}^2 + \|\nabla\mu\|_{L^\infty}^2 + \|\partial_t\phi\|_{L^2}^2)\|\hat{p}\|_{L^2}^2\,ds. \end{aligned}$$

Subsequently, using a Gronwall argument, see [**53, Lemma 3.1**] with $\alpha = 0$, we arrive at the conclusion that

$$\|\hat{p}\|_{L^\infty(L^2)\cap L^2(H^1)} + \|\hat{q}\|_{L^2(L^2)} \leq 0.$$

This establishes the uniqueness of the solution (p,q) for the adjoint state problem. □

4.4.2. Representation of the adjoint operator $F'(x)^*$

Now, we are in the position to derive a representation for the adjoint operator $F'(x)^*$. As a brief reminder, the Fréchet derivative is the linear operator

$$F'(b,f) : (H^2(I))^2 \to L^2(0,T;L^2(\Omega)), \quad (\hat{b},\hat{f}) \mapsto \psi.$$

The adjoint operator is then defined as a mapping $L^2(0,T;L^2(\Omega)) \to (H^2(I))^2$ by the following expression

$$(F'(b,f)^* r, (\hat{b},\hat{f}))_{H^2} := (r, F'(b,f)(\hat{b},\hat{f}))_{L^2(L^2)} = (r,\psi)_{L^2(L^2)} \tag{4.49}$$

for any $r \in L^2(0,T;L^2(\Omega))$ and $(\hat{b},\hat{f}) \in (H^2(I))^2$. This definition is implicit, and we will now establish a representation that can be used for the implementation to compute the outcome $g := (g_1,g_2) := F'(b,f)^* r \in (H^2(I))^2$.

To achieve this, we will utilise the linearised state equations (4.25)–(4.26) and the adjoint state equations (4.39)–(4.40). We have the following result.

Theorem 4.4.2. *Let Assumptions 4.1.1 hold and $r \in L^2(0,T;L^2(\Omega))$. Further, let (b,f) be admissible parameter functions with associated solution (ϕ,μ) of the Cahn-Hilliard system. Then there exists (p,q) as the solution to the adjoint problem* (4.39)–(4.40)*, which depends on $(\phi,\mu),(b,f)$ and r. The result of an application of the adjoint operator, i.e. the outcome $g = (g_1,g_2) = F'(b,f)^* r$, is then defined as the solution of the following variational problem:*

$$(g,(\hat{b},\hat{f}))_{H^2} = (\hat{b}(\phi)\nabla\mu, \nabla p)_{L^2(L^2)} - (\hat{f}(\phi), q)_{L^2(L^2)}$$

for all directions $(\hat{b},\hat{f}) \in (H^2(I))^2$.

Proof. Let $(\hat{b},\hat{f}) \in (H^2(I))^2$, (ψ,ξ) be the corresponding solution of the linearised problem, and let (p,q) be the solution of the adjoint problem associated with the data r.

By the definition of the adjoint operator, it holds

$$(F'(b,f)^* r, (\hat{b},\hat{f}))_{H^2} := (r, F'(b,f)(\hat{b},\hat{f}))_{L^2(L^2)} = (r,\psi)_{L^2(L^2)} =: (i).$$

To begin, we select $v = \psi$ as the test function for the identity (4.41) derived in Theorem 4.4.1, i.e. the first equation of the adjoint system. Note that ψ possesses sufficient regularity for this testing. We obtain

$$(i) = -\int_0^T \langle -\partial_t p, \psi\rangle_{H^2} + (b'(\phi)\nabla\mu\nabla p, \psi)_{L^2} - (f'(\phi)q,\psi)_{L^2} + \gamma(q,\Delta\psi)_{L^2}\, ds.$$

We derive from the second equation of the linearised system (4.31), tested with $w = q$, the equation

$$\int_0^T (\gamma\Delta\psi - f'(\phi)\psi, q)_{L^2}\, ds = \int_0^T (\hat{f}(\phi) - \xi, q)_{L^2}\, ds,$$

and insert it into the previous identity, which yields

$$(i) = -\int_0^T \langle -\partial_t p, \psi\rangle_{H^2} + (b'(\phi)\nabla\mu\nabla p, \psi)_{L^2} + (\hat{f}(\phi) - \xi, q)_{L^2}\, ds.$$

Now by applying integration-by-parts in the time direction, more details on this at the end, also using the boundary conditions $\psi(0,x) = p(T,x) = 0$, we derive

$$(i) = -\int_0^T \langle \partial_t \psi, p\rangle_{H^1} + (b'(\phi)\nabla\mu\nabla p, \psi)_{L^2} + (\hat{f}(\phi) - \xi, q)_{L^2}\, ds.$$

On the other side, we test (4.31) derived in Theorem 4.3.2, i.e. the first equation of the linearised system, with test function $v = p$. Note that p is sufficiently regular for this testing. This yields,

$$\int_0^T \langle \partial_t \psi, p\rangle_{H^1} + (b'(\phi)\psi\nabla\mu, \nabla p)_{L^2}\, ds = \int_0^T -(b(\phi)\nabla\xi + \hat{b}(\phi)\nabla\mu, \nabla p)_{L^2}\, ds.$$

By inserting into the previous identity, we obtain

$$(i) = -\int_0^T -(b(\phi)\nabla\xi + \hat{b}(\phi)\nabla\mu, \nabla p)_{L^2} + (\hat{f}(\phi) - \xi, q)_{L^2}\, ds.$$

Moreover, by testing the second equation of the adjoint system (4.40) with $w = \xi$, we observe that the sum $(\xi, q)_{L^2} + (b(\phi)\nabla\xi, \nabla p)_{L^2}$ evaluates to zero and we arrive at

$$(F'(b,f)^* r, (\hat{b}, \hat{f}))_{H^2} = \int_0^T (\hat{b}(\phi)\nabla\mu, \nabla p)_{L^2} - (\hat{f}(\phi), q)_{L^2}\, ds.$$

It is left to consider some details on the integration-by-parts in the time direction. To this end, let us first recall that both p and ψ belong to $H^1(0,T;(H^2(\Omega))') \cap L^2(0,T;H^2(\Omega))$, allowing us to apply integration-by-parts with respect to time, i.e.

$$\int_0^T \langle -\partial_t p, \psi\rangle_{H^2}\, ds = -\int_\Omega \psi(T)p(T) + \psi(0)p(0)\, dx + \int_0^T \langle \partial_t \psi, p\rangle_{H^2}\, ds.$$

The first integral vanishes due to the boundary conditions $\psi(0,x) = 0$, $p(T,x) = 0$. Further recall that $\partial_t \psi \in L^2(0,T;(H^1(\Omega))')$ and $p \in L^2(0,T;H^1(\Omega))$, such that we deduce

$$\int_0^T \langle -\partial_t p, \psi\rangle_{H^2}\, ds = \int_0^T \langle \partial_t \psi, p\rangle_{H^1}\, ds,$$

which we used before. □

Summary

We discussed the Tikhonov regularisation approach for the inverse problem $F(b,f) = \phi^\delta$ and showed its well-posedness by continuity and weak-to-strong continuity of the solution operator $S(\cdot)$. Then, we proposed a Gauss-Newton approach for the realisation of the Tikhonov minimisation problem. To do this, we established the differentiability of the forward operator $F(\cdot)$, again by claims on the solution operator $S(\cdot)$. Further, we investigated an adjoint system to derive a representation of the adjoint operator $F'(b,f)^*$. In the following chapter, we will consider the discretisation and implementation of the previous theoretical results and present numerical tests.

5. Numerical approximation of the output least squares method

In the previous chapter, we studied the parameter identification problem of $b(\cdot)$ and $f(\cdot)$ in the Cahn-Hilliard equation

$$\partial_t \phi = \operatorname{div}\left(b(\phi)\nabla\mu\right), \tag{5.1}$$

$$\mu = -\gamma\Delta\phi + f(\phi), \tag{5.2}$$

by an output least squares approach. To this end, we considered the forward operator $F(b,f) = \phi$ and studied the parameter identification of $b(\cdot)$ and $f(\cdot)$ from measurements of ϕ, i.e. $F(b,f) = \phi^\delta$, which is a nonlinear inverse problem in Hilbert spaces. We showed continuity and weak continuity of the operator $F(b,f)$ and considered Tikhonov regularisation to derive stable approximations of the solution, i.e. we considered the minimisation of the Tikhonov functional

$$\min_{(b,f)\in\mathcal{D}(F)} J_\alpha(b,f) := \frac{1}{2}\|F(b,f)-\phi^\delta\|_Y^2 + \frac{\alpha}{2}\|(b,f)-(b^*,f^*)\|_X^2 \,. \tag{5.3}$$

We showed that this output-least-squares approach is well-defined and suggested a Gauss-Newton approach to solve the minimisation problem. As preparation for this iterative approach, we established differentiability of $F(b,f)$ and we derived a representation of the adjoint operator $F'(b,f)^*$.

In this chapter, we will now consider the numerical realisation of the previous theoretical results. Initially, we have to discuss the numerical approximation of the Cahn-Hilliard equation (5.1)–(5.2).

Literature

The main challenges arise from the non-convex double-well potential, i.e. the anti-derivative of the function $f(\cdot)$. One has to carefully select a time-stepping method such that the interactions within the interfacial regime are resolved while the energy stability of the discrete method is ensured. The literature has extensively discussed feasible schemes using various methods. The equations (5.1)–(5.2) consider the Cahn-Hilliard equation as a system of two second-order differential equations. Hence, the phase fraction ϕ and chemical potential μ are discretised separately. In the context of finite element approximations, this approach is recognised as a mixed finite element method. It was introduced for the Cahn-Hilliard equation in [**42**] and further analysed in works such as [**30, 33, 44**]. Besides finite element methods, alternative discretisation methods have also been considered. Notably, discontinuous Galerkin methods have been examined in [**70, 76, 93**], and Fourier spectral methods have been used in [**59, 75**].

We will consider a finite element approximation. As previously indicated, the primary challenges arise from the non-convex potential. Conventional explicit time-stepping schemes, for instance, Euler schemes, suffer from severe time-step restrictions, while implicit formulations lead to ill-conditioned non-linear algebraic systems. The reason for this is the interfacial dynamic of the Cahn-Hilliard equation. An additional objective is to preserve the energy structure at the discrete level.

Classical time-integration methods such as Runge-Kutta or multi-step schemes do not generally preserve the structure. This has led to extensive research into the development of energy-stable schemes, which aim to preserve energy dissipation while potentially introducing some artificial numerical energy dissipation. One approach involves decomposing the potential function into a convex and a concave component, which are then treated explicitly and implicitly to establish unconditionally energy-stable schemes. This is illustrated and discussed in works like [**32, 55, 56**]. Alternatively, another strategy involves introducing an additional variable, hence an additional differential equation, which leads to an artificial quadratic energy of the new system. This approach is known in the literature as invariant energy quadratisation (IEQ) or as scalar auxiliary variable (SAV), as discussed in works like [**84, 85, 86**]. Those methods can be interpreted as a relaxation of the energy and can be extended to more complex systems as demonstrated in e.g. [**87**].

Structure preserving discretisation

In [**36**], we described a general framework to preserve the underlying structure of a particular class of abstract evolution problems. Notably, the gradient-flow structure of the Cahn-Hilliard system is included in this class. This structure-preserving property remains intact when considering a fully discrete approximation by a Petrov-Galerkin approach. In [**36**][Sec. 4.2], this approach is demonstrated on a Cahn-Hilliard equation with constant mobility. Moreover, in [**19**], we applied the framework to the Cahn-Hilliard system (5.1)–(5.2), notably including the solution-dependent mobility. As a result of this approximation, the conservation of mass and an energy-dissipation relation are achieved up to machine precision in numerical tests. Furthermore, using relative energy estimates, it was shown that this discretisation approach yields second-order convergence, which is optimal with respect to the considered finite element spaces, see [**19**]. Most importantly, conditions for the uniqueness of the discrete solution were also derived.

Outline

This chapter addresses the numerical realisation of the previous theoretical results. In Section 5.1, we will outline the discretisation of the Cahn-Hilliard equation employing the structure-preserving approach of [**36**]. Using this, we will define the discrete solution operator and deduce that it is well-defined from results in [**19**]. This discretisation scheme will naturally lead to a discretisation of the scalar products of the Hilbert spaces involved in the nonlinear identification problem. Subsequently, we introduce the discrete forward operator and the discrete analogue of the Tikhonov problem (5.3) in Section 5.2 and establish the well-posedness of the discrete problem. Afterwards, we consider the discretisation of the linearised and the adjoint problem, which follows naturally from the structure-preserving approach. Numerical examples will illustrate the application of the discrete approach in Section 5.3. Concluding the chapter, we provide a discussion of the results and a comparison to the results of the equation error method in Section 5.3.4.

5.1. Discretisation of the solution operator $S(\cdot)$

We consider the Cahn-Hilliard system (5.1)–(5.2) on a periodic domain Ω complemented with periodic boundary conditions. Let us recall the main assumptions used in the previous analysis, which we here repeat for the convenience of the reader.

Assumptions 5.1.1. We impose the following assumptions on the domain and on the parameters:

(A0) $\Omega \simeq \mathbb{T}^d$, is the d-dimensional torus; functions defined on Ω are assumed to be periodic.

(A1) $\gamma > 0$ is a positive constant;

(A2) $b : \mathbb{R} \to \mathbb{R}_+$ satisfies $b \in C^2(\mathbb{R})$ with $0 < c_b \leq b(s) \leq C_b$ for all $s \in \mathbb{R}$ and $\|b'\|_\infty \leq C_{b'}$, $\|b''\|_\infty \leq C_{b''}$;

(A3) $f(s) = \lambda'(s)$ with $\lambda \in C^4(\mathbb{R})$ such that $\lambda(s), \lambda''(s) \geq -c_{\lambda_1}$, for some $c_{\lambda_1} \geq 0$. Furthermore, λ and its derivatives are bounded by $|\lambda^{(k)}(s)| \leq C_{\lambda_2}^{(k)} + C_{\lambda_3}^{(k)}|s|^{4-k}$ for $0 \leq k \leq 4$ with constants $C_{\lambda_2}^{(k)}, C_{\lambda_3}^{(k)} \geq 0$.

In addition, we assume $\phi_0 \in H^3(\Omega)$.

In this setting, we consider the following the Petrov-Galerkin approximation for the Cahn-Hilliard equation (5.1)–(5.2).

Finite element spaces

Let $\mathcal{T}_h$ denote a conforming partition of the domain $\Omega \in \mathbb{R}^d$, $d = 2$ into triangles. For simplicity, we assume a uniform mesh size h for all elements $K \in \mathcal{T}_h$. Further, we consider a periodic mesh $\mathcal{T}_h$ in the sense that it can be extended periodically to periodic extensions of the domain Ω. Then, we denote by

$$\mathcal{V}_h := \{v \in H^1(\Omega) : v|_K \in P_2(K)^d, \forall K \in \mathcal{T}_h\},$$

the space of continuous piecewise quadratic polynomials over the mesh $\mathcal{T}_h$. Next, we introduce the time discretisation. Given a time step size $\tau = T/N$, where $N \in \mathbb{N}$, we define discrete time points $t^n := n\tau$, and denote the corresponding partition of the time interval $[0,T]$ as $\mathcal{I}_\tau := \{0 = t^0, t^1, \ldots, t^N = T\}$. We will denote by $\Pi_k(\mathcal{I}_\tau; \mathcal{V}_h)$ the space of piecewise polynomials of degree k over the time grid $\mathcal{I}_\tau$ with values in $\mathcal{V}_h$, and denote by $\Pi_k^c(\mathcal{I}_\tau; \mathcal{V}_h) = \Pi_k(\mathcal{I}_\tau; \mathcal{V}_h) \cap C(0,T; \mathcal{V}_h)$ the corresponding sub-space of continuous functions. Furthermore, we will use a bar symbol $\bar{g}$ to denote piecewise constant functions in time.

Discretisation of the Cahn-Hilliard equation

Our aim is to compute approximations $(\phi_{h,\tau}, \bar{\mu}_{h,\tau})$ of (ϕ, μ) within the spaces

$$\mathbb{Y}_{h,\tau}(0,T) := \Pi_1^c(\mathcal{I}_\tau; \mathcal{V}_h) \quad \text{and} \quad \mathbb{Q}_{h,\tau}(0,T) := \Pi_0(\mathcal{I}_\tau; \mathcal{V}_h).$$

Let us emphasise that functions in $\mathbb{Y}_{h,\tau}(0,T)$ are continuous and piecewise linear in time, while functions $\bar{q} \in \mathbb{Q}_{h,\tau}(0,T)$ are piecewise constant in time, which is indicated by the bar symbol. We consider the following fully discrete approximation for the Cahn-Hilliard system (5.1)–(5.2).

Problem 5.1.2. *Let $\phi_{h,0} \in \mathcal{V}_h$ be given. Find $(\phi_{h,\tau}, \bar{\mu}_{h,\tau}) \in \mathbb{Y}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$, with $\phi_{h,\tau}(0) = \phi_{h,0}$ and such that*

$$\int_{t^{n-1}}^{t^n} (\partial_t \phi_{h,\tau}, \bar{v}_{h,\tau}) + (b(\phi_{h,\tau}) \nabla \bar{\mu}_{h,\tau}, \nabla \bar{v}_{h,\tau})\, ds = 0, \tag{5.4}$$

$$\int_{t^{n-1}}^{t^n} (\bar{\mu}_{h,\tau}, \bar{w}_{h,\tau}) - (\gamma \nabla \phi_{h,\tau}, \nabla \bar{w}_{h,\tau}) - (f(\phi_{h,\tau}), \bar{w}_{h,\tau})\, ds = 0. \tag{5.5}$$

for all test functions $(\bar{v}_{h,\tau}, \bar{w}_{h,\tau}) \in \mathbb{Q}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$ and for $n \geq 1$.

Well-posedness of the discrete scheme has been considered in [**19**], which we recall here.

Theorem 5.1.3 ([**19**])**.** *Let Assumptions 5.1.1 hold. Then any for $\phi_{0,h} \in \mathcal{V}_h$ and any $\tau > 0$, Problem 5.1.2 has at least one solution $(\phi_{h,\tau}, \bar{\mu}_{h,\tau})$ satisfying the uniform bounds*

$$\|\phi_{h,\tau}\|_{L^\infty(H^1)} + \|\bar{\mu}_{h,\tau}\|_{L^2(H^1)} \leq C(\|\phi_{h,0}\|_{H^1}).$$

Further, let (ϕ, μ) denote a regular periodic weak solution of (5.1)–(5.2) *with initial value $\phi_0 \in H^3(\Omega)$ satisfying additionally*

$$\begin{aligned} &\phi \in H^2(0,T; H^1(\Omega)) \cap H^1(0,T; H^3(\Omega)), \\ &\mu \in H^2(0,T; H^1(\Omega)) \cap L^\infty(0,T; W^{1,3}(\Omega)), \end{aligned}$$

and let $(\phi_{h,\tau}, \bar{\mu}_{h,\tau})$ be a solution to Problem 5.1.2 with initial value $\phi_{0,h}(0) = \pi_h^1 \phi_0 \in \mathcal{V}_h$, where $\pi_h^1 : H^1 \to \mathcal{V}_h$ denotes the H^1-elliptic projection. Then

$$\max_{t^n \in \mathcal{I}_\tau} \|\phi_{h,\tau}(t^n) - \phi(t^n)\|_1^2 + \|\bar{\mu}_{h,\tau} - \bar{\mu}\|_{L^2(0,T;H^1)}^2 \leq C_T'(h^4 + \tau^4),$$

with C_T' depending on the norms of the solution (ϕ, μ), but independent of h and τ. If $\tau \sim h$, then the discrete solution $(\phi_{h,\tau}, \bar{\mu}_{h,\tau})$ is unique.

We refer to [**19**] for the proof. In short terms, the authors investigated the stability of solutions to the Cahn-Hilliard equation. By relative energy estimates, they derived bounds for the discretisation error and established order-optimal a-priori error estimates of the previous approximation scheme, summarised in the theorem. The uniqueness of the solution follows from a Gronwall argument using inverse inequalities and the convergence rate estimates. For further insights, we again refer to [**19**].

From Theorem 5.1.3, we can deduce that if the more regular solution (ϕ, μ) exists, the initial value is set as described, and $\tau \sim h$, then the estimates also imply the existence of an interval I, such that $\phi_{h,\tau}(x,t) \in I$ until at least some time T.

Discretisation of the solution operator $S(\cdot)$

Let us start by summarising the assumptions used to define the solution operator $S(\cdot)$.

Assumptions 5.1.4. We impose the following assumptions on the parameter functions and the discretisation parameters:

(S1) let Assumptions 5.1.1 hold,

(S2) let $\mathcal{T}_h$ be a uniform triangulation of the domain Ω,

(S3) let a more regular weak solution (ϕ, μ) of (5.1)–(5.2) exist, with regularity as described in Theorem 5.1.3,

(S4) let $\tau \sim h$,

(S5) let the interval I be large enough, such that it holds $\phi_{h,\tau}(x,t) \in I$ for solutions of Problem 5.1.2.

Recall that the solution operator was defined as a mapping

$$S : \mathcal{D}(S) \subset (H^2(I))^2 \to (L^2(0,T;L^2(\Omega)))^2.$$

By the discrete scheme for the Cahn-Hilliard equation, we have already chosen the discrete subset $\mathbb{Y}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$ for the space $(L^2(0,T;L^2(\Omega)))^2$. We proceed to consider as discrete space for the parameter function space $(H^2(I))^2$ the space of natural cubic splines on a uniform grid of the interval $I := [a_1, a_2]$ with a grid size σ, denoted by $\mathbb{X}_\sigma$. The discrete solution operator is subsequently defined by

$$S_{\sigma,h,\tau} : \mathcal{D}(S_{\sigma,h,\tau}) \subset \mathbb{X}_\sigma \to \mathbb{Y}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T), \quad (b_\sigma, f_\sigma) \mapsto (\phi_{h,\tau}, \bar{\mu}_{h,\tau}),$$

where $(\phi_{h,\tau}, \bar{\mu}_{h,\tau})$ is the solution to the discrete forward problem, i.e. Problem 5.1.2, with (b_σ, f_σ) employed for (b, f). The operator is defined on the domain

$$\mathcal{D}(S_{\sigma,h,\tau}) := \{(b_\sigma, f_\sigma) \in \mathbb{X}_\sigma : \text{Assumptions 5.1.1 hold}\}.$$

From our considerations, we can now readily deduce the following lemma.

Lemma 5.1.5. *Let Assumptions 5.1.4 hold. Then the solution operator $S_{\sigma,h,\tau}(\cdot)$ is well-posed.*

Note that the condition $\tau \sim h$ guarantees the uniqueness of the solution $\phi_{h,\tau}$ and is necessary for the well-posedness of the operator.

Implementation of the solution operator $S(\cdot)$

Remark 5.1.6 (On the resulting time-stepping scheme)**.** As $\phi_{h,\tau}$ is piecewise linear in time, it is determined by the values ϕ_h^{n-1} and ϕ_h^n. Hence, by considering ϕ_h^{n-1} and ϕ_h^n in

Problem 5.1.2, one derives an implicit scheme of for the variables $(\phi_h^n, \mu_h^{n-1/2})$ by computing the integrals over the interval $[t^{n-1}, t^n]$. In practice, by using a quadrature rule $(\varepsilon_j, \omega_j), 0 \leq j \leq J$ with sufficiently high accuracy, the integrals can be approximated, e.g.

$$\int_{t^{n-1}}^{t^n} f_\sigma(\phi_{h,\tau})\bar{w}_{h,\tau}\, ds \approx \tau \sum_{j=0}^{J} \omega_j f_\sigma(\phi_{h,\tau}(t_j^n))\bar{w}_{h,\tau},$$

where $t_j^n = t^{n-1} + \varepsilon_j(t^n - t^{n-1})$ denotes intermediate time points. By utilising suitable quadrature rules, we can achieve exact integration, such that, for instance, the energy dissipation identity remains valid and mass is conserved, both up to machine precision; as discussed in [**14, 36**]. Overall, the resulting system is nonlinear, and we use Newton's method to compute the solution. The time average involving the mobility $b(\cdot)$ can be substituted by a midpoint approximation, which still yields second-order convergence of the scheme, see [**19**]. However, we emphasise that the exact integration of the term involving $f_\sigma(\phi_{h,\tau})$ remains necessary to ensure exact conservation of the energy-dissipation identity.

Remark 5.1.7 (Implementation time averaged integrals)**.** Let us comment in more detail on the implementation, especially regarding the time-averaged integral. Let v_j denote the j-th basis function of $\mathcal{V}_h$, then as usual the discrete representation of $(g(x)v_h, w_h)$ is a matrix $\mathtt{M}$ with entries

$$\mathtt{M}_{i,j} = (g(x)v_j, v_i) = \int_\Omega g(x)v_jv_i\, dx = \sum_{K\in\mathcal{T}_h} \int_K g(x)v_jv_i\, dx.$$

Therein, the integrals over the single elements are calculated via quadrature formulas, e.g. $(\omega_{m,K}, x_{m,K}), m = 1, \ldots, M$, such that

$$\sum_{K\in\mathcal{T}_h} \int_K g(x)v_jv_i\, dx \approx \sum_{K\in\mathcal{T}_h} \sum_{m=1}^{M} \omega_{m,K} g(x_{m,K})v_j(x_{m,K})v_{i,K}(x_{m,K}) = \mathtt{I}_i^\top \mathtt{D} \mathtt{I}_j,$$

where $\mathtt{I}_j$ is a column vector containing the evaluations of the basis function v_j at all the quadrature points $x_{m,K}$, and $\mathtt{D}$ is a diagonal matrix where the entries are the evaluation of the function $g(x)$ at each quadrature point $x_{m,K}$ multiplied with the corresponding weight $\omega_{m,K}$ of the quadrature formula. Hence we observe that we can decompose the matrix assembling into $\mathtt{M} = \mathtt{I}^\top\mathtt{D}\mathtt{I}$, where $\mathtt{I}$ is a matrix with columns $\mathtt{I}_j$, i.e. one column for every degree of freedom, where the entries are the evaluations of the basis functions on the quadrature points. This decomposition should be understood as a pre-assembling simplifying the handling of the integrals in time. As already pointed out, the exact calculation of the time integrals is necessary for the structure-preserving scheme, and is achieved using suitable quadrature rules $(\omega_j, t_j), j = 0, \ldots, J$. Using the previous decomposition of the assembling in space, the time integrals can be computed as follows:

$$\int_{t^1}^{t^2} (g(s)v_h, w_h)\, ds \approx \int_{t^1}^{t^2} \mathtt{w}^\top\mathtt{I}^\top\mathtt{D}(g(s))\mathtt{I}\mathtt{v}\, ds \approx \mathtt{w}^\top\mathtt{I}^\top \left(\sum_{j=0}^{J} \omega_j \mathtt{D}(g(t_j))\right) \mathtt{I}\mathtt{v}.$$

Besides the pre-assembling aspect to safe computational cost, it is a practical form in order to derive a full Newton scheme for our time-stepping problems. Analogue to this, we use pre-assembling steps to compute stiffness matrices. In addition, if $v_{h,\tau}$ is piecewise linear in time, as in the Petrov-Galerkin scheme, one has to consider some additional factors $s, (1-s)$ which can be considered as additional factors in the diagonal matrix $\mathtt{D}$.

5.2. Discretisation of Tikhonov regularisation

We will now consider the discretisation of the Tikhonov regularisation approach. At first, we discretise the forward operator $F(\cdot)$ and then the Tikhonov minimisation problem (5.3).

Discretisation of the forward operator $F(\cdot)$

Recall that the forward operator was defined as

$$F : \mathcal{D}(F) \subset (H^2(I))^2 \to L^2(0,T; L^2(\Omega)),$$

and has the special structure $F(\cdot) = L(S(\cdot))$. The discrete forward operator is subsequently defined as the mapping $F_{\sigma,h,\tau}(\cdot) = L_h(S_{\sigma,h,\tau}(\cdot))$, where $L_h(\cdot)$ denotes the linear operator

$$L_h : \mathbb{Y}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T) \to \mathbb{Y}_{h,\tau}(0,T), \quad (v_{h,\tau}, \bar{w}_{h,\tau}) \mapsto v_{h,\tau}.$$

This leads to the definition of the discrete forward operator

$$F_{\sigma,h,\tau} : \mathcal{D}(F_{\sigma,h,\tau}) \subset \mathbb{X}_\sigma \to \mathbb{Y}_{h,\tau}(0,T), \quad (b_\sigma, f_\sigma) \mapsto \phi_{h,\tau},$$

where $\phi_{h,\tau}$ is the solution to the discrete forward problem, i.e. Problem 5.1.2, with (b_σ, f_σ) employed for (b, f). The operator is defined on the domain

$$\mathcal{D}(F_{\sigma,h,\tau}) := \{(b_\sigma, f_\sigma) \in \mathbb{X}_\sigma : \text{Assumptions 5.1.1 hold } \}.$$

As $L_h(\cdot)$ is a linear operator and $S_{\sigma,h,\tau}(\cdot)$ is well-defined by Lemma 5.1.5, we can directly deduce that $F_{\sigma,h,\tau}(\cdot)$ is well-posed.

Lemma 5.2.1. *Let Assumptions 5.1.4 hold. Then, the discretised forward operator $F_{\sigma,h,\tau}(\cdot)$ is well-posed.*

In the following, we will use the shorthand notation $F_h(\cdot)$ to refer to $F_{\sigma,h,\tau}(\cdot)$.

Discretisation of Tikhonov problem

We are now in the position to establish the discrete Tikhonov problem to achieve the computation of stable approximations of the parameter functions. First, we assume that the measurements $\phi^\delta_{h,\tau}$ satisfy

$$\|\phi_{h,\tau} - \phi^\delta_{h,\tau}\|_{Y_{h,\tau}} \leq \delta$$

with known noise level $\delta > 0$. Then we consider the minimisation problem

$$\min_{(b_\sigma, f_\sigma)\in\mathcal{D}(F_h)} J^\delta_{\alpha,h}(x) := \frac{1}{2}\|F_h(b_\sigma, f_\sigma) - \phi^\delta_{h,\tau}\|^2_{Y_{h,\tau}} + \frac{\alpha}{2}\|(b_\sigma, f_\sigma) - (b^*_\sigma, f^*_\sigma)\|^2_{\mathbb{X}_\sigma}, \tag{5.6}$$

where $\alpha > 0$ is the regularisation parameter and (b^*_σ, f^*_σ) are initial guesses of the parameters functions. The existence of discrete solutions follows from standard arguments of nonlinear optimisation theory.

Lemma 5.2.2. *Let assumptions 5.1.4 hold. Then the discretised version* (5.6) *of Tikhonov regularisation has a solution.*

Projected Gauss-Newton iteration

Following the derivation of the iterative scheme in Section 4.2, we use the following iteration to derive the update of the parameters $x^n_\sigma = (b^n_\sigma, f^n_\sigma)$:

$$\begin{aligned}(F'_h(x^n_\sigma)^* F'_h(x^n_\sigma) + \alpha I)\Delta x^n_\sigma &= F'_h(x^n_\sigma)^*(\phi^\delta_{h,\tau} - F_h(x^n_\sigma)) - \alpha x^n_\sigma\\ x^{n+1}_\sigma &= P_{\mathcal{D}(F_h)}(x^n_\sigma + \omega\Delta x^n_\sigma),\end{aligned}$$

where $0 < \omega \le 1$, and $P_{\mathcal{D}(F_h)}$ denotes the projection to $\mathcal{D}(F_h)$ in order to incorporate the constraints of the parameter functions. The iteration is then stopped by the discrepancy principle, i.e. we stop when $\|F_{\sigma,h,\tau}(b_\sigma, f_\sigma) - \phi^\delta\|_{Y_{h,\tau}} \le \tau\delta$ is satisfied, with $\tau = 1.1$. A preconditioned conjugate gradient algorithm is used to solve the resulting linear system.

For the realisation of the iteration, we once again require to establish the derivative $F'_h(b_\sigma, f_\sigma)$ and a representation of the adjoint operator $F'_h(b_\sigma, f_\sigma)^*$.

Discrete linearised problem and derivative of $F'(b, f)$

The discretisation for the Cahn-Hilliard equation, i.e. Problem 5.1.2, leads, by differentiation, readily to the corresponding discrete linearised problem. Hence, we examine the following discrete approximation of the equations (4.25)–(4.26) to derive $S'_h(b, f)$, and from $F_h(\cdot) = L_h(S_h(\cdot))$ we then deduce the existence of $F'_h(b, f)$.

Problem 5.2.3. *Let $(\phi_{h,\tau}, \bar\mu_{h,\tau}) \in \mathbb{Y}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$ be the solution of the discrete forward problem for parameter functions $(b_\sigma, f_\sigma) \in \mathcal{D}(F_h) \subset \mathbb{X}_\sigma$, and let $(\hat b_\sigma, \hat f_\sigma) \in \mathbb{X}_\sigma$. Find $(\psi_{h,\tau}, \bar\xi_{h,\tau}) \in \mathbb{Y}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$, with $\psi_{h,\tau}(x,0) = 0$ and such that*

$$\begin{aligned}\int_{t^{n-1}}^{t^n} &(\partial_t\psi_{h,\tau}, \bar v_{h,\tau}) + (b'_\sigma(\phi_{h,\tau})\psi_{h,\tau}\nabla\bar\mu_{h,\tau}, \nabla\bar v_{h,\tau}) + (b_\sigma(\phi_{h,\tau})\nabla\bar\xi_{h,\tau}, \nabla\bar v_{h,\tau})\\ &+ (\hat b_\sigma(\phi_{h,\tau})\nabla\bar\mu_{h,\tau}, \nabla\bar v_{h,\tau})\, ds = 0,\end{aligned} \tag{5.7}$$

$$\int_{t^{n-1}}^{t^n} (\bar\xi_{h,\tau}, \bar w_{h,\tau}) - (\gamma\nabla\psi_{h,\tau}, \nabla\bar w_{h,\tau}) - (f'_\sigma(\phi_{h,\tau})\psi_{h,\tau}, \bar w_{h,\tau}) - (\hat f_\sigma(\phi_{h,\tau}), \bar w_{h,\tau})\, ds = 0, \tag{5.8}$$

for all test functions $(\bar v_{h,\tau}, \bar w_{h,\tau}) \in \mathbb{Q}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$ and for $n \ge 1$.

This is a linear problem with respect to the variables $(\psi_{h,\tau}, \bar\xi_{h,\tau})$, and as a result, the existence of solutions can be established by standard arguments.

Lemma 5.2.4. *Let Assumptions 5.1.4 hold. Then, for any $(\hat{b}_\sigma, \hat{f}_\sigma) \in X_\sigma$ Problem 5.2.3 has a unique solution.*

Proof. In order to show the existence of solutions, we use an induction argument. Let $\psi_{h,\tau}(t_{n-1})$ be given and consider the n-th timestep, i.e. we need to determine the function $\psi^n_{h,\tau} := \psi_{h,\tau}(t_n)$ and $\xi^{n-1/2}_{h,\tau} := \xi_{h,\tau}(t_n - \tau/2) \in \mathcal{V}_h$. We can now repeat the testing procedure from the proof of Theorem 4.3.1 on the discrete level, i.e. we test with $(\bar{v}_{h,\tau}, \bar{w}_{h,\tau}) = (\bar{\xi}_{h,\tau}, \partial_t \psi_{h,\tau})$ and derive a-priori-bounds of solutions with constants depending on the bounds in Assumptions 5.1.1, and the norms of $(\hat{b}, \hat{f})$ and $\psi_{h,\tau}(t_{n-1})$. As this is a linear system, it is sufficient to show, that a vanishing right-hand side implies that the solution is zero. Hence, by the previous a-priori bounds, we conclude the existence of a unique solution.

□

We conclude that the discrete derivative of the discrete solution operator $S_h(\cdot)$ is defined as $S'_h(b_\sigma, f_\sigma)(\hat{b}_\sigma, \hat{f}_\sigma) := (\psi_{h,\tau}, \bar{\xi}_{h,\tau})$. Consequently, by the chain rule, the discrete derivative of $F_h(\cdot)$ is defined as

$$F'_h(b_\sigma, f_\sigma) : \mathbb{X}_\sigma \to \mathbb{Y}_{h,\tau}(0,T), \quad (\hat{b}_\sigma, \hat{f}_\sigma) \mapsto \psi_{h,\tau},$$

where $\psi_{h,\tau}$ is the first component of the solution obtained from Problem 5.2.3 using $(\hat{b}_\sigma, \hat{f}_\sigma)$.

Lemma 5.2.5. *Let Assumptions 5.1.4 hold. Then the derivative of $F_h(\cdot)$ is defined by $F'_h(b_\sigma, f_\sigma)(\hat{b}_\sigma, \hat{f}_\sigma) = \psi_{h,\tau}$.*

Remark 5.2.6. On the continuous level, we showed in the proof of Theorem 4.3.2 quadratic convergence of the residuals. We verified in our numerical experiments that our discretisation approach preserves this convergence.

Discrete adjoint problem

Let us now derive the discrete version of the adjoint state equations (4.39)–(4.40). The systematic way to derive the adjoint problem involves again the Lagrangian function. By following the derivation analogue to the continuous level, we obtain the discretisation scheme of the adjoint state problem. Consequently, we consider the following fully discrete approximation for the equations (4.39)–(4.40).

Problem 5.2.7. *Let $(\phi_{h,\tau}, \bar{\mu}_{h,\tau}) \in \mathbb{Y}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$ be the solution of the discrete forward problem for parameter functions $(b_\sigma, f_\sigma) \in \mathcal{D}(F_h)$, and let $r^\delta_{h,\tau} \in \mathbb{Y}_{h,\tau}(0,T)$. Find $(\bar{p}_{h,\tau}, \bar{q}_{h,\tau}) \in \mathbb{Q}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$, with $\bar{p}_{h,\tau}(x,0) = 0$ and such that*

$$\begin{aligned}\int_{t^{n-1}}^{t^n} (\bar{p}_{h,\tau}, \partial_t v_{h,\tau}) + (b'_\sigma(\phi_{h,\tau}) \nabla \bar{\mu}_{h,\tau} \nabla \bar{p}_{h,\tau}, v_{h,\tau}) - (\gamma \nabla \bar{q}_{h,\tau}, \nabla v_{h,\tau}) \\ -(f'_\sigma(\phi_{h,\tau}) \bar{q}_{h,\tau}, v_{h,\tau}) + (r^\delta_{h,\tau}, v_{h,\tau})\, ds = 0\end{aligned} \tag{5.9}$$

$$\int_{t^{n-1}}^{t^n} (\bar{q}_{h,\tau}, \bar{w}_{h,\tau}) + (b_\sigma(\phi_{h,\tau}) \nabla \bar{p}_{h,\tau}, \nabla \bar{w}_{h,\tau})\, ds = 0, \tag{5.10}$$

for all test functions $(v_{h,\tau}, \bar{w}_{h,\tau}) \in \mathbb{Y}_{h,\tau}(0,T) \times \mathbb{Q}_{h,\tau}(0,T)$ and for $n \geq 1$.

Remark 5.2.8. While this formulation serves as a convenient formulation for deriving the discrete adjoint formula for $F_h'(b_\sigma, f_\sigma)^*$, it is not directly recognised as a discretisation of equations (4.39)–(4.40). Hence, let us provide a brief explanation of this scheme. The variables p and q are discretised as piecewise constants in time. The first equation (5.9) is then tested with piecewise linear elements, while the second one (5.10) is tested with piecewise constant functions. In order to derive a standard time-stepping scheme, one utilises for the time direction a basis of the space of piecewise linear functions in time. By collecting the integrals (5.9)–(5.10) for all time steps, rearranging terms, and noting that the time derivative of the test functions is constant on each interval, one derives a formulation with the following structure

$$\frac{1}{\tau}(p^{n+1/2} - p^{n-1/2}, \bar{w}_{h,\tau}) + \int_{t^n}^{t^{n+1}} (g_1 \nabla p^{n+1/2}, \bar{w}_{h,\tau})\, ds + \int_{t^{n-1}}^{t^n} (g_2 \nabla p^{n-1/2}, \bar{w}_{h,\tau})\, ds + \dots$$

where g_1, g_2 are some functions depending on space and time.

Note that this is a linear problem in p and q. By reformulating the Problem 5.2.7 into a time-stepping scheme, the existence of solutions can be established using similar arguments as for the discrete linearised problem.

Lemma 5.2.9. *Let Assumptions 5.1.4 hold. Then for any $r^\delta_{h,\tau} \in \mathbb{Y}_{h,\tau}(0,T)$, the Problem 5.2.7 has a unique solution.*

Discrete representation of the adjoint $F'(b,f)^*$

Due to the chosen discretisation, one can derive the formula for the discrete adjoint operator $F_h'(b_\sigma, f_\sigma)^*$ following the same arguments as on the continuous level in Section 4.4.2. As a result, we arrive at the following discrete representation.

Lemma 5.2.10. *Let Assumptions 5.1.4 hold, and $r^\delta_{h,\tau} \in \mathbb{Y}_{h,\tau}(0,T)$. Further, let $(b_\sigma, f_\sigma) \in \mathcal{D}(F_h)$ be parameter functions with associated discrete solution $(\phi_{h,\tau}, \bar{\mu}_{h,\tau})$ of the Cahn-Hilliard system. Then there exist $(\bar{p}_{h,\tau}, \bar{q}_{h,\tau})$ as the solution to the discrete adjoint problem (5.9)–(5.10), which depends on $(\phi_{h,\tau}, \bar{\mu}_{h,\tau})$, (b_σ, f_σ) and $r^\delta_{h,\tau}$. The result of an application of the discrete adjoint operator, i.e. the outcome $g_\sigma := (g_{\sigma,1}, g_{\sigma,2}) := F_h'(b_\sigma, f_\sigma)^* r^\delta_{h,\tau}$, is then defined as the solution of the following variational problem:*

$$(g_\sigma, (\hat{b}_\sigma, \hat{f}_\sigma))_{\mathbb{X}_\sigma} = (\hat{b}_\sigma(\phi_{h,\tau}) \nabla \bar{\mu}_{h,\tau}, \nabla \bar{p}_{h,\tau})_{\mathbb{Y}_{h,\tau}} - (\hat{f}_\sigma(\phi_{h,\tau}), \bar{q}_{h,\tau})_{\mathbb{Y}_{h,\tau}}$$

for all $(\hat{b}_\sigma, \hat{f}_\sigma) \in \mathbb{X}_\sigma$.

Remark 5.2.11 (Separate identification)**.** The previous schemes cover the simultaneous identification of the parameters $b(\cdot)$ and $f(\cdot)$. The schemes for the separate identification of the parameters follow from a straightforward reduction of the previous analysis. This leads to minor modifications of the previous schemes. In the linearised Problem 5.2.3, the direction of the derivative of the known parameter vanishes, i.e. $\hat{b}(\cdot)$ or $\hat{f}(\cdot)$. The adjoint Problem 5.2.7 does not change, but the adjoint formula in Problem 5.2.10. In the separate case, we seek only one function g_σ, while on the right-hand side, the term corresponding to the known parameter vanishes.

5.3. Numerical illustration

For the equation error method, we had to impose strong conditions on the measurements of ϕ. In comparison, the output least squares method can handle less regular data and a larger noise level, which we will demonstrate in this section. For comparison, we will use a similar setup for the numerical tests as for the equation error method in Section 3.4.4. The domain for our test problems is chosen as $\Omega = (0,1)^d$, where $d = 1, 2$ depends on the experiment.

5.3.1. One dimensional test problem

As the initial experiment, we use the model parameters described in Subsection 3.4.1. Hence, we select the parameter functions

$$f(s) = 2(s + 0.99)^3(s - 0.99)(3s - 0.99),$$

where f is the derivative of the double well potential $\lambda(s) = (s - 0.99)^2(s + 0.99)^4$, and consider the mobility function

$$b(s) = (1 - s)^4(1 + s)^2 + 0.2,$$

while we set $\gamma = 0.003$ for the interface parameter. The initial value of the phase fraction is prescribed by

$$\phi_0(x) = 0.1\sin(2\pi x) - 0.1\sin(4\pi x) + 0.1\sin(12\pi x) + 0.1.$$

Up to modifications, we note again that these functions satisfy the Assumptions 5.1.1, see also Subsection 3.4.1. As discretisation parameters of the finite element spaces, we select $\sigma = 0.1$ for the parameter functions, and for the Cahn-Hilliard system, we choose for the spatial discretisation $h = 0.01$ and the time step size $\tau = 4 \cdot 10^{-5}$. The final time is set to $T = 0.004$. The artificial measurements for our test are generated by an application of the forward operator, using $f_\sigma(\cdot)$ and $b_\sigma(\cdot)$ as prescribed, computing $\phi_{h,\tau}$, which is then perturbed by white noise with magnitude $\delta := \|\phi_{h,\tau} - \phi^\delta_{h,\tau}\|_{L^2(0,T;L^2(\Omega))}$. The precise noise level is specified below.

Remark 5.3.1. The grid of the reconstruction corresponds to the configuration in Subsection 3.4.4. However, therein, we simulated the data on the distinct grid and subsequently used interpolated measurements for the reconstruction. Thus, a direct comparison of the two methods is not feasible already because of the assumption on the data perturbation, but we will qualitatively comment on it.

We perform numerical tests for each of the three identification problems. For the iterative scheme, we choose as initial values of the parameters $b(\cdot)$ and $f(\cdot)$, depending on the identification problem,

$$b_0(s) \equiv 1, \qquad f_0(s) = 4s(s^2 - 0.99^2),$$

where the later is the derivative of a symmetric potential $\lambda_0(s) = (s - 0.99)^2(s + 0.99)^2$. Further we set $b^*(\cdot) \equiv f^*(\cdot) \equiv 0$. The results of the reconstructions are depicted below.

Remark 5.3.2 (Identifiability)**.** In Subsection 3.4.4, we depicted the solution to infer information regarding the intervals where the parameter functions can be identified. Again, this information will be used to determine the intervals where identification is feasible and is depicted as a grey background in our figures. Beyond the intervals where unique identification is ensured, the regularisation term determines the solution.

Identification of $f(\cdot)$

We assume that γ and the mobility function $b(\cdot)$ are known, defined as prescribed, and consider the identification of $f(\cdot)$. As outlined in Lemma 2.3.1, and already discussed in Section 3.4, only the derivative $f'(\cdot)$ can be identified. Moreover, the function $f'(\cdot)$ can only be uniquely determined within the range $R = \{s = \phi(x,t) : x \in \Omega, t \in [0, 004]\}$. In Figure 5.1, we depict the true value of $f'(\cdot)$ and the corresponding reconstruction $(f_\alpha^\delta)'(\cdot)$, derived from our computations. The Tikhonov regularisation approach yields stable and

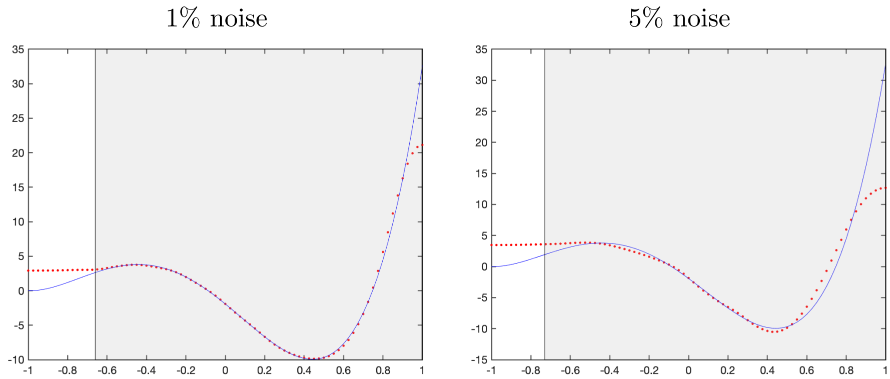

Figure 5.1.: Reconstructions of $f'(\cdot)$ using perturbed data $\phi_{h,\tau}^\delta(\cdot,t)$ where $t \in [0, 0.004]$. The noise level δ is specified in the title of the plots. The range of the observations $\phi_{h,\tau}^\delta$ is depicted in grey. The solid blue line depicts the true function $f'(\cdot)$, while the dotted red line illustrates the reconstruction $(f_\alpha^\delta)'(\cdot)$ obtained by the output least squares method outlined in Subsection 5.2. The regularisation parameter α was determined using the discrepancy principle, with $\tau = 1.1$.

accurate reconstructions for both noise levels. As expected from Theorem 2.4.1, the function $f'(\cdot)$ is reliably reconstructed only on the range R. The regularisation enforces stability but also a certain bias in the regions where less data is available.

Identification of $b(\cdot)$

We assume that γ and the potential derivative $f(\cdot)$ are known and consider the identification of the mobility $b(\cdot)$. As shown in Theorem 2.4.5, the mobility $b(\cdot)$ can only be identified on the range $\tilde{R}_t = \{s = \phi(x,t) : x \in \Omega,\ \partial_x \mu(x,t) \neq 0\}$ of the attained data, where the gradient of the chemical potential μ is non-zero. In Figure 5.2, we depict the reconstructed functions $b_\alpha^\delta(\cdot)$ derived from the perturbed data $\phi_{h,\tau}^\delta$ by the output least

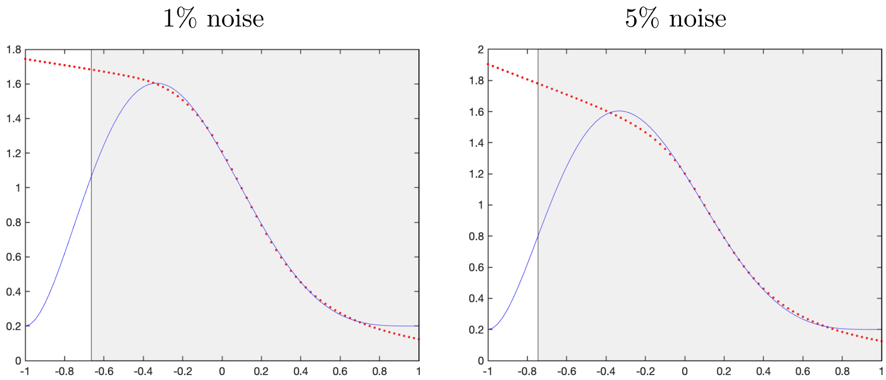

Figure 5.2.: Reconstructions of the mobility function $b(\cdot)$ derived from perturbed data $\phi^\delta_{h,\tau}(\cdot, t)$ with $t \in [0, 0.004]$. The noise level δ is specified in the title of the plots. The range of the observations $\phi^\delta_{h,\tau}$ is once more depicted in grey. The solid blue line depicts the true parameter, while the dotted red line represents the reconstructions $b^\delta_\alpha(\cdot)$. The regularisation parameter α was chosen by the discrepancy principle, with $\tau = 1.1$.

squares method. Once more, the reconstructed mobility aligns well with the true parameter $b(\cdot)$ on the range of attained data, while the reconstructions outside this range are stable but biased by the regularisation term in the Tikhonov functional.

Identification of $f(\cdot)$ and $b(\cdot)$

Here, we only assume that the interface parameter γ is known and consider the identification of both parameter functions. According to Theorem 2.4.7, the simultaneous identification of both parameters $b(\cdot)$ and $f(\cdot)$ requires observations at multiple time steps, which is naturally satisfied by the Tikhonov regularisation approach. Moreover, the observability condition stated in Theorem 2.4.7 has to be valid. For our numerical test, we verified the required linear independence. In Figure 5.3, we depict reconstructions $b^\delta_\alpha(\cdot)$ and $(f^\delta_\alpha)'(\cdot)$ obtained from observations $\phi^\delta_{h,\tau}$, acquired under two distinct noise levels.

As expected, the parameter functions are reliably and accurately determined on the range of available data. While the separate identification maintains stability and accuracy even at higher noise levels, the simultaneous identification exhibits a comparatively reduced accuracy.

5.3.2. Two dimensional test problem

We use the same setup as in Subsection 3.4.5 for our model problem in dimension $d = 2$. Hence, we consider as computational domain the unit square Ω. We select, similar to the experiment in one dimension, the following parameter functions

$$f(s) = 0.3(2(s + 0.99)^3(s - 0.99)(3s - 0.99)), \qquad b(s) = (1 - s)^4(1 + s)^2 + 0.1,$$

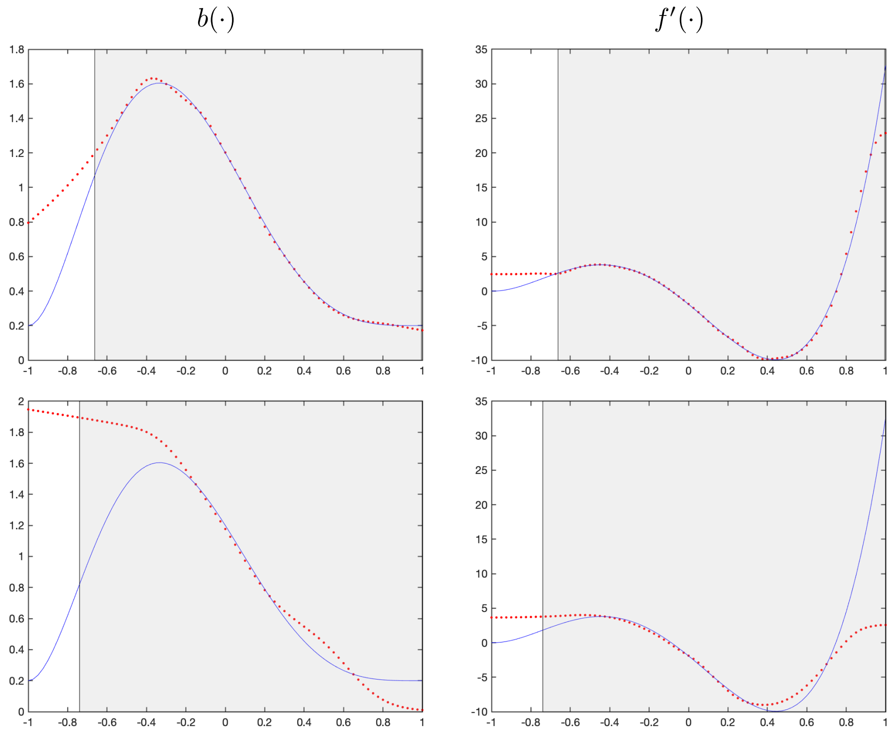

Figure 5.3.: Simultaneous reconstructions of $b(\cdot)$ and $f'(\cdot)$ from perturbed data $\phi^\delta_{h,\tau}(\cdot, t)$ with $t \in [0, 0.004]$. Here, the noise level δ is 1% in the top row and 5% in the bottom row. The range of the attained data is again depicted in grey. The solid blue line depicts the true parameter functions, while the corresponding reconstructions $b^\delta_\alpha(\cdot)$ and $(f^\delta_\alpha(\cdot))'$ are denoted by dotted red lines. The regularisation parameter was determined using the discrepancy principle, with $\tau = 1.1$.

where f is the derivative of the double well potential $\lambda(s) = 0.3(s-0.99)^2(s+0.99)^4$, and we set $\gamma = 0.003$ for the interface parameter. Once again, note that Assumptions 5.1.1 are satisfied up to modifications. As the initial distribution of the phase fraction, we choose

$$\phi_0(x,y) = -0.1\cos(4\pi x)\sin(2\pi y) + 0.05\sin(2\pi x)\sin(4\pi y).$$

The discretisation parameters of the finite element spaces are chosen as $\sigma = 0.1$ for the parameter functions, and, for the Cahn-Hilliard equation (5.1)–(5.2), we choose for the triangulation in space $h = 1/32$ and as time step size $\tau = 4 \cdot 10^{-3}$. The final time is set to $T = 0.08$, which amounts to the computation of 20 time steps. The artificial measurements for our tests are generated as follows: We apply the forward operator using the parameter functions $f(\cdot)$ and $b(\cdot)$ as prescribed to compute $\phi_{h,\tau}$, which is then perturbed by white noise with magnitude $\delta := \|\phi_{h,\tau} - \phi^\delta_{h,\tau}\|_{L^2(0,T;L^2(\Omega))}$. The precise noise level is specified in the tests.

Again, we compute reconstructions for each of the three identification problems. For the iterative solution procedure, we choose as initial values of the parameters $b(\cdot)$ and

$f(\cdot)$, depending on the identification problem, the functions

$$b_0(s) \equiv 1, \qquad f_0(s) = 0.8s(s^2 - 0.99^2)$$

where the later is the derivative of a symmetric potential $\lambda_0(s) = 0.2(s-0.99)^2(s+0.99)^2$. Further we set $b^*(\cdot) \equiv f^*(\cdot) \equiv 0$. The results of the reconstructions are depicted below.

Remark 5.3.3 (Identifiability)**.** In Subsection 3.4.4, we depicted the evolution of the phase fraction and the energy to infer information regarding the intervals where the parameter functions can be identified. From this, the identifiability conditions can be verified. These areas are depicted as grey backgrounds in our figures. Beyond the intervals where unique identification is ensured, the regularisation term determines the solution.

The obtained approximations for the identification of either $f'(\cdot)$ of $b(\cdot)$ are depicted in Figures 5.4 and 5.5, respectively. We observe that the reconstructions again are in good agreement with the true parameter functions on the range of attained data. Outside of this interval, the regularisation leads to a certain bias, as expected.

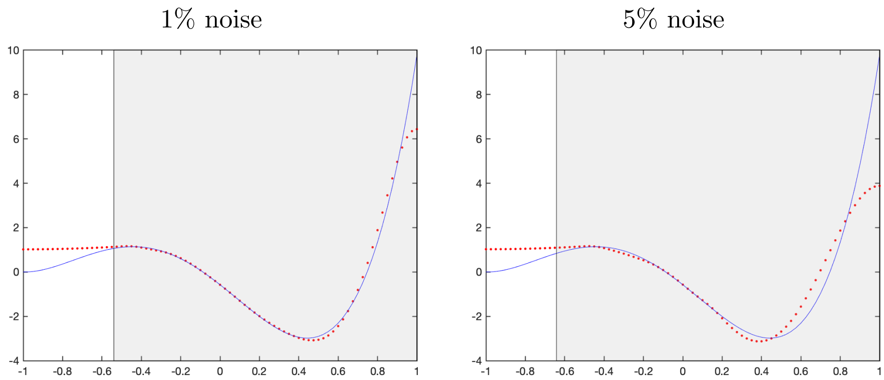

Figure 5.4.: Reconstructions of $f'(\cdot)$ using perturbed data $\phi^\delta_{h,\tau}(\cdot,t)$ where $t \in [0, 0.08]$. The noise level δ is specified in the title of the plots. The range of the observations $\phi^\delta_{h,\tau}$ is depicted in grey. The solid blue line depicts the true function $f'(\cdot)$, while the dotted red line illustrates the reconstruction $(f^\delta_\alpha)'(\cdot)$ obtained by the output least squares method outlined in Subsection 5.2. The regularisation parameter α was determined using the discrepancy principle, with $\tau = 1.1$.

In Figure 5.6, we depict the result of the simultaneous identification of both parameter functions.

5.3.3. Comparison to the equation error method

As previously stated, a direct comparison between the two methods is unfeasible. However, we computed the interpolation error of the data utilised in the equation error method, subsequently deriving the noise level. This approach allows a qualitative comparison of the two methods. In doing so, we derived a noise level of approximately 0.1%. By employing this noise level for the output least squares method, the resulting reconstructions are almost indistinguishable from the true parameter functions and surpass the results

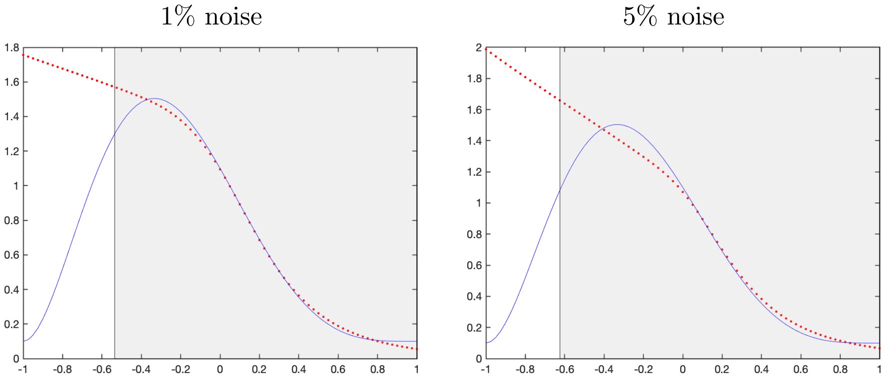

Figure 5.5.: Reconstructions of the mobility function $b(\cdot)$ derived from perturbed data $\phi^{\delta}_{h,\tau}(\cdot, t)$ with $t \in [0, 0.08]$. The noise level δ is specified in the title of the plots. The range of the observations $\phi^{\delta}_{h,\tau}$ is once more depicted in grey. The solid blue line depicts the true parameter, while the dotted red line represents the reconstructions $b^{\delta}_{\alpha}(\cdot)$. The regularisation parameter α was chosen by the discrepancy principle, with $\tau = 1.1$.

from the equation error method. On the other hand, the equation error method has fewer computation costs and thus is a cheap-to-apply method if sufficiently regular data is available.

Furthermore, the equation error method does not yield qualitatively good reconstructions for higher noise levels. This is expected, considering that the interpolation of the data does not effectively prevent noise amplification, mainly due to the calculation of the higher derivatives used in the equation error method. Although this behaviour can be mitigated to a certain extent through presmoothing of the data, this becomes unfeasible at some point.

Let us note that the nonlinear method is a more versatile approach, and it is more transparent how to extend the method to more complex models. In contrast, the extension of the equation error method might be more involved as the approach was fine-tuned to the Cahn-Hilliard equation in a certain sense.

5.3.4. Final remarks

Let us provide some final remarks on additional numerical tests we conducted.

Remark 5.3.4 (Degenerate parameter functions)**.** In our numerical examples, we considered non-degenerate polynomial parameter functions which satisfy Assumptions 5.1.1. Moreover, as indicated in Remark 2.2.3, it is also possible to consider e.g. logarithmic potentials by regularising the degenerate regions, which are expected not to be attained by the data. Further numerical tests show that our approach yields reconstructions comparable to the examples we have presented.

Remark 5.3.5 (Convergence rates)**.** By assuming that suitable source conditions are valid, see e.g. the assumptions of Theorem A.1.3, the best rates we can expect for

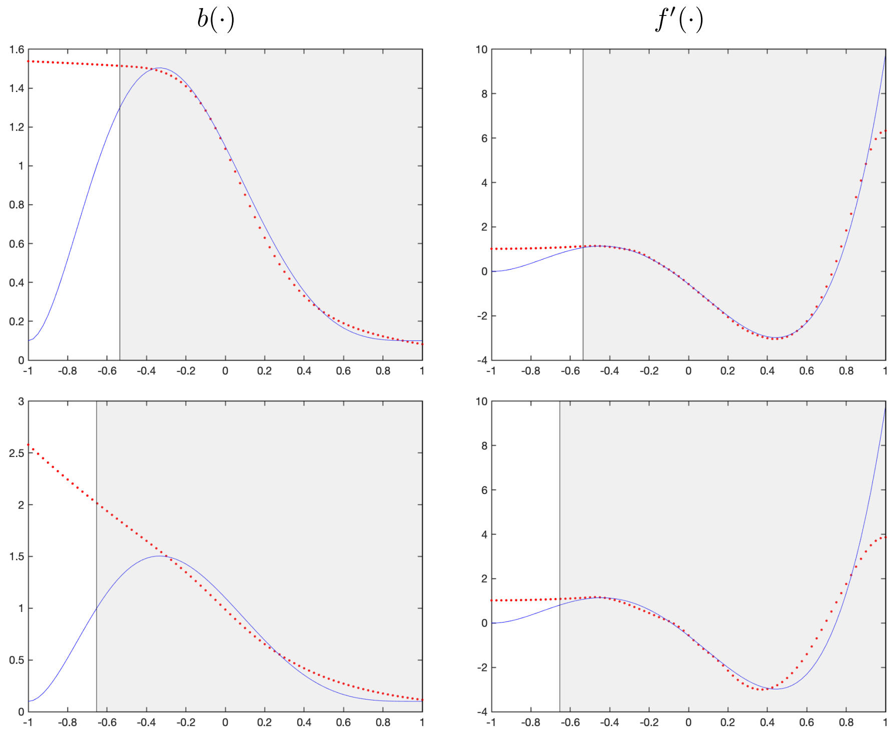

Figure 5.6.: Simultaneous reconstructions of $b(\cdot)$ and $f'(\cdot)$ from perturbed data $\phi^{\delta}_{h,\tau}(\cdot,t)$ with $t \in [0, 0.08]$. Here, the noise level δ is 1% in the top row and 5% in the bottom row. The range of the attained data is again depicted in grey. The solid blue line depicts the true parameter functions, while the corresponding reconstructions $b^{\delta}_{\alpha}(\cdot)$ and $(f^{\delta}_{\alpha})'(\cdot)$ are denoted by dotted red lines. The regularisation parameter was determined using the discrepancy principle, with $\tau = 1.1$.

Tikhonov regularisation are

$$\|x^{\delta}_{\alpha} - x^{\dagger}\|_{H^2(I)} = O(\sqrt{\delta}) \quad \text{and} \quad \|F(x^{\delta}_{\alpha}) - \phi^{\delta}\|_{L^2(0,T;L^2(\Omega))} = O(\delta).$$

We attained these rates in a numerical test using the set-up of the experiment in one dimension at the beginning of this Section 5.3. A detailed investigation of the source conditions is open and is a possible direction for future research.

Remark 5.3.6 (Tests in three dimensions)**.** We previously noted that our analysis does not include dimension $d = 3$. As the existence of solutions of the Cahn-Hilliard equation only holds up to a small time T, the analysis of the inverse problems is also restricted to a small time frame. However, in practice, one expects the identification method also to yield good reconstructions beyond T if we have measurements in three dimensions. Indeed, we did some tests and can confirm that the output least squares method also yields reconstructions in three dimensions, which are comparable to the results in two dimensions.

Conclusion

In this chapter, we have studied the realisation of the output least squares method to identify the parameter functions $f(\cdot)$ and $b(\cdot)$. We discussed a suitable discretisation of the approach by a Petrov-Galerkin framework and presented numerical results demonstrating the feasibility of the method. Compared to the equation error method, the output least squares approach yields reconstructions for less regular data and higher noise levels. This comes with increased computational costs.

Let us mention some directions for possible future research. We have already indicated that it is possible to obtain convergence rates; hence, one might investigate the source conditions. Moreover, we used fully distributed measurements for our presentation, but one might consider other data. Another direction is to use the presented framework above and apply it to more complex models, for example [**1**], [**20**], [**21**], [**29**] or [**62**] and references therein. In the next chapter, we apply the output least squares method to two more complex models to support this claim.

6. Extensions to more complex models

In the previous chapters, we discussed in detail the parameter identification problem in the Cahn-Hilliard equation from measurements of distributed phase fraction data. Future research might also consider extensions of those approaches to more realistic models which incorporate more parameters to identify or include more physical variables.

We will now present preliminary results of applying the output least squares approach to two extended models, i.e. a Cahn-Hilliard model incorporating a matrix-valued mobility function in Section 6.1 and a Cahn-Hilliard-Allen-Cahn phase-field model incorporating a generalised mobility in Section 6.2. Therein, we will consider the identification of the mobility and will assume that the other parameter functions are known. As we aim to illustrate the feasibility of the method from Chapter 4 and 5, we will present numerical results without proofs. Instead, we will refer to the literature and suggest future research directions.

6.1. Cahn-Hilliard with matrix-valued mobility

We consider the following modified Cahn-Hilliard model

$$\partial_t \phi = \operatorname{div}\left(\mathbf{B}\nabla\mu\right), \tag{6.1}$$

$$\mu = -\gamma\Delta\phi + f(\phi), \tag{6.2}$$

where the mobility $\mathbf{B}$ is now a matrix with values in $\mathbb{R}^{d\times d}$ and may depend on the phase fraction ϕ and its gradient $\nabla\phi$. For our illustration of the applicability of the output least squares approach, we only consider the dependence on $\nabla\phi$. The system is complemented with periodic boundary conditions and an initial distribution ϕ_0. We choose the following assumptions for the parameter functions of the modified Cahn-Hilliard model.

Assumptions 6.1.1. We impose the following assumptions on the model parameters:

(A1) $\gamma > 0$ is a positive constant;

(A3) $f(s) = \lambda'(s)$ with $\lambda \in C^4(\mathbb{R})$ such that $\lambda(s), \lambda''(s) \geq -c_{\lambda_1}$, for some $c_{\lambda_1} \geq 0$. Furthermore, λ and its derivatives are bounded by $|\lambda^{(k)}(s)| \leq C^{(k)}_{\lambda_2} + C^{(k)}_{\lambda_3}|s|^{4-k}$ for $0 \leq k \leq 4$ with constants $C^{(k)}_{\lambda_2}, C^{(k)}_{\lambda_3} \geq 0$.

(A4) for any $\nabla\phi$, the matrix $\mathbf{B} : \nabla\phi \to \mathbf{B}(\nabla\phi) \in \mathbb{R}^{d\times d}$ is symmetric and positive definite with

$$\lambda_1|\xi|^2 \leq \xi^\top \mathbf{B}(\nabla\phi)\xi \leq \lambda_2|\xi|^2, \quad \forall \xi \in \mathbb{R}^d.$$

Moreover, every component $b_{ij}(\cdot)$ of $\mathbf{B}(\cdot)$ is a function in $C^2(\mathbb{R})$ of its arguments, with derivatives which are uniformly bounded by some constants, i.e. $\|b'_{ij}\|_\infty \leq C_{b'}$, $\|b''_{ij}\|_\infty \leq C_{b''}$.

The existence of solutions can then be derived using standard techniques analogue to Lemma 2.2.1, compare also to [**20**].

The inverse problem

We consider the parameter-to-measurement operator

$$F : \mathcal{D}(F) \subset X \to Y, \quad \mathbf{B} \mapsto \phi,$$

where ϕ is first component of the solution to the problem (6.1)–(6.2). In this section, the inverse problem under consideration is the following: given spatially measurements ϕ^δ find a mobility $\mathbf{B}$ such that

$$F(\mathbf{B}) = \phi^\delta.$$

This is a non-linear parameter identification problem between Hilbert spaces X and Y, which we define now. By $X = H^2(\Omega_{\mathbf{B}})^{d\times d}$ we denote the space of $d \times d$ matrices with entries from the Hilbert space $H^2(\Omega_{\mathbf{B}})$, where $\Omega_{\mathbf{B}}$ is a two dimensional domain, such that $\nabla\phi(x,t) \in \Omega_{\mathbf{B}}$. On this space, we consider the inner product

$$(\mathbf{B}(\cdot), \tilde{\mathbf{B}}(\cdot))_X := \sum_{i,j=1}^{d} (b_{ij}(\cdot), \tilde{b}_{i,j}(\cdot))_{H^2},$$

and the corresponding norm

$$\|\mathbf{B}(\cdot)\|_X^2 = \sum_{i,j=1}^{d} \|b_{ij}(\cdot)\|_{H^2}^2.$$

For the image space, we choose $Y = L^2(0,T; L^2(\Omega))$. Hence, we define the domain of the forward operator as follows:

$$\mathcal{D}(F) := \{\mathbf{B} \in X : \text{ Assumptions 6.1.1 hold}\}.$$

Remark 6.1.2 (Identifiability)**.** In principle, our identifiability results from Section 2.4.2 can be generalised to the extended model, with some additional assumptions on the set $\tilde{R}_t$. The question on the identifiability of a matrix diffusion coefficient has been addressed in a recent publication [**79**], which goes back to ideas of [**94**]. These works are a good starting point to formulate an identifiability result for the extended model (6.1)–(6.2).

Tikhonov regularisation

We assume that the measurements ϕ^δ satisfy the following condition

$$\|\phi - \phi^\delta\|_{L^2(L^2)} \le \delta,$$

with known noise level $\delta > 0$. As in Chapter 4, we consider the Tikhonov regularisation approach. Consequently, we will obtain stable approximations to the true parameter function $\mathbf{B}^\dagger$, which fulfils $F(\mathbf{B}^\dagger) = \phi$, by minimising the Tikhonov functional

$$\min_{\mathbf{B}\in\mathcal{D}(F)} J_\alpha^\delta(\mathbf{B}) := \frac{1}{2}\|F(\mathbf{B}) - \phi^\delta\|_{L^2(L^2)}^2 + \frac{\alpha}{2}\|\mathbf{B} - \mathbf{B}^*\|_{H^2}^2 \ ,$$

where $\alpha > 0$ is a regularisation parameter and $\mathbf{B}^*$ is an initial guess of the parameter functions. At this point, we now would have to discuss the properties of the forward operator $F(\cdot)$ to ensure the existence of a minimiser, which we leave out. To solve the minimisation problem, we employ the Gauss-Newton iteration from the previous chapters, i.e.

$$\begin{aligned}(F'(\mathbf{B}^k)^* F'(\mathbf{B}^k) + \alpha I)\Delta\mathbf{B}^k &= F'(\mathbf{B}^k)^*(y^\delta - F(\mathbf{B}^k)) - \alpha(\mathbf{B}^k - \mathbf{B}^*),\\ \mathbf{B}^{k+1} &= \mathbf{B}^k + \omega\Delta\mathbf{B}^k,\end{aligned}$$

where $0 < \omega < 1$. Note, we did not include a projection back to $\mathcal{D}(F)$ here. We comment on this again in the following. For the implementation of the iteration, we state the linearised problem of the system (6.1)–(6.2), which is used to define the derivative $F'(\mathbf{B})$, and an adjoint problem, which leads to a representation of $F'(\mathbf{B})^*$. Both are derived analogue to the derivation in Section 4.3 and 4.4, and we do not discuss proofs.

Linearised problem and derivative of $F(\cdot)$

Let Assumptions 6.1.1 hold, and consider a fixed matrix $\mathbf{B}(\cdot) \in \mathcal{D}(F)$ with corresponding solution (ϕ, μ). Moreover, we assume for a matrix function $\hat{\mathbf{B}} \in X$ that $\mathbf{B} + \hat{\mathbf{B}}$ remains in $\mathcal{D}(F)$, hence also satisfying Assumptions 6.1.1. In this setting, the linearised problem of the extended Cahn-Hilliard model (6.1)–(6.2) for the variables (ψ, ξ) reads as follows

$$\begin{aligned}\partial_t\psi - \operatorname{div}(\partial\mathbf{B}(\nabla\phi)\nabla\psi\nabla\mu) - \operatorname{div}(\mathbf{B}(\nabla\phi)\nabla\xi) &= \operatorname{div}(\hat{\mathbf{B}}(\nabla\phi)\nabla\mu) && \text{in } \Omega\times(0,T), && (6.3)\\ \xi + \gamma\Delta\psi - f'(\phi)\psi &= 0 && \text{in } \Omega\times(0,T), && (6.4)\end{aligned}$$

with initial condition $\psi(0, x) = 0$ and complemented with periodic boundary conditions. Here, by $\partial\mathbf{B}$ we denote the component-wise total derivative of $\mathbf{B}$, i.e.

$$(\partial\mathbf{B})_{ij} := \sum_{n=1}^{d} \frac{\partial\mathbf{B}_{ij}}{\partial x_n}.$$

Subsequently, we define the derivative of $F(\cdot)$ as follows

$$F'(\mathbf{B}) : H^2(\Omega_{\mathbf{B}})^{d\times d} \to L^2(0, T; L^2(\Omega)), \quad \hat{\mathbf{B}} \mapsto \psi,$$

where ψ is the first component of the solution to the linearised problem.

Remark 6.1.3 (Convergence rate of the remainder)**.** In the proof of Fréchet differentiability in Section 4.3, we derived quadratic convergence of the residual $\bar{\phi} = \phi_2 - \phi_1 - \psi$. For the extended model, we analogously performed a numerical test also yielding the quadratic convergence of the residual.

Adjoint problem

Let Assumptions 6.1.1 hold, and let $\mathbf{B} \in \mathcal{D}(F)$ be a fixed matrix with corresponding solution (ϕ, μ) of the extended model (6.1)–(6.2). Then one derives in the same way as in Section 4.4, i.e. using the Lagrangian function, the following problem for the adjoint states (p, q):

$$-\partial_t p + \operatorname{div}(\partial \mathbf{B}(\nabla\phi)\nabla\mu\nabla p) + \gamma \operatorname{div}(\nabla q) - f'(\phi)q = -(\phi - \phi^\delta) \quad \text{in } \Omega \times (0,T), \tag{6.5}$$
$$q - \operatorname{div}(\mathbf{B}(\nabla\phi)\nabla p) = 0 \quad \text{in } \Omega \times (0,T), \tag{6.6}$$

with $p(T, x) = 0$ in Ω, periodic boundary conditions and data $\phi^\delta \in L^2(0,T; L^2(\Omega))$.

Representation of the Adjoint operator $F'(\mathbf{B})^*$

The representation of the adjoint operator $F'(\mathbf{B})^*$ is derived as in Theorem 4.4.2. Let Assumptions 6.1.1 hold, and $\phi^\delta \in L^2(0,T; L^2(\Omega))$. Further, let $\mathbf{B}(\cdot)$ be an admissible matrix with associated solution (ϕ, μ) of the extended Cahn-Hilliard equation, and let (p, q) be the solution to the adjoint problem (6.5)–(6.6), which depends on (ϕ, μ), $\mathbf{B}(\cdot)$ and ϕ^δ. Then, one formally defines the adjoint operator via

$$(F'(\mathbf{B})^* r, \hat{\mathbf{B}})_X := (r, F'(\mathbf{B})(\hat{\mathbf{B}}))_Y = (r, \psi)_Y,$$

for all $r \in Y$ and $\hat{\mathbf{B}} \in X$. Analogue to the derivation in Section 4.4, one deduces that the result of an application of the adjoint operator, i.e. the outcome of $\mathbf{G} := F'(\mathbf{B})^* r \in X$, is then defined as the solution of the variational problem:

$$(\mathbf{G}, \hat{\mathbf{B}})_X = (\hat{\mathbf{B}}(\nabla\phi)\nabla\mu, \nabla p)_{L^2(L^2)}$$

for all $\hat{\mathbf{B}} \in X$.

Numerical results

For the discretisation of the previous schemes, we proceed in the same way as described in Section 5.1, i.e. utilising the Petrov-Galerkin approach, with obvious modifications due to the new mobility matrix. We omit the details and continue with a numerical example of the output least squares approach.

The domain of our test problem is chosen as $\Omega = (0,1)^2$, we set $\gamma = 0.003$ for the interface parameter and select

$$f(s) = 0.2(2(s + 0.99)^3(s - 0.99)(3s - 0.99)),$$

which is the derivative of the double-well potential $\lambda(s) = 0.2(s - 0.99)^2(s + 0.99)^2$. For the mobility matrix, we select

$$\mathbf{B}(x, y) = \mathbf{I} + \frac{0.2}{10 + x^2 + y^2}\begin{pmatrix} x^2 & xy \\ xy & y^2 \end{pmatrix}$$

where $\mathbf{I}$ denotes the identity matrix. As the initial distribution of the phase fraction, we choose

$$\phi_0(x, y) = 0.05\cos(4\pi x)\sin(2\pi y) + 0.1.$$

Together, these functions satisfy Assumptions 6.1.1. As discretisation parameters of the finite element spaces, we choose for the extended Cahn-Hilliard model (6.1)–(6.2) the

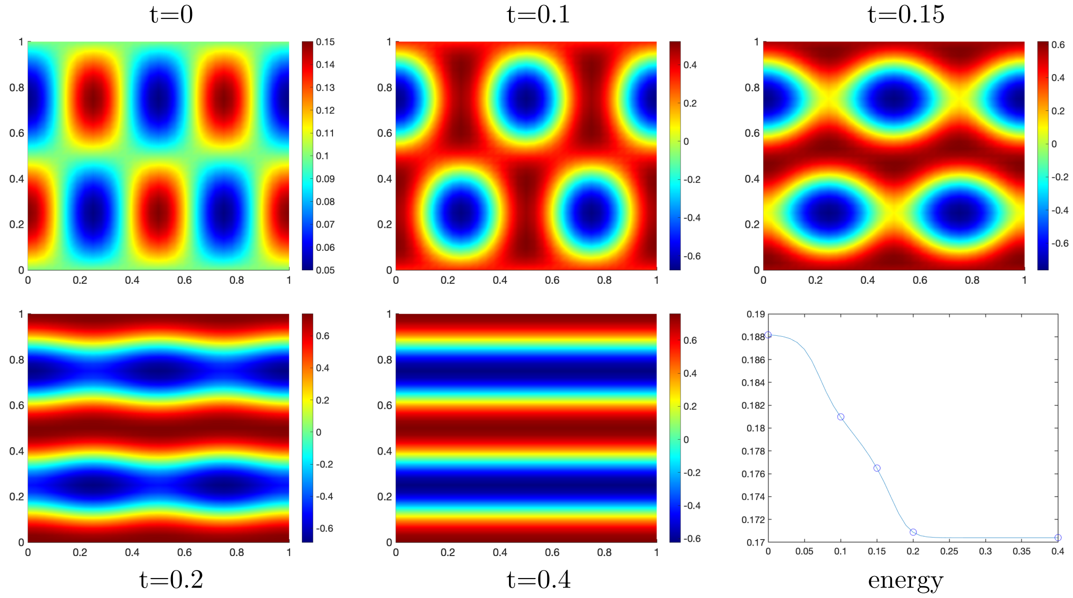

Figure 6.1.: Snapshots of the phase fraction $\phi_{h,\tau}$ for time points t specified in the title of the plots. The evolution of the energy $\mathcal{E}(\phi) = \int_\Omega \frac{\gamma}{2}|\nabla\phi|^2 + \lambda(\phi)\,dx$ is depicted with additional markers which correspond to the time points of the snapshots.

spacial discretisation $h = 1/32$ and as time step size $\tau = 1 \cdot 10^{-2}$. The final time is set to $T = 0.4$, which amounts to 40 time steps. The evolution of the phase fraction $\phi_{h,\tau}$ is depicted in Figure 6.1.

Let us now turn to the inverse problem. The components of the mobility matrix are discretised by the tensor product of one-dimensional cubic splines with natural boundary conditions, and we choose $X_\sigma = H^2([a,b]^2)^{2\times 2}$ with discretisation parameter $\sigma = 1$, while the interval is chosen as $a = -10, b = 10$. The choice of a, b stems from the range of $\nabla\phi$. Note that the matrix is said to be symmetric. Thus, only three discrete parameter functions are needed in practice.

The artificial measurements for our test are generated as follows: We apply the forward operator using the parameter $\mathbf{B}(\cdot)$ as prescribed to compute $\phi_{h,\tau}$, which is then perturbed by white noise with magnitude $\delta := \|\phi_{h,\tau} - \phi^\delta_{h,\tau}\|_{L^2(L^2)}$. For the noise level, we choose 1%.

For our iterative solution procedure, we choose as the initial values of the mobility matrix $\mathbf{B}(\cdot)$ the identity, i.e. $\mathbf{B}_0 = \mathbf{I}$. Further, we set $\mathbf{B}^* = \mathbf{I}$, as we used no measures to impose the positive definiteness of the mobility matrix. Once more, we apply the discrepancy principle to determine the regularisation parameter α. The resulting reconstructions of the parameter functions in $\mathbf{B}(\cdot)$ are depicted in Figure 6.2.

The Tikhonov regularisation approach yields stable and accurate reconstructions in regions where data is available. A closer look at the data ϕ reveals that the range of the derivative $\partial_y\phi$ is much larger than the range of the derivative $\partial_x\phi$, see Figure 6.1. This is (on purpose) a consequence of the chosen example. Considering the reconstructions in Figure 6.2, we observe that the function $(\mathbf{B}^\delta_\alpha)_{22}$ agrees well with the true parameter function, while the function $(\mathbf{B}^\delta_\alpha)_{11}$ is reconstructed on a smaller region. This reflects our observation that more data is available in the y-direction. We conclude that the

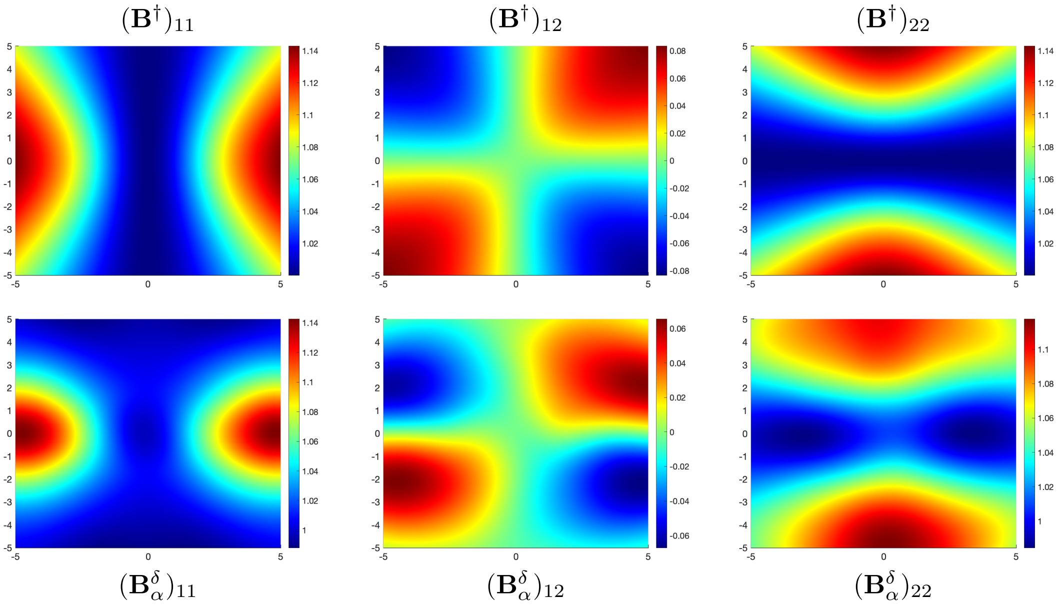

Figure 6.2.: Reconstructions of $\mathbf{B}(\cdot)$ using perturbed data $\phi^\delta_{h,\tau}$. The noise level δ is set to 1%. The reconstructions are depicted on the range of the observations $\nabla\phi$. The upper row depicts the true parameter functions, while the corresponding reconstructions are shown in the lower row. The regularisation parameter α was determined by the discrepancy principle, with $\tau = 1.1$.

reconstructions agree well in regions where much data is available. In regions with no available data, the regularisation and the chosen $\mathbf{B}^*$ determine the reconstructions. This demonstrates the applicability of the method to the extended Cahn-Hilliard model (6.1)–(6.2), but also highlights that observability conditions are now more involved.

Remark 6.1.4 (Challenges of future research)**.** For the rigorous analysis of the parameter identification problem in the extended Cahn-Hilliard model (6.1)–(6.1), there are two main differences or challenges compared to the standard Cahn-Hilliard System (1.1)–(1.2). First, the mobility is now matrix-valued and may depend on the gradient of the phase-fraction. Using the techniques in the recent works [**20, 17**] should lead to the existence of solutions, i.e. the forward operator, and should further lead to continuity results. Second, the dependence on the gradients leads to a $\nabla\phi$ term in the linearised problem. In principle, the previous proof strategy in Section 4.3 should also apply here, but a careful investigation has to be done.

6.2. Cahn-Hilliard/Allen-Cahn system with cross-kinetic coupling

In this section, we apply the Tikhonov regularisation approach of Chapter 4 to a coupled system of Cahn-Hilliard and Allen-Cahn equations with a strong coupling through gradient-dependent mobility matrices. We consider the following coupled system [**20, 17**]:

$$\partial_t\rho = \operatorname{div}(\mathbf{L}_{11}\nabla\mu_\rho + \mathbf{L}_{12}\nabla\mu_\eta), \qquad \mu_\rho = -\gamma_\rho\Delta\rho + \lambda_\rho(\rho,\eta), \tag{6.7}$$

$$\partial_t\eta = -\mathbf{L}_{12}\cdot\nabla\mu_\rho - \mathbf{L}_{22}\mu_\eta, \qquad \mu_\eta = -\gamma_\eta\Delta\eta + \lambda_\eta(\rho,\eta), \tag{6.8}$$

where ρ and η are conserved and non-conserved quantities, γ_ρ, γ_η are the corresponding interface parameters, and $\lambda(\rho,\eta)$ is a free energy density, whose partial derivatives are denoted by $\lambda_\rho(\rho,\eta)$ and $\lambda_\eta(\rho,\eta)$. We complement the system with periodic boundary conditions and initial distributions of ρ and η. Moreover, $\mathbf{L}(\cdot)$ denotes a generalised mobility matrix, which is symmetric, positive definite and depends on the gradient of the phase field ρ. In [**20, 17**], the authors allow the mobility matrix $\mathbf{L}$ to depend on ρ, η and its gradients. However, we do not consider the general case for our demonstration of applicability. For a detailed description and analysis of the model problem, we refer to [**20, 17**]. Let us now formulate the assumptions on the domain and the parameters ensuring the well-posedness of the problem.

Assumptions 6.2.1 ([**17**])**.** We assume

(A0) $\Omega \simeq \mathbb{T}^d$, is the d-dimensional torus; functions defined on Ω are assumed to be periodic.

(A5) the interface parameters γ_ρ and γ_η are positive constants;

(A6) for any $\nabla\rho$, the matrix $\mathbf{L}(\nabla\rho) \in \mathbb{R}^{(d+1)\times(d+1)}$ is symmetric and positive definite with

$$\lambda_1|\xi|^2 \le \xi^\top\mathbf{L}(\nabla\rho)\xi \le \lambda_2|\xi|^2, \quad \forall\xi \in \mathbb{R}^{d+1}.$$

Moreover, every component $b_{i,j}(\cdot)$ of $\mathbf{L}(\cdot)$ is a function in $C^2(\mathbb{R})$ of its argument $\nabla\rho$, with derivatives which are uniformly bounded by some constant λ_3.

(A7) the potential $\lambda(\cdot,\cdot)$ is smooth with $\lambda(\rho,\eta) > 0$ and satisfies

$$\left|\frac{\partial^{k+l}\lambda(\rho,\eta)}{\partial^k\rho\,\partial^l\eta}\right| \le C_1\sum|\rho|^{4-k} + |\eta|^{4-l} + C_2$$

for all $0 \le k, l, k+l \le 4$. Furthermore, the shifted potential

$$\lambda(\rho,\eta) + \frac{\alpha}{2}(|\rho|^2 + |\eta|^2)$$

is strictly convex for some $\alpha > 0$.

In addition, we assume $\rho_0, \eta_0 \in H^1(\Omega)$.

Under these assumptions, the existence and regularity of solutions and their discretisation have been discussed in [**20, 17**].

The inverse problem

We consider the parameter-to-measurement operator

$$F : \mathcal{D}(F) \subset X \to Y, \quad \mathbf{L} \to (\rho, \eta),$$

where (ρ, η) are the first and third components of a solution to the problem (6.7)–(6.8). The inverse problem under consideration in this section is the following: given measurements $(\rho^\delta, \eta^\delta)$ find a generalised mobility $\mathbf{L}(\cdot)$ such that

$$F(\mathbf{L}) = (\rho^\delta, \eta^\delta).$$

Again, this is a non-linear parameter identification problem between Hilbert spaces X and Y, which we define as follows

$$X = (H^2(\Omega_{\mathbf{L}}))^{(d+1)\times(d+1)}, \quad Y = L^2(0, T; L^2(\Omega))^2,$$

where $\Omega_{\mathbf{L}}$ is a two dimensional domain, such that $\nabla\rho \in \Omega_{\mathbf{L}}$. We define the domain of the forward operator as

$$\mathcal{D}(F) := \{\mathbf{L} \in X : \text{Assumptions 6.2.1 hold }\}.$$

Remark 6.2.2 (Identifiability)**.** In Section 2.4.2, we formulated and proved identifiability conditions for the Cahn-Hilliard equation. Those results can adjusted to derive similar identifiability conditions for the Allen-Cahn equation, where now the set $\tilde{R}_t$ depends on the chemical potential instead of its gradient. In Section 6.1, we outlined proof ideas in the case of a matrix-valued mobility. However, the identifiability of the parameters in the coupled Cahn-Hilliard/Allen-Cahn system is an open problem. The previous ideas should be a starting point for further investigations.

Tikhonov regularisation

We assume that the measurements $(\rho^\delta, \eta^\delta)$ satisfy the following condition

$$\|\rho - \rho^\delta\|_{L^2(L^2)} + \|\eta - \eta^\delta\|_{L^2(L^2)} \leq \delta,$$

with known noise level $\delta > 0$. Again, we consider the Tikhonov regularisation approach and will compute stable approximations to the true parameter functions $\mathbf{L}^\dagger(\cdot)$, which fulfils $F(\mathbf{L}^\dagger) = (\rho, \eta)$, by minimising the Tikhonov functional

$$\min_{\mathbf{L}\in\mathcal{D}(F)} J_\alpha^\delta(\mathbf{L}) := \frac{1}{2}\|F(\mathbf{L}) - (\rho^\delta, \eta^\delta)\|^2_{L^2(L^2)} + \frac{\alpha}{2}\|\mathbf{L} - \mathbf{L}^*\|^2_X \ ,$$

where $\alpha > 0$ is a regularisation parameter and $\mathbf{L}^*(\cdot)$ is an initial guess of the parameter functions. Again, at this point, we now would have to discuss the properties of the forward operator $F(\cdot)$ to ensure the existence of a minimiser, which we leave out. For the solution we employ the Gauss-Newton iteration from the previous chapters, i.e

$$\begin{aligned}(F'(\mathbf{L}^k)^* F'(\mathbf{L}^k) + \alpha I)\Delta\mathbf{L}^k &= F'(\mathbf{L}^k)^*(y^\delta - F(\mathbf{L}^k)) - \alpha(\mathbf{L}^k - \mathbf{L}^*),\\ \mathbf{L}^{k+1} &= \mathbf{L}^k + \omega\Delta\mathbf{L}^k,\end{aligned}$$

where $0 < \omega < 1$. Note, we did not include a projection back to $\mathcal{D}(F)$ here. To implement the iterative scheme, we state the linearised problem of (6.7)–(6.8), which is used to define $F'(\mathbf{L})$, and an adjoint problem, which leads to a representation of $F'(\mathbf{L})^*$. Both are derived analogue to the derivation in Section 4.3 and 4.4.

Linearised problem and derivative of $F(\cdot)$

Let Assumptions 6.2.1 hold, and consider a generalised mobility $\mathbf{L}(\cdot) \in \mathcal{D}(F)$ with corresponding solution $(\rho, \mu_\rho, \eta, \mu_\eta)$. Moreover, we assume that for a matrix $\hat{\mathbf{L}} \in X$ that $\mathbf{L} + \hat{\mathbf{L}}$ remains in $\mathcal{D}(F)$, hence also satisfying Assumptions 6.2.1. In this setting, the linearised problem of the coupled Cahn-Hilliard/Allen-Cahn model (6.7)–(6.8) for the variables $(\tilde{\rho}, \tilde{\mu}_\rho, \tilde{\eta}, \tilde{\mu}_\eta)$ reads as follows:

$$
\begin{aligned}
\partial_t \tilde{\rho} - \operatorname{div}(\partial_\rho \mathbf{L}_{11} \nabla \tilde{\rho} \nabla \mu_\rho + \partial_\rho \mathbf{L}_{12} \nabla \tilde{\rho} \mu_\eta + \mathbf{L}_{11} \nabla \tilde{\mu}_\rho + \mathbf{L}_{12} \tilde{\mu}_\eta) &= R_1, && (6.9)\\
\tilde{\mu}_\rho + \gamma_\rho \Delta \tilde{\rho} - \partial_\rho \lambda_\rho \tilde{\rho} - \partial_\eta \lambda_\rho \tilde{\eta} &= 0, && (6.10)\\
\partial_t \tilde{\eta} + \partial_\rho \mathbf{L}_{12} \cdot \nabla \tilde{\rho} \nabla \mu_\rho + \partial_\rho \mathbf{L}_{22} \nabla \tilde{\rho} \mu_\eta + \mathbf{L}_{12} \cdot \nabla \tilde{\mu}_\rho + \mathbf{L}_{22} \tilde{\mu}_\eta &= R_2, && (6.11)\\
\tilde{\mu}_\eta + \gamma_\eta \Delta \tilde{\eta} - \partial_\rho \lambda_\eta \tilde{\rho} - \partial_\eta \lambda_\eta \tilde{\eta} &= 0, && (6.12)
\end{aligned}
$$

in $\Omega \times (0, T)$, where $R_1 = -\operatorname{div}(\hat{\mathbf{L}}_{11} \nabla \mu_\rho + \hat{\mathbf{L}}_{12} \mu_\eta)$ and $R_2 = -(\hat{\mathbf{L}}_{12} \cdot \nabla \mu_\rho + \hat{\mathbf{L}}_{22} \mu_\eta)$, and initial conditions $\rho(0, x), \eta(0, x) = 0$ complemented with periodic boundary conditions. Subsequently, we define the derivative of $F(\cdot)$ as follows

$$
F'(\mathbf{L}) : H^2(\Omega_{\mathbf{B}})^{(d+1)\times(d+1)} \to (L^2(0, T; (\Omega)))^2, \quad \hat{\mathbf{L}} \mapsto (\tilde{\rho}, \tilde{\eta}),
$$

where $(\tilde{\rho}, \tilde{\eta})$ are the first and third components of the solution to the linearised problem.

Remark 6.2.3 (Convergence rate of the remainder)**.** We performed a convergence test of the remainder, which now includes $\bar{\rho} := \rho_2 - \rho_1 - \tilde{\rho}$ and $\bar{\eta} := \eta_2 - \eta_1 - \tilde{\eta}$, and observed quadratic convergence.

Adjoint problem

Let Assumptions 6.2.1 hold, and let $\mathbf{L} \in \mathcal{D}(F)$ be a fixed matrix with corresponding solution $(\rho, \mu_\rho, \eta, \mu_\eta)$ of the Cahn-Hilliard/Allen-Cahn model (6.7)–(6.8). By using the Lagrangian function similar as in Section 4.4, we derive the following problem for the adjoint states (p, q, r, s):

$$
\begin{aligned}
\partial_t p + (\partial_\rho \mathbf{L}_{11} \nabla \mu_\rho + \partial_\rho \mathbf{L}_{12} \mu_\eta) \nabla p + \gamma_\rho \Delta q - \partial_\rho \lambda_\rho q - \partial_\rho \lambda_\eta s &\\
+ (\partial_\rho \mathbf{L}_{12} \cdot \nabla \mu_\rho + \partial_\rho \mathbf{L}_{22} \mu_\eta) r &= -(\rho - \rho^\delta), && (6.13)\\
q - \operatorname{div}(\mathbf{L}_{11} \nabla p + \mathbf{L}_{12} \cdot r) &= 0, && (6.14)\\
-\partial_t r + \gamma_\eta \Delta s - \partial_\eta \lambda_\eta s - \partial_\eta \lambda_\rho q &= -(\eta - \eta^\delta), && (6.15)\\
\mathbf{L}_{22} r + s + \mathbf{L}_{12} \nabla p &= 0, && (6.16)
\end{aligned}
$$

with $p(T, x), r(T, x) = 0$ for $x \in \Omega$, data $\rho^\delta, \eta^\delta \in L^2(0, T; L^2(\Omega))$ and complemented with periodic boundary conditions.

Representation of the adjoint operator $F'(\mathbf{L})^*$

The representation of the adjoint operator $F'(\mathbf{L})^*$ is derived as in Theorem 4.4.2. Let Assumptions 6.2.1 hold, and $\rho^\delta, \eta^\delta \in L^2(0,T;L^2(\Omega))$. Further, let $\mathbf{L}(\cdot)$ be an admissible matrix with associated solutions $(\rho, \mu_\rho, \eta, \mu_\eta)$ of the Cahn-Hilliard/Allen-Cahn model (6.7)–(6.8). Moreover, let (p,q,r,s) be the solution to the adjoint problem (6.13)–(6.16), which depends on the solution $(\rho, \mu_\rho, \eta, \mu_\eta)$, the parameters $\mathbf{L}(\cdot)$ and the data ρ^δ, η^δ. Then, one formally defines the adjoint operator via

$$(F'(\mathbf{L})^* y, \hat{\mathbf{L}})_X := (y, F'(\mathbf{L})(\hat{\mathbf{L}}))_Y = (y, (\tilde{\rho}, \tilde{\eta}))_Y,$$

for $y \in Y$ and $\hat{\mathbf{L}} \in X$. Similar as in Section 4.4, one deduces that the result of an application of the adjoint operator, i.e. the outcome $\mathbf{G} := F'(\mathbf{L})^* y \in X$, is then defined as the solution of the variational problem:

$$\begin{aligned}(\mathbf{G}, \hat{\mathbf{L}})_X =& (\hat{\mathbf{L}}_{11}(\nabla\rho)\nabla\mu_\rho, \nabla p)_{L^2(L^2(\Omega))} + (\hat{\mathbf{L}}_{12}(\nabla\rho)\mu_\eta, \nabla p)_{L^2(L^2(\Omega))} \\ &+ (\hat{\mathbf{L}}_{12}(\nabla\rho)\nabla\mu_\rho, r)_{L^2(L^2(\Omega))} + (\hat{\mathbf{L}}_{22}(\nabla\rho)\mu_\eta, r)_{L^2(L^2(\Omega))}\end{aligned}$$

for all $\hat{\mathbf{L}} \in X = (H^2(\Omega_{\mathbf{L}}))^{(d+1)\times(d+1)}$.

Numerical results

The previous schemes are discretised using the Petrov-Galerkin approach described in Section 5.1; consider also [**17**]. We omit the details and continue with a numerical example.

The following parameter choices resemble the numerical example in [**17**]. We consider the domain $\Omega = (0,1)^2$, set $\gamma_\rho = \gamma_\eta = 0.001$ for the interface parameters and select as potential function

$$\begin{aligned}\lambda(\rho,\eta) = C\rho^2(1-\rho)^2 + D[\rho^2 + 6(1-\rho)(\eta^2 + (1-\eta)^2) - 4(2-\rho)(\eta^3 + (1-\eta)^3) \\ + 3(\eta^2 + (1-\eta)^2)^2],\end{aligned}$$

where $C = 1$ and $D = 0.062$. For the generalised mobility matrix, we choose

$$\mathbf{L}_{11}(x,y) = \mathbf{I} + \frac{1}{10 + x^2 + y^2}\begin{pmatrix} x^2 & xy \\ xy & y^2 \end{pmatrix}, \mathbf{L}_{12}(x,y) = \frac{\sqrt{100}}{\sqrt{10 + x^2 + y^2}}\begin{pmatrix} x \\ y \end{pmatrix}, \mathbf{L}_{22} = 100,$$

where $\mathbf{I}$ denotes the identity matrix. As the initial distribution of the quantities ρ and η, we choose

$$\rho_0(x,y) = 0.5 + 0.45\sin(2\pi x)\sin(2\pi y), \quad \eta_0(x,y) = 0.5 + 0.45\sin(4\pi x)\sin(2\pi y).$$

Together, these functions satisfy Assumptions 6.2.1. As discretisation parameters of the finite element spaces, we choose for the Cahn-Hilliard/Allen-Cahn system (6.7)-(6.8) the spacial discretisation $h = 1/32$ and as time step size $\tau = 1 \cdot 10^{-4}$. The final time is set to $T = 0.06$, which amounts to 600 time steps. The evolution of the quantities $\rho_{h,\tau}$ and $\eta_{h,\tau}$ are depicted in Figures 6.3 and 6.4.

Now, we consider the inverse problem. The components of the generalised mobility matrix are again discretised by the tensor product of one-dimensional cubic splines with

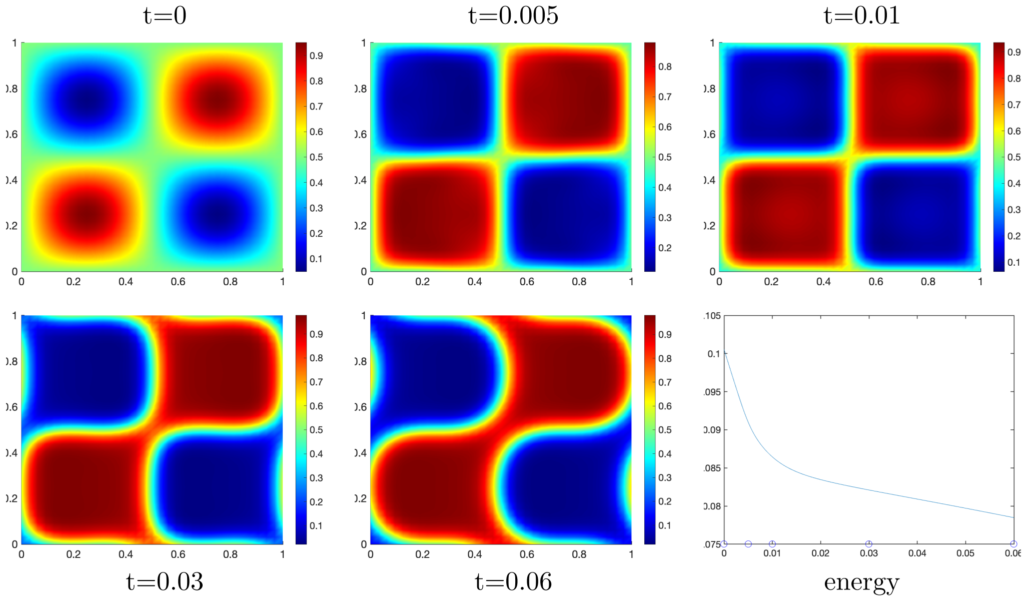

Figure 6.3.: Snapshots of the phase fraction $\rho_{h,\tau}$ for time points t specified in the title of the plots. The evolution of the energy $\mathcal{E}(\rho,\eta) = \int_\Omega \frac{\gamma}{2}|\nabla\rho|^2 + \frac{\gamma}{2}|\nabla\eta|^2 + \lambda(\rho,\eta)\,dx$ is depicted with additional markers on the x-axis which correspond to the time points of the snapshots.

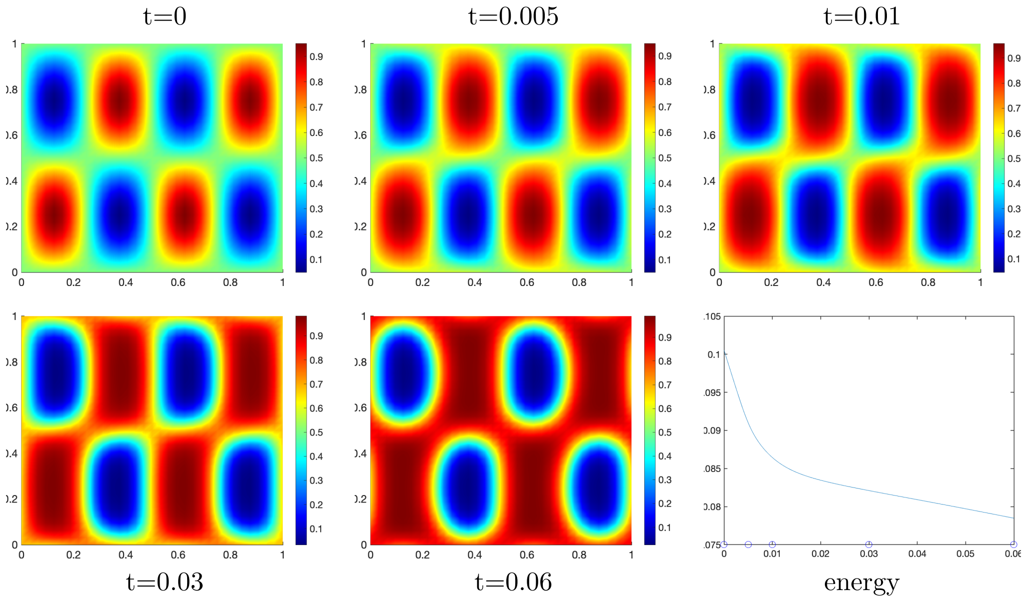

Figure 6.4.: Snapshots of the phase fraction $\eta_{h,\tau}$ for time points t specified in the title of the plots. The evolution of the energy $\mathcal{E}(\rho,\eta) = \int_\Omega \frac{\gamma}{2}|\nabla\rho|^2 + \frac{\gamma}{2}|\nabla\eta|^2 + \lambda(\rho,\eta)\,dx$ is depicted with additional markers on the x-axis which correspond to the time points of the snapshots.

natural boundary conditions. We choose for the parameter space $H^2([a,b]^2)$ the discretisation parameter $\sigma = 0.1$, while $a = -10, b = 10$. The choice of a, b stems from the range of $\nabla\rho$. Note that the matrix $\mathbf{L}(\cdot)$ has to be symmetric. Thus, only six discrete parameter functions are needed in practice. Further, we assume that $\mathbf{L}_{22}(\cdot)$ is just a real number.

The perturbed data for our test are generated as before: We apply the forward operator using the previous parameters to compute $\rho_{h,\tau}$ and $\eta_{h,\tau}$, to which we then add white noise with magnitude $\delta_\phi = \|\rho_{h,\tau} - \rho^\delta_{h,\tau}\|_{L^2(L^2)}$, $\delta_\eta = \|\eta_{h,\tau} - \eta^\delta_{h,\tau}\|_{L^2(L^2)}$. As noise level, we choose 1% for both.

For our iterative solution procedure, we choose as the initial values of the generalised mobility $\mathbf{L}(\cdot)$:

$$\mathbf{L}_{11,0} = \mathbf{I},\ \mathbf{L}_{12,0} = 0,\ \mathbf{L}_{22,0} = 1,$$

and we set

$$\mathbf{L}^*_{11,0} = \mathbf{I},\ \mathbf{L}^*_{12,0} = 0,\ \mathbf{L}^*_{22,0} = 1.$$

We used no further measures to impose the positive definiteness of the matrix. The discrepancy principle is then applied to determine the regularisation parameter α. The resulting reconstruction of $\mathbf{L}_{11}(\cdot)$ is depicted in Figure 6.5, while the result for $\mathbf{L}_{12}(\cdot)$ is shown in Figure 6.6. The real number $\mathbf{L}_{22}$ was determined to $\mathbf{L}^{\alpha,\delta}_{22} = 98.3342$ ($\mathbf{L}^\dagger_{22} = 100$).

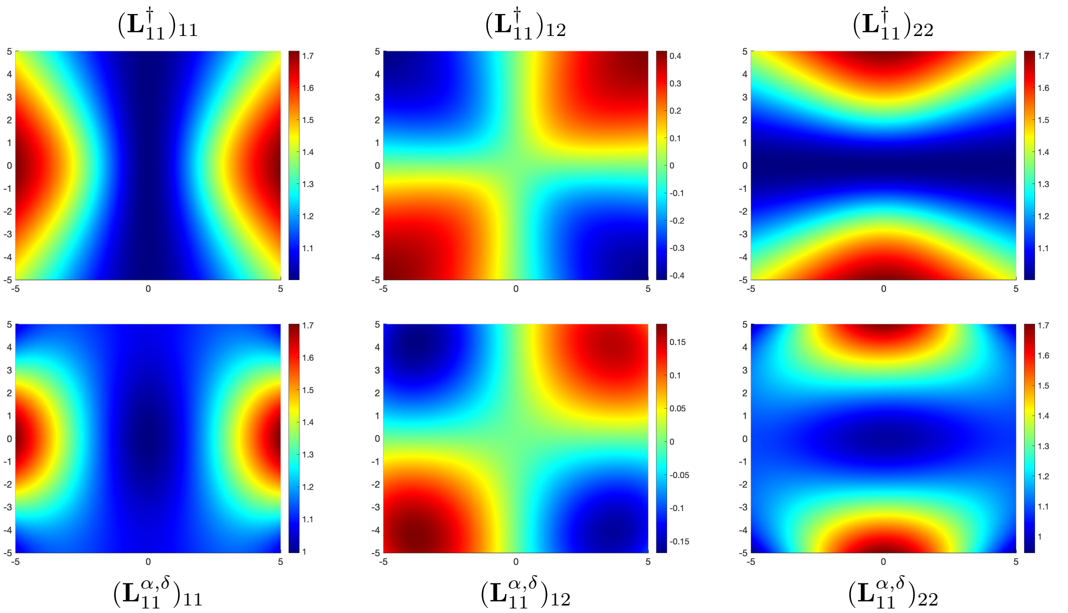

Figure 6.5.: Reconstructions of $\mathbf{L_{11}}(\cdot)$ using perturbed data $\rho^\delta_{h,\tau}, \eta^\delta_{h,\tau}$. The noise level δ is set to 1%. The reconstructions are depicted on the range of $\nabla\rho$. The upper row depicts the true parameter functions, while the corresponding reconstructions are shown in the lower row. The regularisation parameter α was determined by the discrepancy principle, with $\tau = 1.1$.

Also, for this more complex model, we derive stable and accurate reconstructions demonstrating the applicability of the method to the Cahn-Hilliard/Allen-Cahn model (6.7)-(6.8). A closer look at the data ρ reveals that the reconstructions agree well in regions where data is available and are biased by the regularisation and the initial guess where less or no data is available.

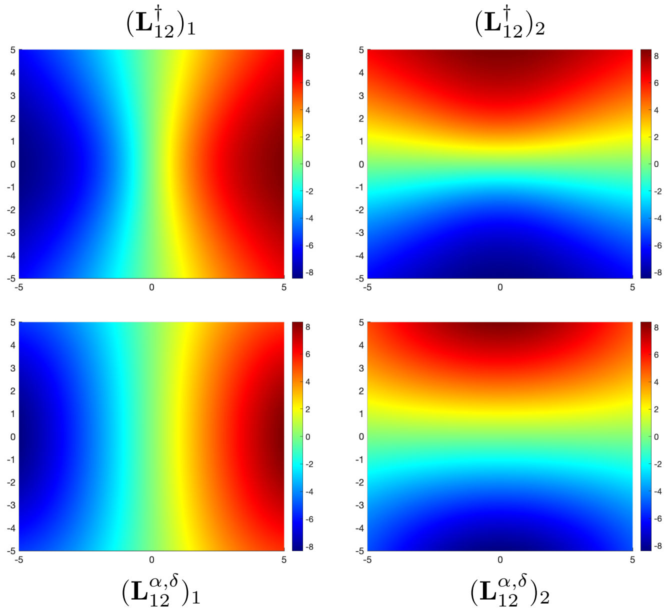

Figure 6.6.: Reconstructions of $\mathbf{L_{12}}(\cdot)$ using perturbed data $\rho_{h,\tau}^{\delta}, \eta_{h,\tau}^{\delta}$. The noise level δ is set to 1%. The reconstructions are depicted on the range of $\nabla\rho$. The upper row depicts the true parameter functions, while the corresponding reconstructions are shown below in the lower row. The regularisation parameter α was determined by the discrepancy principle, with $\tau = 1.1$.

Remark 6.2.4 (Challenges of future research)**.** For the rigorous analysis of the parameter identification problem in the Cahn-Hilliard/Allen-Cahn model (6.7)–(6.8), there are several challenges compared to the standard Cahn-Hilliard System (1.1)–(1.2). Similar to the generalised Cahn-Hilliard model in the previous section, the generalised mobility is now matrix-valued and depends on the gradient of the phase-fraction. Using the techniques in the recent works [**20, 17**], one derives the existence of solutions, and one should further be able to obtain the required continuity results using similar techniques. However, this is now a coupled model and identifiability results in this case are an open problem. Moreover, the dependence on the gradients again leads to a $\nabla\rho$ term in the linearised problem. In principle, the previous proof strategy in Section 4.3 might apply here, but a careful investigation is necessary.

7. Conclusion

In this thesis, we considered the identification of the phase fraction dependent parameter functions in the Cahn-Hilliard equation from the knowledge of distributed phase fraction data. We established identifiability results and derived a linear and a nonlinear approach for the stable reconstruction of the parameter functions. The approaches were investigated analytically, and we demonstrated the numerical realisation. Finally, we considered preliminary results using our approach to identify parameters in more complex models. Let us now summarise our main contributions and some directions for future research.

Identifiability

We established an inherent non-uniqueness of the parameter identification problem in the Cahn-Hilliard equation, which led to the exclusion of the interface parameter γ from our considerations. We then proved that the mobility $b(\cdot)$ and the potential derivative $f(\cdot)$ can be identified uniquely under realistic observability conditions. Further, we derived a conditional identifiability result to uniquely identify both parameters simultaneously.

Equation error method

We employed an equation error approach to solve the parameter identification problems. The insertion of the data into the Cahn-Hilliard equation led to linear operator equations with perturbed operators. As the problem is ill-posed, we applied Tikhonov regularisation to derive stable reconstructions of the parameter functions. Here, we used an abstract result as a theoretical backup and showed that our problems satisfied the prescribed assumptions, establishing the well-posedness of the approach. In the numerical tests, we demonstrated the feasibility of the method and discussed the limitations of this approach due to its dependence on the quality of the available data.

Output least squares

In order to circumvent the problems of the previous method, we also considered an output least squares approach. This led to a nonlinear inverse problem in Hilbert spaces, and we applied Tikhonov regularisation to derive approximations to the solution. We carried out a complete analysis of this approach. Hence, we considered the well-posedness and continuity properties of the forward operator, leading to the existence of a solution to the Tikhonov minimisation problem. A Gauss-Newton-type iteration was suggested to compute the solution to the Tikhonov problem. To facilitate this iteration, we established the differentiability of the forward operator and derived a representation for the adjoint of the derivative. For those results, we defined auxiliary variational problems and showed the existence of solutions via Galerkin approximation and additional energy estimates. The key to those results was the sufficient smoothness of solutions to the Cahn-Hilliard equation. Afterwards, we considered the discretisation of this method using a Petrov-Galerkin approximation. We discussed the discretisation of the forward operator, the Tikhonov problem and the required auxiliary problems. Numerical results were presented, which backed the claim that this method addresses the issues of the previous linear approach.

Outlook

Future research might consider extensions of those approaches to more realistic models incorporating more parameters to identify or include more physical variables. As examples, we considered a matrix-valued mobility in the Cahn-Hilliard system and a Cahn-Hilliard/Allen-Cahn system [**20**], where the coupling of the system is realised through state and gradient-dependent matrices. In principle, our preliminary tests indicate that the output least squares approach could be extended to those models. However, a careful investigation is required due to the new dependency of the mobility matrix, i.e. including gradients. Therefore, a good starting point is to study the Cahn-Hilliard system with mobility matrices incorporating the new dependencies and then examine the coupled model. Especially for the coupled model, identifiability is an open problem, although recent works indicate how to generalise our identifiability results. To conclude, our preliminary analysis and numerical tests of both models suggest that this is a promising direction for continuing the work of this thesis. Other more complex models are the Cahn-Hilliard-Navier-Stokes system [**18**] and a viscoelastic phase-field model [**14, 21**], which have been studied in our research cooperation and the results could be used for the analysis of the nonlinear inverse problem. As a final direction for future research, we would like to mention the analysis of convergence rates, which we did not cover in this thesis.

A. Appendix

A.1. Tikhonov regularisation for nonlinear inverse problems

This section addresses the stable derivation of solutions to ill-posed non-linear inverse problems. For this, we provide a condensed overview of the analysis of such problems on the abstract level, and we recall the established theory following [**45**][Chapter 10].

At the abstract level, we aim to find a solution $x \in X$ that satisfies

$$F(x) = y^\delta \tag{A.1}$$

where $F : \mathcal{D}(F) \subset X \to Y$ is a non-linear operator between two Hilbert spaces X and Y with $\mathcal{D}(F) := \{x \in X : x \text{ admissible } \}$ denoting the domain of the operator $F(\cdot)$, which we assume to be closed and convex. The observations y^δ are considered as perturbed measurements of a true distribution $y^\dagger = F(x^\dagger)$, where $x^\dagger$ denotes the true solution. We assume that the noise level δ is known, i.e.

$$\|y^\dagger - y^\delta\|_Y \leq \delta$$

The problem of finding a solution to (A.1) is typically ill-posed, which requires regularisation techniques. Here, we consider Tikhonov regularisation, the standard approach in connection with output least squares problems, resulting in a standard minimisation problem. Thus, in order to compute stable approximations to the true solution $y^\dagger$, we consider the minimisation of the Tikhonov functional, i.e.

$$\min_{x \in \mathcal{D}(F)} J_\alpha^\delta := \frac{1}{2}\|F(x) - y^\delta\|_Y^2 + \frac{\alpha}{2}\|x - x^*\|_X^2, \tag{A.2}$$

where $\alpha > 0$ is the regularisation parameter and $x^* \in X$ an initial guess. It is important to note that, in general, the minimisers of the non-linear Tikhonov functional are not unique. In the case of multiple solutions, the initial guess x^* acts as a selection criterion, as discussed in [**45, Section 10.1**]. Here, we denote any solution of the minimisation problem (A.2) by $x_\alpha^\delta \in \mathcal{D}(F)$.

Existence and convergence results:

The existence of a solution x_α^δ for any $\alpha > 0$ follows from standard theory, as shown in for instance [**45, 60**].

Theorem A.1.1 ([**45, 60**]). *Let the forward operator $F : \mathcal{D}(F) \subset X \to Y$ be continuous and weakly continuous. Further, assume that the domain $\mathcal{D}(F)$ is weakly closed and non-empty. Then for every $\alpha > 0$, the minimisation problem* (A.2) *has at least one solution x_α^δ.*

Note that if $\mathcal{D}(F)$ is closed and convex, then it is weakly closed. Although the solutions are not unique, it can be shown that the Tikhonov problem (A.2) is stable in the sense of a certain continuous dependence of the solutions on the data y^δ [**45, Theorem 10.2**]. By imposing similar conditions on $\alpha(\delta)$ as in the linear case, the convergence of the solutions of (A.2) toward a solution of (A.1) can be ensured, as stated in the following theorem.

Theorem A.1.2 ([**45, Theorem 10.3**]). *Let $y^\delta \in Y$ with $\|y - y^\delta\|_Y \leq \delta$ and let $\alpha(\delta)$ be such that $\alpha(\delta) \to 0$ and $\delta^2/\alpha(\delta) \to 0$ as $\delta \to 0$. Then every sequence $\{x_{\alpha_k}^{\delta_k}\}$, where $\delta_k \to 0$, $\alpha_k := \alpha(\delta_k)$ and $x_{\alpha_k}^{\delta_k}$ is a solution of* (A.2)*, has a convergent subsequence. The limit of every convergent subsequence is an x^*-minimum-norm solution. If in addition, the x^*-minimum-norm solution $x^\dagger$ is unique, then*

$$\lim_{\delta \to 0} x_{\alpha(\delta)}^\delta = x^\dagger \quad \textit{in } X.$$

Here, an x^*-minimum-norm solution, is defined by

$$\|x^\dagger - x^*\|_X := \min\{\|x - x^*\|_X : F(x) = y\}.$$

Achieving convergence rates in the non-linear case requires additional assumptions on $F(\cdot)$, which are automatically satisfied in the linear case. One finds the following theorem in the literature.

Theorem A.1.3 ([**45, Theorem 10.4**]). *Let $\mathcal{D}(F)$ be convex, let $y^\delta \in Y$ with $\|y - y^\delta\|_Y \leq \delta$ and let $x^\dagger$ be an x^*-minimum solution. Moreover, let the following conditions hold:*

(i) F is Fréchet differentiable,

(ii) there exists $\gamma > 0$ such that $\|F'(x^\dagger) - F'(x)\| \leq \gamma \|x^\dagger - x\|_X$ for all $x \in \mathcal{D}(F)$ in a sufficiently large ball around $x^\dagger$,

(iii) there exists $w \in Y$ satisfying $x^\dagger - x^* = F'(x^\dagger)^* w$ and

(iv) $\gamma \|w\|_Y < 1$.

Then for the choice $\alpha \sim \delta$, we obtain

$$\|x_\alpha^\delta - x^\dagger\|_X = O(\sqrt{\delta}) \quad \textit{and} \quad \|F(x_\alpha^\delta) - y^\delta\|_Y = O(\delta)$$

The assertion of the theorem remains valid when the regularisation $\alpha = \alpha(\delta, y^\delta)$ is chosen according to the discrepancy principle; see [**45, Section 10.3**]. The discrepancy principle is a parameter choice rule for the regularisation parameter α; see [**45**]. It reads as follows: Choose $\overline{\alpha} = \alpha(\delta, y^\delta)$ such that

$$\overline{\alpha} = \sup\{\alpha > 0 : \|F(x_\alpha^\delta) - y^\delta\|_Y \leq \tau\delta\} \text{ for some } \tau > 1.$$

This concludes our brief overview regarding the existence and convergence of regularised solutions.

A.2. Useful lemmas and inequalities

Let us first recall the well-known Gronwall inequality.

Lemma A.2.1 (Gronwall inequality,[**92**])**.** *Let $T > 0, v, g \in C[0,T]$ and $\lambda \in L^1(0,T)$ be given. Further, assume that*

$$v(t) \leq g(t) + \int_0^t \lambda(s)v(s)\,ds, \quad 0 \leq t \leq T,$$

and that $\lambda(t) \geq 0$ for a.a. $0 \leq t \leq T$. Then

$$v(t) \leq g(t) + \int_0^t g(s)\lambda(s)\exp^{\int_s^t \lambda(r)\,dr}\,ds, \quad 0 \leq t \leq T.$$

Further, we gather some useful inequalities.

Interpolation inequality/Ladyženskaja [73]: Let $\Omega \in \mathbb{R}^2$ be a bounded smooth domain and $f \in H^1(\Omega)$. Then, there exists a positive constant C depending only on Ω such that

$$\|f\|_{L^4(\Omega)} \leq C\left(\|f\|_{L^2(\Omega)}^{\frac{1}{2}}\|\nabla f\|_{L^2(\Omega)}^{\frac{1}{2}} + \|f\|_{L^2(\Omega)}\right). \tag{A.3}$$

Interpolation inequalities [73]: Let $v \in L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;W^{1,2}(\Omega))$. Then $v \in L^4(0,T;L^4(\Omega))$ for $d = 2$.

Elliptic Estimates [46][89]: Let Ω be a smooth domain. Then there exist constants C only dependent on the domain such that

$$\begin{aligned} \|f\|_{H^2(\Omega)} &\leq C(\|f\|_{L^2(\Omega)} + \|\Delta f\|_{L^2(\Omega)}), \\ \|f\|_{H^4(\Omega)} &\leq C(\|f\|_{L^2(\Omega)} + \|\Delta^2 f\|_{L^2(\Omega)}). \end{aligned} \tag{A.4}$$

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