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Nonsmooth Schur–Newton methods for multicomponent Cahn–Hilliard systems

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We present globally convergent nonsmooth Schur–Newton methods for the solution of discrete multicomponent Cahn–Hilliard systems with logarithmic and obstacle potentials. The method solves the nonlinear set-valued saddle-point problems arising from discretization by implicit Euler methods in time and first-order finite elements in space without regularization. Efficiency and robustness of the convergence speed for vanishing temperature is illustrated by numerical experiments.

Keywords: phase field models; variational inequalities; finite elements; convex minimization; descent methods; multigrid methods.

1. Introduction

We consider a multicomponent Cahn–Hilliard system, i.e., a Cahn–Hilliard system with vector-valued order parameter, with logarithmic free energy for positive temperature θ and the associated deep quench limit model for $\theta = 0$ describing the isothermal decomposition and coarsening of multicomponent alloys (Morral & Cahn, 1971; De Fontaine, 1972; Elliott & Luckhaus, 1991). Existence and uniqueness are shown in the pioneering paper of Elliott & Luckhaus (1991). Discretization by an implicit Euler method in time and by piecewise affine finite elements in space is suggested and analysed by Blowey *et al.* (1996) and Barrett & Blowey (1996) for the logarithmic potential and by Barrett & Blowey (1997) in the deep quench limit. Besides the fully implicit Euler method, a globally stable semiimplicit variant taking the concave terms of the logarithmic or obstacle potential explicitly is also considered.

While the numerical analysis of multicomponent Cahn–Hilliard systems with logarithmic free energy and the associated deep quench limit model are well developed, the fast and robust numerical solution of large-scale algebraic systems arising in each time step still seems to be open. Blowey *et al.* (1996) use a nonlinear Gauß–Seidel-type iteration and Barrett & Blowey (1996, 1997) adapt a splitting method of Lions & Mercier (1979) which can be regarded as a type of alternating direction scheme. Both approaches suffer from severe mesh dependence. Boynova & Neytcheva (2012) suggest an inexact Newton method applicable to polynomial or regularized logarithmic free energies, but do not address the influence of the regularization parameter on the convergence speed. Kim & Kang (2009) apply a full approximation storage multigrid algorithm to a ternary system with polynomial free energy but neither article provides a theoretical convergence result nor discusses the convergence speed of their method.

Efficient and reliable, i.e., fast and globally converging, solvers are available for discretized Cahn–Hilliard equations for binary mixtures (Gräser & Kornhuber, 2009b; Blank *et al.*, 2011; Gräser, 2011, 2013; Hintermüller *et al.*, 2011; Banas *et al.*, 2013) or for discretized Allen–Cahn equations with vector-valued order parameter (Kornhuber & Krause, 2003, 2006; Blank *et al.*, 2013), both for logarithmic and

obstacle-type free energy. Moreover, for logarithmic potentials, the convergence behaviour is robust with respect to temperature even in the deep quench limit (Kornhuber & Krause, 2006; Gräser, 2011). To the best knowledge of the authors, efficient, reliable and robust solvers for multicomponent Cahn–Hilliard systems with logarithmic free energy are not known.

In this paper, we present so-called nonsmooth Schur–Newton methods for the spatial problems arising from the discretizations of multicomponent Cahn–Hilliard systems suggested in Barrett & Blowey (1996, 1997) and Blowey *et al.* (1996) up to lumping of lower-order terms. Though our approach is applicable to both implicit and semiimplicit time discretizations (see Gräser, 2011, Section 3.4.2), we concentrate on the semiimplicit variant for ease of presentation. Our starting point is the discrete spatial problems (SI) arising in Barrett & Blowey (1996, 1997) up to lumping of lower-order terms in the case of logarithmic free energy. As (SI) only makes sense for temperature $\theta > 0$, we provide a reformulation ($\widehat{\text{VI}}$) in terms of variational inequalities, which is meaningful for all $\theta \geqslant 0$. Note that ($\widehat{\text{VI}}$) essentially reduces to the discretization suggested and analysed in Barrett & Blowey (1997). From a computational point of view, it is convenient to incorporate the algebraic constraints, i.e., all phases must sum to 1, in a suitable weak form. This leads to the final formulation (VI) that makes sense for all $\theta \geqslant 0$. We prove that solutions of (VI) and (SI) provide the same order parameter, but possibly different chemical potentials. On the nondegeneracy condition that no phase vanishes completely, Theorem 3.5 provides the existence of solutions of (VI) together with uniqueness and continuity of the corresponding order parameter with respect to temperature θ. Finally, Theorem 3.6 states existence, uniqueness and continuity of both the order parameter and the chemical potential on the additional condition that the diffuse interface is resolved sufficiently well.

Nonsmooth Schur–Newton methods have been introduced, analysed and assessed numerically for discretized binary Cahn–Hilliard equations with obstacle potential (Gräser & Kornhuber, 2009b) or logarithmic potential (Gräser, 2011, 2013). They can be regarded as gradient-related descent methods for the Schur complement formulation of set-valued saddle-point problems, as a preconditioned Uzawa iteration or as generalizations of well-known primal–dual active set methods (Hintermüller *et al.*, 2003; Gräser, 2008). No regularization is involved. The presented extension to vector-valued order parameters is robust in the sense that global convergence holds for all temperatures $\theta \geqslant 0$. Moreover, numerical experiments illustrate that the convergence speed is hardly affected by temperature or even by the number of components. Our numerical computations also indicate mesh-independent convergence for initial iterates obtained by nested iteration (Hackbusch, 1985, Chapter 5). Theoretical validation is the subject of current research.

The paper is organized as follows. After presenting the continuous problem and its discretization, Section 3 concentrates on the unified formulation (VI) of the spatial problems that includes both the logarithmic potential and the deep quench limit in terms of a variational inequality. We show existence, uniqueness and equivalence to a (generally set-valued) nonlinear saddle-point problem. In Section 4, we derive truncated nonsmooth Schur–Newton methods for the iterative solution of an algebraic reformulation of (VI), prove global convergence and discuss some algorithmic issues. Numerical experiments, reported in Section 5, illustrate the efficiency and robustness of our approach.

2. Multicomponent Cahn–Hilliard systems

We consider phase separation in isothermal multicomponent systems on a polygonal (polyhedral) domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$. The concentrations of the different constituents $i = 1, \ldots, N$ at $(x, t) \in \Omega \times [0, T_0]$, $T_0 > 0$ are represented by the components $u_i(x, t)$ of the order parameter $u = (u_1, \ldots, u_N)^{\mathrm{T}}$.

Throughout the following, we will make use of the Euclidean scalar product $v \cdot w$ with associated norm $|\cdot|$ in Euclidean vector spaces, of the canonical scalar product $(\cdot,\cdot)$ in $L^2(\Omega)$, of the scalar product

$$(v,w) = \int_\Omega v \cdot w \,\mathrm{d}x$$

in $L^2(\Omega)^N$ with canonical norm $\|\cdot\|_0$ and of the scalar product

$$(v,w)_1 = (v,w) + (\nabla v, \nabla w), \quad (\nabla v, \nabla w) = \sum_{i=1}^N \int_\Omega \nabla v_i \cdot \nabla w_i \,\mathrm{d}x$$

in $H^1(\Omega)^N$ with canonical norm $\|\cdot\|_1$ and seminorm $|\cdot|_1^2 = (\nabla\cdot, \nabla\cdot)$. Generic constants are denoted by c, C and can have different values at different occurrences.

The order parameter u satisfies the constraints

$$u(x,t) \in G = \left\{ v \in \mathbb{R}^N \mid v_i \geqslant 0, \sum_{i=1}^N v_i = 1 \right\} \quad \forall (x,t) \in \Omega \times [0,T_0],$$

because concentrations are non-negative and add up to unity. The closed convex set $G \subset \mathbb{R}^N$ is often called the *Gibbs simplex*. Note that the indicator function χ_G, defined by $\chi_G(u) = 0$ for $u \in G$ and $\chi_G(u) = +\infty$ for $u \notin G$, can be decomposed according to

$$\chi_G(u) = \sum_{i=1}^N \chi_{[0,\infty)}(u_i) + \chi_{V_1}(u), \quad V_1 = \left\{ v \in \mathbb{R}^N \,\middle|\, \sum_{i=1}^N v_i = 1 \right\},$$

with $\chi_{[0,\infty)}$ and χ_{V_1} denoting the indicator functions of $[0,\infty)$ and V_1, respectively. We assume that the Ginzburg–Landau total free energy of our system takes the form

$$\mathcal{E}(u) = \int_\Omega \frac{\varepsilon}{2} \sum_{i=1}^N |\nabla u_i|^2 + \frac{1}{\varepsilon} \Psi(u) \,\mathrm{d}x \tag{2.1}$$

with fixed interface parameter $\varepsilon > 0$. While the quadratic interfacial energy is penalizing steep gradients, the free energy Ψ gives rise to phase separation. We concentrate on a multiphase version of the well-known logarithmic free energy (Barrett & Blowey, 1996; Blowey *et al.*, 1996). More precisely, $\Psi = \Psi_\theta$ is given by

$$\Psi_\theta(u) = \Phi_\theta(u) + \chi_{V_1}(u) + \tfrac{1}{2} K u \cdot u \tag{2.2}$$

with the convex function

$$\Phi_\theta(u) = \begin{cases} \displaystyle\sum_{i=1}^N \theta u_i \ln(u_i) & \text{for } \theta > 0, \\ \displaystyle\sum_{i=1}^N \chi_{[0,\infty)}(u_i) & \text{for } \theta = 0, \end{cases} \tag{2.3}$$

and a symmetric interaction matrix $K = (K_{ij})_{i,j=1}^N$ (cf. De Fontaine, 1972) depending on θ_c. Here, θ and θ_c denote absolute and critical temperature, respectively.

For $\theta < \theta_c$, we assume that Ψ_θ has exactly N distinct local minima on G, corresponding to almost pure components $i = 1, \dots, N$. For example, this is achieved by choosing the interaction matrix

$$K = \theta_c N (1 - \delta_{ij})_{i,j=1}^N \quad \text{(Kronecker-}\delta\text{)}, \tag{2.4}$$

which means that the interaction of all different components is equal and no self-interaction occurs. In the deep quench limit $\theta = 0$, we then obtain the classical obstacle potential (cf. Barrett & Blowey, 1997)

$$\Psi_0(u) = \chi_G(u) + \theta_c \frac{N}{2} \sum_{i=1}^N u_i (1 - u_i).$$

For $\theta > 0$ and $N = 2$ the well-known logarithmic free energy

$$\Psi_\theta(\tilde{u}) = \frac{1}{2}\theta \left[(1 + \tilde{u}) \ln \left(\frac{1 + \tilde{u}}{2} \right) + (1 - \tilde{u}) \ln \left(\frac{1 - \tilde{u}}{2} \right) \right] + \frac{1}{2}\theta_c (1 - \tilde{u}^2)$$

of the scalar order parameter $\tilde{u} := u_2 - u_1 \in [-1, 1]$ is recovered in this way. In the shallow quench, i.e., for $\theta \approx \theta_c$, polynomial free energies generalizing the quartic potential $(1 - \tilde{u}^2)^2$ provide good approximations of Ψ_θ (cf. Steinbach *et al.*, 1996). As polynomials are defined everywhere, the contributions from the nondifferentiable indicator function $\chi_{[0,\infty)}$ are usually skipped in this case.

For $\theta > 0$ the multicomponent Cahn–Hilliard system

$$\begin{aligned} u_t &= L \Delta w, \\ w &= -\varepsilon^2 \Delta u + P \Psi_\theta'(u) \end{aligned} \tag{2.5}$$

is obtained by postulating that u satisfies a conservation law with flux $-L\nabla w$ and w given by the derivative of the total free energy $\mathcal{E}$ defined in (2.1). In this way, the mass of all components u_i is conserved and (2.5) is thermodynamically consistent in the sense that $\mathcal{E}$ decreases monotonically throughout the evolution. We assume that the matrix L is symmetric and positive semidefinite with one-dimensional kernel spanned by $\mathbf{1} = (1, \dots, 1)^{\mathrm{T}} \in \mathbb{R}^N$. The latter condition accounts for the fact that $u \cdot \mathbf{1} \equiv 1$ and therefore $u_t \cdot \mathbf{1} \equiv 0$. For ease of presentation, we concentrate on constant mobilities $L \in \mathbb{R}^{N \times N}$. However, all our algorithms and theoretical considerations presented below extend to discretizations of solution-dependent mobilities as suggested in Barrett & Blowey (2001), where $L = L(u)$ is replaced by a suitable constant.

The orthogonal projection

$$P = I - \frac{1}{N}(\mathbf{1}, \dots, \mathbf{1}) \in \mathbb{R}^{N \times N}$$

maps $\mathbb{R}^N$ onto the linear subspace

$$V_0 = \left\{ v \in \mathbb{R}^N \;\middle|\; \sum_{i=1}^N v_i = 0 \right\} \subset \mathbb{R}^N.$$

It accounts for the fact that admissible variations of $u(x, t) \in V_1$ must be in V_0.

In the singular deep quench limit $\theta = 0$, the second equation in (2.5) becomes

$$w \in -\varepsilon^2 \Delta u + P\partial\Psi_0(u). \tag{2.6}$$

We assume that the initial condition $u_0 \in H^1(\Omega)$ satisfies $u_0(x) \in V_1$ for almost all $x \in \Omega$ and the componentwise inequality

$$0 < \frac{1}{|\Omega|}\int_\Omega u_0(x)\,\mathrm{d}x < \mathbf{1}, \tag{2.7}$$

which means that the given problem is nondegenerate in the sense that exactly N different components actually occur. We further impose Neumann boundary conditions for u and w so that mass conservation

$$\int_\Omega u(x,t)\,\mathrm{d}x = \int_\Omega u_0(x)\,\mathrm{d}x,$$

and

$$(I-P)u(x,t) = \frac{1}{N}\mathbf{1}, \quad (I-P)w(x,t) = 0$$

hold for almost all $x \in \Omega$ and $t > 0$. On these assumptions, existence and uniqueness were shown by Elliott & Luckhaus (1991) for $\theta \geqslant 0$. For sharp interface limits, we refer the reader to Bronsard *et al.* (1998).

3. Discretization

3.1 *Semiimplicit time discretization and finite elements*

Let us first consider the case $\theta > 0$. Then time discretization of a weak formulation of (2.5) by the implicit Euler scheme and subsequent finite element discretization lead to spatial problems of the following form.

(FI) Find $u \in \mathcal{G}, w \in \mathcal{S}^N$ such that

$$\begin{aligned}\varepsilon^2(\nabla u, \nabla v) + (P\Phi_\theta'(u), v)^{\mathcal{T}} + (PKu, v) &= (w, v) \quad \forall v \in \mathcal{S}^N,\\ (u, v) + \tau(L\nabla w, \nabla v) &= (u^{\mathrm{old}}, v) \quad \forall v \in \mathcal{S}^N.\end{aligned}$$

Here, $\tau > 0$ denotes the uniform time-step size, u and w stand for the finite element approximations of the order parameter and the chemical potential in the given time step, respectively, and u^{old} denotes the approximate order parameter in the preceding time step. The finite element space $\mathcal{S}^N$ is the tensor product of scalar, piecewise affine finite elements

$$\mathcal{S} = \{v \in C(\bar{\Omega}) \mid v|_T \text{ is affine } \forall T \in \mathcal{T}\}$$

induced by a simplicial partition $\mathcal{T}$ of Ω. We assume that $\mathcal{T} = \mathcal{T}_j$ together with an underlying hierarchy $\mathcal{T}_0, \ldots, \mathcal{T}_j$ obtained by successive adaptive refinement of a conforming, intentionally coarse partition $\mathcal{T}_0$. During this refinement process, so-called 'hanging' vertices are allowed to occur at the midpoints of certain edges. Each function $v \in \mathcal{S}$ is characterized by its values in $p \in \mathcal{N}$, the set of all 'nonhanging' vertices of simplices $T \in \mathcal{T}$. Therefore, $\mathcal{S}$ is spanned by the nodal basis $\lambda_p \in \mathcal{S}$, $p \in \mathcal{N}$, defined by the condition $\lambda_p(q) = \delta_{p,q}$ for all $q \in \mathcal{N}$. We refer the reader to Gräser (2011) for details.

We have also used the closed convex subset

$$\mathcal{G} = \{v \in \mathcal{S}^N \mid v(p) \in G \ \forall p \in \mathcal{N}\},$$

and the lumped L^2 scalar product

$$(u, v)^{\mathcal{T}} = \int_\Omega I^{\mathcal{T}}(u \cdot v)\,\mathrm{d}x$$

induced by canonical nodal interpolation $I^{\mathcal{T}} v = \sum_{p\in\mathcal{N}} v(p)\lambda_p$. Note that lumping has been applied only to the nonlinear term $(\Phi_\theta'(u), v)$ in order to separate the unknowns associated with different nodes with respect to nonlinearity. Full lumping, i.e., lumping of all other zero-order terms, is quite common in the literature (cf., e.g., Barrett & Blowey, 1996, 1997, 1999, 2001; Blowey *et al.*, 1996) but is avoided here, because it would either destroy symmetry or mass conservation if the underlying grids have changed from the preceding time step to the given time step (Gräser & Sander, 2009, Section 5; Gräser, 2011, Section 3.4.3).

All reasoning presented below extends a fully lumped version of (FI) as proposed and analysed by Blowey *et al.* (1996) and Barrett & Blowey (1996). Existence and uniqueness of corresponding discrete solutions have been shown in Blowey *et al.* (1996, Theorem 2.4) for the fully lumped version on the time-step constraint

$$\tau < 4\varepsilon^2/(\lambda_K^2 \|L\|).$$

Here, λ_K denotes the largest positive eigenvalue of K and $\|L\|$ stands for the spectral norm of L. For example, for K taken from (2.4), the time step τ has to satisfy $\tau < 4\varepsilon^2/(\theta_c^2 N^2 (N-1)^2 \|L\|)$. In order to avoid such severe stability restrictions, the expanding linear part K of $\Psi_\theta' = \Phi_\theta' + K$ on $\mathcal{G}$ is often discretized explicitly (cf., e.g., Blowey & Elliott, 1993; Blowey *et al.*, 1996; Barrett *et al.*, 2004; Gräser *et al.*, 2013). More precisely, Ku is replaced by $Ku^{\mathrm{old}} + (P - I)Ku$, providing the following unconditionally stable semiimplicit scheme.
(SI) Find $u \in \mathcal{G}, w \in \mathcal{S}^N$ such that

$$\begin{aligned} \varepsilon^2(\nabla u, \nabla v) + (P\Phi_\theta'(u), v)^{\mathcal{T}} + (Ku^{\mathrm{old}} + (P - I)Ku, v) &= (w, v) \quad \forall v \in \mathcal{S}^N, \\ (u, v) + \tau(L\nabla w, \nabla v) &= (u^{\mathrm{old}}, v) \quad \forall v \in \mathcal{S}^N. \end{aligned}$$

By construction, $u(p) \in G$ for all $p \in \mathcal{N}$. Orthogonality of P with respect to the Euclidean scalar product immediately provides $(I - P)w \equiv 0$ for the fully implicit discretization (FI). For the semiimplicit version (SI), testing with $v = \lambda_p \mathbf{1}$ and a short calculation shows

$$(w \cdot \mathbf{1}, \lambda_p) = (K(u^{\mathrm{old}} - u) \cdot \mathbf{1}, \lambda_p). \tag{3.1}$$

Hence $(I - P)w \equiv 0$ is no longer true in general but only holds in special cases, e.g., for the choice (2.4) of K.

3.2 *Unified formulation of spatial problems for* $\theta \geqslant 0$

The occurrence of P in the projected derivative $P\Phi_\theta'(\cdot)$ in the discretizations (FI) and (SI) prevents a direct reformulation as a variational inequality that would allow to the deep quench limit $\theta = 0$ to be passed. Utilizing $(I - P)w \equiv 0$, such a formulation can be easily obtained for the fully implicit version

(FI). We therefore concentrate on the semiimplicit variant and first introduce the (affine) subspaces

$$\mathcal{S}_r^N = \{v \in \mathcal{S}^N \mid v(p) \in V_r \forall p \in \mathcal{N}\}, \quad r \in \{0, 1\}.$$

Using the reduced test space $\mathcal{S}_0^N \subset \mathcal{S}^N$ in the first equation of (SI), we obtain

$$\varepsilon^2(\nabla u, \nabla v) + (\Phi_\theta'(u), v)^{\mathcal{T}} + (Ku^{\text{old}}, v) = (w_0, v) \quad \forall v \in \mathcal{S}_0^N$$

with the new variable $w_0 = Pw \in \mathcal{S}_0^N$. We now rewrite this equation as a variational inequality and use the reduced test space $\mathcal{S}_0^N \subset \mathcal{S}^N$ in the second equation of (SI) as well, to obtain the following.

($\widehat{\text{VI}}$) Find $u \in \mathcal{S}_1^N, w \in \mathcal{S}_0^N$ such that

$$\begin{aligned} \varepsilon^2(\nabla u, \nabla(v-u)) + \phi_\theta^{\mathcal{T}}(v) - \phi_\theta^{\mathcal{T}}(u) - (w_0, v-u) &\geqslant -(Ku^{\text{old}}, v-u) \quad \forall v \in \mathcal{S}_1^N, \\ (u, v) + \tau(L\nabla w_0, \nabla v) &= (u^{\text{old}}, v) \quad \forall v \in \mathcal{S}_0^N. \end{aligned}$$

Note that the lumped nonlinearity $(\Phi_\theta'(u), v)^{\mathcal{T}}$ gives rise to the nonlinear functional $\phi_\theta^{\mathcal{T}}$, defined by

$$\phi_\theta^{\mathcal{T}}(v) = \begin{cases} \displaystyle\int_\Omega I^{\mathcal{T}}(\Phi_\theta(v))\,\mathrm{d}x & \text{if } v \geqslant 0, \\ +\infty & \text{otherwise.} \end{cases}$$

The variational problem ($\widehat{\text{VI}}$) has the advantage that it allows for a straightforward extension to the deep quench limit $\theta = 0$. In this case, $\phi_0^{\mathcal{T}}$ just accounts for the inequality constraints $u_i \geqslant 0$. For positive temperature, the variational formulation ($\widehat{\text{VI}}$) is equivalent to (SI) in the following sense.

PROPOSITION 3.1 Let $\theta > 0$. If (u, w) is a solution of (SI), then (u, Pw) is a solution of ($\widehat{\text{VI}}$), and if (u, w_0) is a solution of ($\widehat{\text{VI}}$), then there is a solution (u, w) of (SI) with $w_0 = Pw$.

Proof. Let (u, w) be a solution of (SI). Then (u, Pw) is a solution of ($\widehat{\text{VI}}$) by construction.

Now let (u, w_0) be a solution of ($\widehat{\text{VI}}$). Then we use the decomposition

$$v = Pv + (I - P)v = v_0 + v_1\mathbf{1}, \quad v_0 = Pv \in \mathcal{S}_0^N, \quad v_1 = \frac{1}{N} v \cdot \mathbf{1}$$

of all $v \in \mathcal{S}^N$ to define (cf. (3.1))

$$w = w_0 + w_1\mathbf{1}, \quad (w_1, \lambda_p) = \frac{1}{N}(K(u^{\text{old}} - u) \cdot \mathbf{1}, \lambda_p) \ \ \forall p \in \mathcal{N}.$$

Note that w is well defined because the mass matrix $((\lambda_p, \lambda_q))_{p,q \in \mathcal{N}}$ is invertible. Now exploiting the orthogonality of P and the properties of L, it is easily checked that u, w solve (SI). □

3.3 *Weak formulation of affine constraints*

In order to simplify the algebraic solution, we now derive a version of (SI) that incorporates the affine constraints $u(p) \cdot \mathbf{1} = 1$ in the weak form

$$(u, \mathbf{1}v) = (u \cdot \mathbf{1}, v) = (1, v) \quad \forall v \in \mathcal{S} \tag{3.2}$$

and not in the strong form $u \in \mathcal{S}_1^N$. Introducing the Lagrange multiplier $\mathbf{1}\eta \in \mathcal{S}^N$ associated with (3.2), the solution of ($\widehat{\text{VI}}$) amounts to finding $u \in \mathcal{S}^N, w_0 \in \mathcal{S}_0^N, \eta \in \mathcal{S}$ such that

$$\begin{aligned}\varepsilon^2(\nabla u, \nabla(v-u)) + \phi_\theta^{\mathcal{T}}(v) - \phi_\theta^{\mathcal{T}}(u) - (w_0 + \mathbf{1}\eta, v-u) &\geqslant -(Ku^{\text{old}}, v-u) \quad \forall v \in \mathcal{S}^N,\\ -(u,v) - \tau(L\nabla w_0, \nabla v) &= -(u^{\text{old}}, v) \quad \forall v \in \mathcal{S}_0^N,\\ -(u, \mathbf{1}v) &= -(u^{\text{old}}, \mathbf{1}v) \quad \forall v \in \mathcal{S}.\end{aligned}$$

For the deep quench limit $\theta = 0$ a fully implicit and fully lumped version of this discretization has been suggested and analysed by Barrett & Blowey (1997).

Introducing the new variable $\tilde{w} = w_0 + \mathbf{1}\eta$, adding the last two equations and using $L\mathbf{1} = 0$, we see that this problem is equivalent to finding $u \in \mathcal{S}^N, \tilde{w} \in \mathcal{S}^N$ such that

$$\begin{aligned}\varepsilon^2(\nabla u, \nabla(v-u)) + \phi_\theta^{\mathcal{T}}(v) - \phi_\theta^{\mathcal{T}}(u) - (\tilde{w}, v-u) &\geqslant -(Ku^{\text{old}}, v-u) \quad \forall v \in \mathcal{S}^N,\\ -(u,v) - \tau(L\nabla\tilde{w}, \nabla v) &= -(u^{\text{old}}, v) \quad \forall v \in \mathcal{S}^N.\end{aligned}$$

In the final step, we enforce coercivity of the primal operator by exploiting mass conservation,

$$\int_\Omega u_i(x)\,\mathrm{d}x = \int_\Omega u_i^{\text{old}}(x)\,\mathrm{d}x,$$

in a similar way to that introduced in Gräser (2004, 2011) and Gräser & Kornhuber (2009b). More precisely, we add the equality

$$\varepsilon^2(u, \mathbf{1})(v-u, \mathbf{1}) = \varepsilon^2(u^{\text{old}}, \mathbf{1})(v-u, \mathbf{1}) \quad \forall v \in \mathcal{S}^N$$

to the variational inequality above, to obtain the final form of the following spatial problem.
(VI) Find $(u, w) \in \mathcal{S}^N \times \mathcal{S}^N$ such that

$$\begin{aligned}&\varepsilon^2(\nabla u, \nabla(v-u)) + \varepsilon^2 \int_\Omega u\,\mathrm{d}x \cdot \int_\Omega v-u\,\mathrm{d}x + \phi_\theta^{\mathcal{T}}(v) - \phi_\theta^{\mathcal{T}}(u) - (w, v-u)\\ &\quad\geqslant \varepsilon^2 \int_\Omega u^{\text{old}}\,\mathrm{d}x \cdot \int_\Omega v-u\,\mathrm{d}x - (Ku^{\text{old}}, v-u) \quad \forall v \in \mathcal{S}^N,\\ &\quad\quad -(u,v) - \tau(L\nabla w, \nabla v) = -(u^{\text{old}}, v) \quad \forall v \in \mathcal{S}^N.\end{aligned}$$

In the light of the above considerations and Proposition 3.1, the formulations (SI) and (VI) are equivalent for positive temperature in the following sense.

PROPOSITION 3.2 Let $\theta > 0$. If (u, w) is a solution of (SI), then there is a solution $(u, \tilde{w})$ of (VI) satisfying $Pw = P\tilde{w}$ and vice versa.

The common idea behind the above reformulations is to use the part $(I-P)w \in \mathcal{S}$ as a kind of dustbin, e.g., for the Lagrange parameter in $\eta \in \mathcal{S}$.

3.4 *Existence and uniqueness of discrete solutions*

The variational problem (VI) is equivalent to a saddle-point problem of finding $(u, w) \in \mathcal{S}^N \times \mathcal{S}^N$ such that

$$\mathcal{L}(u, w) = \inf_{v \in \mathcal{S}^N} \sup_{z \in \mathcal{S}^N} \mathcal{L}(v, z) \tag{3.3}$$

holds for the Lagrangian

$$\mathcal{L}(v, z) = \mathcal{J}(v) + (u^{\text{old}} - v, z) - \frac{\tau}{2}(L\nabla z, \nabla z)$$

involving the coercive, convex, lower semicontinuous energy functional

$$\mathcal{J}(v) = \frac{\varepsilon^2}{2}(\nabla v, \nabla v) + \frac{\varepsilon^2}{2}\left|\int_\Omega v - u^{\text{old}}\,\mathrm{d}x\right|^2 + \phi_\theta^{\mathcal{T}}(v) + (Ku^{\text{old}}, v).$$

The Lagrangian $\mathcal{L}$ has finite values on the closed, convex set

$$\text{dom}(\mathcal{J}) \times \mathcal{S}^N = \{v \in \mathcal{S}^N \mid v \geqslant 0\} \times \mathcal{S}^N.$$

In order to show the existence of discrete solutions of (3.3), we will make use of a dual problem for w only. The key ingredient for solutions of the dual problem is the following lemma.

LEMMA 3.3 The functional $h = -\inf_{v \in \text{dom}(\mathcal{J})} \mathcal{L}(v, \cdot)$ is coercive on $\mathcal{S}^N$.

Proof. Let $z \in \mathcal{S}^N$ be arbitrary and define a corresponding $v_0 = v^{(1)} + v^{(2)} \in \mathcal{S}^N$ with $v^{(1)}, v^{(2)} \in \mathcal{S}^N$ given by the nodal values

$$v^{(1)}(p) = \tfrac{1}{2}(1 + \text{sgn}(z^{(1)})), \quad v^{(2)}(p) = \rho(1 + \text{sgn}(\mathbf{1} \cdot z(p)))\mathbf{1}, \quad p \in \mathcal{N}.$$

Here, we have used the componentwise mean value of z,

$$z^{(1)} = |\Omega|^{-1} \int_\Omega z\,\mathrm{d}x, \quad |\Omega| = \int_\Omega \mathrm{d}x,$$

and some positive $\rho \in \mathbb{R}$ to be specified later. In the light of

$$-\inf_{v \in \text{dom}(\mathcal{J})} \mathcal{L}(v, z) \geqslant -\mathcal{L}(v_0, z) = -\mathcal{J}(v_0) - (u^{\text{old}} - v_0, z) + \frac{\tau}{2}(L\nabla z, \nabla z), \tag{3.4}$$

we now derive an upper bound for $(u^{\text{old}} - v_0, z)$. To this end, we first decompose z according to

$$z = z^{(0)} + z^{(1)}, \quad z^{(0)} = z - z^{(1)} = z - |\Omega|^{-1} \int_\Omega z\,\mathrm{d}x.$$

Utilizing $u^{\text{old}}(p) \in V_1$ and the definition of $z^{(0)}$ and $v^{(1)}$, we then have

$$(u^{\text{old}}, (I - P)z^{(0)}) = \frac{1}{N}(\mathbf{1}, z^{(0)}) = 0 = \rho(\mathbf{1}, z^{(0)}), \quad (v^{(1)}, z^{(0)}) = 0.$$

These identities and the properties of P provide

$$\begin{aligned}(u^{\text{old}} - v_0, z) &= (u^{\text{old}}, Pz^{(0)}) + (u^{\text{old}}, (I-P)z^{(0)}) - (v_0, z^{(0)}) + (u^{\text{old}} - v^{(1)}, z^{(1)}) - (v^{(2)}, z^{(1)}) \\ &= (u^{\text{old}}, Pz^{(0)}) - (\rho\mathbf{1}, z^{(0)}) + (u^{\text{old}} - v^{(1)}, z^{(1)}) - (v^{(2)}, z) \\ &= (u^{\text{old}}, Pz^{(0)}) + (u^{\text{old}} - \rho\mathbf{1} - v^{(1)}, z^{(1)}) + (\rho\mathbf{1} - v^{(2)}, z).\end{aligned}$$

Using the Poincaré inequality, the first term can be estimated by

$$(u^{\text{old}}, Pz^{(0)}) \leqslant \|u^{\text{old}}\|_0 \|Pz^{(0)}\|_0 \leqslant C_0 |Pz^{(0)}|_1 = C_0 |Pz|_1 \tag{3.5}$$

with C_0 independent of z. In order to estimate the second term, we now select

$$\rho = \frac{1}{2|\Omega|} \min_{i=1,\dots,N} \int_\Omega u_i^{\text{old}} \,\mathrm{d}x > 0$$

and set $\mu_i = |\Omega|^{-1} \int_\Omega u_i^{\text{old}} - \rho \,\mathrm{d}x$. Note that $0 < \mu_i < 1$. Investigating the three cases $v_i^{(1)} \in \{0, \frac{1}{2}\}$, using the equivalence of norms on $\mathbb{R}^N$ and that the orthogonal projection has unit norm, we obtain

$$\begin{aligned}(u^{\text{old}} - \rho\mathbf{1} - v, z^{(1)}) &= \sum_{i=1}^N (\mu_i - v_i^{(1)}) \int_\Omega z_i \,\mathrm{d}x = -\sum_{i=1}^N |\mu_i - v_i^{(1)}| \left| \int_\Omega z_i \,\mathrm{d}x \right| \\ &\leqslant -c_0 \sum_{i=1}^N \left| \int_\Omega z_i \,\mathrm{d}x \right| \leqslant -c_0 \sqrt{N} \left| \int_\Omega z \,\mathrm{d}x \right| \leqslant -c_0 \sqrt{N} \left| \int_\Omega Pz \,\mathrm{d}x \right|.\end{aligned}$$

Here, c_0 is defined by

$$c_0 = \min_{\substack{i=1,\dots,N \\ z_i^{(1)} \neq 0}} |\mu_i - v_i^{(1)}| > 0$$

if there is at least one i such that $z_i^{(1)} = |\Omega|^{-1} | \int_\Omega z_i \,\mathrm{d}x| \neq 0$ and $c_0 = 1$ otherwise. In order to treat the third term $(\rho\mathbf{1} - v^{(2)}, z)$, we utilize the identities

$$\begin{aligned}(\rho\mathbf{1} - v^{(2)}(p)) \cdot z(p) &= -\rho \operatorname{sgn}[\mathbf{1} \cdot z(p)] \mathbf{1} \cdot (I-P)z(p) = -\rho |\mathbf{1} \cdot z(p)|, \\ |(I-P)z(p)| &= \frac{1}{\sqrt{N}} |\mathbf{1} \cdot z(p)|\end{aligned}$$

to obtain

$$(\rho\mathbf{1} - v^{(2)}, z) = -\rho \int_\Omega |\mathbf{1} \cdot z| \,\mathrm{d}x = -\rho\sqrt{N} \int_\Omega |(I-P)z| \,\mathrm{d}x.$$

Inserting these three estimates and the identity $(L\nabla z, \nabla z) = |Pz|_1^2$ into (3.4), we obtain

$$-\mathcal{L}(v_0, z) \geqslant C \left(|Pz|_1^2 - |Pz|_1 + \left| \int_\Omega Pz \,\mathrm{d}x \right| + \int_\Omega |(I-P)z| \,\mathrm{d}x - 1 \right) \tag{3.6}$$

with a constant C independent of z. In order to show that the right-hand side of this inequality tends to infinity, if (a suitable norm of) z tends to infinity, observe that Poincaré's inequality yields

$$|Pz|_1^2 - |Pz|_1 + \left|\int_\Omega Pz\,\mathrm{d}x\right| \geqslant |Pz|_1 + \left|\int_\Omega Pz\,\mathrm{d}x\right| - 1$$
$$\geqslant c(|Pz|_1 + \|Pz\|_0 - 1) \geqslant c(\|Pz\|_1 - 1)$$

with positive c independent of z. Inserting this estimate into (3.6), we finally obtain

$$-\mathcal{L}(v_0, z) \geqslant C\left(\|Pz\|_1 + \int_\Omega |(I-P)z| - 1\right) \tag{3.7}$$

with a constant C independent of z. This concludes the proof. □

Now we are ready to show existence and uniqueness. Here, the condition

$$0 < \int_\Omega u^{\mathrm{old}}\,\mathrm{d}x \tag{3.8}$$

follows from the nondegeneracy condition (2.7) by componentwise mass conservation of (VI).

THEOREM 3.4 Assume that u^{old} satisfies the nondegeneracy condition (3.8). Then (VI) has a solution (u, w).

Proof. Later, we will show in Proposition 4.2 that (i) the functional h defined in Lemma 3.3 is convex, continuous and finite and (ii) that minimizing h over $\mathcal{S}^N$ is equivalent to (VI). Hence, the existence of a minimizer w of h and thus of a solution (u, w) of (VI) follows from the convexity and continuity stated in Proposition 4.2 together with coercivity stated in Lemma 3.3; see, e.g., Ekeland & Temam (1976a, Chapter II, Proposition 1.2). □

An important feature of (VI) is that it provides a unified formulation for $\theta > 0$ and $\theta = 0$. The following results show that (VI) is robust in the sense that solutions (u, w) depend continuously on θ for all $\theta \geqslant 0$.

THEOREM 3.5 Assume that u^{old} satisfies the nondegeneracy condition (3.8) and let (u, w) be solutions of (VI). Then u and ∇Pw depend Hölder continuously on θ with Hölder exponent 0.5 and a constant only depending on Ω and L. Particularly, u and ∇Pw are unique for each $\theta \geqslant 0$.

Proof. Let $(u^1, w^1) \in \mathcal{S}^N \times \mathcal{S}^N$ and $(u^2, w^2) \in \mathcal{S}^N \times \mathcal{S}^N$ be solutions of (VI) for $\theta_1 \geqslant 0$ and $\theta_2 \geqslant 0$, respectively. Testing the variational inequalities for (u^1, w^1) with u^2 and vice versa, and adding the inequalities yields

$$\varepsilon^2|u^1 - u^2|_1^2 + \varepsilon^2\left|\int_\Omega u^1 - u^2\mathrm{d}x\right|^2 + (w^1 - w^2, u^2 - u^1)$$
$$\leqslant \phi_{\theta_1}^{\mathcal{T}}(u^2) - \phi_{\theta_1}^{\mathcal{T}}(u^1) + \phi_{\theta_2}^{\mathcal{T}}(u^1) - \phi_{\theta_2}^{\mathcal{T}}(u^2). \tag{3.9}$$

Similarly, testing the variational equations with $w^1 - w^2$ yields

$$(u^1 - u^2, w^1 - w^2) + \tau(L\nabla(w^1 - w^2), \nabla(w^1 - w^2)) = 0.$$

Inserting this in (3.9) and using the Poincaré inequality, properties of L, the definition of Φ_θ and the boundedness $-1/e \leqslant \Phi_1 \leqslant 0$ on $[0,1]$ then gives

$$\begin{aligned}\varepsilon^2\|u^1-u^2\|_1^2+\tau|P(w^1-w^2)|_1^2 &\leqslant C(\phi_{\theta_1}^{\mathcal{T}}(u^2)-\phi_{\theta_1}^{\mathcal{T}}(u^1)+\phi_{\theta_2}^{\mathcal{T}}(u^1)-\phi_{\theta_2}^{\mathcal{T}}(u^2))\\ &= C(\theta_1-\theta_2)(\phi_1^{\mathcal{T}}(u^2)-\phi_1^{\mathcal{T}}(u^1)) \leqslant C\frac{N|\Omega|}{e}|\theta_1-\theta_2|\end{aligned}$$

with C being the maximum of the Poincaré constant and the smallest nonzero eigenvalue of L. Using $\theta_1=\theta_2$ shows the uniqueness of u and ∇Pw. □

For the chemical potential w, uniqueness and continuous dependence on θ are available under additional conditions.

THEOREM 3.6 Denote by (u^θ, w^θ) a solution of (VI) for $\theta \geqslant 0$. In addition to the nondegeneracy condition (3.8) of Theorem 3.5, assume that for some fixed $\theta_0 \geqslant 0$ there is a subset

$$\mathcal{B}=\{\eta_{i,j}=e^i-e^j \mid i\neq j \text{ and } \exists p\in\mathcal{N}:\ u_i^{\theta_0}(p),u_j^{\theta_0}(p)>0\}\subset V_0 \tag{3.10}$$

such that $\operatorname{span}\mathcal{B}=V_0$. Then there is a relatively open neighbourhood of θ_0 in $\mathbb{R}_0^+$ where (u^θ,w^θ) is unique and depends continuously on θ.

Proof. By the continuity of $\theta\mapsto u^\theta$ there is a relatively open neighbourhood U of θ_0 in $\mathbb{R}_0^+$ and $\alpha>0$ such that for all $\eta_{i,j}\in\mathcal{B}$ there is a $p\in\mathcal{N}$ with $u_i^\theta(p),u_j^\theta(p)\geqslant\alpha>0$ for all $\theta\in U$. To show the continuity of $\theta\mapsto w^\theta$ in U let (by abuse of notation) $\theta_0\in U$ be arbitrary and fixed and $\theta\in U$ arbitrary.

First, we show $Pw^\theta\to Pw^{\theta_0}$ as $\theta\to\theta_0$. To this end, we consider some arbitrary $\eta_{i,j}\in\mathcal{B}$ with associated vertex $p\in\mathcal{N}$ such that $u_i^\theta(p),u_j^\theta(p)\geqslant\alpha>0$ for all $\theta\in U$. Then $v_\pm^\theta=u^\theta\pm\delta v\geqslant 0$ with $v=\eta_{i,j}\lambda_p$ holds for $\delta<\alpha$ and all $\theta\in U$. Testing the variational inequality for θ with v_+^θ and for θ_0 with $v_-^{\theta_0}$, adding both and dividing by δ yields

$$\begin{aligned}(w^\theta-w^{\theta_0},v) \leqslant{}& \varepsilon^2(\nabla(u^\theta-u^{\theta_0}),\nabla v)+\varepsilon^2\int_\Omega u^\theta-u^{\theta_0}\,\mathrm{d}x\cdot\int_\Omega v\,\mathrm{d}x\\ &+\theta\frac{\phi_1^{\mathcal{T}}(u^\theta+\delta v)-\phi_1^{\mathcal{T}}(u^\theta)}{\delta}-\theta_0\frac{\phi_1^{\mathcal{T}}(u^{\theta_0})-\phi_1^{\mathcal{T}}(u^{\theta_0}-\delta v)}{\delta}.\end{aligned}$$

As $u_i^\theta(p),u_j^\theta(p),u_i^{\theta^0}(p),u_j^{\theta_0}(p)>0$, the scalar functions $\xi\mapsto\phi_\theta^{\mathcal{T}}(u^\theta+\xi v)$ and $\xi\mapsto\phi_\theta^{\mathcal{T}}(u^{\theta_0}-\xi v)$ are differentiable in $\xi=0$. Hence, we can pass to the limit $\delta=0$ and use the Hölder continuity of Theorem 3.5 to obtain

$$(w^\theta-w^{\theta_0},v)\leqslant C(|\theta-\theta_0|^{1/2}\|v\|_1+\theta\Phi_1'(u^\theta)+\theta_0\Phi_1'(u^{\theta_0}))\xrightarrow[\theta\to\theta_0]{}0.$$

Exchanging the role of θ_1 and θ_2 and using $Pv=v$, we finally obtain

$$|(P(w^\theta-w^{\theta_0})\cdot\eta_{i,j},\lambda_p)|=|(w^\theta-w^{\theta_0},v)|\xrightarrow[\theta\to\theta_0]{}0. \tag{3.11}$$

In combination with $\nabla P(w^\theta-w^{\theta_0})\to 0$, the convergence (3.11) provides $P(w^\theta-w^{\theta_0})\cdot\eta_{i,j}\to 0$, since $|\cdot|_1+|(\cdot,\lambda_p)|$ is a norm on $\mathcal{S}$. As $\eta_{i,j}\in\mathcal{B}$ was arbitrarily chosen, we have shown $P(w^\theta-w^{\theta_0})\to 0$. This holds for all solutions w^{θ_0}. Hence, Pw^{θ_0} must be unique.

Finally, we show $w^\theta \to w^{\theta_0}$ as $\theta \to \theta_0$. To this end, we select for each node $p \in \mathcal{N}$ some $1 \leqslant i_p \leqslant N$ such that $u^{\theta_0}_{i_p}(p) \geqslant 2\beta > 0$ for some $\beta > 0$. This is possible because $u^{\theta_0}(p) \cdot \mathbf{1} = 1$ holds for all nodes $p \in \mathcal{N}$. By the continuity of $\theta \mapsto u^\theta$, we also have $u^\theta_{i_p}(p) \geqslant \beta > 0$ for all $\theta \in U' \subset U$ with a possibly smaller neighbourhood U' of θ_0.

For any $p \in \mathcal{N}$, $\theta \in U'$ and $\delta < \beta$ we then have $v^\theta_\pm = u^\theta \pm \delta v > 0$ with $v = e^{i_p}\lambda_p$. Proceeding literally as above, we obtain

$$|((w^\theta - w^{\theta_0})_{i_p}, \lambda_p)| = |(w^\theta - w^{\theta_0}, v)| \underset{\theta \to \theta_0}{\longrightarrow} 0. \tag{3.12}$$

Since $v \mapsto \|P \cdot v\|_1 + \sum_{p\in\mathcal{N}} |(v_{i_p}, \lambda_p)|$ is a norm on $\mathcal{S}^N$, combining (3.12) with $P(w^\theta - w^{\theta_0}) \to 0$ gives $w^\theta - w^{\theta_0} \to 0$. Again, this implies the uniqueness of w^{θ_0}. □

The assumption on $\mathcal{N}$ in Theorem 3.6 essentially means that the discrete interfacial region is rich enough to contain a suitable set of nodal basis functions. This assumption can be replaced by the more instructive, but much stronger condition that at least one of the components that are present at a certain vertex must also be present at each neighbouring one. This property can always be achieved by resolving the diffuse interface sufficiently well.

LEMMA 3.7 Assume that for some fixed $\theta_0 \geqslant 0$ the given u^{old} satisfies the nondegeneracy condition (3.8) and that for any pair (p, q) of neighbouring vertices we have

$$\{1 \leqslant i \leqslant N \mid u_i(p) > 0\} \cap \{1 \leqslant i \leqslant N \mid u_i(q) > 0\} \neq \emptyset. \tag{3.13}$$

Then there is a set $\mathcal{B} \subset V_0$ of vertices satisfying the assumption in Theorem 3.6.

Proof. It is sufficient to construct subsets $\mathcal{B}_i$, $i = 1, \ldots, N$ of the form (3.10), i.e.,

$$\mathcal{B}_i = \{\eta_{k,j} \mid \eta_{k,j} = e^k - e^j \text{ with } k \neq j \text{ and } u_k(p), u_j(p) > 0 \text{ for some } p \in \mathcal{N}\}$$

such that $e^i - e^1 \in \operatorname{span} \mathcal{B}_i$, because then the vectors $e^i - e^1$, $i = 1, \ldots, N$, spanning V_0, are contained in the span of

$$\mathcal{B} := \bigcup_{i=1}^{N} \mathcal{B}_i.$$

Let us consider some fixed $i \in \{1, \ldots, N\}$. By the degeneracy condition (3.8) there are vertices q_1, $q_i \in \mathcal{N}$ such that $u_1(q_1) > 0$, $u_i(q_i) > 0$. Since the grid $\mathcal{T}$ is a connect graph, there is a path $p^1, \ldots, p^K$ of neighbouring vertices with $p^1 = q_1$ and $p^K = q_i$.

We now assign a component $c_k \in \{1, \ldots, N\}$ to each p^k in the following way. We start by setting $c_1 = 1$ so that $u_{c_1}(p^1) > 0$ and assume $u_{c_{k-1}}(p^{k-1}) > 0$ for some $k > 1$. Then we keep $c_k := c_{k-1}$, if $u_{c_{k-1}}(p^k) > 0$, i.e., if the component c_{k-1} is still present at the neighbouring vertex p^k. If this is not the case, then we switch to a new component c_k with $u_{c_k}(p^k) > 0$ and $u_{c_k}(p^{k-1}) > 0$, i.e., to a new component which is present in both vertices p^k and p^{k-1}. This is possible due to assumption (3.13). Finally, we formally set

$c_{K+1} = i$ and define

$$\mathcal{B}_i = \{e^{c_k} - e^{c_{k-1}} \mid c_k \neq c_{k-1}, k = 2, \dots, K+1\}.$$

By construction, $u_{c_k}(p^{k-1})$, $u_{c_{k-1}}(p^{k-1}) > 0$ holds for all $k = 2, \dots, K+1$ so that $\mathcal{B}_i$ is of the desired form. Moreover, we have $e^i - e^1 \in \operatorname{span} \mathcal{B}_i$ using the telescope sum

$$e^i - e^1 = \sum_{k=2}^{K+1} e^{c_k} - e^{c_{k-1}} \in \operatorname{span} \mathcal{B}_i.$$

□

Obviously, the assumption in Lemma 3.7 can be weakened by applying the same arguments to certain paths of not necessarily neighbouring vertices. However, this essentially amounts to a reformulation of the abstract assumption of Theorem 3.6 again.

3.5 *Algebraic formulation*

Now we rewrite the discrete problem (VI) in an algebraic fashion. This will simplify the derivation and convergence analysis of nonsmooth Schur–Newton methods for the iterative solution of (VI) presented in the next section. Starting from an enumeration $\mathcal{N} = \{p_1, \dots, p_m\}$ of the $m = \#\mathcal{N}$ vertices, we enumerate the $n = mN$ nodal basis functions of $\mathcal{S}^N$ according to

$$\{\lambda^1, \lambda^2, \dots, \lambda^n\}, \quad \lambda^{\pi(i,k)} = e^i \lambda_{p_k}, \ \ i = 1, \dots, N, \ k = 1, \dots m,$$

utilizing the bijective index map $\pi\{1, \dots, N\} \times \{1, \dots, m\} \to \{1, \dots, n\}$ defined by $\pi(i,k) = i + N(k-1)$. Utilizing the canonical isomorphism $\mathcal{S}^N \ni v \mapsto V = (V_i) \in \mathbb{R}^n$ induced by the basis representation

$$v = \sum_{i=1}^{n} V_i \lambda^i, \quad v \in \mathcal{S}^N,$$

the solution of (VI) amounts to finding $U, W \in \mathbb{R}^n$ such that

$$\begin{aligned} AU \cdot (V - U) + \varphi(V) - \varphi(U) + BW \cdot (V - U) &\geqslant f \cdot (V - U) \quad \forall V \in \mathbb{R}^n, \\ BU - CW &= g. \end{aligned} \tag{3.14}$$

Here, we have used the matrices $A = (A_{ij})$, $B = (B_{ij})$, $C = (C_{ij}) \in \mathbb{R}^{n,n}$ given by

$$A_{ij} = \varepsilon^2 (\nabla \lambda^j, \nabla \lambda^i) + (M^{\mathrm{T}} M)_{ij}, \quad B_{ij} = -(\lambda^j, \lambda^i), \quad C_{ij} = \tau (L \nabla \lambda^j, \nabla \lambda^i), \tag{3.15}$$

where the definition

$$M_{i,j} = \varepsilon \left(\int_\Omega \lambda^j \right)_i, \quad i = 1, \dots, N, \ \ j = 1, \dots n \tag{3.16}$$

of $M = (M_{ij}) \in \mathbb{R}^{N,n}$ provides $M^{\mathrm{T}} M U \cdot V = \varepsilon^2 \int_\Omega u \, \mathrm{d}x \cdot \int_\Omega v \, \mathrm{d}x$. The algebraic representation

$$\varphi(V) = \sum_{i=1}^{n} \varphi_i(V_i), \quad \text{with} \quad \varphi_i(\xi) = \Phi_\theta(\xi) \int_\Omega \lambda^i \, \mathrm{d}x, \tag{3.17}$$

of the nonlinearity ϕ_θ satisfies $\varphi(V) = \phi_\theta(v)$ and the right-hand sides $f = (f_i)$, $g = (g_i) \in \mathbb{R}^n$ are given by

$$f_i = -(Ku^{\text{old}}, \lambda^i) + \left(M^{\mathrm{T}} M \int_\Omega u^{\text{old}} \, \mathrm{d}x \right)_i, \quad g_i = -(u^{\text{old}}, \lambda^i). \tag{3.18}$$

In analogy to (3.3) the variational problem (3.14) can be reformulated as the saddle-point problem

$$\mathcal{L}(U, W) = \inf_{V \in \mathbb{R}^n} \sup_{Z \in \mathcal{S}^N} \mathcal{L}(V, Z) \tag{3.19}$$

for the Lagrangian

$$\mathcal{L}(U, W) = \tfrac{1}{2} AU \cdot U - f \cdot U + \varphi(U) + (BU - g) \cdot W - \tfrac{1}{2} CW \cdot W.$$

The construction and convergence analysis of nonsmooth Schur–Newton methods presented below will rely on the following reformulation.

Proposition 3.8 The discrete spatial problem (VI) is equivalent to the following set-valued saddle-point problem.

(VIA) Find U, $W \in \mathbb{R}^n$ such that

$$\begin{pmatrix} A + \partial\varphi & B^{\mathrm{T}} \\ B & -C \end{pmatrix} \begin{pmatrix} U \\ W \end{pmatrix} \ni \begin{pmatrix} f \\ g \end{pmatrix}$$

with the symmetric, positive definite matrix $A \in \mathbb{R}^{n,n}$, $B \in \mathbb{R}^{n,n}$, the symmetric, positive semidefinite matrix $C \in \mathbb{R}^{n,n}$, the subdifferential $\partial\varphi$ of the lower semicontinuous, proper convex functional $\varphi : \mathbb{R}^n \to \mathbb{R}$ and f, $g \in \mathbb{R}^n$ given in (3.15–3.18).

4. Nonsmooth Schur–Newton methods

In this section, we consider the efficient algebraic solution of set-valued saddle-point problems of the form (VIA) with a symmetric, positive definite matrix $A \in \mathbb{R}^{n,n}$, some matrix $B \in \mathbb{R}^{n,n}$, a symmetric, positive semidefinite matrix $C \in \mathbb{R}^{n,n}$, the subdifferential $\partial\varphi$ of a lower semicontinuous, proper convex functional $\varphi : \mathbb{R}^n \to \mathbb{R}$ and f, $g \in \mathbb{R}^n$ by nonsmooth Schur–Newton methods. This approach was introduced and applied to discretized binary Cahn–Hilliard equations with obstacle potential in Gräser & Kornhuber (2009b). It was extended to more general nonsmooth nonlinearities and applied to a binary Cahn–Hilliard equation with logarithmic potential in Gräser (2011, 2013) and Gräser & Sander (2013). For completeness, we present the basic ideas and convergence results, referring the reader to Gräser (2013) and Gräser & Kornhuber (2009b) for details.

4.1 *Nonlinear Schur complement and unconstrained minimization*

Nonsmooth Schur–Newton methods are based on the reformulation of the set-valued saddle-point problem (VIA) as a dual, unconstrained minimization problem. In a first step, we eliminate the primal variable U from (VIA).

LEMMA 4.1 The set-valued saddle-point problem (VIA) is equivalent to the nonlinear system

$$H(W) = 0 \tag{4.1}$$

with the single-valued, Lipschitz-continuous nonlinear Schur complement

$$H(W) = -B(A + \partial\varphi)^{-1}(f - B^{\mathrm{T}}W) + CW + g \tag{4.2}$$

in the sense that (U, W) is a solution of (VIA) if and only if W solves (4.1) and $U = (A + \partial\varphi)^{-1}(f - B^{\mathrm{T}}W)$.

Proof. The inverse $(A + \partial\varphi)^{-1}$ of $A + \partial\varphi$ is single valued and Lipschitz continuous with Lipschitz constant given by the inverse of the coercivity constant of A, because A is symmetric and positive definite, and φ is lower semicontinuous, proper convex (Ekeland & Temam, 1976b, Part One, Chapter II). Now the assertion follows from straightforward computation. □

In the linear case $\partial\varphi \equiv 0$, it is well known that the Schur complement $BA^{-1}B^{\mathrm{T}} + C$ is symmetric and positive definite. We now provide an extension of this property to the present nonlinear case.

PROPOSITION 4.2 There is a Fréchet-differentiable convex functional $h : \mathbb{R}^n \to \mathbb{R}$ such that $H = \nabla h$.

Proof. Using Ekeland & Temam (1976a, p. 22, Corollary 5.2), it follows that $H = \partial h$ is the subdifferential of

$$h(W) = -\inf_{V \in \mathbb{R}^n} \mathcal{L}(V, W) = -\mathcal{L}((A + \partial\varphi)^{-1}(f - B^{\mathrm{T}}W), W).$$

As $\partial h = H$ is single valued and continuous, h is even Fréchet-differentiable and $H = \nabla h$ is the Fréchet derivative of h. □

As a direct consequence of Lemma 4.1 and Proposition 4.2, the set-valued saddle-point problem (VIA) is equivalent to finding $W \in \mathbb{R}^n$ such that

$$h(W) \leqslant h(V) \quad \forall V \in \mathbb{R}^n \tag{4.3}$$

and then solving $AU + \partial\varphi(U) \ni f - B^{\mathrm{T}}W$. We emphasize that (4.3) now is an unconstrained convex minimization problem for an LC^1 function to which classical gradient-related descent methods can be applied.

4.2 *Gradient-related descent methods*

We give a short summary of this approach referring to textbooks like, e.g., Ortega & Rheinboldt (1970), for the general theory or to Gräser (2011) and Gräser & Kornhuber (2009b) for a more specific presentation.

We consider iterative methods for the approximation of minimizers of a given functional $h : \mathbb{R}^n \to \mathbb{R}$ of the form

$$W^{\nu+1} = W^\nu + \rho_\nu D^\nu. \tag{4.4}$$

The search directions $D^\nu \in \mathbb{R}^n$ are called gradient related if for any sequence $(W^\nu) \subset \mathbb{R}^n$ the conditions

$$\nabla h(W^\nu) = 0 \quad \Longleftrightarrow \quad D^\nu = 0$$

and

$$-\nabla h(W^\nu) \cdot D^\nu \geqslant c_D |\nabla h(W^\nu)|\, |D^\nu|$$

hold for all $\nu \in \mathbb{N}$ with a constant $c_D > 0$ independent of ν. For example, the gradients $D^\nu = -\nabla h(W^\nu)$ are gradient related, and we obtain the classical gradient method for this choice. Faster convergence can be expected for preconditioned gradient methods resulting from search directions of the form

$$D^\nu = -S_\nu^{-1} \nabla h(W^\nu) \tag{4.5}$$

with a sequence $(S_\nu) \subset \mathbb{R}^{n,n}$ of suitable symmetric, positive definite preconditioners. Such search directions are gradient related if there are constants $\gamma, \Gamma > 0$ such that

$$\gamma |V|^2 \leqslant S_\nu V \cdot V \leqslant \Gamma |V|^2 \tag{4.6}$$

holds uniformly in $\nu \in \mathbb{N}$.

While the search directions D^ν are constructed to allow for suitable descent of the functional h, the step sizes ρ_ν should guarantee that this descent is actually realized. A sequence $(\rho_\nu) \subset \mathbb{R}$ of step sizes is called *efficient* if

$$h(W^\nu + \rho_\nu D^\nu) \leqslant h(W^\nu) - c_S \left(\frac{\nabla h(W^\nu) \cdot D^\nu}{|D^\nu|} \right)^2 \tag{4.7}$$

holds with a constant $c_S > 0$ independent of ν.

THEOREM 4.3 Assume that the search directions take the form $D^\nu = -S_\nu^{-1} \nabla h(W^\nu)$ with symmetric, positive definite preconditioners $S_\nu \in \mathbb{R}^{n,n}$ satisfying (4.6), that the step sizes ρ_ν are efficient in the sense of (4.7) and that h has a unique minimizer. Then the sequence (W^ν) produced by (4.4) converges to the minimizer of h for $\nu \to \infty$.

Proof. See Gräser (2011, Theorems 5.2 and 5.7). The proof presented there is based on the fact that the uniqueness of the minimizer implies the compactness of the sublevel set $\{W \in \mathbb{R}^n \,|\, h(W) \leqslant h(W^0)\}$. Using this the rest can essentially be shown with standard arguments as, e.g., in Ortega & Rheinboldt (1970). □

Efficiency of the step sizes ρ_ν can be guaranteed by various strategies such as, e.g., the Armijo rule (see, e.g., Deuflhard, 2004, Chapter 3 for a detailed discussion). In order to reduce the number of tuning parameters involved, we propose a strategy that approximates the minimizer of h along $W^\nu + \rho D^\nu$, $\rho \in \mathbb{R}$.

PROPOSITION 4.4 Assume that the search directions in the descent method (4.4) take the form $D^\nu = -S_\nu^{-1} \nabla h(W^\nu)$ and that

$$\nabla h(W^\nu + \rho_\nu D^\nu) \cdot D^\nu \in [\alpha \nabla h(W^\nu) \cdot D^\nu, 0]$$

holds for all $\nu \in \mathbb{N}$ with some $\alpha \in [0, 1)$ independent of ν. Then the step sizes ρ_ν are efficient.

Proof. For the proof, see Gräser (2011, Proposition 5.4). □

REMARK 4.5 Utilizing Proposition 4.4 with fixed $\alpha \in (0,1)$, efficient step sizes ρ_ν can be computed by a simple bisection algorithm. However, as each iteration step requires the evaluation of $H = \nabla h$ and thus of $(A+\varphi)^{-1}$, this procedure might be quite costly. The actual computation of ρ_ν can be avoided if the monotonicity test

$$|D^\nu| \leqslant \sigma |D^{\nu-1}| \tag{4.8}$$

holds with some fixed $\sigma < 1$. In this case, convergence is preserved for $\rho_\nu = 1$. We refer the reader to Gräser (2011, Theorem 5.4) for details.

REMARK 4.6 The above convergence results also remain valid if the descent directions D^ν are replaced by approximations $\tilde{D}^\nu$ which are sufficiently accurate in the sense that the conditions

$$\tilde{D}^\nu \cdot \nabla h(W^\nu) < 0, \quad |D^\nu - \tilde{D}^\nu| / |\tilde{D}^\nu| \to 0$$

are satisfied. For a detailed analysis of such inexact versions we refer the reader to Gräser (2011).

In particular, Remark 4.6 allows for inexact evaluation of the preconditioner S_ν^{-1}.

4.3 *Nonsmooth Newton-like descent directions*

In the light of Theorem 4.3, the gradient-related descent method (4.4) with search directions of the form (4.5) converges globally for any sequence of symmetric, positive definite preconditioners S_ν with the property (4.6). We now aim at selecting S_ν in such a way that the convergence is locally fast. For a sufficiently smooth functional h, the Jacobian $S_\nu = \nabla^2 h(W^\nu)$ would clearly be a desirable choice because it leads to the classical Newton method with asymptotically quadratic convergence. Since for the given problem we cannot expect $\nabla h = H$ to be differentiable but only to be Lipschitz, the choice $S_\nu \in \partial_C H(W^\nu)$ with ∂_C denoting the generalized Jacobian in the sense of Clarke (1983) would be a natural generalization. However, an element of $\partial_C H(W^\nu)$ is difficult to obtain since, in general, we cannot make use of the chain rule. Following Gräser (2011) and Gräser & Kornhuber (2009b), we will therefore construct related nonsmooth Newton-like preconditioners S_ν by *postulating* the chain rule. We will focus on the basic ideas of construction and present the resulting preconditioner for the given problem (4.1), referring the reader to Gräser (2011) and Gräser & Kornhuber (2009b) for details.

Our starting point is the observation that some of the components of $(A+\partial\varphi)^{-1}$ are smooth in a given $Y \in \mathbb{R}^n$, while the others are not. To be precise, we introduce the inactive set

$$\bar{\mathcal{I}}(Y) := \{1 \leqslant i \leqslant n \mid \partial\varphi_i \text{ is single valued and differentiable in } Y_i\}.$$

For the given φ defined in (3.17), we obtain

$$\bar{\mathcal{I}}(Y) = \{1 \leqslant i \leqslant n \mid Y_i > 0\}. \tag{4.9}$$

It turns out that the ith component of the inverse $(A+\partial\varphi)^{-1}$ is differentiable in Y if $i \in \bar{\mathcal{I}}((A+\partial\varphi)^{-1}Y)$. This observation motivates the linearization

$$\partial(A+\partial\varphi)^{-1}(Y) := (A+\varphi''(X))^{+}_{\bar{\mathcal{I}}(X)} \tag{4.10}$$

of $(A+\partial\varphi)^{-1}$ at a given $Y \in (A+\partial\varphi)(X)$. Here, $\varphi''(X)$ denotes the diagonal matrix with diagonal entries $\varphi_i''(X_i)$, the matrix $M^+ \in \mathbb{R}^{n,n}$ stands for the Moore–Penrose pseudoinverse of $M \in \mathbb{R}^{n,n}$ and

$M_{\bar{\mathcal{I}}} \in \mathbb{R}^{n,n}$ denotes the so-called truncated matrix

$$(M_{\bar{\mathcal{I}}})_{i,j} = \begin{cases} M_{i,j} & \text{if } i,j \in \bar{\mathcal{I}}, \\ 0 & \text{otherwise.} \end{cases}$$

Truncation of a matrix means that certain lines and columns are set to zero. Note that the multiplication of the matrix $(A + \varphi''(X))^{+}_{\bar{\mathcal{I}}(X)}$ with a vector amounts to the solution of a *truncated linear system*, i.e., of a reduced linear system with a coefficient matrix consisting of the ith row and column unit vector in $\mathbb{R}^n$ if $i \notin \bar{\mathcal{I}}(X)$ and remaining entries taken from $A + \varphi''(X)$, respectively.

The definition (4.9) of inactive sets is well suited to the deep quench limit $\theta = 0$ because then the second derivatives of $\varphi_i(Y_i)$ are uniformly bounded, in fact equal to zero. This is different for the logarithmic potential, where the property $\varphi(Y_i) \to \infty$ for $Y_i \to 0$ might lead to badly scaled linearizations of the form (4.10). As a remedy we modify the definition of the active set according to

$$\mathcal{I}(Y) := \{1 \leqslant i \leqslant n \mid Y_i > \delta\} \tag{4.11}$$

with some fixed $\delta > 0$ such that $\varphi_i(Y_i) \leqslant c_T$ holds with a corresponding fixed constant c_T. We will use $c_T = 10^8$ in our numerical computations. Against this background, we finally define the linearization

$$\partial(A + \partial\varphi)^{-1}(Y) = (A + \varphi''(X))^{+}_{\mathcal{I}(X)}, \quad X = (A + \partial\varphi)^{-1}(Y)$$

of $(A + \partial\varphi)^{-1}$ at some given $Y \in \mathbb{R}^n$. Now, postulating the chain rule with $\partial(A + \partial\varphi)^{-1}$ as inner derivative, we obtain the nonsmooth Newton-like linearization

$$\partial H(Y) = B(A + \varphi''(X))^{+}_{\mathcal{I}(X)} B^{\mathrm{T}} + C, \quad X = (A + \partial\varphi)^{-1}(f - B^{\mathrm{T}}Y)$$

of H defined in (4.2) at some given $Y \in \mathbb{R}^n$.

The candidate $\partial H(W^\nu)$ for a preconditioner S_ν is symmetric and positive definite if and only if $\mathcal{I}(U^\nu) \neq \emptyset$ holds with $U^\nu = (A + \partial\varphi)^{-1}(W^\nu)$ because we get $\partial H(W^\nu) = C$ otherwise, and C is only positive semidefinite. Hence, in the nongeneric case $\mathcal{I}(U^\nu) = \emptyset$, we regularize $\partial H(W^\nu)$, e.g., by adding the scaled mass matrix τB to obtain

$$S_\nu = \begin{cases} \partial H(W^\nu) & \text{if } \mathcal{I}(U^\nu) \neq \emptyset, \\ \partial H(W^\nu) + \tau B & \text{otherwise.} \end{cases} \tag{4.12}$$

Definition 4.7 The gradient-related descent method (4.4) with search directions $D^\nu = -S_\nu^{-1} H(W^\nu)$, preconditioners $S_\nu \in \mathbb{R}^{n,n}$ defined in (4.12) and efficient step sizes ρ_ν is called a *nonsmooth Schur–Newton iteration* for the set-valued saddle-point problem (VIA).

Recall that efficient step sizes ρ_ν can be computed utilizing Proposition 4.4.

Theorem 4.8 Assume that (VIA) has a unique solution (U, W). Then, for any initial iterate $W^0 \in \mathbb{R}^n$, the nonsmooth Schur–Newton iteration converges to the solution W and $U = (A + \partial\varphi)^{-1}(f - B^{\mathrm{T}}W)$.

Proof. In the light of Theorem 4.3, it only remains to show that the preconditioners S_ν defined in (4.12) are symmetric and positive definite and satisfy condition (4.6). We refer the reader to Gräser (2011, Theorem 5.7). □

Recall that sufficient conditions for uniqueness are given in Theorem 3.6. Global convergence also holds for suitable inexact versions of (4.4) according to Remark 4.6.

By construction, we generally cannot expect $\partial H(W^\nu)$ to be contained in the set of generalized Jacobians in the sense of Clarke. Hence, the general theory of semismooth Newton methods cannot be applied to show local quadratic convergence. However, exploiting that the underlying solution space is finite-dimensional, related results can be easily shown directly.

REMARK 4.9 Assume that the parameter $\delta > 0$ in (4.11) is sufficiently small and that the monotonicity test in (4.8) is not used. Then the nonsmooth Schur–Newton method applied to the set-valued saddle-point problem (VIA) locally reduces to a classical Newton iteration in case of the logarithmic potential $\theta > 0$, and is even locally exact in the deep quench limit $\theta = 0$.

The numerical relevance of these asymptotic results is limited: for $\theta > 0$, sufficiently small parameters $\delta > 0$ typically lead to severe ill conditioning of the arising Hessian matrices and to convergence radii of the Newton iteration that are smaller than machine precision.

The general convergence analysis of nonsmooth Schur–Newton methods is based on arguments restricted to finite-dimensional spaces (see Gräser & Kornhuber, 2009b and Gräser, 2011 for a detailed discussion). Convergence results in function spaces are available only in special cases (Hinze & Vierling, 2012). However, numerical computations indicate mesh-independent convergence speed for initial iterates provided by nested iteration (cf. Gräser & Kornhuber, 2009b; Gräser, 2011 and the numerical experiments reported below). Theoretical validation of such local mesh independence is still open.

4.4 *Algorithmic aspects*

Rewriting the nonsmooth Schur–Newton iteration introduced in Definition 4.7 in the primal–dual form

$$U^\nu = (A + \partial\varphi)^{-1}(f - B^{\mathrm{T}}W^\nu),$$
$$W^{\nu+1} = W^\nu + \rho_\nu S_\nu^{-1}(BU^\nu + CW^\nu + g),$$

we obtain a preconditioned Uzawa method. Each iteration step amounts to the update of the primal variable U^ν, the evaluation of the preconditioned residual $S_\nu^{-1}(BU^\nu + CW^\nu + g)$ and the selection of a suitable step size ρ_ν.

The first substep is equivalent to the solution of the minimization problem

$$U^\nu = \arg\min_{V\in\mathbb{R}^n} \tfrac{1}{2}AV\cdot V + \varphi(V) - (f - B^{\mathrm{T}}W^\nu)\cdot V. \tag{4.13}$$

While there is a vast literature about elliptic obstacle problems emerging in the deep quench limit $\theta = 0$ (cf., e.g., Dostál, 2009; Gräser & Kornhuber, 2009a and the references therein), fast solvers for the logarithmic potential $\theta > 0$ that show robust convergence behaviour for $\theta \to 0$ are still rare (see, however, Kornhuber, 2002 and Kornhuber & Krause, 2006). In the numerical experiments reported below, we apply the *truncated nonsmooth Newton method* (TNNMG) (Gräser & Kornhuber, 2009a; Gräser *et al.*, 2009; Gräser, 2011) that combines robustness for $\theta \to 0$ with similar efficiency observed for classical multigrid methods in the linear self-adjoint case. Note that optimal complexity of each iteration step even for the dense matrix A is achieved by exploiting that A is the sum of a sparse matrix and a dense low-rank matrix with a known product representation (Gräser, 2004).

The preconditioned residual $W^{\nu+1/2} = S_\nu^{-1}(BU^\nu + CW^\nu + g)$ can be computed by (approximately) solving a truncated linear saddle-point problem of the form

$$\begin{pmatrix} \hat{A} & \hat{B}^{\mathrm{T}} \\ \hat{B} & -\hat{C} \end{pmatrix} \begin{pmatrix} \hat{U} \\ W^{\nu+1/2} \end{pmatrix} = \begin{pmatrix} \hat{f} \\ g \end{pmatrix} \tag{4.14}$$

with the symmetric, positive definite matrix $\hat{A} \in \mathbb{R}^{\hat{n},\hat{n}}$, $\hat{n} = n - \#\mathcal{I}(U^\nu)$, obtained by eliminating the ith row and column of A for all $i \in \mathcal{I}(U^\nu)$, the matrix $\hat{B} \in \mathbb{R}^{\hat{n},n}$ obtained by eliminating the ith row of B for all $i \in \mathcal{I}(U^\nu)$ and $\hat{C} = C$ if $\hat{n} > 0$ or $C = C + \tau B$ otherwise. In the numerical experiments reported below, we use a preconditioned GMRES iteration with a truncated version of the multigrid method with successive Vanka smoothers, suggested by Schöberl & Zulehner (2003) as a preconditioner. For an overview of other methods for the numerical solution of linear saddle-point problems, we refer the reader to Benzi *et al.* (2005).

Efficient step sizes ρ^ν can be computed utilizing Remark 4.5 which requires the evaluation of $\nabla h(W^\nu + \rho D^\nu) = H(W^\nu + \rho D^\nu)$ and thus the solution of a minimization problem of the form (4.13) in each bisection step. Recall that this costly procedure can be avoided for iterates that are sufficiently accurate in the sense that the monotonicity test (4.8) is passed.

5. Numerical experiments

5.1 *Problem, discretization and subproblem solvers*

We consider the multicomponent Cahn–Hilliard system (2.5) with $L = P = I - (1/N)(\mathbf{1}, \dots, \mathbf{1})$, $\varepsilon^2 = 5 \cdot 10^{-3}$ and logarithmic potential Ψ_θ defined by (2.2), where K is given by (2.4) with $\theta_c = 1.0$, on the computational domain $\Omega = (-1, 1) \times (-1, 1)$. We select $N = 4$ components and the temperature $\theta = 0.1$ if not stated otherwise. To obtain initial conditions with similar granularity for varying N, 200 circles with radius $0.1 - 0.15$ are randomly distributed over Ω and randomly assigned to the different components.

Throughout the following, we use the uniform time-step size $\tau = 10^{-3}$ and a grid hierarchy $\mathcal{T}_1, \dots, \mathcal{T}_j$ obtained by successive refinement of the initial triangulation $\mathcal{T}_0$ consisting of two triangles with hypotenuse oriented from the upper-left to lower-right vertex of Ω. Though adaptivity is clearly mandatory in practical applications and would not affect any of the algorithms or results presented above, we assume for simplicity that the triangulations are uniformly refined, i.e., the edges of all triangles are bisected in each refinement step. If not stated otherwise, we select $j = 8$ refinement steps, providing the triangulation $\mathcal{T}_8$ with $n_8 = 66049$ vertices and the mesh size $h_j = 2^{-7} \approx \varepsilon/9$. In this case, we found that the interface is resolved by about 11 grid points.

For the iterative solution of the resulting algebraic subproblems, we consider the nonsmooth Schur–Newton method (NSNMG) presented in Section 4 with multigrid solution of the nonlinear nonsmooth subproblems (4.13) and a preconditioned GMRES iteration for the linearized saddle-point problems (4.14).

More precisely, nonsmooth subproblems (4.13) are solved by a truncated nonsmooth Newton multigrid method (TNNMG) (Gräser & Kornhuber, 2009a; Gräser *et al.*, 2009; Gräser, 2011). Throughout the following, the iteration is executed almost up to machine precision, i.e., we use the stopping criterion

$$\|U^{\nu,k+1} - U^{\nu,k}\|_A < 10^{-13} \tag{5.1}$$

for the iterates $U^{\nu,k}$, $k = 1, \dots,$ with $\|\cdot\|_A$ denoting the energy norm induced by the matrix A.

The linear saddle-point problems (4.14) are solved by a preconditioned GMRES iteration with restart after 50 steps. The preconditioner is based on a straightforward extension of a truncated multigrid method with block-Gauß–Seidel smoother as suggested in Kornhuber (2002) and Schöberl & Zulehner (2003) for the case of vector-valued order parameters. In the light of Remark 4.6, the iteration is stopped if the ratio of the Euclidean norms of the preconditioned residual and the actual iterate is less than $\min(\zeta_1^\nu,\ \zeta_2\|W^\nu - W^{\nu-1}\|_{C,B}^2)$. Here, we chose $\zeta_1 = 10^{-1}$ and $\zeta_2 = 10^{-2}$ and the corrections $W^\nu - W^{\nu-1}$ of the overall NSNMG iteration are measured in the norm

$$\|V\|_{C,B} = \|V\|_C + \tau\|V\|_B, \quad V \in \mathbb{R}^n, \tag{5.2}$$

generated by the positive semidefinite matrix C and the mass matrix B defined in (3.15).

The step sizes ρ^ν are computed according to Proposition 4.4.

The overall NSNMG iteration is terminated once its target, the dual variable W, is approximated sufficiently well, i.e., once the stopping criterion

$$\|W^{\nu+1} - W^\nu\|_{C,B} < \kappa 10^{-11} \tag{5.3}$$

is satisfied with some $\kappa > 0$. We chose the default value $\kappa = 1$ if not stated otherwise.

5.2 *Evolution and distribution of computational work*

In our first experiment, we consider the evolution of $N = 6$ components. Here, we chose $\kappa = 2$ in the stopping criterion (5.3) in order to avoid the influence of round-off errors in our linear saddle-point solver.

The evolution over 1000 time steps is illustrated in Fig. 1. As expected, we observe fast separation in the beginning and slower dynamics in the course of the evolution. Triple, quadruple and even quintuple junctions occur with nicely equilibrated angles. It is also interesting to see that the evolution tends to a hexagonal structure of grains with equilibrated mass. Mass conservation is fulfilled up to 0.0053% over all time steps, which is in good accordance with our prescribed algebraic accuracy.

To illustrate the amount of computational work, Fig. 2 shows the total number of iterations of NSNMG (red), TNNMG (blue) and preconditioned GMRES (green) for each spatial problem, scaled by their respective values in the first time step (6 (NSNMG), 45 (TNNMG) and 281 (preconditioned GMRES)), over the number of time steps. The initial iterate is obtained by nested iteration in each case. We observe exactly 6 NSNMG iterations for all spatial problems and only slight changes in the performance of TNNMG and preconditioned GMRES. No damping was needed throughout the evolution. Hence, the solution of each subproblem (4.13) only required about 7 iterations of TNNMG. This is in accordance with previous computations, where TNNMG exhibited linear multigrid efficiency and mesh-independent convergence rates for initial iterates provided by nested iteration (Gräser *et al.*, 2009; Gräser, 2011). Preconditioned GMRES needed more than 40 iterations for each linear solve and thus strongly dominates the overall computational work. Moreover, we found that our straightforward multigrid preconditioning did not provide mesh independence. Hence, the overall efficiency of NSNMG will benefit from more sophisticated linear saddle-point solvers as have been studied elsewhere (see, e.g., Murphy *et al.*, 2000).

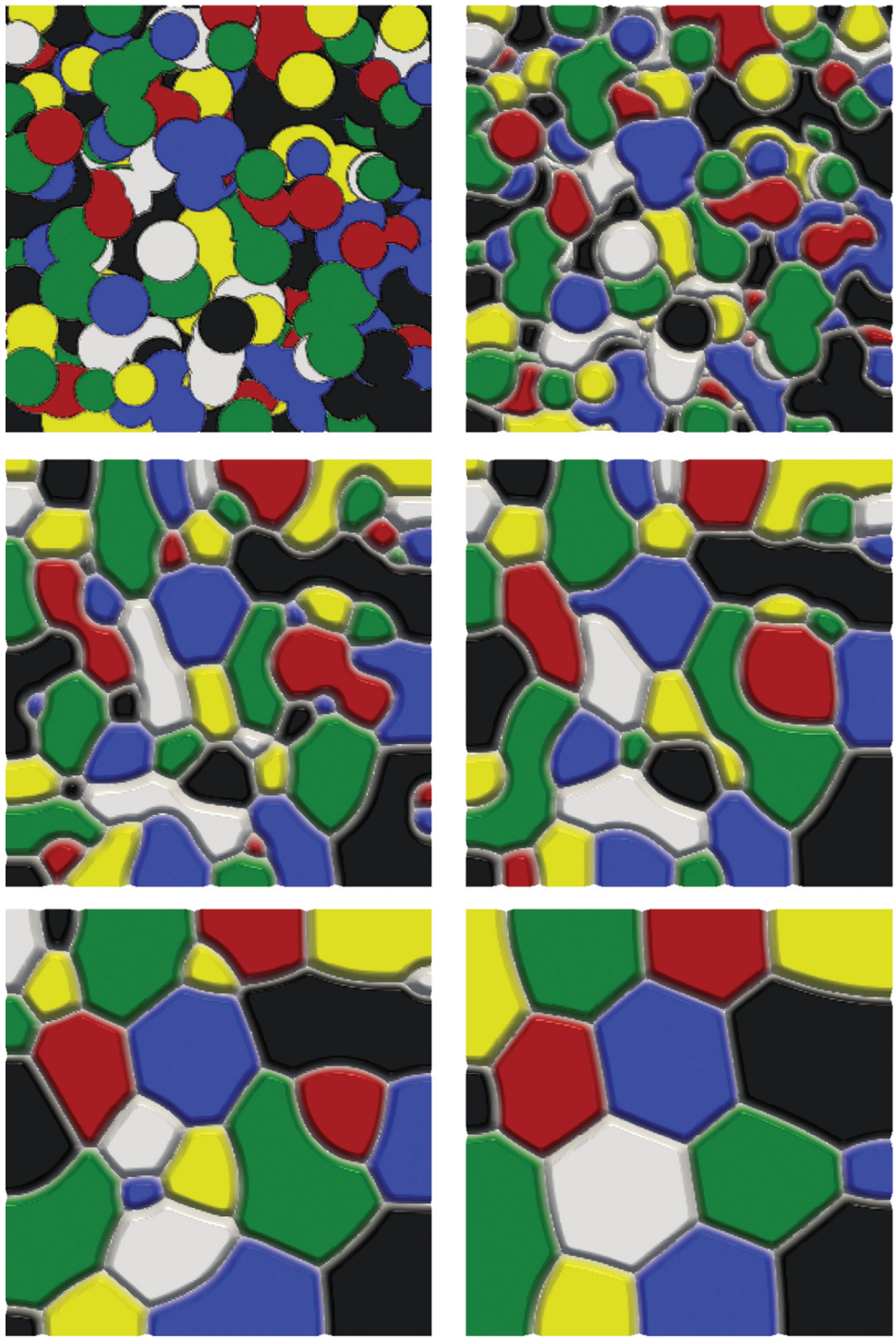

FIG. 1. Initial condition u_0 and approximate order parameter $u(\cdot, t)$ at time $t = 1\tau,\ 20\tau,\ 50\tau,\ 200\tau,\ 1000\tau$.

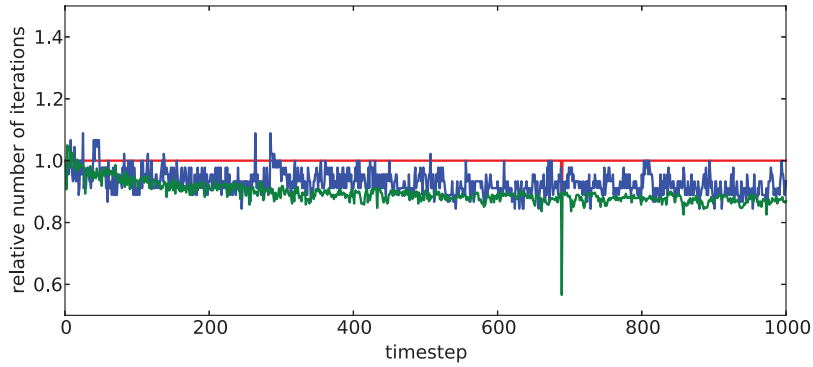

FIG. 2. Total number of iterations by NSNMG (red), TNNMG (blue) and preconditioned GMRES (green), scaled by their value in the first time step (6 (NSNMG), 45 (TNNMG) and 281 (preconditioned GMRES)), over the number of time steps.

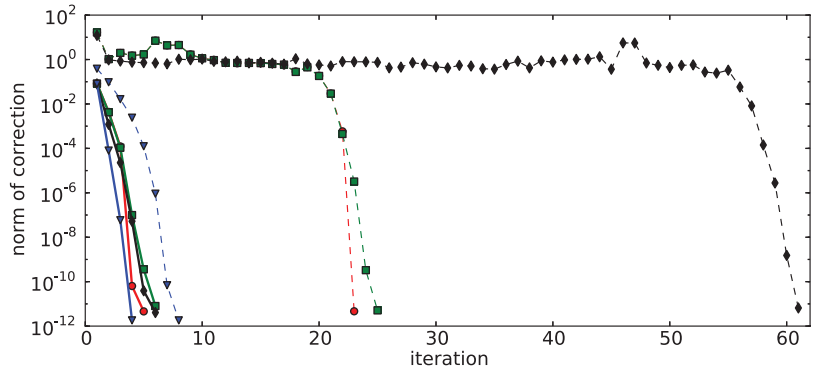

FIG. 3. Approximate algebraic error $\|W^{\nu} - W^{\nu-1}\|_{C,B}$ over the number of NSNMG iterations for the temperatures $\theta = 0.0$ (red •), 0.001 (green), 0.1 (black), 0.5 (blue) with initial iterates $W^0 = 0$ (dashed lines) and nested iteration (solid lines) for the first spatial problem.

5.3 *Influence of initial iterate, temperature, number of components and spatial mesh size on the convergence speed*

In our next experiment, we come back to $N = 4$ components and study the influence of initial iterates W^0 and temperature θ on the convergence speed of NSNMG. As the performance of NSNMG hardly changed for different spatial problems (cf. Section 5.2), we concentrate on the first one. Figure 3 shows the approximate algebraic error $\|W^{\nu} - W^{\nu-1}\|_{C,B}$ over the number of NSNMG iterations for the temperatures $\theta = 0.5$ (blue), 0.1 (black), 0.001 (green), 0.0 (red) with 'bad' initial iterates $W^0 = 0$ (dashed lines) and 'good' initial iterates obtained by nested iteration (solid lines). For bad initial iterates, the iteration history can be separated into an asymptotic phase with slow convergence and step sizes $\rho^{\nu} < 1$ and into an asymptotic phase with superlinear convergence speed. The asymptotic phase is entered immediately for initial iterates obtained by nested iteration. While we observe a strong influence of the temperature θ on the duration of the asymptotic phase, it hardly seems to affect the asymptotic superlinear convergence speed.

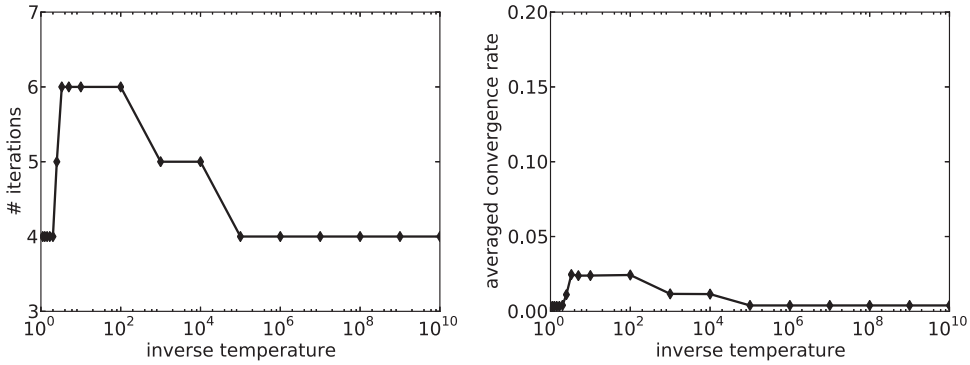

FIG. 4. Number of NSNMG iterations over inverse temperature $1/\theta$ (left) and averaged convergence rates of NSNMG over $1/\theta$ (right).

This suggests robustness of NSNMG with respect to temperature θ for initial iterates obtained by nested iteration, which is confirmed by our next experiment, illustrated in Fig. 4. The left-hand picture shows the number of iterations required to meet the stopping criterion (5.3) with $\kappa = 1$ over the inverse temperature $1/\theta$. We chose the values $\theta = i \cdot 10^{-1}$, $i = 1, \ldots, 9$ and $\theta = 10^{-i}$, $i = 2, \ldots, 10$. The corresponding averaged convergence rates are shown in the right-hand picture. In a sense, problems with $\theta \approx \theta_c = 1$ and $\theta \approx 0$ seem to be a little easier to solve than problems with medium temperatures, such as, e.g., $\theta = 0.1$. Observe that the convergence behaviour for $\theta = 10^{-5}$ cannot be distinguished from the deep quench limit $\theta = 0$. At most 6 NSNMG iterations were required to reduce the approximate error by ten orders of magnitude. The averaged NSNMG convergence rate is always far below 0.05 so that usually one or two NSNMG steps would be enough to reduce the algebraic error below the discretization accuracy. Each NSNMG step amounts to the total number of at most 23 TNNMG iterations and one inexact linear saddle-point solution. This means that the average number of TNNMG iterations for each occurring subproblem (4.13) is less than 6, which nicely confirms efficiency and robustness of this method (Gräser *et al.*, 2009; Gräser, 2011). Again the overall computational work is strongly dominated by the inexact linear saddle-point solution which is partly due to the larger number of unknowns.

In the next experiment, we assess the influence of the number N of components on the convergence speed of NSNMG. Here, we had to choose $\kappa = 7$ in the stopping criterion (5.3) in order to avoid the influence of round-off errors in our linear saddle-point solver. The left-hand picture of Fig. 5 shows the number of NSNMG iterations over N, while the right-hand picture shows the corresponding averaged convergence rates. Again, the initial iterates are obtained by nested iteration. The number of NSNMG iterations varies between 5 and 6 over $N = 2, \ldots, 10$ components, indicating considerable robustness of the convergence speed of NSNMG with respect to the number of components. This robustness is preserved by TNNMG, which required less than a total number of 45 TNNMG iterations in each NSNMG step to solve the nonlinear nonsmooth subproblems (4.13) almost up to machine accuracy.

As the convergence theory presented in Section 4.2 is partly based on arguments that are restricted to finite-dimensional spaces, we now investigate the mesh dependence of NSNMG. As we are interested in the local asymptotic convergence speed, the initial iterates are obtained by nested iteration. The left-hand picture of Fig. 6 shows the number of NSNMG iterations over the number n_j of vertices of the triangulations $\mathcal{T}_j$ on the levels $j = 4, \ldots, 8$, while the right-hand picture shows the corresponding averaged convergence rates. For the mesh size ranging from $h_4 = 2^{-3}$ to $h_8 = 2^{-7}$, the number of NSNMG

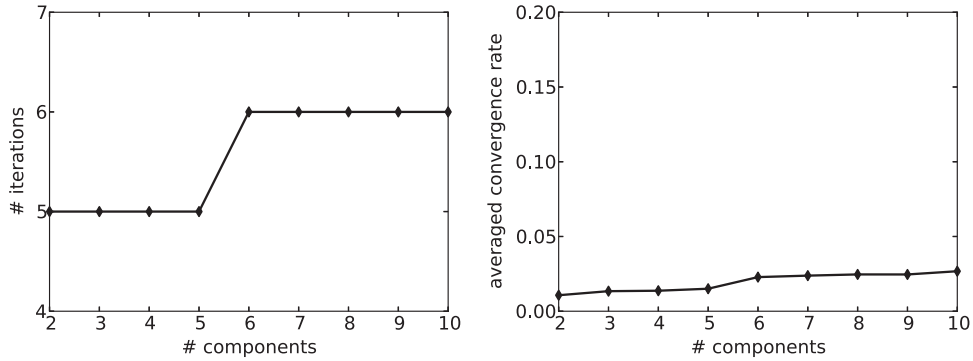

FIG. 5. Number of NSNMG iterations over the number N of components (left) and averaged convergence rates of NSNMG over N (right).

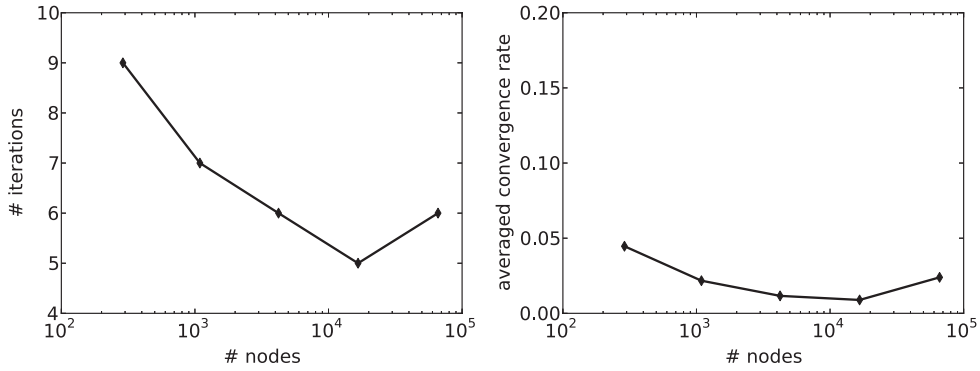

FIG. 6. Number of NSNMG iterations over the number of vertices n_j on the refinement levels $j = 4, \ldots, 8$, (left) and averaged convergence rates of NSNMG over n_j, $j = 4, \ldots, 8$, (right).

iterations is bounded by 9, suggesting local mesh-independent convergence of NSNMG and even local convergence of a related approach in function space (see Hinze & Vierling, 2012 for a first result in this direction). Theoretical justification will be the subject of future research.

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