On preconditioned Uzawa-type iterations for a saddle point problem with inequality constraints

Carsten Gräser[1] and Ralf Kornhuber[1]

FU Berlin, FB Mathematik und Informatik
(http://www.math.fu-berlin.de/rd/we-02/numerik/)

Summary. We consider preconditioned Uzawa iterations for a saddle point problem with inequality constraints as arising from an implicit time discretization of the Cahn-Hilliard equation with obstacle potential. We present a new class of preconditioners based on linear Schur complements associated with successive approximations of the coincidence set. In numerical experiments, we found superlinear convergence and finite termination.

1 Introduction

Since their first appearance in the late fifties, Cahn-Hilliard equations have become the prototype class of phase-field models for separation processes, e.g., of binary alloys [7, 11, 19]. As a model problem, we consider the scalar Cahn-Hilliard equation with isotropic interfacial energy, constant mobilities and obstacle potential [3, 4]. In particular, we concentrate on the fast solution of the algebraic spatial problems as resulting from an implicit time discretization and a finite element approximation in space [4]. Previous block Gauß-Seidel schemes [2] and the very popular ADI-type iteration by Lions and Mercier [18] suffer from rapidly deteriorating convergence rates for increasing refinement. In addition, the Lions-Mercier algorithm requires the solution of an unconstrained saddle point problem in each iteration step.

Our approach is based on a recent reformulation of the spatial problems in terms of a saddle point problem with inequality constraints [15]. Similar problems typically arise in optimal control. In contrast to interior point methods [22] or classical active set strategies we do not regularize or linearize the inequality constraints but directly apply a standard Uzawa iteration [14]. In order to speed up convergence, appropriate preconditioning is essential.

Preconditioning is well-understood in the linear case [1, 6, 12, 16] and variants for nonlinear and nonsmooth problems have been studied as well [8, 9]. However, little seems to be known about preconditioning of saddle point problems with inequality constraints or corresponding set-valued operators. For

such kind of problems a reduced linear problem is recovered, once the exact coincidence set is known. In this case, preconditioning by the associated Schur complement would provide the exact solution in a single step. As the exact coincidence set is usually not available, our starting point for preconditioning is to use the Schur complement with respect to some approximation. General results by Glowinski et al. [14] provide convergence. To take advantage of the successive approximation of the coincidence set in course of the iteration, it is natural to update the preconditioner in each step. In our numerical computations the resulting updated version shows superlinear convergence and finite termination. Previous block Gauß-Seidel schemes [2] are clearly outperformed. The convergence analysis and related inexact variants are considered elsewhere [15].

This paper is organized as follows. After a short revision of the continuous problem and its discretization, we introduce the basic saddle point formulation. In Section 4 we present the Uzawa iterations and Section 5 is devoted to the construction of preconditioners. We conclude with some numerical experiments.

2 The Cahn-Hilliard equation with obstacle potential

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain. Then, for given $\gamma > 0$, final time $T > 0$ and initial condition $u_0 \in \mathcal{K} = \{v \in H^1(\Omega) : |v| \leq 1\}$, we consider the following initial value problem for the Cahn-Hilliard equation with obstacle potential [3].

(P) Find $u \in H^1(0,T;(H^1(\Omega))') \cap L^\infty(0,T;H^1(\Omega))$ and $w \in L^2(0,T;H^1(\Omega))$ with $u(0) = u_0$ such that $u(t) \in \mathcal{K}$ and

$$\begin{aligned} \left\langle \frac{du}{dt}, v \right\rangle_{H^1(\Omega)} + (\nabla w, \nabla v) &= 0, && \forall v \in H^1(\Omega), \\ \gamma\,(\nabla u, \nabla v - \nabla u) - (u, v-u) &\geq (w, v-u)\,, && \forall v \in \mathcal{K} \end{aligned}$$

holds for a.e. $t \in (0,T)$.

Here $(\cdot,\cdot)$ stands for the L^2 scalar product and $\langle\cdot,\cdot\rangle_{H^1(\Omega)}$ is the duality pairing of $H^1(\Omega)$ and $H^1(\Omega)'$. The unknown functions u and w are called order parameter and chemical potential, respectively. The following existence and uniqueness result was shown by Blowey and Elliott [3].

Theorem 1. *Let $u_0 \in \mathcal{K}$ with $|(u_0, 1)| < |\Omega|$. Then* **(P)** *has a unique solution.*

For simplicity, we assume that Ω has a polygonal boundary. Let $\mathcal{T}_h$ denote a triangulation of Ω with maximal diameter h and vertices $\mathcal{N}_h$. Then $\mathcal{S}_h$ is the corresponding space of linear finite elements spanned by the standard nodal basis φ_p, $p \in \mathcal{N}_h$. Using the lumped L^2 scalar product $\langle\cdot,\cdot\rangle$, we define the

affine subspace $\mathcal{S}_{h,m} = \{v \in \mathcal{S}_h \mid \langle v, 1\rangle = m\}$ with fixed mass m. Finally, $\mathcal{K}_h = \mathcal{K} \cap \mathcal{S}_h$ is an approximation of $\mathcal{K}$ and we set $\mathcal{K}_{h,m} = \mathcal{K} \cap \mathcal{S}_{h,m}$.

Semi-implicit Euler discretization in time and finite elements in space [2, 4, 13]) lead to the following discretized problem.

($\mathbf{P}^h$) For each $k = 1, \dots, N$ find $u_h^k \in \mathcal{K}_h$ and $w_h^k \in \mathcal{S}_h$ such that

$$\begin{aligned} \left\langle u_h^k, v\right\rangle + \tau\left(\nabla w_h^k, \nabla v\right) &= \left\langle u_h^{k-1}, v\right\rangle, && \forall v \in \mathcal{S}_h, \\ \gamma\left(\nabla u_h^k, \nabla(v - u_h^k)\right) - \left\langle w_h^k, v - u_h^k\right\rangle &\geq \left\langle u_h^{k-1}, v - u_h^k\right\rangle, && \forall v \in \mathcal{K}_h. \end{aligned}$$

We select the uniform time step $\tau = T/N$. The initial condition $u_h^0 \in \mathcal{S}_h$ is the discrete L^2 projection of $u_0 \in \mathcal{K}$ given by $\langle u_h^0, v\rangle = (u_0, v)\ \forall v \in \mathcal{S}_h$. Note that the mass $m = \langle u_h^k, 1\rangle = (u_0, 1)$, $k \geq 1$, is conserved in this way.

The following discrete analogue of Theorem 1 is contained in [4], where optimal error estimates can be found as well.

Theorem 2. *There exists a solution (u_h^k, w_h^k) of $(\mathbf{P}^h)$ with uniquely determined u_h^k, $k = 1, \dots, N$. Moreover, w_h^k is also unique, if there is a $p \in \mathcal{N}_h$ with $|u_h^k(p)| < 1$.*

Note that non-uniqueness of w_h^k means that either the diffuse interface is not resolved by $\mathcal{T}_h$ or that u_h^k is constant.

3 A saddle point problem with inequality constraints

We consider the discrete Cahn-Hilliard system

(CH) Find $\mathbf{u} = (u, w) \in \mathcal{K}_h \times \mathcal{S}_h$ such that

$$\begin{aligned} \langle u, v\rangle + \tau\left(\nabla w, \nabla v\right) &= \left\langle u^{old}, v\right\rangle, && \forall v \in \mathcal{S}_h, \\ \gamma\left(\nabla u, \nabla(v - u)\right) - \langle w, v - u\rangle &\geq \left\langle u^{old}, v - u\right\rangle, && \forall v \in \mathcal{K}_h, \end{aligned}$$

for given $u^{old} \in \mathcal{S}_h$. Such kind of problem is arising in each time step of $(\mathbf{P}^h)$.

Following [4, 15], we introduce the pde-constrained minimization problem

(M) Find $\mathbf{u_0} = (u, w_0) \in \mathcal{V} \subset \mathcal{K}_h \times \mathcal{S}_{h,0}$ such that

$$\mathcal{J}(\mathbf{u_0}) \leq J(\mathbf{v}) \qquad \forall \mathbf{v} \in \mathcal{V},$$

$$\mathcal{V} = \{(v_u, v_w) \in \mathcal{K}_h \times \mathcal{S}_{h,0} \mid \left\langle u^{old} - v_u, v\right\rangle - \tau(\nabla v_w, \nabla v) = 0\ \forall v \in \mathcal{S}_h\}.$$

Denoting $\mathbf{u_0} = (u, w_0), \mathbf{v} = (v_u, v_w)$, the bivariate energy functional

$$\mathcal{J}(\mathbf{u_0}) = \tfrac{1}{2} a(\mathbf{u_0}, \mathbf{u_0}) - \ell(\mathbf{u_0}), \qquad \mathbf{u_0} \in \mathcal{K}_h \times \mathcal{S}_{h,0}, \tag{1}$$

is induced by the bilinear form

$$a(\mathbf{u_0}, \mathbf{v}) = \gamma \left(\nabla u, \nabla v_u\right) + \gamma \left\langle u, 1\right\rangle \left\langle v_u, 1\right\rangle + \tau \left(\nabla w_0, \nabla v_w\right) \tag{2}$$

and the bounded linear functional

$$\ell(\mathbf{v}) = \gamma m \left\langle v_u, 1\right\rangle + \left\langle u^{old}, v_u\right\rangle. \tag{3}$$

The bilinear form $a(\cdot,\cdot)$ is symmetric and, by Friedrich's inequality, coercive with a constant independent of h on the Hilbert space $\mathcal{S}_h \times \mathcal{S}_{h,0}$ equipped with the inner product

$$(\mathbf{u_0}, \mathbf{v})_{\mathcal{S}_h \times \mathcal{S}_{h,0}} = \langle u, v_u\rangle + (\nabla u, \nabla v_u) + (\nabla w_0, \nabla v_w).$$

Hence, **(M)** has a unique solution (cf., e.g., [10, p. 34]).

Incorporating the pde-constraint $\mathbf{u_0} \in \mathcal{V}$ occuring in **(M)** by a Lagrange multiplier $\lambda \in \mathcal{S}_h$ we obtain the saddle point problem

(S) Find $(\mathbf{u_0}, \lambda) \in (\mathcal{K}_h \times \mathcal{S}_{h,0}) \times \mathcal{S}_h$ such that

$$\mathcal{L}(\mathbf{u_0}, \mu) \le \mathcal{L}(\mathbf{u_0}, \lambda) \le \mathcal{L}(\mathbf{v}, \lambda) \qquad \forall\, (\mathbf{v}, \mu) \in (\mathcal{K}_h \times \mathcal{S}_{h,0}) \times \mathcal{S}_h$$

with the Lagrange functional

$$\mathcal{L}(\mathbf{v}, \mu) = \mathcal{J}(\mathbf{v}) + \left\langle u^{old} - v_u, \mu\right\rangle - \tau(\nabla v_w, \nabla \mu).$$

It turns out that **(S)** is an equivalent reformulation of **(CH)** where the Lagrange parameter λ is identical with the chemical potential w. The following result is taken from [15].

Theorem 3. *Let $\mathbf{u} = (u, w) \in \mathcal{K}_h \times \mathcal{S}_h$ be a solution of* **(CH)**. *Then $\mathbf{u_0} = (u, w_0)$ with $w_0 = w - \int_\Omega w\, dx/|\Omega| \in \mathcal{S}_{h,0}$ is the unique solution of* **(M)** *and $(\mathbf{u_0}, w)$ is a solution of* **(S)**. *Conversely, if $(\mathbf{u_0}, \lambda) = ((u, w_0), \lambda)$ is a solution of* **(S)**, *then $\mathbf{u} = (u, \lambda)$ solves* **(CH)**.

4 Preconditioned Uzawa-type iterations

From now on, we concentrate on Uzawa-type iterations for the saddle point formulation (**S**) of the discrete Cahn-Hilliard system **(CH)**. In the light of Theorem 3, the Lagrange multiplier λ is identified with the chemical potential w. We first express the Lagrangian terms by a suitable operator Φ_S.

Lemma 1. *Let $\langle\cdot,\cdot\rangle_S$ be some inner product on $\mathcal{S}_h$. Then there is a unique Lipschitz continuous function $\Phi_S : \mathcal{S}_h \times \mathcal{S}_{h,0} \to \mathcal{S}_h$ with the property*

$$\left\langle u^{old} - v_u, \mu\right\rangle - \tau(\nabla v_w, \nabla \mu) = \langle \Phi_S(\mathbf{v}), \mu\rangle_S \qquad \forall \mu \in \mathcal{S}_h.$$

Furthermore $\langle \Phi_S(\cdot), \mu\rangle_S : \mathcal{S}_h \times \mathcal{S}_{h,0} \to \mathbb{R}$ is Lipschitz continuous and convex.

Proof. Existence and uniqueness follows directly from the representation theorem of Fréchet-Riesz. Since Φ_S is affine linear on the finite dimensional space $\mathcal{S}_h \times \mathcal{S}_{h,0}$, it is Lipschitz continuous. The same argument provides Lipschitz continuity and convexity of $\langle \Phi_S(\cdot), \mu \rangle_S$. □

Of course, Φ_S depends on the choice of the inner product $\langle \cdot, \cdot \rangle_S$ which plays the role of a preconditioner. For given $w^0 \in \mathcal{S}_h$ and $\rho > 0$ the corresponding Uzawa iteration reads as follows [14, p. 91].

Algorithm 1. (Preconditioned Uzawa iteration)

$$\begin{aligned} \mathbf{u_0}^\nu \in \mathcal{K}_h \times \mathcal{S}_{h,0} : \quad \mathcal{L}(\mathbf{u_0}^\nu, w^\nu) \leq \mathcal{L}(\mathbf{v}, w^\nu) \quad \forall \mathbf{v} \in \mathcal{K}_h \times \mathcal{S}_{h,0} \\ w^{\nu+1} = w^\nu + \rho \Phi_S(\mathbf{u_0}^\nu). \end{aligned} \tag{4}$$

As $a(\cdot, \cdot)$ is symmetric positive definite on $\mathcal{S}_h \times \mathcal{S}_{h,0}$ and $\mathcal{K}_h \times \mathcal{S}_{h,0}$ is a closed, convex subset, we can apply Theorem 4.1 in Chapter 2 of [14] to obtain

Theorem 4. *There are positive constants α_0, α_1 such that the iterates $\mathbf{u_0}^\nu$ provided by Algorithm 1 converge to $\mathbf{u_0}$ for $\nu \to \infty$ and all $\rho \in [\alpha_0, \alpha_1]$.*

In order to derive a more explicit formulation of Algorithm 1, it is convenient to introduce the identity I and the operators $A, C : \mathcal{S}_h \to \mathcal{S}_h$ according to

$$\langle Au, v \rangle = \gamma \left(\nabla u, \nabla v \right) + \gamma \left\langle u, 1 \right\rangle \left\langle v, 1 \right\rangle, \quad \langle Cw, v \rangle = \tau \left(\nabla w, \nabla v \right) \qquad \forall v \in \mathcal{S}_h$$

and the functions $f, g \in \mathcal{S}_h$ by

$$\langle f, v \rangle = \gamma m \left\langle v, 1 \right\rangle + \left\langle u^{old}, v \right\rangle \quad \forall v \in \mathcal{S}_h, \qquad g = -u^{old}.$$

Finally, $\partial I_{\mathcal{K}_h}$ is the subdifferential of the indicator function of $\mathcal{K}_h$. With this notation, the discrete Cahn-Hilliard system **(CH)** can be rewritten as the inclusion

$$\begin{pmatrix} A + \partial I_{\mathcal{K}_h} & -I \\ -I & -C \end{pmatrix} \begin{pmatrix} u \\ w \end{pmatrix} \ni \begin{pmatrix} f \\ g \end{pmatrix}. \tag{5}$$

Reformulating the minimization problem occuring in the first step of Algorithm 1 as a variational inclusion, we can eliminate w_0 and then insert the above operator notation to obtain the following explicit formulation

$$\begin{aligned} u^\nu &= (A + \partial I_{\mathcal{K}_h})^{-1}(f + w^\nu) \\ w^{\nu+1} &= w^\nu + \rho S^{-1}(-u^\nu - Cw^\nu - g) \end{aligned} \quad . \tag{6}$$

The preconditioner $S : \mathcal{S}_h \to \mathcal{S}_h$ is the symmetric positive definite operator defined by

$$\langle Sr, v \rangle = \langle r, v \rangle_S \qquad \forall v \in \mathcal{S}_h.$$

Observe that (6) turns out to be a classical Uzawa iteration for the nonlinear, perturbed saddle point problem (5) with the preconditioner S.

5 Towards efficient preconditioning

In order to construct efficient preconditioners S, we have to find good approximations of the nonlinear Schur complement, i.e.,

$$S \approx (A + \partial I_{\mathcal{K}_h})^{-1} + C.$$

Our construction is based on the observation that the discrete Cahn-Hilliard system (5) degenerates to a reduced linear problem once the solution u on the coincidence set

$$\mathcal{N}_h^\bullet(u) = \{p \in \mathcal{N}_h \mid |u(p)| = 1\},$$

is known. To be more precise, we define the reduced linear operators

$$\left\langle \widehat{A}(u)\varphi_p, \varphi_q \right\rangle = \begin{cases} \delta_{p,q} \langle \varphi_p, \varphi_q \rangle & \text{if } q \in \mathcal{N}_h^\bullet(u) \\ \langle A\varphi_p, \varphi_q \rangle & \text{else} \end{cases}$$
$$\left\langle \widehat{I}(u)\varphi_p, \varphi_q \right\rangle = \begin{cases} 0 & \text{if } q \in \mathcal{N}_h^\bullet(u) \\ \langle \varphi_p, \varphi_q \rangle & \text{else} \end{cases} \qquad p \in \mathcal{N}_h$$

and the right hand side

$$\left\langle \widehat{f}(u), \varphi_q \right\rangle = \begin{cases} u(q) \langle \varphi_q, \varphi_q \rangle & \text{if } q \in \mathcal{N}_h^\bullet(u) \\ \langle f, \varphi_q \rangle & \text{else} \end{cases}.$$

Recall that φ_p, $p \in \mathcal{N}_h$, denotes the standard nodal basis of $\mathcal{S}_h$. Then, by construction, the discrete Cahn-Hilliard system (5) has the same solution as the reduced linear system

$$\begin{pmatrix} \widehat{A}(u) & -\widehat{I}(u) \\ -I & -C \end{pmatrix} \begin{pmatrix} u \\ w \end{pmatrix} = \begin{pmatrix} \widehat{f}(u) \\ g \end{pmatrix}$$

with the Schur complement $S(u) = \widehat{A}(u)^{-1}\widehat{I}(u) + C$. Replacing the exact solution u by some approximation $\tilde{u} \approx u$, we obtain the preconditioner

$$S(\tilde{u}) = \widehat{A}(\tilde{u})^{-1}\widehat{I}(\tilde{u}) + C. \tag{7}$$

Proposition 1. *The operator $S(\tilde{u})$ is symmetric and positive semidefinite. $S(\tilde{u})$ is positive definite, if and only if $\mathcal{N}_h^\bullet(\tilde{u}) \neq \mathcal{N}_h$.*

Proof. First note that $\widehat{I}(\tilde{u}) : \mathcal{S}_h \to \mathcal{S}_h^\circ = \{v \in \mathcal{S}_h \mid v(p) = 0 \ \forall p \in \mathcal{N}_h^\bullet(\tilde{u})\}$ is orthogonal with respect to $\langle \cdot, \cdot \rangle$. The range of the restriction $A^\circ = \widehat{A}(\tilde{u})|_{\mathcal{S}_h^\circ}$ is contained in $\mathcal{S}_h^\circ$, because, for all $v \in \mathcal{S}_h^\circ$, we have by definition

$$\left\langle \widehat{A}(\tilde{u})v, \varphi_q \right\rangle = \sum_{p \in \mathcal{N}_h \setminus \mathcal{N}_h^\bullet(\tilde{u})} v(p)\delta_{p,q} \langle \varphi_p, \varphi_q \rangle = 0 \qquad \forall q \in \mathcal{N}_h^\bullet(\tilde{u}).$$

Similarly, we get $\langle A^\circ v, v' \rangle = \langle Av, v' \rangle \ \forall v, v' \in \mathcal{S}_h^\circ$ so that A° is symmetric and positive definite on $\mathcal{S}_h^\circ$. As a consequence, $\widehat{A}^{-1}(\tilde{u})\widehat{I}(\tilde{u})$ is symmetric and positive semidefinite on $\mathcal{S}_h$, because

$$\left\langle \widehat{A}^{-1}(\tilde{u})\widehat{I}(\tilde{u})v, v' \right\rangle = \left\langle (A^\circ)^{-1}\widehat{v}, v' \right\rangle = \left\langle \widehat{I}(\tilde{u})(A^\circ)^{-1}\widehat{v}, v' \right\rangle = \left\langle (A^\circ)^{-1}\widehat{v}, \widehat{v}' \right\rangle$$

denoting $\widehat{v} = \widehat{I}(\tilde{u})v$, $\widehat{v}' = \widehat{I}(\tilde{u})v'$. As C is also symmetric and positive semidefinite, the first assertion follows. It is easy to see that the kernels of $\widehat{A}^{-1}(\tilde{u})\widehat{I}(\tilde{u})$ and C have trivial intersection, if and only if $\mathcal{N}_h^\bullet(\tilde{u}) \neq \mathcal{N}_h$. This concludes the proof. □

In the light of Theorem 4, Proposition 1 guarantees convergence of the preconditioned Uzawa iteration (6) with $S = S(\tilde{u})$ and suitable damping. The condition $\mathcal{N}_h^\bullet(u^\nu) \neq \mathcal{N}_h$ reflects the criterion $\mathcal{N}_h^\bullet(u) \neq \mathcal{N}_h$ for uniqueness of w (cf. Theorem 2). It could be removed, e.g., by imposing mass conservation $\langle w^{\nu+1}, 1 \rangle = \langle w^\nu, 1 \rangle$ in the singular case $\mathcal{N}_h^\bullet(\tilde{u}) = \mathcal{N}_h$.

As a straightforward approximation of u one may choose the first iterate $\tilde{u} = u^1$. It is natural to update $\tilde{u}$ in each iteration step, selecting $S = S(u^\nu)$. However, in this case convergence no longer follows from Theorem 4, because the preconditioner now depends on ν.

The following proposition is obtained by straightforward computation.

Proposition 2. *Let $\mathcal{N}_h^\bullet(u^\nu) \neq \mathcal{N}_h$. Then, for $S = S(u^\nu)$ and $\rho = 1$ the preconditioned Uzawa iteration* (6) *takes the form*

$$\begin{aligned} u^\nu &= (A + \partial I_{\mathcal{K}_h})^{-1}(f + w^\nu) \\ w^{\nu+1} &= S(u^\nu)^{-1}\left(-\widehat{A}(u^\nu)^{-1}\widehat{f}(u^\nu) - g\right) \end{aligned} \quad . \tag{8}$$

Note that only the actual coincidence set $\mathcal{N}_h^\bullet(u^\nu)$ and the values of u^ν on $\mathcal{N}_h^\bullet(u^\nu)$ enter the computation of $w^{\nu+1}$. Hence, (8) has the flavour of an active set strategy. As an important consequence, the Uzawa iteration (8) provides the exact solution, once the exact coincidence set $\mathcal{N}_h^\bullet(u)$ is detected. In the numerical experiments to be reported below, this required only a finite (quite moderate) number of steps. A theoretical justification will be discussed elsewhere [15].

Multigrid solvers for the subproblems. Each step of the preconditioned Uzawa iteration (8) requires a) the solution of a discretized symmetric elliptic obstacle problem with box constraints and b) the evaluation of the linear preconditioner $S(u^\nu)$.

For subproblem (8a), we apply monotone multigrid methods whose convergence speed is comparable to classical multigrid algorithms for unconstrained problems [17]. Moreover, in the non-degenerate case, the actual coincidence set $\mathcal{N}_h^\bullet(u^\nu)$ is detected after a finite number of steps. This means that we can stop the iteration on (8a) after a finite (usually quite moderate) number of steps without loosing exactness of the iteration (8). Using the Lipschitz-continuity

$$\langle A(u-u^\nu), u-u^\nu\rangle \le \langle w-w^\nu, w-w^\nu\rangle$$

of (8a) with respect to w^ν, the *potential* accuracy of u^ν can be controlled by a posteriori estimates of the algebraic error of w^ν. Hence, the Uzawa iteration could be stopped and u^ν computed up to the desired accuracy (only once!) as soon as w^ν is accurate enough.

The substep (8b) amounts to the solution of the following symmetric saddle point problem

$$\begin{pmatrix} \widehat{A}(u^\nu)\widehat{I}(u^\nu) & -\widehat{I}(u^\nu) \\ -\widehat{I}(u^\nu) & -C \end{pmatrix} \begin{pmatrix} \widehat{u} \\ w^{\nu+1} \end{pmatrix} = \begin{pmatrix} \tilde{f}(u^\nu) \\ \tilde{g}(u^\nu) \end{pmatrix} \tag{9}$$

with an auxiliary variable $\widehat{u}$ satisfying $\widehat{u} = u^\nu$ on $\mathcal{N}_h^\bullet(u^\nu)$ and the modified right-hand sides $\tilde{f}(u^\nu) = \widehat{f}(u^\nu) - \widehat{A}(u^\nu)(I-\widehat{I}(u^\nu))u^\nu$, $\tilde{g}(u^\nu) = g+(I-\widehat{I}(u^\nu))u^\nu$. For the iterative solution of (9) we apply a multigrid method with block Gauß-Seidel smoother and canonical restriction and prolongation. Related algorithms have been investigated in [5, 20, 21, 23, 24]. In particular, multigrid convergence for a block Jacobi smoother is proved in [20].

6 Numerical experiments

We consider the Cahn-Hilliard equation **(P)** on the unit square $\Omega = (0,1)^2$ in the time interval $(0,T)$, $T = 0.5$, with $\gamma = 10^{-4}$ and its discretization by $\mathbf{(P}^h\mathbf{)}$. The underlying triangulation $\mathcal{T}_{h_j}$ with meshsize $h_j = 2^{-j}$ is resulting from $j = 8$ uniform refinements applied to the initial triangulation $\mathcal{T}_{h_0}$ consisting of two congruent triangles. We choose the time step $\tau = \gamma$. Figure 2 illustrates the approximate solution for the initial condition u_0 as depicted in Figure 1.

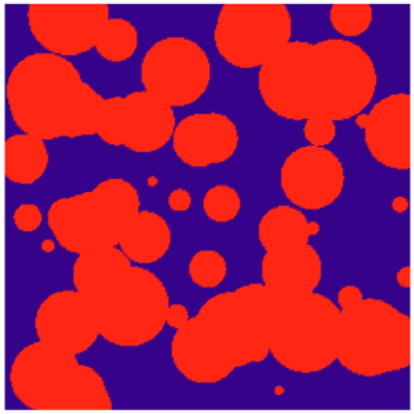


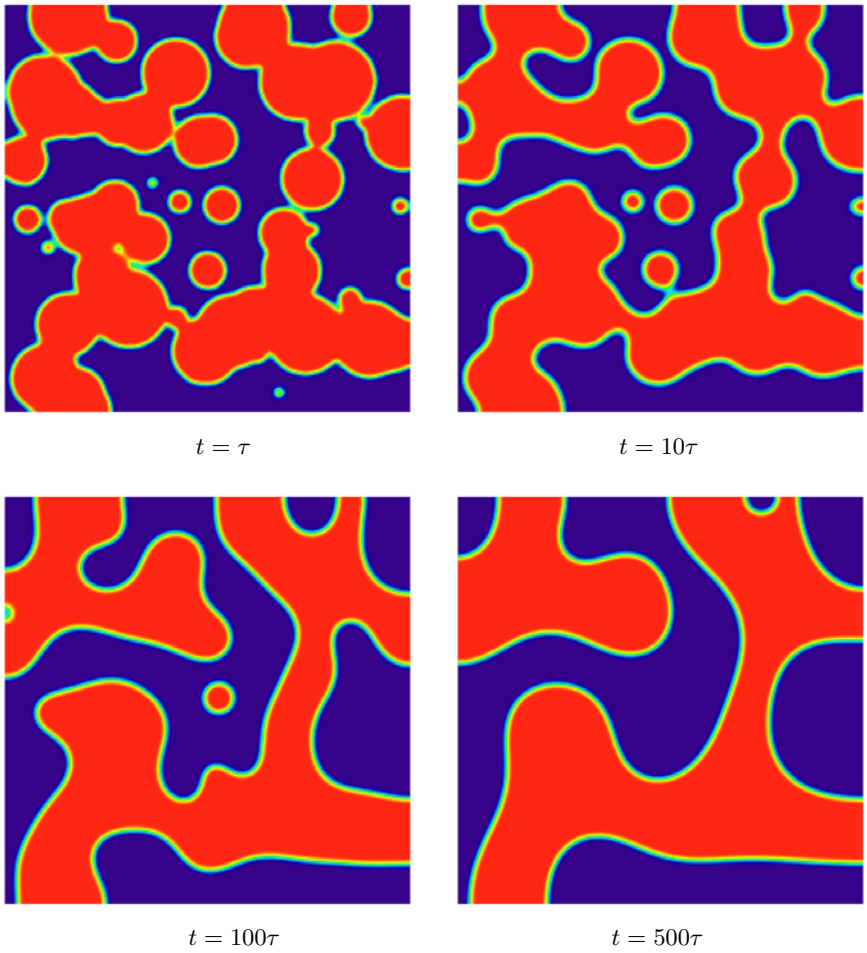
Fig. 1. Initial condition u_0

Observe that the initially fast dynamics slows down with decreasing curvature of the interface.

We now investigate the performance of the preconditioned Uzawa iteration (6). In all our experiments, we select $\rho = 1$, i.e. no damping is applied. As initial iterates w^0 we use the final approximations from the previous time step. The first time step is an exception, because no initial condition is prescribed for the chemical potential w. Here, we start with the the solution of the unconstrained reduced problem (9). Reduction takes place with respect to $\mathcal{N}_h^\bullet(u^0)$. The algebraic error is measured by the energy-type norm

$$\|\mathbf{v}\|^2 = a(\mathbf{v},\mathbf{v}) + \tau \langle v_w, v_w \rangle, \quad v = (v_u, v_w) \in \mathcal{S}_h \times \mathcal{S}_h,$$

with $a(\cdot,\cdot)$ defined in (2).



$t = \tau$ $t = 10\tau$

$t = 100\tau$ $t = 500\tau$

Fig. 2. Evolution of the phases

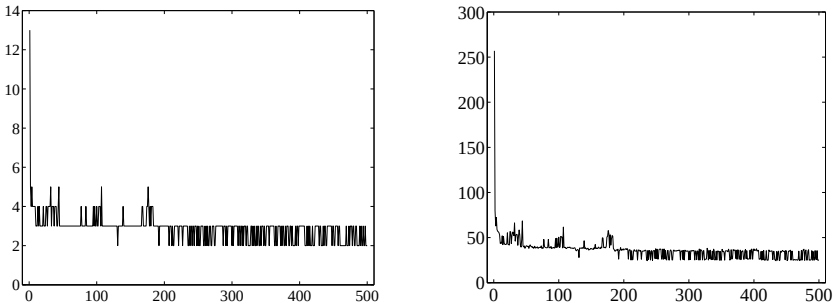


Fig. 3. Preconditioned Uzawa steps and cpu time over the time levels

It turns out that preconditioning by $S(u^1)$ does not speed up, but slows down convergence considerably. Without preconditioning, the first spatial problem is solved up to machine accuracy by about 3000 Uzawa steps. Using $S(u^1)$ as a preconditioner, 3000 steps only provide an error reduction by 10^{-1}.

From now on we only consider the preconditioner $S(u^\nu)$ which is updated in each iteration step $\nu \geq 0$. The resulting preconditioned Uzawa iteration is called UUZAWA. Figure 3 illustrates the computational work for the solution of the spatial problems on the time levels $k = 1, \ldots, 500$. The iteration is stopped as soon as the exact coincidence set is detected. The left picture shows the required number ν_0 of UUZAWA steps. From 13 steps on the first time level, ν_0 drops down to 4 or 5 and later even to 2 or 3. This behavior clearly reflects the quality of the initial iterates w^0. The right picture shows the elapsed cpu time measured in terms of work units. One work unit is the cpu time required by one multigrid $V(3,3)$ cycle as applied to the unconstrained saddle point problem (9) on the actual refinement level j. About 15 multigrid steps are necessary to solve (9) up to machine accuracy. Comparing both pictures, we find that the computational cost for each spatial problem is obtained approximately by multiplying that number with the number of Uzawa steps. The cpu time for the 4 to 7 monotone multigrid steps for detecting the actual coincidence set from each obstacle problem (8a) only plays a minor role.

To take a closer look at the convergence behavior of UUZAWA, we now consider the iteration history on the first two time levels, using the refined mesh $\mathcal{T}_{h_j}$ with $j = 9$. Figure 4 shows the algebraic error $\|\mathbf{u} - \mathbf{u}^\nu\|$ over the cpu time measured in terms of work units. The "exact" solution $\mathbf{u}$ is precomputed up to roundoff errors. For a comparison, we consider a recent block Gauß-Seidel iteration [2]. Reflecting the increasing accuracy of $\mathcal{N}_h^\bullet(u^\nu)$, UUZAWA shows superlinear convergence throughout the whole iteration process, ending up with an error reduction by about 10^{-5} in the last iteration step. For bad initial iterates w^0, as encountered on the first time level, the efficiency of UUZAWA

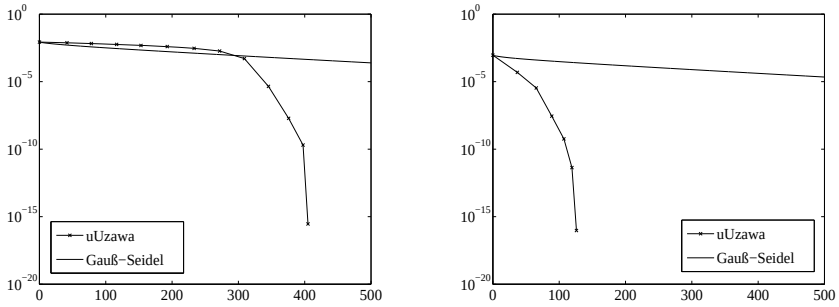


Fig. 4. Iteration history for the first 2 time levels

and Gauß-Seidel is comparable in the beginning of the iteration. However, UZAWA speeds up considerably as soon as the coincidence set is approximated sufficiently well. For good initial iterates, as available on the second and all later time levels, such fast convergence takes place immediately. Even better initial iterates could be expected from nested iteration. While the convergence rates of the Gauß-Seidel scheme rapidly degenerate with decreasing mesh size, the convergence speed of UZAWA hardly depends on the refinement level. For example, the first spatial problem on the refinement levels $j = 7, 8, 9$ was solved up to machine accuracy by $\nu_0 = 10, 12, 13$ iteration steps.

References

[1] R.E. Bank, B.D. Welfert, and H. Yserentant. A class of iterative methods for solving saddle point problems. *Numer. Math.*, 56(7):645–666, 1990.

[2] J.W. Barrett, R. Nürnberg, and V. Styles. Finite element approximation of a phase field model for void electromigration. *SIAM J. Numer. Anal.*, 42(2):738–772, 2004.

[3] J.F. Blowey and C.M. Elliott. The Cahn-Hilliard gradient theory for phase separation with non-smooth free energy Part I: Mathematical analysis. *Euro. Jnl of Applied Mathematics*, 2:233–280, 1991.

[4] J.F. Blowey and C.M. Elliott. The Cahn-Hilliard gradient theory for phase separation with non-smooth free energy Part II: Numerical analysis. *Euro. Jnl of Applied Mathematics*, 3:147–179, 1992.

[5] D. Braess and R. Sarazin. An efficient smoother for the Stokes problem. *Appl. Numer. Math.*, 23(1):3–19, 1997.

[6] J.H. Bramble, J.E. Pasciak, and A.T. Vassilev. Analysis of the inexact Uzawa algorithm for saddle point problems. *SIAM J. Numer. Anal.*, 34(3):1072–1092, 1997.
[7] J.W. Cahn and J.E. Hilliard. Free energy of a nonuniform system I. Interfacial energy. *J. Chem. Phys.*, 28:258–267, 1958.
[8] X. Chen. Global and superlinear convergence of inexact Uzawa methods for saddle point problems with nondifferentiable mappings. *SIAM J. Numer. Anal.*, 35(3):1130–1148, 1998.
[9] X. Chen. On preconditioned Uzawa methods and SOR methods for saddle-point problems. *J. Comput. Appl. Math.*, 100(2):207–224, 1998.
[10] I. Ekeland and R. Temam. *Convex analysis and variational problems*. North-Holland, Amsterdam, 1976.
[11] C.M. Elliott. The Cahn-Hilliard model for the kinetics of phase separation. In J.F. Rodrigues, editor, *Mathematical models for phase change problems*, pages 35 – 73, Basel, 1989. Birkhäuser.
[12] H.C. Elman and G.H. Golub. Inexact and preconditioned Uzawa algorithms for saddle point problems. *SIAM J. Numer. Anal.*, 31(6):1645–1661, 1994.
[13] D.J. Eyre. An unconditionally stable one-step scheme for gradient systems. Preprint, University of Utah, Salt Lake City, 1997.
[14] R. Glowinski, J.L. Lions, and R. Trémolières. *Numerical Analysis of Variational Inequalities*. Number 8 in Studies in Mathematics and its Applications. North-Holland Publishing Company, Amsterdam New York Oxford, 1981.
[15] C. Gräser and R. Kornhuber. Preconditioned Uzawa iterations for the Cahn-Hilliard equation with obstacle potential. *to appear*.
[16] Q. Hu and J. Zou. Two new variants of nonlinear inexact Uzawa algorithms for saddle-point problems. *Numer. Math.*, 93(2):333–359, 2002.
[17] R. Kornhuber. Monotone multigrid methods for elliptic variational inequalities I. *Numer. Math.*, 69(2):167–184, 1994.
[18] P.L. Lions and B. Mercier. Splitting algorithms for the sum of two nonlinear operators. *Siam J. Numer. Anal.*, 16:964–979, 1979.
[19] A. Novick-Cohen. The Cahn-Hilliard equation: Mathematical and modeling perspectives. *Adv. Math. Sci.*, 8:965–985, 1998.
[20] J. Schöberl and W. Zulehner. On Schwarz-type smoothers for saddle point problems. *Numer. Math.*, 95(2):377–399, 2003.
[21] S.P. Vanka. Block-implicit multigrid solution of Navier-Stockes equations in primitive variables. *J. Comput. Phys.*, 65:138–158, 1986.
[22] S. Wright. *Primal-dual interior-point methods*. SIAM, Philadelphia, 1997.
[23] W. Zulehner. A class of smoothers for saddle point problems. *Computing*, 65(3):227–246, 2000.
[24] W. Zulehner. Analysis of iterative methods for saddle point problems: A unified approach. *Math. Comput.*, 71(238):479–505, 2002.