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inequalities with non-local constraints**

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Preprint Nr. 11/2010

PRECONDITIONING FOR ALLEN-CAHN VARIATIONAL INEQUALITIES WITH NON-LOCAL CONSTRAINTS

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Abstract. The solution of Allen-Cahn variational inequalities with mass constraints is of interest in many applications. This problem can be solved both in its scalar and vector-valued form as a PDE-constrained optimization problem by means of a primal-dual active set method. At the heart of this method lies the solution of linear systems in saddle point form. In this paper we propose the use of Krylov-subspace solvers and suitable preconditioners for the saddle point systems. Numerical results illustrate the competitiveness of this approach.

AMS subject classifications. Primary 65F10, 65N22, 65F50 Secondary 76D07

Key words. PDE-constrained optimization, Allen-Cahn model, Newton method, Saddle point systems, Preconditioning, Krylov subspace solver.

1. Introduction. The solution of Allen-Cahn variational inequalities with non-local constraints can be formulated as an optimal control problem, which can be solved using a primal-dual active set method [4, 6, 7]. This method has proven very efficient in a variety of applications [27, 29, 35, 36]. As we will show in the course of this paper the solution to a linear system of the form $\mathcal{K}x = b$ with \mathcal{K} a real symmetric matrix is at the heart of this method. The sparse linear systems are usually of very large dimension and in combination with 3-dimensional experiments the application of direct solvers such as UMFPack [11] becomes infeasible. As a result iterative methods have to be employed (see e.g. [24, 43] for introductions to this field). For symmetric and indefinite systems the Minimal Residual method (MINRES) [39] is a common solver as it minimizes the 2-norm of the residual $r_k = b - \mathcal{K}x_k$ over the Krylov subspace $\text{span}\{r_0, \mathcal{K}r_0, \dots, \mathcal{K}^{k-1}r_0\}$. The convergence behaviour of the iterative scheme depends on the conditioning of the problem and the clustering of the eigenvalues and can usually be enhanced with preconditioning techniques. $\mathcal{P}^{-1}\mathcal{K}x = \mathcal{P}^{-1}b$ In this paper, we provide an efficient preconditioner \mathcal{P} for the solution of Allen-Cahn variational inequalities combining methods for indefinite problems [31, 39, 48, 3] and algebraic multigrid developed for elliptic systems [15, 43, 42]. The arising linear systems lead to matrices \mathcal{K} which have the following saddle point block-structure which arise in a variety of applications [3]

$$\mathcal{K} = \begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \quad (1.1)$$

with A being symmetric and positive definite. Hence, MINRES is our method of choice. With some restrictions on \mathcal{P} it is also possible to apply variants of CG [7, 5, 9, 40, 46]. For moderate sizes of \mathcal{K} and 2D problems direct solvers such as UMFPACK [11] or HSL_MA57 [12] can show outstanding performance.

The paper is organized as follows. In Section 2 we introduce the Allen-Cahn variational inequalities in scalar and vector-valued form with nonlocal constraints.

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We briefly introduce the primal-dual active set method and derive the linear systems giving rise to the matrix \mathcal{K} in question. In Section 3 we analyze the linear systems and propose preconditioning strategies for the saddle point problems in combination with well-known techniques for some of the underlying operators, as e.g. algebraic multigrid. In addition, we show how the active set method can lead to a reduction in problem size and how this can be implemented efficiently. We also discuss a semi-implicit formulation that promises greater flexibility with respect to the choice of the timestep size. Section 4 illustrates the competitiveness of our approach.

2. Problem setups.

2.1. Allen-Cahn equation with obstacle potential. The Allen-Cahn model, which is used to describe the motion of an interface, plays an important role in many applications [8, 16, 49]. Here the interface in which a phase field or order parameter changes its value rapidly is modelled with thickness $\varepsilon > 0$ with ε being small. The energy functional of interest is given by the Ginzburg-Landau energy

$$E(u) = \int_{\Omega} \frac{\gamma\varepsilon}{2} |\nabla u|^2 + \frac{\gamma}{\varepsilon} \psi(u) \quad (2.1)$$

where $\Omega \subset \mathbb{R}^d$ is a bounded domain, $\gamma > 0$ is a parameter related to the interfacial energy and $u : \Omega \rightarrow \mathbb{R}$ is the phase field. The potential function $\psi : \mathbb{R} \rightarrow \mathbb{R}_0^+ \cup \{\infty\}$ has two global minima at ± 1 which describe the pure phases, e.g. the double well $\psi(u) = (1 - u^2)^2$ or the double obstacle potential $\psi(u) = \psi_0(u) + I_{[-1,1]}(u)$ with

$$\psi_0(u) = \frac{1}{2}(1 - u^2) \text{ and } I_{[-1,1]}(u) = \begin{cases} 0 & \text{if } |u| \leq 1 \\ \infty & \text{otherwise} \end{cases} \quad (2.2)$$

which is considered in the following.

Given an initial phase distribution $u(., 0) = u_0$ and assuming that ψ is smooth the interface motion can be modelled by the scaled steepest descent of E with respect to the L^2 -norm and we obtain the Allen-Cahn equation

$$\varepsilon \partial_t u = \gamma \varepsilon \Delta u - \frac{\gamma}{\varepsilon} \psi'(u) \quad (2.3)$$

with homogeneous Neumann boundary conditions on $\partial\Omega$. In the case that the total spatial amount of the phases is conserved the steepest descent of E under the constraint $\int_{\Omega} u = m$, where $\int_{\Omega} f(x) dx := \frac{1}{|\Omega|} \int_{\Omega} f(x) dx$ with $|\Omega|$ being the Lebesgue measure of Ω , becomes

$$\varepsilon \partial_t u = \gamma \varepsilon \Delta u - \frac{\gamma}{\varepsilon} \psi'(u) + \frac{\gamma}{\varepsilon} \int_{\Omega} \psi'(u). \quad (2.4)$$

For the obstacle potential (2.2) the following problem has to be solved where $\langle ., . \rangle$ denotes the L^2 -inner product (see e.g. [6]):

OS 2.1. *Given $u(., 0) = u_0 \in H^1(\Omega)$ with $|u_0| \leq 1$ and $\int_{\Omega} u_0 = m$ find $u \in H^1(\Omega_T)$ such that $\int_{\Omega} u = m$ and $|u| \leq 1$ a.e. in $\Omega_T := \Omega \times (0, T)$ and*

$$\varepsilon \langle \partial_t u, \chi - u \rangle + \gamma \varepsilon \langle \nabla u, \nabla(\chi - u) \rangle + \frac{\gamma}{\varepsilon} \langle \psi'_0(u), \chi - u \rangle \geq 0 \quad (2.5)$$

which has to hold for almost all t and all $\chi \in H^1(\Omega)$ with $|\chi| \leq 1$ and $\int_{\Omega} \chi = m$. In [6] it is shown that (2.5) can be reformulated as follows

$$\begin{aligned} \varepsilon^2 \partial_t u - \varepsilon^2 \gamma \Delta u + \gamma \psi'_0(u) + \mu - \lambda &= 0 & \text{a.e. in } \Omega \\ \frac{\partial u}{\partial \nu} &= 0 & \text{a.e. on } \partial\Omega \\ \int_{\Omega} u &= m \end{aligned} \quad (2.6)$$

together with the complementary conditions

$$\begin{aligned} \mu_+ \geq 0, \quad \mu_- \geq 0, \quad |u| \leq 1 & \quad \text{a.e. in } \Omega, \\ \mu_+(u-1) = \mu_-(u+1) = 0 & \quad \text{a.e. in } \Omega, \end{aligned} \quad (2.7)$$

where λ is the scaled multiplier for $\int_{\Omega} u = m$ and $\mu := \mu_+ - \mu_-$ is the scaled Lagrange multiplier for $|u| \leq 1$. Note that (2.7) is equivalent to

$$\begin{aligned} u &= 1 & \text{a.e. in } \mathcal{A}_+(t) := \{x \in \Omega : c(u(x, t) - 1) + \mu(x, t) > 0\}, \\ u &= -1 & \text{a.e. in } \mathcal{A}_-(t) := \{x \in \Omega : c(u(x, t) + 1) + \mu(x, t) < 0\}, \\ \mu &= 0 & \text{a.e. in } \mathcal{I}(t) := \Omega \setminus (\mathcal{A}_-(t) \cup \mathcal{A}_+(t)) \end{aligned} \quad (2.8)$$

for an arbitrary $c > 0$. Here $\mathcal{A}_+, \mathcal{A}_-, \mathcal{I}$ are the primal-dual active and inactive sets respectively.

A primal-dual active set method for OS 2.1 is introduced in [6] and we now briefly discuss this method. In order to solve OS 2.1 we employ a backward Euler discretization where for simplicity we denote $u^{(k)} := u(\cdot, k\tau)$ by u with τ being the time step. In space we discretize the problem using finite elements. Let \mathcal{T}^h be a regular triangulation of Ω with maximal element size h and let \mathcal{J} be the set of nodes of \mathcal{T}^h . Associated with \mathcal{T}^h is the finite element space

$$S_h := \{\phi \in C^0(\bar{\Omega}) : \phi|_{\sigma} \text{ is linear } \forall \sigma \in \mathcal{T}^h\} \subset H^1(\Omega).$$

Furthermore, we denote the standard nodal basis functions of S_h by χ_j for all $j \in \mathcal{J}$. Then a function $u_h \in S_h$ is given by $u_h = \sum_{j \in \mathcal{J}} u_j \chi_j$ and the vector of coefficients is denoted by \mathbf{u} . We introduce also the lumped mass scalar product $\langle f, g \rangle_h = \int_{\Omega} I_h(fg)$ instead of $\langle f, g \rangle$. The interpolation operator $I_h : C^0(\bar{\Omega}) \rightarrow S_h$ is defined by $(I_h f)(p_j) = f(p_j)$ for all nodes $j \in \mathcal{J}$ where p_j denotes the coordinates corresponding to the node j . Using this discrete inner product, Green's identity and $\psi'_0(u) = -u$ the first equation in (2.6) can be written as

$$\frac{\varepsilon^2}{\tau} \langle u_h - u_h^{(k-1)}, \phi \rangle_h + \varepsilon^2 \gamma \langle \nabla u_h, \nabla \phi \rangle - \gamma \langle u_h, \phi \rangle_h + \langle \mu_h, \phi \rangle_h - \lambda \langle 1, \phi \rangle = 0 \quad \forall \phi \in S_h. \quad (2.9)$$

In linear algebra terms this becomes

$$((\frac{\varepsilon^2}{\tau} - \gamma)M + \varepsilon^2 \gamma K) \mathbf{u} + M \boldsymbol{\mu} - \lambda \mathbf{m} = \frac{\varepsilon^2}{\tau} M \mathbf{u}^{(k-1)} \quad (2.10)$$

where $K := (\langle \nabla \chi_j, \nabla \chi_i \rangle)$ is the stiffness matrix, $\mathbf{m} = [m_1, m_2, \dots, m_n]^T$ with $m_i := \langle 1, \chi_i \rangle$ is the mass vector and $M := (\langle \chi_j, \chi_i \rangle_h) = \text{diag}(\mathbf{m})$ is the lumped mass matrix. The discretization of the constraint $\int_{\Omega} u_h = m$ uses the fact that $|\Omega| = \sum m_j = \mathbf{m}^T \mathbf{1}$ and hence

$$\mathbf{m}^T \mathbf{u} = m |\Omega|. \quad (2.11)$$

We also discretize the complementarity conditions (2.8) which give

$$\begin{aligned} u_j &= 1 & \text{if } j \in \mathcal{A}_+ &:= \{j \in \mathcal{J} : c(u_j - 1) + \mu_j > 0\}, \\ u_j &= -1 & \text{if } j \in \mathcal{A}_- &:= \{j \in \mathcal{J} : c(u_j + 1) + \mu_j < 0\}, \\ \mu_j &= 0 & \text{if } j \in \mathcal{I} &:= \mathcal{J} \setminus (\mathcal{A}_+ \cup \mathcal{A}_-). \end{aligned} \quad (2.12)$$

Altogether, considering a partitioning in $\mathcal{A}_+, \mathcal{A}_-, \mathcal{I}$ and defining $\mathbf{b} = \frac{\varepsilon^2}{\tau} M \mathbf{u}^{(k-1)}$ and

$$L := (\frac{\varepsilon^2}{\tau} - \gamma)M + \varepsilon^2 \gamma K \quad (2.13)$$

this leads to the following linear system

$$\begin{bmatrix} L_{\mathcal{I}, \mathcal{I}} & L_{\mathcal{I}, \mathcal{A}_+} & L_{\mathcal{I}, \mathcal{A}_-} & M_{\mathcal{I}, \mathcal{I}} & 0 & 0 & -\mathbf{m}_{\mathcal{I}} \\ L_{\mathcal{A}_+, \mathcal{I}} & L_{\mathcal{A}_+, \mathcal{A}_+} & L_{\mathcal{A}_+, \mathcal{A}_-} & 0 & M_{\mathcal{A}_+, \mathcal{A}_+} & 0 & -\mathbf{m}_{\mathcal{A}_+} \\ L_{\mathcal{A}_-, \mathcal{I}} & L_{\mathcal{A}_-, \mathcal{A}_+} & L_{\mathcal{A}_-, \mathcal{A}_-} & 0 & 0 & M_{\mathcal{A}_-, \mathcal{A}_-} & -\mathbf{m}_{\mathcal{A}_-} \\ 0 & 0 & 0 & I & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & I & 0 & 0 & 0 & 0 \\ \mathbf{m}_{\mathcal{I}}^T & \mathbf{m}_{\mathcal{A}_+}^T & \mathbf{m}_{\mathcal{A}_-}^T & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}_{\mathcal{I}} \\ \mathbf{u}_{\mathcal{A}_+} \\ \mathbf{u}_{\mathcal{A}_-} \\ \boldsymbol{\mu}_{\mathcal{I}} \\ \boldsymbol{\mu}_{\mathcal{A}_+} \\ \boldsymbol{\mu}_{\mathcal{A}_-} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{b}_{\mathcal{I}} \\ \mathbf{b}_{\mathcal{A}_+} \\ \mathbf{b}_{\mathcal{A}_-} \\ \mathbf{0}_{\mathcal{I}} \\ \mathbf{1}_{\mathcal{A}_+} \\ -\mathbf{1}_{\mathcal{A}_-} \\ m|\Omega| \end{bmatrix}.$$

Given (2.12), i.e. $\mathbf{u}_{\mathcal{A}_+} = \mathbf{1}, \mathbf{u}_{\mathcal{A}_-} = -\mathbf{1}$ and $\boldsymbol{\mu}_{\mathcal{I}} = \mathbf{0}$, this linear system can be reduced to the following form

$$\begin{bmatrix} L_{\mathcal{I}, \mathcal{I}} & -\mathbf{m}_{\mathcal{I}} \\ -\mathbf{m}_{\mathcal{I}}^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}_{\mathcal{I}} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{b}_{\mathcal{I}} - L_{\mathcal{I}, \mathcal{A}_+} \mathbf{u}_{\mathcal{A}_+} - L_{\mathcal{I}, \mathcal{A}_-} \mathbf{u}_{\mathcal{A}_-} \\ -m|\Omega| + \mathbf{m}_{\mathcal{A}_+}^T \mathbf{u}_{\mathcal{A}_+} + \mathbf{m}_{\mathcal{A}_-}^T \mathbf{u}_{\mathcal{A}_-} \end{bmatrix}. \quad (2.14)$$

The Lagrange multipliers $\boldsymbol{\mu}$ on \mathcal{A}_{\pm} are then given by

$$\begin{aligned} M_{\mathcal{A}_+, \mathcal{A}_+} \boldsymbol{\mu}_{\mathcal{A}_+} &= \mathbf{b}_{\mathcal{A}_+} - L_{\mathcal{A}_+, \mathcal{I}} \mathbf{u}_{\mathcal{I}} - L_{\mathcal{A}_+, \mathcal{A}_+} \mathbf{u}_{\mathcal{A}_+} - L_{\mathcal{A}_+, \mathcal{A}_-} \mathbf{u}_{\mathcal{A}_-} + \lambda \mathbf{m}_{\mathcal{A}_+} \\ M_{\mathcal{A}_-, \mathcal{A}_-} \boldsymbol{\mu}_{\mathcal{A}_-} &= \mathbf{b}_{\mathcal{A}_-} - L_{\mathcal{A}_-, \mathcal{I}} \mathbf{u}_{\mathcal{I}} - L_{\mathcal{A}_-, \mathcal{A}_+} \mathbf{u}_{\mathcal{A}_+} - L_{\mathcal{A}_-, \mathcal{A}_-} \mathbf{u}_{\mathcal{A}_-} + \lambda \mathbf{m}_{\mathcal{A}_-}. \end{aligned} \quad (2.15)$$

For practical purposes we look at the system matrix

$$\mathcal{K} := \begin{bmatrix} L & -\mathbf{m} \\ -\mathbf{m}^T & 0 \end{bmatrix} \quad (2.16)$$

as we do not form the matrix $L_{\mathcal{I}, \mathcal{I}}$ but rather use L and implicitly work only on the free variables $\mathbf{u}_{\mathcal{I}}$ (see [41, 48] for details). In short, we want to create a Krylov subspace for the matrix given in (2.14). Therefore, we make sure the Lanczos process for \mathcal{K} is started with zeros corresponding to all elements in the active sets \mathcal{A}_+ and \mathcal{A}_- in the vector r_0 . Then at every step of the algorithm we have to carry out a multiplication with \mathcal{K} that maintains these zeros, i.e.,

$$\mathcal{K}p = \begin{bmatrix} L_{\mathcal{I}, \mathcal{I}} & L_{\mathcal{I}, \mathcal{A}_+} & L_{\mathcal{I}, \mathcal{A}_-} & -\mathbf{m}_{\mathcal{I}} \\ L_{\mathcal{A}_+, \mathcal{I}} & L_{\mathcal{A}_+, \mathcal{A}_+} & L_{\mathcal{A}_+, \mathcal{A}_-} & -\mathbf{m}_{\mathcal{A}_+} \\ L_{\mathcal{A}_-, \mathcal{I}} & L_{\mathcal{A}_-, \mathcal{A}_+} & L_{\mathcal{A}_-, \mathcal{A}_-} & -\mathbf{m}_{\mathcal{A}_-} \\ \mathbf{m}_{\mathcal{I}}^T & \mathbf{m}_{\mathcal{A}_+}^T & \mathbf{m}_{\mathcal{A}_-}^T & 0 \end{bmatrix} \begin{bmatrix} p_{\mathcal{I}}^{(1)} \\ p_{\mathcal{A}_+}^{(1)} = 0 \\ p_{\mathcal{A}_-}^{(1)} = 0 \\ p^{(2)} \end{bmatrix} \quad (2.17)$$

where p represents the vector in the iterative solver that has to be multiplied by \mathcal{K} . It can easily be seen that if we eliminate the entries of $\mathcal{K}p$ corresponding to the sets \mathcal{A}_+ and \mathcal{A}_- working with system 2.16 is a feasible approach.

In general, the primal-dual active sets of the solution are unknown. Hence not only the variables but also $\mathcal{A}_\pm, \mathcal{I}$ are unknowns in (2.14). The primal-dual active set method proposed in [6] as solver for the Allen-Cahn problem iterates now with regards to the active sets. This algorithm can be written as follows and is applied in each time step iteration.

```

1: Given  $\mathcal{A}_+^{(0)}$  and  $\mathcal{A}_-^{(0)}$ 
2: for  $n = 0, 1, \dots$  do
3:   Set  $u_{(n)} = \pm 1$  on  $\mathcal{A}_\pm^{(n)}$  and  $\mu_{(n)} = 0$  on  $\mathcal{I}^{(n)}$ 
4:   Solve (2.14) to obtain  $u_{(n)}$  on  $\mathcal{I}^{(n)}$  and  $\lambda_{(n)}$ 
5:   Compute  $\mu_{(n)}$  on  $\mathcal{A}_\pm^{(n)}$  using (2.15)
6:   Compute  $\mathcal{A}_\pm^{(n+1)}$  using (2.12) with  $u_{(n)}$  and  $\mu_{(n)}$ 
7:   if  $\mathcal{A}_+^{(n+1)} = \mathcal{A}_+^{(n)}$  and  $\mathcal{A}_-^{(n+1)} = \mathcal{A}_-^{(n)}$  then
8:     STOP (Algorithm converged)
9:   end if
10: end for

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Algorithm 1: Primal dual active set method (PDAS)

2.2. Vector-valued Allen-Cahn equation with multi obstacle potential.

The scalar Allen-Cahn equation describes the motion of an interface separating two phases. In practical applications often more than two phases occur [7, 18, 30] and the phase field concept has been extended to deal with multi phase systems [17]. There a vector-valued order parameter $u : \Omega \rightarrow \mathbb{R}^N$ is introduced, where each u_i describes one phase, i.e. if $u_i = 0$ then the phase i is absent in that region, if $u_i = 1$ only phase i is present in that region. Hence $\sum_{i=1}^N u_i = 1$ and $u_i \geq 0$ is required. The motion of the interfaces separating N bulk regions can be modelled again with the Ginzburg Landau energy (2.1) where the potential function $\psi : \mathbb{R}^N \rightarrow \mathbb{R}_0^+ \cup \{\infty\}$ is now a multi obstacle potential given by

$$\psi(\xi) = \begin{cases} \psi_0(\xi) = -\frac{1}{2}\xi \cdot W\xi & \text{for } \xi \geq 0, \xi \cdot \mathbf{1} = 1 \\ \infty & \text{otherwise} \end{cases} \quad (2.18)$$

with a symmetric matrix $W \in \mathbb{R}^{N,N}$. In [2] it is discussed that W must have at least one positive eigenvalue. Taking the scaled L^2 -gradient of the energy (2.1) leads to the vector valued Allen-Cahn variational inequality

$$\varepsilon \langle \partial_t u, \chi - u \rangle + \gamma \varepsilon \langle \nabla u, \nabla (\chi - u) \rangle - \frac{\gamma}{\varepsilon} \langle Wu, \chi - u \rangle \geq 0 \quad (2.19)$$

which has to hold for all $\chi \in \mathcal{G} := \{\chi \in (H^1(\Omega))^N : \chi \cdot \mathbf{1} = 1, \chi_i \geq 0 \text{ a.e. in } \Omega\}$ and for almost all t .

Again systems where the total spatial amount of the phases is conserved are considered, i.e.,

$$\int_{\Omega} u = m = [m^1, m^2, \dots, m^N]^T$$

where $m^i \in (0, 1)$ and $\sum_{i=1}^N m^i = 1$ due to $u \in \mathcal{G}$. Defining $\mathcal{G}^m := \{u \in \mathcal{G} : \int_{\Omega} u = m\}$ the following problem can be obtained

OS 2.2. *For a given $u(\cdot, 0) = u_0 \in \mathcal{G}^m$ find $u \in L^2(0, T; \mathcal{G}^m) \cap H^1(0, T; (L^2(\Omega))^N)$ such that for almost all $t \in (0, T)$*

$$\varepsilon \langle \partial_t u, \chi - u \rangle + \gamma \varepsilon \langle \nabla u, \nabla (\chi - u) \rangle - \frac{\gamma}{\varepsilon} \langle Wu, \chi - u \rangle \geq 0 \quad \forall \chi \in \mathcal{G}^m.$$

Similar to OS 2.1 a primal-dual active set method can be employed and we quickly review some of the details for OS 2.2. In [7, 5] the following formulation of OS 2.2 is given

$$\begin{aligned} \varepsilon^2 \partial_t u - \varepsilon^2 \gamma \Delta u - \gamma Wu - \mu - \lambda - \eta \mathbf{1} &= 0 && \text{a.e. in } \Omega \\ \frac{\partial u}{\partial \nu} &= 0 && \text{a.e. on } \partial \Omega \\ \int_{\Omega} u = m, \quad \sum_{i=1}^N u_i = 1, \quad \sum_{i=1}^N \lambda_i = 0 \end{aligned} \quad (2.20)$$

together with the complementary conditions $u \geq 0$, $\mu \geq 0$ a.e. in Ω and $\langle \mu, u \rangle = 0$. Here μ is the Lagrange multiplier associated with $u \geq 0$, λ is the Lagrange multiplier for $\int_{\Omega} u = m$ with $\sum_{i=1}^N \lambda_i = 0$ and η is the Lagrange multiplier for $\sum_{i=1}^N u_i = 1$. Note that $\lambda(t) \in \mathbb{R}^N$, $\eta(x, t) \in \mathbb{R}$, $\mu(x, t) \in \mathbb{R}^N$ and $u(x, t) \in \mathbb{R}^N$ for a.e. $(x, t) \in \Omega \times [0, T]$. For each component u_i we have an active set and the complementarity conditions can be reformulated for $i = 1, \dots, N$ as

$$\begin{aligned} u_i(\cdot, t) &= 0 && \text{a.e. in } \mathcal{A}_i(t) := \{x \in \Omega : c(u(x, t))_i - (\mu(x, t))_i < 0\} \\ \mu_i(\cdot, t) &= 0 && \text{a.e. in } \mathcal{I}_i(t) := \Omega \setminus \mathcal{A}_i(t). \end{aligned} \quad (2.21)$$

Again in order to solve the underlying optimization problem we discretize the equations using the backward Euler method in time and finite elements in space and then employ a slight modification of Algorithm 1. We obtain the discretized problem: Given $u^{(k-1)}$ find $\lambda \in \mathbb{R}^N$, $u, \mu \in (S_h)^N$, $\eta \in S_h$ such that $\int_{\Omega} u = m$, $\sum_{i=1}^N u_i = 1$, $\sum_{i=1}^N \lambda_i = 0$, furthermore (2.21) is fulfilled in each node $j \in \mathcal{J}$ and the following equation holds for all $\phi \in S_h$ and $i = 1, \dots, N$:

$$\frac{\varepsilon^2}{\tau} \langle u_i - u_i^{(k-1)}, \phi \rangle_h + \varepsilon^2 \gamma \langle \nabla u_i, \nabla \phi \rangle - \langle \gamma (Wu)_i + \mu_i + \eta, \phi \rangle_h - \lambda_i \langle 1, \phi \rangle = 0. \quad (2.22)$$

Using $u_i = \sum_{j=1}^N (\mathbf{u}_i)_j \chi_j \in S_h$ for $i = 1, \dots, N$ with the nodal basis functions χ_j of S_h (2.22) can be written in linear algebra terms as

$$\left(\frac{\varepsilon^2}{\tau} M + \varepsilon^2 \gamma K \right) \mathbf{u}_i - \gamma M \sum_{l=1}^N w_{il} \mathbf{u}_l - M \boldsymbol{\mu}_i - \lambda_i \mathbf{m} - M \boldsymbol{\eta} = \frac{\varepsilon^2}{\tau} M \mathbf{u}_i^{(k-1)}. \quad (2.23)$$

Moreover, we have the constraints

$$\mathbf{m}^T \mathbf{u}_i = m^i |\Omega|, \quad \sum_{i=1}^N \mathbf{u}_i = 1, \quad \sum_{i=1}^N \lambda_i = 0. \quad (2.24)$$

In addition we have $\lambda_N = -\sum_{i=1}^{N-1} \lambda_i$. As in the scalar case we work implicitly only on the free variables $(\mathbf{u}_i)_{\mathcal{I}_i}$, λ_i , $\boldsymbol{\eta}$. The variables $(\boldsymbol{\mu}_i)_{\mathcal{A}_i}$ are then determined by (2.23). Hence using L as defined in (2.13) we can reduce (2.23) to the following system, where

we take $W = I$ and $N = 3$ to simplify matters (see [7]):

$$\begin{bmatrix} L_{\mathcal{I}_1, \mathcal{I}_1} & 0 & 0 & -\mathbf{m}_{\mathcal{I}_1} & 0 & -M_{\mathcal{I}_1, :} \\ 0 & L_{\mathcal{I}_2, \mathcal{I}_2} & 0 & 0 & -\mathbf{m}_{\mathcal{I}_2} & -M_{\mathcal{I}_2, :} \\ 0 & 0 & L_{\mathcal{I}_3, \mathcal{I}_3} & \mathbf{m}_{\mathcal{I}_3} & \mathbf{m}_{\mathcal{I}_3} & -M_{\mathcal{I}_3, :} \\ -\mathbf{m}_{\mathcal{I}_1}^T & 0 & \mathbf{m}_{\mathcal{I}_3}^T & 0 & 0 & 0 \\ 0 & -\mathbf{m}_{\mathcal{I}_2}^T & \mathbf{m}_{\mathcal{I}_3}^T & 0 & 0 & 0 \\ -M_{:, \mathcal{I}_1}^T & -M_{:, \mathcal{I}_2}^T & -M_{:, \mathcal{I}_3}^T & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} (\mathbf{u}_1)_{\mathcal{I}_1} \\ (\mathbf{u}_2)_{\mathcal{I}_2} \\ (\mathbf{u}_3)_{\mathcal{I}_3} \\ \lambda_1 \\ \lambda_2 \\ \boldsymbol{\eta} \end{bmatrix} = \begin{bmatrix} \left(\frac{\varepsilon^2}{\tau} M \mathbf{u}_1^{(k-1)}\right)_{\mathcal{I}_1} \\ \left(\frac{\varepsilon^2}{\tau} M \mathbf{u}_2^{(k-1)}\right)_{\mathcal{I}_2} \\ \left(\frac{\varepsilon^2}{\tau} M \mathbf{u}_3^{(k-1)}\right)_{\mathcal{I}_3} \\ (m^3 - m^1) |\Omega| \\ (m^3 - m^2) |\Omega| \\ -\mathbf{m} \end{bmatrix}. \quad (2.25)$$

For a different choice of W the first 3 by 3 block changes and might lose the diagonal structure but remains symmetric.

To solve this system for unknown active sets we again apply a PDAS-algorithm like Algorithm 1, i.e. in the n -th iteration we update the sets $\mathcal{A}_i^{(n)}$, $\mathcal{I}_i^{(n)}$ using (2.21), solve with these sets the equation system (2.25), set $(\mathbf{u}_i)_{\mathcal{A}_i^{(n)}} = 0$, $(\boldsymbol{\mu}_i)_{\mathcal{I}_i^{(n)}} = 0$, $\lambda_N = -\sum_{i=1}^{N-1} \lambda_i$ and finally $(\boldsymbol{\mu}_i)_{\mathcal{A}_i^{(n)}}$ is obtained from equation (2.23). For one iteration the main numerical effort is therefore the solution of the system (2.25).

Again, assembling the matrices on the free variables or reassigning parts of the matrix blocks in (2.25) is not feasible. Hence, using reordering and $(\mathbf{u}_i)_{\mathcal{A}_i} = 0$ and $(\boldsymbol{\mu}_i)_{\mathcal{I}_i} = 0$ we work with the full blocks which are given by the following system

$$\begin{bmatrix} L & 0 & 0 & -M & -\mathbf{m} & 0 \\ 0 & L & 0 & -M & 0 & -\mathbf{m} \\ 0 & 0 & L & -M & \mathbf{m} & \mathbf{m} \\ -M^T & -M^T & -M^T & 0 & 0 & 0 \\ -\mathbf{m}^T & 0 & \mathbf{m}^T & 0 & 0 & 0 \\ 0 & -\mathbf{m}^T & \mathbf{m}^T & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \mathbf{u}_3 \\ \boldsymbol{\eta} \\ \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} M\boldsymbol{\mu}_1 + \frac{\varepsilon^2}{\tau} M \mathbf{u}_1^{(k-1)} \\ M\boldsymbol{\mu}_2 + \frac{\varepsilon^2}{\tau} M \mathbf{u}_2^{(k-1)} \\ M\boldsymbol{\mu}_3 + \frac{\varepsilon^2}{\tau} M \mathbf{u}_3^{(k-1)} \\ -\mathbf{m} \\ (m^3 - m^1) |\Omega| \\ (m^3 - m^2) |\Omega| \end{bmatrix}. \quad (2.26)$$

The system matrix in (2.26) is denoted by \mathcal{K}_{vv} for the remainder of the paper.

3. Preconditioning. As for any meaningful computation the assembly of the matrices on the free variables (see (2.25) and (2.14)) will be unfeasible, we consider in the following the preconditioning of the matrices \mathcal{K} and \mathcal{K}_{vv} . Numerical results illustrate the efficiency of this approach.

3.1. \mathcal{K} -The scalar case. To clarify some ideas we first consider the scalar case. In (2.16) a linear symmetric and indefinite system in saddle point form is shown to be at the heart of the computation. Systems of this form have been analyzed carefully in [3, 14]. A common ansatz for preconditioning a saddle point matrix of the form (1.1) is given in [38]. Here the preconditioning matrix is given by an approximation, respectively of the inverse of

$$\mathcal{P} = \begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix} \quad (3.1)$$

where S is the Schur-complement $-B^T A^{-1} B$. If one is willing to approximate the Schur-complement, which is in this case $-\mathbf{m}^T L^{-1} \mathbf{m} \in \mathbb{R}$, techniques based on the Lanczos process [37] and its connection to Gauss quadrature [20] can be used [19].

Then a few steps of the Lanczos process applied to L and an eigenvalue calculation for a tridiagonal matrix [22] should provide a good approximation to the Schur-complement.

However we would like to avoid the approximation of S . Therefore, let us for the moment assume that the preconditioner for (2.16) is given by

$$\mathcal{P}_{BD} = \begin{bmatrix} L & 0 \\ 0 & 1 \end{bmatrix}. \quad (3.2)$$

Here we employ that L is symmetric and positive definite which we show in Section 3.3. Assuming that $\left(\lambda, \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}\right)$ represents an eigenpair of the preconditioned saddle point matrix \mathcal{K} , that means of $\mathcal{P}_{BD}^{-1}\mathcal{K}$, we get

$$Lv_1 - \mathbf{m}v_2 = \lambda Lv_1 \quad (3.3)$$

$$-\mathbf{m}^T v_1 = \lambda v_2. \quad (3.4)$$

For $\lambda = 1$ we get from (3.3) $v_2 = 0$ and hence (3.4) becomes $-\mathbf{m}^T v_1 = 0$. I.e. the hyperplane given by \mathbf{m}^\perp determines the eigenspace and the multiplicity $n-1$ of $\lambda = 1$. Now, for $\lambda \neq 1$ we get for the remaining two eigenvalues $\lambda_{1/2}$

$$v_1 = \frac{1}{1-\lambda}L^{-1}\mathbf{m}v_2, \quad -\frac{1}{1-\lambda}\mathbf{m}^T L^{-1}\mathbf{m}v_2 = \lambda v_2 \quad \Rightarrow \lambda_{1/2} = \frac{1}{2} \pm \sqrt{\frac{1}{4} + \sigma}$$

where σ is $\mathbf{m}^T L^{-1}\mathbf{m}$.

This analysis indicates that for the Allen-Cahn variational inequality with volume constraint the preconditioning of the $(1, 1)$ block L of \mathcal{K} given by (2.13) is crucial as it can result in a clustering of the eigenvalues that guarantees fast convergence. Thus, we will only focus on efficient preconditioning strategies for the Allen-Cahn equation and then consider a preconditioner

$$\mathcal{P}_{BD} = \begin{bmatrix} A_0 & 0 \\ 0 & 1 \end{bmatrix} \quad (3.5)$$

where A_0 approximates the Allen-Cahn block L .

We also want to discuss one other way of solving the given linear system

$$\mathcal{K} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ -c \end{bmatrix}$$

that is used in [23, 34]. The linear system is the first order condition of

$$\min \frac{1}{2}x^T Lx - b^T x \text{ s.t. } \mathbf{m}^T x = c. \quad (3.6)$$

This optimization problem is equivalent to $\min x^T (L + \mathbf{m}\mathbf{m}^T) x - (b + c\mathbf{m}^T)x$ and hence to solving the linear system

$$(L + \mathbf{m}\mathbf{m}^T) x = b + c\mathbf{m}. \quad (3.7)$$

Since $L + \mathbf{m}\mathbf{m}^T$ is a symmetric and positive definite matrix one can employ the classical CG method [26] with a preconditioner for L (see Section 2.1). In the idealized case we would get the preconditioned matrix $L^{-1}(L + \mathbf{m}\mathbf{m}^T) = I + L^{-1}\mathbf{m}\mathbf{m}^T$ and as the

matrix $L^{-1}\mathbf{m}\mathbf{m}^T$ is a rank-one matrix the disturbance with term $\mathbf{m}\mathbf{m}^T$ would result in one additional CG iteration. It is also possible to construct a multigrid method for the matrix $L + \mathbf{m}\mathbf{m}^T$. However, the rank-one perturbation might make the multigrid convergence slow as the eigenvalues of $L + \mathbf{m}\mathbf{m}^T$ might be close to 1 (see [28] for eigenvalue bounds on rank-one perturbed matrices). Again a good preconditioner for L will provide a fast solution of this reformulation.

3.2. \mathcal{K}_{vv} —the vector-valued case. As in the previous section we focus on the properties of the symmetric and indefinite system matrix \mathcal{K}_{vv} of (2.26) and devise suitable preconditioning strategies. Going back to the notation of the classical 2×2 saddle point problem we have to decide how to split \mathcal{K}_{vv} to achieve the best preconditioning strategy. Here, we propose the following splitting, formulated for three phases

$$A = \begin{bmatrix} L & 0 & 0 & -M \\ 0 & L & 0 & -M \\ 0 & 0 & L & -M \\ -M^T & -M^T & -M^T & 0 \end{bmatrix} \text{ and } B = \begin{bmatrix} -\mathbf{m}^T & 0 & \mathbf{m}^T \\ 0 & -\mathbf{m}^T & \mathbf{m}^T \end{bmatrix} \quad (3.8)$$

which we motivate by the following eigenvalue analysis. A is of size $n_N := (N+1)n$, B has rank $r := N-1$ and \mathcal{K}_{vv} is of size $n_N + r$, where N is the number of phases and $n = |J|$ the number of nodal basis functions of S_h . Assume that an eigenpair (λ, v) of the generalized eigenvalue problem, respectively of the preconditioned matrix \mathcal{K}_{vv} , is given

$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} v = \lambda \begin{bmatrix} A & 0 \\ 0 & I \end{bmatrix} v \quad (3.9)$$

one can show [31, 38, 47] that there are $n_N - r = (N+1)n - (N-1)$ eigenvalues at 1, i.e. clustering takes place. The remaining $2r = 2(N-1)$ eigenvalues can be found based on the eigenvalues of the Schur-complement of $BA^{-1}B^T$. A good preconditioner for \mathcal{K}_{vv} is hence

$$\mathcal{P}_{vv} = \begin{bmatrix} A & 0 \\ 0 & I \end{bmatrix} \quad (3.10)$$

and built on a good preconditioner of A . The matrix A itself is of saddle point structure

$$A = \begin{bmatrix} \tilde{A} & \tilde{B}^T \\ \tilde{B} & 0 \end{bmatrix}$$

with $\tilde{A} = \text{blkdiag}(L, \dots, L)^1$ and the “skinny” matrix $\tilde{B} = \begin{bmatrix} -M^T & \dots & -M^T \end{bmatrix}$. As mentioned before a preconditioner of A can be built upon a good approximation of the inverse of \tilde{A} and of the inverse of the Schur-complement S of A , which is given by

$$S = N(M^T L^{-1} M).$$

¹Using Matlab notation

The inverse of the Schur-complement can be used exactly since

$$S^{-1} = \frac{1}{N}(M^T L^{-1} M)^{-1} = \frac{1}{N} \left\{ \left(\frac{\varepsilon^2}{\tau} - \gamma \right) M^{-T} + \varepsilon^2 \gamma M^{-1} K M^{-T} \right\}$$

where M is a diagonal matrix and hence can be inverted easily. A good approximation (or preconditioner) to \tilde{A} is naturally based on how to approximate or precondition the relevant Allen-Cahn block L . This discussion we defer to the next Section.

Again, if one is willing to put more effort into preconditioning using instead of the identity block in \mathcal{P}_{vv} the Schur-complement $-B^T A^{-1} B$ of \mathcal{K}_{vv} , then for the approximation of $-B^T A^{-1} B$ Block-Lanczos techniques as used in [19, 21] to approximate $B^T f(A) B$ can be employed. The techniques are similar to the ones mentioned in the scalar case, but typically rely on block methods.

3.3. Preconditioning for the Allen-Cahn equation. In this subsection we comment on the preconditioning of the block L , which is essential for the scalar as well as for the vector valued case. The system matrix $L = (\frac{\varepsilon^2}{\tau} - \gamma)M + \varepsilon^2 \gamma K$ reflects the space discretization of the time discretized Allen-Cahn type equation (2.3), namely

$$-\varepsilon^2 \gamma \Delta u + \left(\frac{\varepsilon^2}{\tau} - \gamma \right) u = \frac{\varepsilon^2}{\tau} u^{(k-1)}.$$

As K is the finite element discretization of the Laplace operator we know that it is symmetric and positive semidefinite and M being the lumped mass matrix is symmetric and positive definite. Hence L is symmetric and positive definite whenever

$$\varepsilon^2 > \gamma \tau. \quad (3.11)$$

Therefore the interface thickness ε and the time-step τ of the implicit Euler scheme are coupled. This time step restriction is due to the implicit treatment of the non-convex potential term and similar restrictions are obtained for other choices of ψ , see e.g. [34].

Explicit treatment of the potential: So far we considered only the implicit time discretization, i.e. we implicitly treated the terms coming from the discretization of $\psi'_0(u)$. This leads to restrictions on the time step τ . If the term $\psi'_0(u)$ is discretized explicitly, equation (2.10) becomes

$$\left(\frac{\varepsilon^2}{\tau} M + \varepsilon^2 \gamma K \right) \mathbf{u} + M \boldsymbol{\mu} - \lambda \mathbf{m} = \left(\frac{\varepsilon^2}{\tau} + \gamma \right) M \mathbf{u}^{(k-1)}$$

Respectively the equation (2.23) of the vector valued case changes. Hence L is given as $\frac{\varepsilon^2}{\tau} M + \varepsilon^2 \gamma K$ in the considerations, which is positive definite for all time steps τ . The same preconditioning techniques proposed earlier can be applied. Even though the time-step can be arbitrarily large for the linear algebra considerations, computations show that the results obtained for large time-steps are highly inaccurate [6].

Larger τ for implicit discretization: For the scalar Allen-Cahn case we can relax the time step restriction to some extent, which is argued now. The invertibility of the system matrix (2.16) is given whenever L is positive definite on $\ker(\mathbf{m}^T) = \mathbf{m}^\perp$. The space \mathbf{m}^\perp reflects the condition $\int_{\Omega} v = 0$ for $v \in S_h$. For the function space $\{v \in H^1(\Omega_h) \mid \int_{\Omega} v = 0\}$ the Poincare inequality $\|v\|_{L^2(\Omega_h)} \leq \tilde{c}_p \|\nabla v\|_{L^2(\Omega_h)}$ holds with a Poincare constant \tilde{c}_p for appropriate conditions on $\partial\Omega_h$ [10]. If one applies this inequality and incorporates mass lumping, we obtain

$$\lambda_{\min}^M \|\mathbf{u}\|^2 \leq \mathbf{u}^T M \mathbf{u} \leq c_p \mathbf{u}^T K \mathbf{u} \quad \forall \mathbf{u} \in \mathbf{m}^\perp \quad (3.12)$$

where $\lambda_{\min}^M > 0$ is the minimal eigenvalue (here the minimal coefficient) of M . Consequently we obtain

$$\mathbf{u}^T L \mathbf{u} \geq \left(\frac{\varepsilon^2}{\tau} - \gamma + \frac{\varepsilon^2 \gamma}{c_p} \right) \lambda_{\min}^M \|\mathbf{u}\|^2 \quad \forall \mathbf{u} \in \mathbf{m}^\perp$$

and L is positive definite on $\ker(\mathbf{m}^T)$ if

$$\varepsilon^2 > \gamma \tau \left(1 - \frac{\varepsilon^2}{c_p} \right).$$

If one is more specific and considers the system (2.14), hence the positive definiteness of $L_{\mathcal{I}, \mathcal{I}}$ on $\mathbf{m}_{\mathcal{I}}^\perp$, then in one space dimension one can show in a similar way as above that no time restriction is necessary due to $c_p = \frac{1}{4}\varepsilon^2$ (see [6]).

As a **preconditioning strategy** for L we propose an algebraic multigrid (AMG) preconditioner for the Allen-Cahn equation. Algebraic multigrid methods typically exhibit geometric multigrid-like properties by only using algebraic information. This has the advantage that it works well in general even for complicated geometries and meshes. We refer to [42, 15] for more information on AMG. We illustrate the performance of AMG for the Allen-Cahn equation in Section 4.

However geometric multigrid methods are possible too. In [32, 33] a multigrid method is developed to solve discrete elliptic variational inequalities arising from obstacle problems. The monotone multigrid algorithm is based on a subspace correction approach (see [50]) where a subspace is decomposed into smaller spaces, which leads to a polygonal Gauss-Seidel relaxation (see [50]) as the fine grid smoother. This is combined with a coarse grid correction. This idea has been extended for the vector-valued Allen-Cahn equation [34]. Recently, in [30] this technique is applied to problems in image segmentation. A review on various multigrid methods for obstacle problems can be found in [23]. A comparison of multigrid methods in case of Allen-Cahn equations is still missing due to the lack of comparable software.

3.4. Choice of Krylov-subspace solver. As the saddle point systems are symmetric and indefinite we choose MINRES [39]. For the preconditioned version of MINRES the preconditioner \mathcal{P} has to be symmetric and positive definite, which is fulfilled by the block-diagonal preconditioners presented earlier. An implementation of MINRES with preconditioning can be found in [14]. In its standard version MINRES minimizes the 2-norm of the residual $\|r_k\|_2$ and with the preconditioner \mathcal{P} symmetric and positive definite the residual is now minimized in the \mathcal{P}^{-1} -norm. In this paper we only present results based on MINRES but other Krylov subspace solvers might also be applicable. One other option is the Bramble-Pasciak CG method [9] which uses a block-triangular preconditioner

$$\mathcal{P}_{BT} = \begin{bmatrix} A_0 & 0 \\ B & -I \end{bmatrix} \quad (3.13)$$

where A_0 here approximates the saddle point block A , which we developed previously. The resulting preconditioned matrix $\mathcal{P}^{-1}\mathcal{K}$ is symmetric in the non-standard inner product given by

$$\mathcal{H} = \begin{bmatrix} A_0 - A & 0 \\ 0 & I \end{bmatrix} \quad (3.14)$$

and is positive definite under certain conditions on the preconditioner which allows the implementation of a non-standard inner product version of the CG method (see [9, 40, 13]).

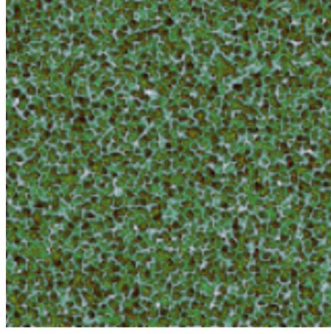
Another alternative solver would be to use SYMMLQ [39] as this can sometimes be advantageous to MINRES (see [45]).

4. Numerical results. For the numerical results presented in this section we choose $\varepsilon = 0.09$, $\tau = 0.0001$ and $\gamma = 1$. The domain Ω is set to be $[-1, 1]^d$ but different domains provide no additional difficulty for the preconditioners. The tolerance in MINRES was set to $1e-6$ in all examples. As a preconditioner for the block L we chose the Trilinos AMG [25]. For one application of the preconditioner we take in general 5 steps of a Gauss-Seidel smoother and one V-cycle. The implementation of the primal-dual active set method is performed with deal.II [1], which allows the use of the Trilinos library. This reasons the fact that all numerical experiments listed here are generated with finite elements on rectangles, while above results are stated for a regular triangulation \mathcal{T}^h . However, two dimensional numerical results using triangulations, which are implemented with the finite element toolbox Alberta 2.0 [44], generate similar results. Unfortunately, Alberta 2.0 does not provide any interfaces to external linear algebra routines such as Trilinos AMG [25], which limits its efficiency for more complex problems.

4.1. Results for the scalar problem. In this section we show results for the scalar problem. We start with a random data problem in two space dimensions where we set the initial value $u_0(x)$ for the order parameter randomly between -0.1 and 0.1 , i.e. no pure phases are present at time $t = 0$. The volume constraint is chosen to be $m = 0.4$. Figure 4.1 shows the initial configuration and the result of the Allen-Cahn evolution after 300 time steps. For this problem we considered various uniform mesh-sizes and we compared the average number of MINRES iterations needed per Newton iteration with (Figure 4.2a) and without (Figure 4.2b) preconditioning. In the legend the number of unknowns and the total time for computation is listed. As can be seen from this the preconditioned version always outperforms the unpreconditioned method. Especially when the number of mesh points is very large the preconditioning reduces the number of iterations significantly, e.g. for roughly one million number of unknowns from 72 to 14 iterations at the last time step. Also, at the beginning of the computation when no pure phases are present and all mesh points are inactive the preconditioning works extremely well. In all our computations we use the solution from the previous Newton iteration or time step iteration as the initial guess x_0 for MINRES. Hence we note that when the phases and consequently the solution from one time-step to the next are hardly changing the initial guess x_0 is sufficiently close to the new solution and only very few iterations with or without preconditioning will be needed.

It can be seen that in the first time steps the preconditioned results have very low MINRES iteration numbers (sometimes even one iteration). In not listed numerical test without preinitialization of x_0 , i.e. x_0 set to zero, the iteration numbers in the first time steps are slightly larger but typically less than 5 iterations.

The next example, starts with a 2D dumbbell as the initial configuration. Table 4.1 shows the average number of MINRES iterations per Newton iteration. For this computation we used an adaptively refined and coarsened mesh with the minimal size of an element $h_{min} = 1/512$ and the maximal size $h_{max} = 1/16$. We also used uniform mesh sizes and compared the average number of MINRES iterations for the first 20 time steps. Figure 4.3 shows that the average number of MINRES iterations stays

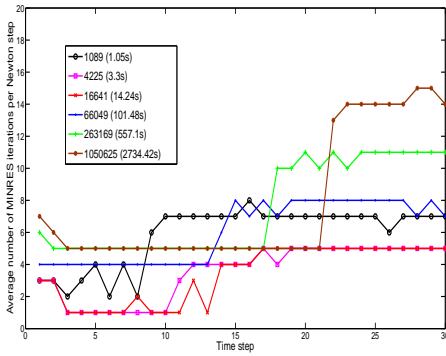


(a) Initial state of the phase

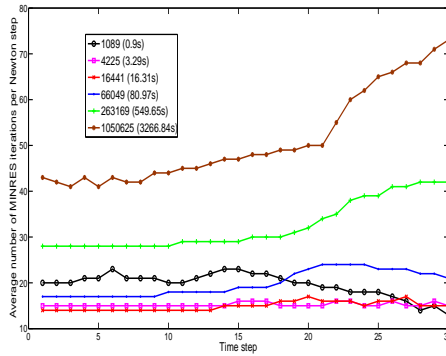


(b) After 300 time steps

Figure 4.1: Computation with random initial data



(a) with preconditioning



(b) no preconditioning

Figure 4.2: Results for 30 time steps of a random data with different mesh-sizes

(almost) constant for one mesh size. For all the dumbbell computations we used the preconditioned MINRES. We observe a very benign mesh dependence. However the number of iterations stay low with at most 16 iterations for a mesh with roughly one million unknowns.

In the last computation for the scalar case we consider a three dimensional domain and we choose a Doughnut as initial state, see Figure 4.4. Figure 4.4c shows the average number of MINRES iterations with and without preconditioning for the first 30 time step iterations. It can clearly be seen that the preconditioned version outperforms the unpreconditioned version. However, the effect in this case is not as drastic as in the random data case. A reason for this is that the active sets do not change very much from one Newton iteration to the next which means that the previous solution provides a good initial guess for MINRES and hence only a relatively

| time step | dimension | Newton | MINRES per Newton |
|-----------|-----------|--------|-------------------|
| 0 | 16641 | 4 | 5 |
| 1 | 28509 | 5 | 8 |
| 2 | 35589 | 7 | 11 |
| 3 | 51390 | 10 | 16 |
| 4 | 75936 | 9 | 17 |
| 5 | 73456 | 10 | 17 |
| 6 | 78339 | 10 | 17 |
| 7 | 75430 | 10 | 17 |
| 8 | 77710 | 10 | 17 |
| 9 | 75061 | 10 | 16 |
| 10 | 77036 | 10 | 17 |
| 11 | 75113 | 10 | 16 |
| 12 | 76800 | 10 | 17 |
| 13 | 74908 | 10 | 17 |
| 14 | 76604 | 10 | 18 |
| 15 | 75411 | 10 | 17 |
| 16 | 76359 | 10 | 18 |
| 17 | 74921 | 10 | 17 |
| 18 | 75633 | 10 | 18 |
| 19 | 74852 | 10 | 16 |

Table 4.1: Number of Newton and MINRES iterations for the dumbbell computation with adaptive mesh

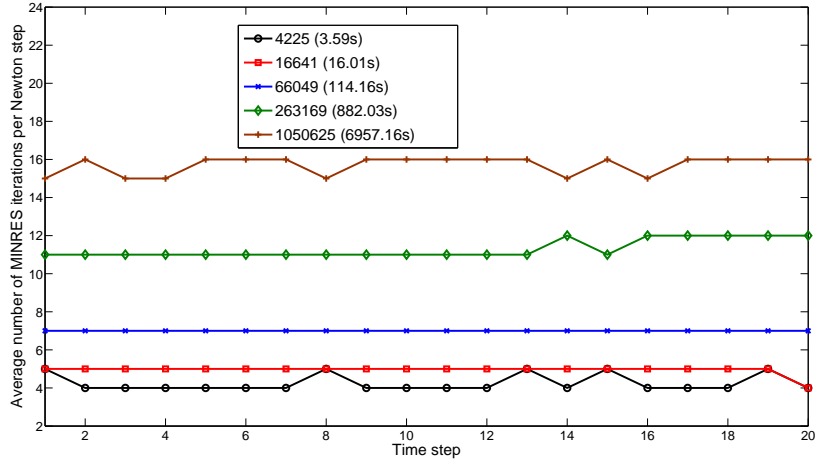


Figure 4.3: Dumbbell computation: 20 time steps for different uniform mesh sizes

small number of iterations is needed in general.

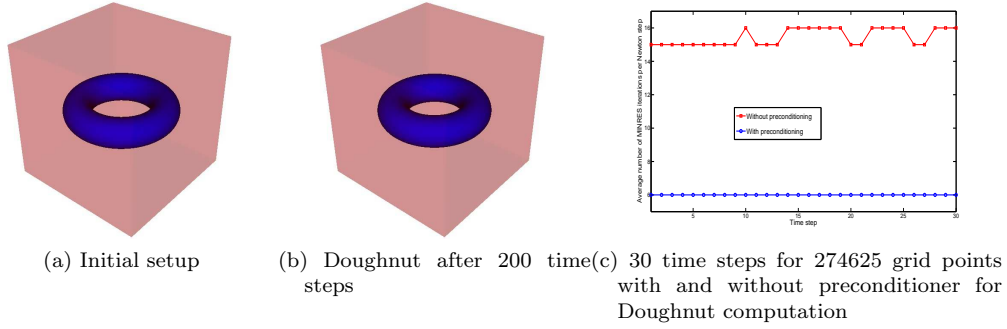


Figure 4.4: Results for 3D doughnut

4.2. Results for the vector-valued problem. In this section we present results for the vector-valued problem with three phases ($N = 3$). The parameters for τ , ε and γ remain unchanged. Our first example is the so-called double bubble as shown in Figure 4.5. We use a non-adaptive strategy and start with a uniform partitioning of the hypercube $[-1, 1]^3$ that has 274625 degrees of freedom. For this example we consider preconditioning and no preconditioning and we compare the results. Figure 4.5c shows the average number of MINRES iterations per Newton step for 50 time steps. The effect of using a preconditioner is much more dramatic than in the scalar case (a factor of 10 in iteration numbers could often be observed). We would expect this to be even more significant if a larger number of phases is simulated. The computation times are given by 18413 seconds with 4651.22 seconds for the AMG setup plus application in the case with preconditioning and 72825 seconds without preconditioner.

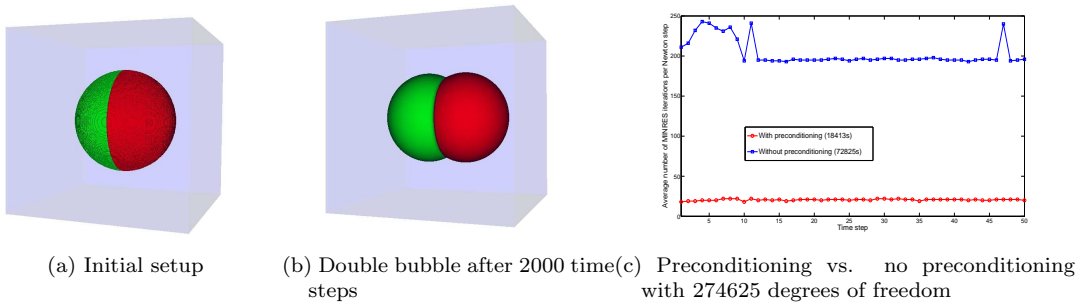
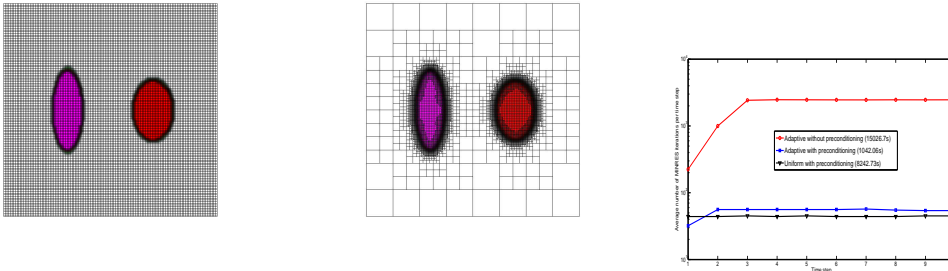


Figure 4.5: Initial configuration, evolution and iteration numbers of the 3D double bubble

The next example is concerned with a configuration of $N = 3$ phases in $[-1, 1]^2$ where two phases represent an ellipse each and we focus on a comparison between an adaptive mesh and a uniform mesh. The initial configuration and the adaptively refined mesh are shown in Figure 4.6 with $h_{\max} = 1/16$ and $h_{\min} = 1/256$. The

results of 10 time steps are shown in Figure 4.6c where we compare a uniform grid with 263169 degrees of freedom against an adaptively refined mesh (around 34000 unknowns after initial refining and coarsening), where the uniform mesh is of size h_{\min} . In this example we used 10 steps of the Chebyshev smoother rather than 5 Gauss-Seidel smoother steps. The Chebyshev smoother is rather cheap to apply and we can see that the preconditioning results using this type of smoother produce satisfactory results. The computation times for the uniform vs. adaptive grid with and without preconditioning are shown in Figure 4.6c, where the dramatic difference in computation times and average MINRES iteration numbers can be observed.



(a) Initial setup with uniform mesh (b) Adaptive mesh after 4 time steps (c) Uniform grid vs. adaptive grid

Figure 4.6: Results for two 2D ellipses

4.3. Conclusions. In this paper we analyzed the linear systems arising from the primal-dual active set method for the scalar and vector-valued Allen-Cahn equation with volume constraints. In order to make the primal-dual active set method more efficient we proposed to use the linear algebra solver MINRES and hence we analyzed block-diagonal preconditioners. We further showed that for both problems the crucial part is a good approximation of the block coming from the discretization of the Allen-Cahn equation. We chose an algebraic multigrid as preconditioner for the Allen-Cahn equation and the numerical results for both the scalar and the vector-valued case justify this choice.

Acknowledgment. The authors would like to thank Ralf Kornhuber for fruitful discussions in Oberwolfach. This publication is partially based on work supported by Award No. KUK-C1-013-04, made by King Abdullah University of Science and Technology (KAUST)

REFERENCES

- [1] W. BANGERTH, R. HARTMANN, AND G. KANSCHAT, *deal.II—a general-purpose object-oriented finite element library*, ACM Trans. Math. Software, 33 (2007), pp. Art. 24, 27.
- [2] J.W. BARRET AND J.F. BLOWEY, *Finite element approximation of a model for phase separation of a multi-component alloy with non-smooth free energy*, Num. Math., 77 (1997), pp. 11–34.
- [3] M. BENZI, G.H. GOLUB, AND J. LIESEN, *Numerical solution of saddle point problems*, Acta Numer., 14 (2005), pp. 1–137.
- [4] M. BERGOUNIOUX, K. ITO, AND K. KUNISCH, *Primal-dual strategy for constrained optimal control problems*, SIAM J. Control Optim., 37 (1999), pp. 1176–1194.

- [5] L. BLANK, M. BUTZ, H. GARCKE, L. SARBU, AND V. STYLES, *Allen-Cahn and Cahn-Hilliard variational inequalities solved with optimization techniques*, (2010). to be published in: K.H. Hoffmann and G. Leugering (Eds.): Optimization with Partial Differential Equations, ISNM, Birkhäuser Verlag, in press end of (2010).
- [6] L. BLANK, H. GARCKE, L. SARBU, AND V. STYLES, *Primal-dual active set methods for Allen-Cahn variational inequalities with non-local constraints*, Preprint SPP1253-09-01.
- [7] ———, *Primal-dual active set methods for vector-valued Allen-Cahn variational inequalities with non-local constraints*, Draft.
- [8] J.F. BLOWEY AND C.M. ELLIOTT, *Curvature dependent phase boundary motion and parabolic double obstacle problems*, in Degenerate diffusions (Minneapolis, MN, 1991), vol. 47 of IMA Vol. Math. Appl., Springer, New York, 1993, pp. 19–60.
- [9] J.H. BRAMBLE AND J.E. PASCIAK, *A preconditioning technique for indefinite systems resulting from mixed approximations of elliptic problems*, Math. Comp, 50 (1988), pp. 1–17.
- [10] C. SUSANNE BRENNER AND L. RIDGWAY SCOTT, *The Mathematical Theory of Finite Element Methods*, vol. 15 of Texts in Applied Mathematics, Springer, New York, 2008.
- [11] T.A. DAVIS, *Umpack version 4.4 user guide*, tech. report, Dept. of Computer and Information Science and Engineering Univ. of Florida, Gainesville, FL, 2005.
- [12] I.S. DUFF, *MA57—a code for the solution of sparse symmetric definite and indefinite systems*, ACM Transactions on Mathematical Software (TOMS), 30 (2004), pp. 118–144.
- [13] H.C. ELMAN, *Multigrid and Krylov subspace methods for the discrete Stokes equations*, in Seventh Copper Mountain Conference on Multigrid Methods, N. D. Melson, T. A. Manteuffel, S. F. McCormick, and C. C. Douglas, eds., vol. CP 3339, Hampton, VA, 1996, NASA, pp. 283–299.
- [14] H.C. ELMAN, D.J. SILVESTER, AND A.J. WATHEN, *Finite elements and fast iterative solvers: with applications in incompressible fluid dynamics*, Numerical Mathematics and Scientific Computation, Oxford University Press, New York, 2005.
- [15] R.D. FALGOUT, *An Introduction to Algebraic Multigrid*, Computing in Science and Engineering, 8 (2006), pp. 24–33. Special Issue on Multigrid Computing.
- [16] H. GARCKE, B. NESTLER, B. STINNER, AND F. WENDLER, *Allen-Cahn systems with volume constraints*, Math. Models Methods Appl. Sci., 18 (2008), pp. 1347–1381.
- [17] H. GARCKE, B. NESTLER, AND B. STOTH, *A multi phase field concept: Numerical simulations of moving phase boundaries and multiple junctions*, SIAM J. Appl. Math., 60 (1999), pp. 295–315.
- [18] H. GARCKE AND V. STYLES, *Bi-directional diffusion induced grain boundary motion with triple junctions*, Interfaces and Free Boundaries, 6 (2004).
- [19] G.H. GOLUB AND G. MEURANT, *Matrices, moments and quadrature*, in Numerical analysis 1993 (Dundee, 1993), Griffiths DF; Watson GA, ed., Longman Sci. Tech.
- [20] ———, *Matrices, moments and quadrature with applications*. Draft, 2007.
- [21] G.H. GOLUB AND R. UNDERWOOD, *The block Lanczos method for computing eigenvalues*, in Mathematical software, III (Proc. Sympos., Math. Res. Center, Univ. Wisconsin, Madison, Wis., 1977), J. R. Rice, ed.
- [22] G.H. GOLUB AND J.H. WELSCH, *Calculation of Gauss quadrature rules*, Math. Comp. 23 (1969), 221–230; addendum, *ibid.*, 23 (1969), pp. A1–A10.
- [23] C. GRÄSER AND R. KORNUBER, *Multigrid methods for obstacle problems*, J. Comput. Math., 27 (2009), pp. 1–44.
- [24] A. GREENBAUM, *Iterative methods for solving linear systems*, vol. 17 of Frontiers in Applied Mathematics, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1997.
- [25] M. HEROUX, R. BARTLETT, V.H.R. HOEKSTRA, J. HU, T. KOLDA, R. LEHOUCQ, K. LONG, R. PAWLOWSKI, E. PHIPPS, A. SALINGER, H. THORNQUIST, R. TUMINARO, J. WILLENBRING, AND A. WILLIAMS, *An Overview of Trilinos*, Tech. Report SAND2003-2927, Sandia National Laboratories, 2003.
- [26] M.R. HESTENES AND E. STIEFEL, *Methods of conjugate gradients for solving linear systems*, J. Res. Nat. Bur. Stand, 49 (1952), pp. 409–436 (1953).
- [27] M. HINTERMÜLLER, V. A. KOVTUNENKO, AND K. KUNISCH, *The primal-dual active set method for a crack problem with non-penetration*, IMA J. Applied Math., 69 (2004), pp. 1–26.
- [28] I.C.F. IPSEN AND B. NADLER, *Refined perturbation bounds for eigenvalues of Hermitian and non-Hermitian matrices*, SIAM J. Matrix Anal. Appl., 31 (2009), pp. 40–53.
- [29] K. ITO AND K. KUNISCH, *The primal-dual active set method for nonlinear optimal control problems with bilateral constraints*, SIAM J. Contr. and Opt., 43 (2004), pp. 357–376.
- [30] D.A. KAY AND A. TOMASI, *Colour image segmentation by the vector-valued Allen-Cahn phase-field model: a multigrid solution*, IEEE Trans. Image Proc., 18 (2007).

- [31] C. KELLER, N.I.M. GOULD, AND A.J. WATHEN, *Constraint Preconditioning for Indefinite Linear Systems*, SIAM J. Matrix Anal. Appl., 21 (2000), pp. 1300–1317.
- [32] R. KORNHUBER, *Monotone multigrid methods for elliptic variational inequalities I.*, Num. Math., 69 (1994), pp. 167–184.
- [33] ———, *Monotone multigrid methods for elliptic variational inequalities II.*, Num. Math., 72 (1996), pp. 481–499.
- [34] R. KORNHUBER AND R. KRAUSE, *Robust multigrid methods for vector-valued Allen-Cahn equations with logarithmic free energy*, Comput. Vis. Sci., 9 (2006), pp. 103–116.
- [35] D. KRISHNAN, P. LIN, AND A.M. YIP, *A primal-dual active-set method for non-negativity constrained total variation deblurring problems*, IEEE Trans. on Image Processing, 16 (2007), pp. 2766–2777.
- [36] D. KRISHNAN, Q.V. PHAM, AND A. M. YIP, *A primal-dual active-set algorithm for bilaterally constrained total variation deblurring and piecewise constant Mumford-Shah segmentation problems*, Advances in Comp. Math., 31 (2009), pp. 237–266.
- [37] C. LANCZOS, *An iteration method for the solution of the eigenvalue problem of linear differential and integral operators*, J. Res. Nat. Bur. Stand., 45 (1950), pp. 255–282.
- [38] M.F. MURPHY, G.H. GOLUB, AND A.J. WATHEN, *A note on preconditioning for indefinite linear systems*, SIAM J. Sci. Comput., 21 (2000), pp. 1969–1972.
- [39] C.C. PAIGE AND M.A. SAUNDERS, *Solutions of sparse indefinite systems of linear equations*, SIAM J. Numer. Anal., 12 (1975), pp. 617–629.
- [40] T. REES AND M. STOLL, *Block triangular preconditioners for PDE constrained optimization*, Accepted to Numer. Linear Algebra Appl., (2009).
- [41] T. REES, M. STOLL, AND A. WATHEN, *All-at-once preconditioners for PDE-constrained optimization*, Accepted to Kybernetika, (2009).
- [42] J.W. RUGE AND K. STÜBEN, *Algebraic multigrid*, in Multigrid methods, vol. 3 of Frontiers Appl. Math., SIAM, Philadelphia, PA, 1987, pp. 73–130.
- [43] Y. SAAD, *Iterative methods for sparse linear systems*, Society for Industrial and Applied Mathematics, Philadelphia, PA, 2003.
- [44] A. SCHMIDT AND K.G. SIEBERT, *Design of adaptive finite element software. the finite element toolbox alberta*, Lecture Notes in Computational Science and Engineering 42. Springer-Verlag, Berlin xii+315, (2005).
- [45] G.L.G. SLEIJPEN, H.A. VAN DER VORST, AND J. MODERSITZKI, *Differences in the Effects of Rounding Errors in Krylov Solvers for Symmetric Indefinite Linear Systems*, SIAM J. Matrix Anal. Appl., 22 (2001), pp. 726–751.
- [46] M. STOLL, *Solving Linear Systems using the Adjoint*, PhD thesis, University of Oxford, 2009.
- [47] M. STOLL AND A. WATHEN, *Combination preconditioning and the Bramble–Pasciak⁺ preconditioner*, SIAM J. Matrix Anal. Appl., 30 (2008), pp. 582–608.
- [48] M. STOLL AND A. WATHEN, *Preconditioning for active set and projected gradient methods as semi-smooth Newton methods for PDE-constrained optimization with control constraints*, Submitted, (2009).
- [49] J.E. TAYLOR AND J.W. CAHN, *Linking anisotropic sharp and diffuse surface motion laws via gradient flows*, J. Statist. Phys., 77 (1994), pp. 183–197.
- [50] J. XU, *Iterative methods by space decomposition and subspace correction*, SIAM Rev., 34 (1992), pp. 581–613.