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30. On multigrid methods for vector–valued Allen–Cahn equations with obstacle potential

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1. Introduction. Phase field models provide a well–established framework for the mathematical description to free boundary problems for phase transitions. In contrast to sharp interface models, the phase field approach postulates a diffuse interface with a small but finite thickness. Approximations of the interface are recovered as level sets of a function u, called order parameter or phase field. The main advantage of this approach is that topological changes of the approximate interface cause no problems, because bulk phases and interface are treated in the same manner. In this paper, we consider multicomponent phase transitions as described by a vector–valued Allen–Cahn equation with obstacle potential [2, 3]. Semi–implicit discretization in time is unconditionally stable but, after finite element discretization in space, leads to large non–smooth algebraic systems. So far, fast solvers for such kind of problems were not available. As a consequence, explicit schemes are applied, in spite of severe stability restrictions on the time step [4]. We present a new class of multigrid methods based on successive minimization in the direction of well selected search directions and prove global convergence. Similar multigrid techniques have been applied in [6, 8] in a different context. Numerical experiments illustrate the reliability and efficiency of our method.

2. Vector–valued Allen–Cahn equations and discretization. We consider isothermal, multicomponent phase transitions in a polygonal (polyhedral) domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$. Each phase at a particular point $(x, t) \in Q = \Omega \times [0, T_0]$, $T_0 > 0$, is represented by the value of a component $u_i(x, t)$ of the order parameter $u = (u_1, \ldots, u_N)^T$. In practical applications the components u_i may represent concentrations or volume fractions of the different phases in the system. Hence, we impose the condition that values of u_i are non–negative and add up to unity [3], i.e.

$$u(x,t) \in G = \{v \in \mathbb{R}^N \mid v_i \geq 0,\ \textstyle\sum_i v_i = 1\} \qquad \forall (x,t) \in Q.$$

We further assume that the Ginsburg–Landau total free energy of our system is given by

$$\mathcal{E}(u) = \int_\Omega \tfrac{1}{2}\varepsilon^2 \textstyle\sum_i |\nabla u_i|^2 + \Psi(u)\, dx, \qquad \varepsilon > 0.$$

The quadratic term describes interfacial energy and the non–convex free energy functional Ψ has N distinct local minima on G giving rise to phase separation. Phase kinetics should satisfy the second law of thermodynamics stating that total free energy is non–increasing along solution paths. The vector–valued Allen–Cahn equation

$$u_t = -\frac{d}{du}\mathcal{E}(u) = \varepsilon^2 \Delta u - T\nabla_u \Psi(u) \tag{2.1}$$

is the most simple model with this property. Denoting $\mathbf{1} = (1, 1, \ldots, 1) \in \mathbb{R}^N$, the projection $T : \mathbb{R}^N \to \Sigma_0 = \{v \in \mathbb{R}^N \mid \sum_i v_i = 0\}$, defined by

$$Tv = v - \tfrac{1}{N}(v \cdot \mathbf{1})\mathbf{1},$$

accounts for the fact that the values $u(x, t) \in G \subset \Sigma = \{v \in \mathbb{R}^N \mid \sum_i v_i = 1\}$ must only vary on the affine hyperplane Σ. See [3] for details.

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From now on, we concentrate on the obstacle potential $\Psi = \Psi_\infty$,

$$\Psi_\infty(u) = \begin{cases} \sum_{i<j} u_i u_j, & u \in G, \\ +\infty, & \text{else.} \end{cases}$$

Minimal values of Ψ_∞ on G are attained at the N unit vectors $e_1, \dots, e_N \in \mathbb{R}^N$ which are associated with pure phases. Imposing Neumann boundary conditions, a weak formulation of (2.1) takes the form

$$\frac{d}{dt}(u,v) + \varepsilon^2(\nabla u, \nabla(v-u)) - (u, v-u) \geq -\tfrac{1}{N}(\mathbf{1}, v-u) \qquad \forall v \in \mathcal{G}, \tag{2.2}$$

where the time derivative is understood in an appropriate weak sense and

$$u(\cdot,t) \in \mathcal{G} := \{v \in H^1(\Omega)^N \mid v(x) \in G \text{ a.e. in } \Omega\}, \quad 0 < t \leq T_0.$$

In addition, we prescribe initial conditions $u(\cdot,0) = u_0 \in \mathcal{G}$.

Let $\mathcal{T}_J$ be a given partition of $\overline{\Omega}$ into triangles (tetrahedra) with minimal diameter $h_J = \mathcal{O}(2^{-J})$. The set of vertices is denoted by $\mathcal{N}_J$ and we set

$$\mathcal{S}_J = \{v \in C(\overline{\Omega}) \mid v_i|_t \text{ is linear } \forall t \in \mathcal{T}_J\}.$$

Now we discretize (2.2) in time by backward Euler with step size $\tau > 0$. The concave part $-(u,\cdot)$ of Ψ_∞ is taken explicitly (cf. e.g. [1]). Discretization in space by piecewise linear finite elements then leads to the discrete variational inequality

$$\begin{aligned} u_{J,k} \in \mathcal{G}_J : \quad \langle u_{J,k}, v - u_{J,k}\rangle + \tau\varepsilon^2(\nabla u_{J,k}, \nabla(v-u_{J,k})) \geq \\ \langle (1+\tau)u_{J,k-1} - \tfrac{\tau}{N}\mathbf{1}, v - u_{J,k}\rangle \quad \forall v \in \mathcal{G}_J \end{aligned} \tag{2.3}$$

to be solved in the k–th time step. Here, $\langle\cdot,\cdot\rangle$ stands for the lumped L^2–product and the continuous constraints $\mathcal{G}$ are approximated by

$$\mathcal{G}_J = \{v \in \mathcal{S}_J^N \mid v(p) \in G \ \forall p \in \mathcal{N}_J\}. \tag{2.4}$$

As $\mathcal{G}_J$ is a non–empty, closed, convex subset of $\mathcal{S}_J^N$ and the bilinear form appearing on the left hand side of (2.3) is symmetric, positive definite on $\mathcal{S}_J^N$ there is a unique solution $u_{J,k}$ for arbitrary step size $\tau > 0$, see [5].

3. Polygonal relaxation. We now derive a Gauß–Seidel type relaxation scheme for discrete variational inequalities of the form

$$u_J \in \mathcal{G}_J : \quad a(u_J, v - u_J) \geq \ell(u_J, v - u_J) \quad \forall v \in \mathcal{G}_J \tag{3.1}$$

with a symmetric, positive definite bilinear form $a(\cdot,\cdot)$ on $\mathcal{S}_J^N$, $\ell \in (\mathcal{S}_J^N)'$ and $\mathcal{G}_J$ defined in (2.4). Of course, (2.3) is a special case of (3.1).

Note that $\mathcal{G}_J$ is a subset of an affine subspace of $\mathcal{S}_J^N$ spanned by the hyperplane $\mathcal{H}_J = \{v \in \mathcal{S}_J^N \mid \sum_j v_j(p) = 0\}$. Hence, each splitting of $\mathcal{H}_J$ gives rise to a successive subspace correction method for (3.1). We consider the splitting

$$\mathcal{H}_J = \sum_{l=1}^{m_J} V_l, \quad V_l = \operatorname{span}\{\mu_l\}, \qquad \mu_{l(i,j)} = \lambda_{p_i}^{(J)} E_j, \ \ l = 1, \dots, m_J, \tag{3.2}$$

where $\lambda_{p_i}^{(J)}$, $i = 1, \dots, n_J$, denotes the nodal basis of $\mathcal{S}_J$, the vectors $E_j \in \mathbb{R}^N$, $i = 1, \dots, M := \frac{1}{2}N(N-1)$ are given by the edges of G, $l = l(i,j)$ is some enumeration and $m_J := n_J M$.

The resulting successive subspace correction method reads as follows. Starting with the given ν–th iterate $u_J^\nu =: w_0^\nu \in \mathcal{G}_J$, we compute a sequence of intermediate iterates $w_l^\nu = w_{l-1}^\nu = v_l^*$, $l = 1, \ldots, m_J$. The corrections v_l^* are the unique solutions of the local subproblems

$$v_l^* \in \mathcal{D}_l^* \quad a(v_l^*, v - v_l^*) \geq \ell(v - v_l^*) - a(w_{l-1}^\nu, v - v_l^*) \quad \forall v \in \mathcal{D}_l^*, \tag{3.3}$$

where the closed convex subsets $\mathcal{D}_l^* = \mathcal{D}_l^*(w_{l-1}^\nu)$ are defined by

$$\mathcal{D}_l^*(w_{l-1}^\nu) = \{v \in V_l \mid w_{l-1}^\nu + v \in \mathcal{G}_J\}.$$

Finally, we obtain the next iterate $u_J^{\nu+1}$,

$$u_J^{\nu+1} = \mathcal{M}(u_J^\nu) := w_{m_J}^\nu = u_J^\nu + \sum_{l=1}^{m_J} v_l^*. \tag{3.4}$$

It is well–known from, e.g., [5] that (3.1) is equivalent to the constrained minimization problem

$$u_J \in \mathcal{G}_J : \quad \mathcal{J}(u_J) \leq \mathcal{J}(v) \quad \forall v \in \mathcal{G}_J \tag{3.5}$$

for the quadratic energy functional

$$\mathcal{J}(v) = \tfrac{1}{2} a(v, v) - \ell(v), \quad v \in \mathcal{S}_J^N.$$

Successive subspace correction (3.4) can be regarded as a successive minimization of $\mathcal{J}$ in the direction of μ_l, $l = 1, \ldots, m_J$. In particular, we have

$$\mathcal{J}(u_J^{\nu+1}) \leq \mathcal{J}(w_l^\nu) \leq \mathcal{J}(u_J^\nu), \qquad \forall l = 1, \ldots, m_J, \;\; \nu = 0, 1, \ldots \; . \tag{3.6}$$

The following lemma is crucial for the convergence of (3.4).

Lemma 3.1 *For any given $U, W \in G$ there is a decomposition*

$$W = U + \sum_{j=1}^{M} \omega_j E_j, \tag{3.7}$$

which is feasible in the sense that

$$U + \omega_j E_j \in G \qquad \forall j = 1, \ldots, M.$$

Proof. We only sketch the basic idea of the proof which is easy for $N = 2, 3, 4$, but becomes technical for arbitrary N. Let $U, W \in G$ be given. Recall that $e_1, \ldots, e_N \in \mathbb{R}^N$ denote the unit vectors in $\mathbb{R}^N$. By definition of G, there are coefficients $\alpha_1, \ldots, \alpha_N$ with the properties

$$w = \sum_{i=1}^{N} \alpha_i e_i, \qquad \alpha_i \geq 0, \quad \alpha_1 + \cdots + \alpha_N = 1. \tag{3.8}$$

Now it can be shown that the unit vectors e_i can be decomposed in such a way that insertion in (3.8) provides the desired feasible decomposition (3.7). ■

We are ready to prove convergence.

Theorem 3.1 *For any initial iterate $u_J^0 \in \mathcal{G}_J$, the polygonal relaxation (3.4) converges to the solution u_J of (3.1).*

Proof. We only sketch the proof based on similar arguments as the proof of Theorem 2.1 in [7]. Utilizing (3.6), we have $\mathcal{J}(u_J^\nu) \le \mathcal{J}(u_J^0) < \infty$ for all $\nu \ge 0$. As a consequence, the sequence of iterates $(u_J^\nu)_{\nu\in\mathbb{N}}$ is bounded. As $\mathcal{S}_J^N$ has finite dimension, any subsequence of $(u_J^\nu)_{\nu\in\mathbb{N}}$ has a subsubsequence $(u_J^{\nu_k})_{k\in\mathbb{N}}$ that converges to some $u_J^* \in \mathcal{G}_J$. We now show that $u_J^* = u_J$. Observe that (3.6) leads to

$$\mathcal{J}(u_J^{\nu_{k+1}}) \le \mathcal{J}(\mathcal{M}(u_J^{\nu_k})) \le \mathcal{J}(u_J^{\nu_k}) \qquad \forall k = 1, \dots ,$$

where $\mathcal{M}$ is defined in (3.4). As $\mathcal{J}$, $\mathcal{M}$ are continuous on $\mathcal{G}_J$, we can pass to the limit in order to obtain

$$\mathcal{J}(\mathcal{M}(u_J^*)) = \mathcal{J}(u_J^*).$$

Hence, starting with $w_0 = u_J^*$, all corrections v_l^* computed from (3.3) are zero, giving

$$0 \ge \ell(v) - a(u_J^*, v) \qquad \forall v \in \mathcal{D}_l^*(u_J^*), \;\; l = 1, \dots, m_J. \tag{3.9}$$

Now, let $w \in \mathcal{G}_J$ be arbitrary chosen. As an immediate consequence of Lemma 3.1, there is a decomposition $w = u_J^* + \sum_{l=1}^{m_J} v_l$ such that $v_l \in V_l$ and $u_J^* + v_l \in \mathcal{G}_J$, i.e. $v_l \in \mathcal{D}_l^*(u_J^*)$. Inserting $v = v_l$ in (3.9) and summing up for $l = 1, \dots, m_J$, we obtain

$$a(u_J^*, w - u_J) \ge \ell(w - u_J).$$

Hence, u_J^* is a solution of (3.1). As u_J is the unique solution of (3.1), we get $u_J^* = u_J$. We have shown that any subsequence has a subsubsequence converging to u_J. Hence, the whole sequence $(u_J^\nu)_{\nu\in\mathbb{N}}$ must converge to u_J. ■

Implementation of (3.4) is based on the representation

$$\mathcal{D}_{l(i,j)}^* = \{v \in V_l \mid v = z\lambda_{p_i}^{(J)} E_j, \; \underline{\psi}_{i,j} \le z \le \overline{\psi}_{i,j}\}$$

with local obstacles $\underline{\psi}_{i,j} \le 0 \le \overline{\psi}_{i,j}$ depending on the actual intermediate iterate w_l^ν. In contrast to box constraints, each correction $v_{l(i,j)}$ requires an update of *all* local obstacles $\underline{\psi}_{i,s}, \overline{\psi}_{i,s}$ $s = 1, \dots, M$. As a consequence, each iteration step of the polygonal relaxation requires $\mathcal{O}(M^2 n_J) = \mathcal{O}(N^4 n_J)$ point operations.

4. Extended polygonal relaxation. The convergence speed of Gauß–Seidel type relaxation (3.4) deteriorates rapidly with decreasing mesh size h_J. In order to accelerate convergence, we consider the extended splitting

$$\mathcal{H}_J = \sum_{l=1}^{m_J} V_l + \sum_{l=m_J+1}^{M_J^\nu} V_l^\nu, \qquad V_l^\nu = \operatorname{span}\{\mu_l^\nu\}, \quad \mu_l^\nu \in \mathcal{H}_J, \tag{4.1}$$

with V_l, $l = 1, \dots, m_J$, defined in (3.2). The additional search directions μ_l^ν are intended to improve the representation of the low–frequency contributions of the error and therefore should have large support. The μ_l^ν might be iteratively adjusted to the unknown solution u_J and, for this reason, are allowed to vary in each iteration step.

We consider the resulting *extended polygonal relaxation* defined as follows. Starting from a given iterate $u_J^\nu \in \mathcal{G}_J$, we first compute a *smoothed iterate* $\bar{u}_J^\nu = w_{m_J}^\nu = \mathcal{M}(u_J^\nu)$ by fine grid smoothing (3.4). Successive "coarse grid corrections" v_l are then obtained from

$$v_l \in \mathcal{D}_l : \quad a(v_l, v - v_l) \ge \ell(v - v_l) - a(w_{l-1}^\nu, v - v_l) \quad \forall v \in \mathcal{D}_l, \tag{4.2}$$

denoting $w_l^\nu = w_{l-1}^\nu + v_l$, $l = m_J + 1, \dots, M_J^\nu$. Due to large support of μ_l^ν, it might be too costly to check whether some $v \in V_l^\nu$ is contained in $\mathcal{D}_l^*$ or not. Hence, we may use approximate closed convex subsets $\mathcal{D}_l$, satisfying

$$0 \in \mathcal{D}_l \subset \mathcal{D}_l^* = \{v \in V_l^\nu \mid w_{l-1}^\nu + v \in \mathcal{G}_J\}.$$

The next iterate is given by

$$u_J^{\nu+1} = w_{M_J^\nu}^\nu = \bar{u}_J^\nu + \sum_{l=m_J+1}^{M_J^\nu} v_l. \tag{4.3}$$

The convergence proof is almost literally the same as for Theorem 2.1 in [6].

Theorem 4.1 *For any initial iterate $u_J^0 \in \mathcal{G}_J$, the extended polygonal relaxation (4.3) converges to the solution u_J of (3.1).*

The subset of all nodes with vanishing i–th phase is denoted by

$$\mathcal{N}_{J,i}^\bullet(u_J) = \{p \in \mathcal{N}_J \mid u_{J,i}(p) = 0\}, \quad i = 1, \dots, N.$$

It would be interesting to know whether

$$\mathcal{N}_{J,i}^\bullet(u_J^\nu) = \mathcal{N}_{J,i}^\bullet(u_J), \qquad \nu \geq \nu_0, \tag{4.4}$$

holds for some $\nu_0 \in \mathbb{N}$. In fact, assuming reasonable search directions μ_l^ν, a non–degeneracy condition of the form

$$a(u_J, \lambda_p^{(J)} E_j) < (-1)^{r_j} \ell(\lambda_p^{(J)} E_j) \qquad \forall j \text{ with } (e_i \cdot E_j) \neq 0 \quad \forall p \in \mathcal{N}_{J,i}^\bullet(u_J)$$

with suitable r_j depending on the orientation of E_j and finally that $u_J(p) \neq e_j$ holds for all $j \neq i$ and $p \in \mathcal{N}_{J,i}^\bullet(u_J)$, convergence of phases (4.4) can be shown in a similar way as Lemma 2.2 in [6]. Unfortunately, this result is of minor relevance for discretized vector–valued Allen–Cahn equation (2.3), because $u_J(p) = e_j$ stands for pure phase j. Recall that pure phases are local minima of Ψ_∞.

5. Monotone multigrid. Assume that $\mathcal{T}_J$ is resulting from J refinements of an intentionally coarse triangulation $\mathcal{T}_0$. In this way, we obtain a sequence of triangulations $\mathcal{T}_0 \subset \cdots \subset \mathcal{T}_J$ and corresponding nested finite element spaces $\mathcal{S}_0 \subset \cdots \subset \mathcal{S}_J$. Though the algorithms to be presented can be easily generalized to the non–uniform case, we assume for simplicity that the triangulations are uniformly refined. More precisely, each triangle $t \in \mathcal{T}_k$ is subdivided into four congruent subtriangles in order to produce the next triangulation $\mathcal{T}_{k+1}$.

Using the nodal basis functions $\lambda_p^{(k)}$, $p \in \mathcal{N}_k$ on all levels $k = J, \dots, 0$, we define the search directions μ_l^ν appearing in the splittings (3.2) and (4.1) by

$$\mu_{l(i,j,k)} = \lambda_{p_i}^{(k)} E_j, \qquad l = 1, \dots, M_J := M(n_J + \cdots + n_0).$$

The enumeration $l(i,j,k)$ is taken from fine to coarse, i.e. $l(i,j,k) > l'(i',j',k')$ implies $k \leq k'$. Approximate constraints in (4.2) have the form

$$\mathcal{D}_l = \{v = z\lambda_{p_i}^{(k)} E_j \in V_{l(i,j,k)} \mid \underline{\psi}_l \leq z \leq \overline{\psi}_l\}, \quad l = Mn_J + 1, \dots, M_J.$$

Local obstacles $\underline{\psi}_l$, $\overline{\psi}_l$ can be constructed by quasioptimal monotone restriction [6]. As a consequence of Theorem 4.1, the resulting *standard monotone multigrid method* converges for all initial iterates $u_J^0 \in \mathcal{G}_J$. It can be implemented as a multigrid V–cycle. Smoothing

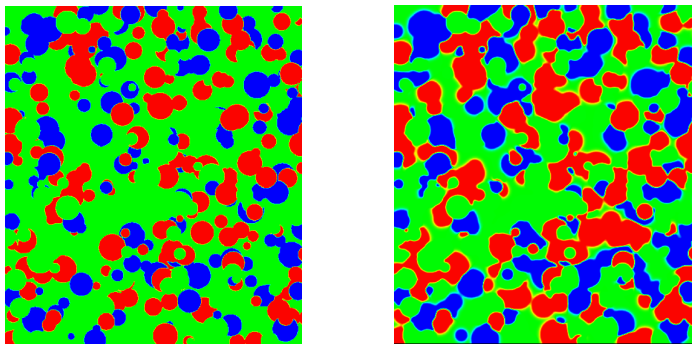

Figure 6.1: Initial condition u_0 and approximate solution at $t = 4$

is performed by polygonal relaxation (3.4) on each level. Restriction of stiffness matrix and residual and prolongation of corrections are canonical, if representation in terms of search directions $\lambda_p^{(k)} E_j$ is used. The numerical complexity of each iteration step is $\mathcal{O}(N^4 n_J)$, i.e. of the same order as fine–grid smoothing. Asymptotic multigrid convergence rates could be derived in the framework of linear successive subspace correction (cf. [6, 9]), provided that convergence of phases (4.4) holds for all $i = 1, \ldots, N$.

In related algorithms, convergence speed of standard monotone multigrid could be improved by so–called truncation of coarse grid nodal basis functions [6, 7, 8]. In the present case, truncation leads to the coarse grid search directions

$$\tilde{\mu}^{\nu}_{l(i,j,k)} = T^{\nu}_{J,k,j} \lambda^{(k)}_{p_i} E_j, \qquad l = M n_J + 1, \ldots, M_J.$$

For each direction E_j, the truncation operators $T^{\nu}_{J,k,j} : \mathcal{S}_J \to \mathcal{S}_k$ are defined according to [6]. Truncation is implemented by modification of quasioptimal restriction and canonical restriction and prolongation: All entries from $\mathcal{N}^{\bullet}_{J,i}(\bar{u}^{\nu}_J)$ are set to zero. In this way, we obtain a *truncated monotone multigrid method*. Again, convergence follows from Theorem 4.1 and asymptotic multigrid convergence rates could be derived, if all phases $i = 1, \ldots, N$ converge according to (4.4). Mesh independent *global bounds* for convergence rates of monotone multigrid methods, e.g. from [6], are still an open problem.

6. Numerical experiments. We consider grain growth as described by the vector–valued Allen–Cahn equation (2.2) on the unit square $\Omega = (0,1) \times (0,1)$ with $N = 3$ and $\varepsilon = 0.002$. For example, each of the $N = 3$ different phases may reflect a different crystalline structure. The initial condition $u_0 \in \mathcal{G}$ is a randomly chosen superposition of 500 circular grains, each of which corresponds to a pure phase. The randomly chosen radii are ranging from 0.01 to 0.04. See the left picture in Figure 6.1 for illustration.

The continuous problem is approximated by the discretization (2.3) with step size $\tau = 1$ and triangulation $\mathcal{T}_J$ resulting from $J = 8$ uniform refinements. The initial triangulation $\mathcal{T}_0$ is obtained by subdivision of Ω into two congruent triangles and a subsequent refinement step. The right picture in Figure 6.1 and Figure 6.2 show the approximate discrete solution at $t = 4$, $t = 100$ and $T_0 = 600$, respectively. Observe that reduction of total free energy goes with a reduction of the (diffuse) interfaces by smoothing and coarsening. Interfaces at triple junctions tend to meet at an angle of 120°. This supports formal asymptotic analysis in [2]. In order to illustrate the convergence behavior of our iterative schemes, we consider the spatial problem to be solved in the first time step. The left picture in Figure 6.3 shows the iteration history of polygonal relaxation (cf. Section 3) as compared to the standard monotone multigrid method with V–cycle and three pre–smoothing and post–smoothing

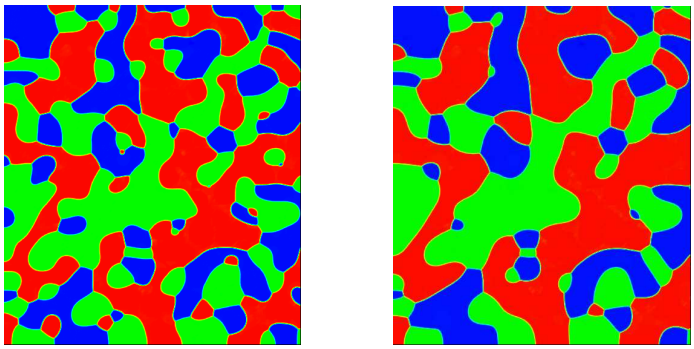

Figure 6.2: Approximate solutions at $t = 100$ and $T_0 = 600$

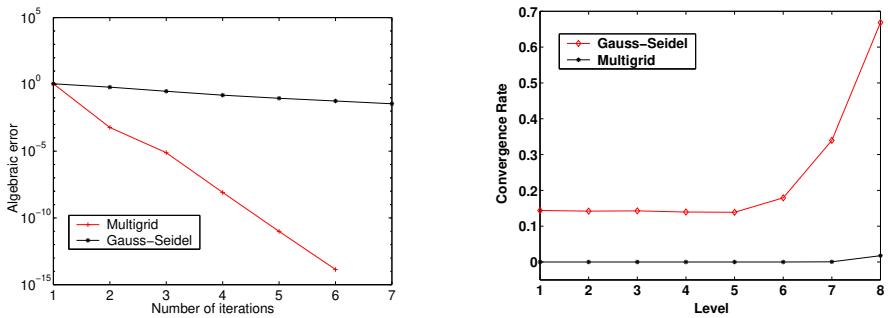

Figure 6.3: Iteration history and averaged convergence rates

steps, respectively (cf. Section 5). The algebraic error $\|u_J - u_J^\nu\|$ is measured by the energy norm $\|\cdot\| = a(\cdot,\cdot)^{1/2}$. The initial iterate $u_J^0 = e_3 \in \mathcal{G}_J$ has little to do with u_J. Nevertheless, we observe very fast convergence of our multigrid method throughout the iteration process. The averaged convergence rate is $\rho_J^{\mathrm{STD}} := \sqrt[\nu_0]{\|u_J - u_J^{\nu_0}\|/\|u_J - u_J^0\|} \approx 0.005$ where ν_0 is chosen such that $\|u_J - u_J^{\nu_0}\| < 10^{-12}$. Taking into account that each iteration step is much cheaper, polygonal relaxation performs reasonably well with averaged convergence rate $\rho_J^{\mathrm{GS}} = 0.56$. This seems to be a consequence of the redundancy of search directions in combination with a moderate number of grid points in the diffuse interface. The right picture in Figure 6.3 illustrates the mesh dependence of averaged convergence rates $\rho_j^{\mathrm{GS}}, \rho_j^{\mathrm{STD}}$, $j = 0, \ldots, 8$. Iteration always starts with the "arbitrary" initial iterate $u_j^0 = e_3 \in \mathcal{G}_j$. As expected, we observe only minor sensitivity of multigrid as compared to single grid. On the other hand, it seems that the mesh size $h_J = 2^{-9} \approx \frac{1}{2}\varepsilon$ is still too large to provide saturation.

7. Conclusion an perspective. We have introduced and analyzed new Gauß–Seidel type relaxation and monotone multigrid methods for systems of variational inequalities with local triangular constraints. Such problems arise in mathematical description of certain free boundary problems by phase field models. Future work will concentrate on more realistic Ginzburg–Landau functionals, involving anisotropic interfacial energy and logarithmic free energy [4]. Of course, adaptive mesh refinement will be indispensable for a better resolution of the diffuse interface. In this case, truncated multigrid might also be profitable.

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