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Angaben zur Veröffentlichung / Publication details:

Hoppe, Ronald H. W. 1993. "A globally convergent multi-grid algorithm for moving boundary problems of two-phase Stefan type." *IMA Journal of Numerical Analysis* 13 (2): 235–53. https://doi.org/10.1093/imanum/13.2.235.

A globally convergent multi-grid algorithm for moving boundary problems of two-phase Stefan type

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In this paper we deal with the numerical solution of moving boundary problems of two-phase Stefan type. Based on an implicit discretization in time and the use of continuous, piecewise linear finite elements in the space variables with respect to the weak formulation of the problem, a globally convergent multi-grid algorithm is developed. That algorithm strongly relies on the variational characterization of the fully discretized problem as the unconstrained minimization of a subdifferentiable convex objective functional. Numerical results indicate a significant improvement in efficiency compared with previous multi-grid approaches.

1. Introduction

We shall be concerned with the efficient numerical solution of a moving boundary problem of two-phase Stefan type described by its fixed-domain formulation as the following degenerate parabolic initial-boundary value problem

$$\partial e/\partial t - \Delta u = f, \qquad e \in H(u) \quad \text{in} \quad Q := \Omega \times (0, T), \tag{1.1a}$$

$$e(0) = e^0 \in H(u^0) \quad \text{in} \quad \Omega, \tag{1.1b}$$

$$u = 0 \quad \text{on} \quad \partial\Omega \times (0, T), \tag{1.1c}$$

holding in the distributional sense.

Here, Ω stands for a bounded domain in Euclidean space $\mathbb{R}^2$ with piecewise smooth boundary $\partial\Omega$ and $H(\cdot)$ is assumed to be a strongly maximal monotone graph in $\mathbb{R}^2$ of the form

$$H(\lambda) = \begin{cases} a_1\lambda - s_1 & \text{if} \quad \lambda < 0 \\ [-s_1, s_2] & \text{if} \quad \lambda = 0 \\ a_2\lambda + s_2 & \text{if} \quad \lambda > 0 \end{cases} \tag{1.2}$$

with positive constants a_i and nonnegative constants s_i, $1 \leq i \leq 2$, such that $s_1 + s_2 > 0$.

An intrinsic feature of the above initial-boundary value problem (1.1a–c) is the occurrence of moving boundaries

$$\Sigma^\alpha = \partial(\overline{\Omega^\alpha}) \cap \overline{\Omega^3}, \quad 1 \leq \alpha \leq 2 \tag{1.3}$$

where

$$\Omega^\alpha = \{(x, t) \in Q \mid (-1)^\alpha u(x, t) > 0\}, \qquad 1 \leq \alpha \leq 2,$$

$$\Omega^3 = \{(x, t) \in Q \mid u(x, t) = 0\}.$$

The set int Ω^3 is referred to as the mushy region which may occur due to superheating or supercooling effects.

Such moving boundary problems model physical processes with a change of phase. A well known example is the determination of the temporal and spatial temperature distribution $\theta(x, t)$, $(x, t) \in Q$, of a heat conducting substance undergoing a change of phase at the nominal change phase temperature $\theta_c = 0$. In this case, denoting by ρ the density, by L the latent heat and by c_i, κ_i, $1 \leqslant i \leqslant 2$, the heat capacities and heat conductivities in both phases, respectively, the function u appears to be a generalized temperature obtained by the standard Kirchhoff transformation $u = \kappa_1 \theta$ for $\theta \leqslant 0$ and $u = \kappa_2 \theta$ for $\theta \geqslant 0$ while $H(u)$ may be viewed as a generalized enthalpy with a_i, s_i, $1 \leqslant i \leqslant 2$, given by $a_i = \rho c_i / \kappa_i$, $s_1 = 0$ and $s_2 = \rho L$ (cf. e.g. Elliott & Ockendon (1982), Friedman (1982) and Jerome (1983)).

Another example is the electromagnetic induction in ferromagnetic media at a constant temperature below the Curie point when modelling the magnetization characteristics by the so called simplified Fröhlich's model (see e.g. Bossavit (1985) and Hoppe & Kornhuber (1989, 1990) for the treatment of a more general coupled system of two-phase Stefan problems arising in induction heating of large steel slabs).

A solution to (1.1a–c) has to be understood in a suitable weak sense. For weak solution concepts and existence, uniqueness and regularity results we refer to Jerome (1983) and the earlier work of Oleinik (1960), Kamenomostskaya (1961) and Friedman (1968).

It should be noted that the existence of a weak solution can be shown in a constructive way as has been done by Kamenomostskaya (1961) using a forward Euler scheme in time and finite difference discretizations in the space variables and by Jerome (1983) whose existence proof is based on an implicit time discretization and a suitable regularization of the enthalpy function H. The above constructive methods also lay the foundations for a numerical solution of (1.1a–c). Meyer (1973) has considered the backward Euler scheme in time and finite difference methods in the space variables applied to (1.1a–c) with a smoothed enthalpy function. Elliott (1981) has also used an implicit time discretization but continuous, piecewise linear finite elements in space directly applied to (1.1a–c) without resorting to regularization techniques. His arguments strongly rely on the close relationship between the semi-discretized problem, elliptic variational inequalities of the second kind and the unconstrained minimization of subdifferentiable convex functionals.

Other numerical approaches are based on an alternative formulation of (1.1a–c) by introducing the enthalpy $v = H(u)$ as a new dependent variable. We refer to Berger, Brézis & Rogers (1970) and Nochetto & Verdi (1987–88, 1988a) for linearization techniques based on nonlinear semigroup theory, to Ciavaldini (1975) for explicit and implicit finite element discretizations and to Nochetto & Verdi (1988b) who treat a more general problem with an additional nonlinear flux term by a semi-implicit time discretization in conjunction with continuous, piecewise linear finite elements and regularization techniques (see Paolini, Sacchi & Verdi (1988) for a comparison of the numerical performance of nonlinear

algorithms and linearization methods). Energy error estimates have been derived by Jerome & Rose (1982), Elliott (1987) and Nochetto & Verdi (1988b). Finally, the practical aspect of solving the algebraic system arising from a full discretization of the enthalpy formulation has been dealt with in White (1982, 1986).

In all the papers on numerical methods cited above, for the solution of the nonlinear algebraic system obtained by implicit finite difference or finite element discretizations some nonlinear SOR-type techniques have been used. As is well known these methods suffer from rapidly deteriorating convergence rates for decreasing mesh sizes but can be used as appropriate smoothing procedures within a multi-grid framework. Hoppe & Kornhuber (1988) have developed a multi-grid algorithm based on a finite difference discretization of the backward in time discretized system (1.1a–c) with respect to a hierarchy of grids. The characteristic features of that algorithm are the use of nonlinear Gauss–Seidel iteration as a smoother, a modified FAS-type coarse grid correction, derived by means of duality arguments from convex analysis, and an adaptive local choice of restrictions and prolongations in the fine-to-coarse and coarse-to-fine transfers of the multi-grid cycles. Meshsize independent local convergence of W-cycles has been established using nonlinear multi-grid convergence theory and subdifferentiable calculus in the spirit of Hackbusch (1981, 1985) and Clarke (1983).

Discretizing by continuous, piecewise linear finite elements in space and taking advantage of the variational characterization of the fully discretized equation as an unconstrained nonsmooth convex minimization problem, in this paper we will improve on the above multi-grid algorithm by introducing a damping factor to the prolongated coarse grid correction. Such a device has recently been proposed by Hackbusch & Reusken (1989) for such nonlinear problems which are optimality conditions for unconstrained minimization problems with differentiable objective functionals. As a result of that damping factor we will get global convergence while retaining the meshsize independent local convergence.

The paper is organized as follows. The damped multi-grid two-phase Stefan problem solver will be developed in full detail in Section 2 while its convergence properties will be established in Section 3. Finally, in Section 4 we will report on some numerical results displaying a significant improvement in asymptotic efficiency rates.

2. The damped multi-grid solver

The implicit time discretization of the degenerate parabolic initial-boundary value problem (1.1a–c) with respect to a uniform partition $\{t_m = m\Delta t \mid 0 \leq m \leq M\}$, $\Delta t = T/M$, $M \in \mathbb{N}$, of the time interval $[0, T]$ requires the successive solution of elliptic differential inclusions

$$b^m - Au^m \in H(u^m) \quad \text{in} \quad \Omega, \tag{2.1a}$$

$$u^m = 0 \quad \text{on} \quad \partial\Omega \tag{2.1b}$$

where $A = -\Delta t\Delta$ and $b^m = H^{m-1} + \Delta t f^m$ with an appropriately chosen $H^{m-1} \in H(u^{m-1})$.

In the sequel, since we will mainly be concerned with the numerical solution of (2.1a–b), for notational convenience the upper index m will be suppressed.

Due to the fact that the enthalpy function H is the subgradient of a piecewise quadratic function Φ, i.e., $H = \partial\Phi$, a weak solution to (2.1a–b) can be characterized by the following elliptic variational inequality of the second kind. Find $u \in H_0^1(\Omega)$ such that

$$a(u, v-u) - (b, v-u) + \phi(v) - \phi(u) \geq 0, \qquad v \in H_0^1(\Omega) \tag{2.2}$$

where $a(\cdot,\cdot) : H_0^1(\Omega) \times H_0^1(\Omega) \to \mathbb{R}$ is the bilinear form associated with the elliptic operator A, $\phi : H_0^1(\Omega) \to \mathbb{R}$ is the subdifferentiable functional given by $\phi(v) = \int_\Omega \Phi(v(x))\,dx$, $v \in H_0^1(\Omega)$, and $(\cdot,\cdot)$ denotes the standard L^2 inner product.

Concerning existence, uniqueness and regularity of a solution to (2.2) we have that, if $b \in L^2(\Omega)$, then there exists a unique solution $u \in H_0^1(\Omega) \cap H^2(\Omega)$ (cf. e.g. Barbu (1976)). Moreover, it is easily shown that (2.2) is the necessary and sufficient optimality condition for the unconstrained subdifferentiable convex minimization problem

$$J(u) + \phi(u) = \inf_{v \in H_0^1(\Omega)} \big(J(v) + \phi(v)\big) \tag{2.3}$$

where $J(v) = a(v, v)/2 - (b, v)$.

We shall now consider a finite element approximation to (2.2) with respect to a hierarchy of triangulations where for the ease of exposition we will assume Ω to have a polygonal boundary $\partial\Omega$. Moreover, we will restrict ourselves to a hierarchy generated by uniform refinement. Given an initial coarse triangulation T_0 with $\bar{\Omega} = \bigcup_{T \in T_0} T$, we create $(T_k)_{k=0}^l$, $l \in \mathbb{N}$, in such a way that T_{k+1} is obtained from T_k by subdividing each triangle $T \in T_k$ into four subtriangles such that the midpoints of the edges of T are the additional vertices. We further assume that T_0 is such that the family $(T_k)_{k=0}^l$ is regular and quasi-uniform with all T_k, $0 \leq k \leq l$, sharing the property of acuteness.

We refer to V_k, $0 \leq k \leq l$, as the finite dimensional subspace of $H_0^1(\Omega)$ generated by continuous, piecewise linear finite elements, i.e. $V_k = \{v_k \in C_0(\Omega) \mid v_k|_T \in P_1(T),\ T \in T_k\}$ where $P_1(T)$ is the set of polynomials on T of degree less than or equal to 1. Denoting by a_i^T, $1 \leq i \leq 3$, the vertices of $T \in T_k$, the set N_k of interior nodal points is given by $N_k = (\bigcup_{T \in T_k} \{a_1^T, a_2^T, a_3^T\}) \cap \Omega$, and we have $\dim V_k = n_k$, $n_k = \operatorname{card} N_k$. Ordering the nodal points lexicographically, we may write $N_k = \{c_1^k, \ldots, c_{n_k}^k\}$, and a suitable basis $\{w_i^k\}_{i=1}^{n_k}$ of V_k is given by $w_i^k(c_j^k) = \delta_{ij}$, $1 \leq i, j \leq n_k$. Then, for a function $v \in C(\bar{\Omega})$ its V_k-interpolate will be denoted by $\Pi_k v$ while for a function $v \in L^2(\Omega)$ we will refer to $Q_k v$ as its L^2-projection onto V_k.

The standard finite element approach to (2.3) is to minimize (2.3) over V_k which, however, is impractical under the present circumstances, since the computation of $\phi|_T$, $T \in T_k$, would require us to determine where $v_k \in V_k$ changes sign on T. Therefore, following Elliott (1981) we approximate the functional ϕ in such a way that we replace the integrand by its V_k-interpolate thus giving

$$\phi_k(v_k) = \int_\Omega (\Pi_k \Phi(v))(x)\,dx = \sum_{T \in T_k} \tfrac{1}{3}\,\text{area}\,(T) \sum_{i=1}^{3} \Phi(v_k(a_i^T)). \tag{2.4}$$

Then the fully discretized problem on level k is to minimize $J + \phi_k$ over V_k, i.e., find $u_k \in V_k$ such that

$$J(u_k) + \phi_k(u_k) = \min_{v_k \in V_k} (J(v_k) + \phi_k(v_k)). \tag{2.5}$$

As in the continuous case, setting

$$\Omega_k^\alpha = \{x \in \Omega \mid (-1)^\alpha u_k(x) > 0\}, \qquad 1 \leq \alpha \leq 2,$$
$$\Omega_k^3 = \{x \in \Omega \mid u_k(x) = 0\},$$

the discrete free boundaries are given by

$$\Sigma_k^\alpha = \partial(\Omega_k^\alpha) \cap \Omega_k^3, \qquad 1 \leq \alpha \leq 2. \tag{2.6}$$

We identify finite element functions in V_k with vectors in $\mathbb{R}^{n_k}$ via the bijective mapping

$$I_k v_k = \sum_{i=1}^{n_k} v_{k,i} w_i^k, \qquad v_k \in \mathbb{R}^{n_k}, \tag{2.7}$$

and we refer to $\langle \cdot, \cdot \rangle_k$ as the discrete inner product on $\mathbb{R}^{n_k}$ given by

$$\langle u_k, v_k \rangle_k = \sum_{i=1}^{n_k} \gamma_i^k u_{k,i} v_{k,i}, \qquad \gamma_i^k = \tfrac{1}{3} \sum_{j=1}^{m_i^k} \text{area}\,(T_{i,j}) \tag{2.8}$$

where $T_{i,j} \in T_k$, $1 \leq j \leq m_i^k$ are the triangles having $c_i^k \in N_k$ as a common vertex. The associated norm will be denoted by $|\cdot|_k$.

Further we denote by I^k the adjoint of I_k with respect to the inner products $(\cdot, \cdot)$ on V_k and $\langle \cdot, \cdot \rangle_k$ on $\mathbb{R}^{n_k}$, i.e.,

$$\langle I^k u_k, v_k \rangle_k = (u_k, I_k v_k), \qquad u_k \in V_k, \quad v_k \in R^{n_k}, \tag{2.9}$$

and we set $A_k = I^k A I_k$, $b_k = I^k Q_k b$ and $\Phi_k(v_k) = \phi_k(I_k v_k)$, $v_k \in \mathbb{R}^{n_k}$. Then, with $J_k : \mathbb{R}^{n_k} \to \mathbb{R}^{n_k}$ given by

$$J_k(v_k) = \tfrac{1}{2} \langle A_k v_k, v_k \rangle_k - \langle b_k, v_k \rangle_k + \Phi_k(v_k), \tag{2.10}$$

the minimization problem (2.5) can be algebraically written in the form

$$J_k(u_k) = \min_{v_k \in \mathbf{R}^{n_k}} J_k(v_k) \tag{2.11}$$

which obviously is equivalent to the algebraic inclusion

$$b_k - A_k u_k \in \partial \Phi(u_k). \tag{2.12}$$

The multi-grid algorithm for the solution of (2.12) on level l will now be exemplarily described in the case of two levels l and $l-1$. It will be designed in such a way that, given an iterate u_l^ν, $\nu \geq 0$, on level l, the result $u_l^{\nu+1}$ of the two-level cycle yields a decrease in the value of the functional J_l. For this purpose we require both ingredients of the multi-grid algorithm, namely the smoothing procedure and the coarse grid correction, to provide a descent direction for J_l. According to the results in Elliott (1981), a natural candidate for the smoothing process is nonlinear Gauss–Seidel iteration which will be used here in its

symmetric variant. In particular, if we perform κ_1 smoothing steps, then, given $z_l^0 := u_l^\nu$, we first obtain $z_l^{\mu+1/2}$ from z_l^μ, $0 \leq \mu \leq \kappa_1 - 1$, by the successive solution of the n_l scalar inclusions

$$d_{l,i} - a_{ii}^l z_{l,i}^{\mu+1/2} \in \partial\Phi(z_{l,i}^{\mu+1/2}), \qquad 1 \leq i \leq n_l \tag{2.13}$$

where

$$d_{l,i} = b_{l,i} - \sum_{j=1}^{i-1} a_{ij}^l z_{l,j}^{\mu+1/2} - \sum_{j=i+1}^{n_l} a_{ij}^l z_{l,j}^{\mu}$$

and a_{ij}^l, $1 \leq i, j \leq n_l$, are the components of A_l.

Secondly, we compute $z_l^{\mu+1}$ from $z_l^{\mu+1/2}$ in essentially the same way but with a reversed ordering of the unknowns.

Note that in view of $\partial\Phi = H$ and (1.2) the inclusions (2.13) can be easily solved by means of

$$z_{l,i}^{\mu+1/2} = \begin{cases} (d_{l,i} + s_1)/(a_{ii}^l + a_1), & \text{if} \quad d_{l,i} < -s_1 \\ 0, \quad \text{if} \quad d_{l,i} \in [-s_1, s_2] & \\ (d_{l,i} - s_2)/(a_{ii}^l + a_2), & \text{if} \quad d_{l,i} > s_2. \end{cases} \tag{2.14}$$

The above smoothing process will be formally described by

$$\bar{u}_l^\nu = S_l^{\kappa_1}(u_l^\nu; b_l). \tag{2.15}$$

Concerning the coarse grid correction, the difficulty to deal with inclusions can be circumvented by the following well known equivalence from convex analysis (cf. e.g. Ekeland & Temam (1976))

$$b_l - A_l u_l \in \partial\Phi(u_l) \Leftrightarrow u_l \in \partial\Phi^*(b_l - A_l u_l) \tag{2.16}$$

where Φ^* denotes the conjugate function to Φ given by

$$\Phi^*(\lambda) = \sup_\mu (\lambda\mu - \Phi(\mu)).$$

In particular, in our case the subgradient $\partial\Phi^*$ turns out to be the continuous, piecewise linear function

$$\partial\Phi^*(\lambda) = \begin{cases} a_1^{-1}(\lambda + s_1), & \text{if} \quad \lambda < -s_1 \\ 0, & \text{if} \quad \lambda \in [-s_1, s_2] \\ a_2^{-1}(\lambda - s_2), & \text{if} \quad \lambda > s_2. \end{cases} \tag{2.17}$$

Consequently, the second inclusion in (2.16) reduces to the non-linear algebraic system

$$F_l(u_l) = u_l - \partial\Phi^*(b_l - A_l u_l) = 0. \tag{2.18}$$

It is that system which will now be subjected to a variant of Brandt's FAS-scheme (cf. e.g. Brandt (1977)) combined with the idea of introducing a damping factor for the prolongated coarse grid correction. Denoting by r_l^{l-1} and p_{l-1}^l an appropriately chosen restriction and prolongation, respectively (this point will be discussed in more detail below), we determine an improved iterate by

$$\bar{u}_l^\nu(\omega_l) = \bar{u}_l^\nu - \omega_l p_{l-1}^l (r_l^{l-1}\bar{u}_l^\nu - u_{l-1}) \tag{2.19}$$

where $u_{l-1} \in R^{n_{l-1}}$ is the solution of the coarse grid correction problem

$$\begin{aligned} F_{l-1}(u_{l-1}) &= u_{l-1} - \partial\Phi^*(\bar{b}_{l-1} - A_{l-1}u_{l-1}), \\ \bar{b}_{l-1} &= A_{l-1}r_l^{l-1}\bar{u}_l^\nu - r_l^{l-1}d_l,\ d_l = A_l\bar{u}_l^\nu - b_l \end{aligned} \tag{2.20}$$

and $\omega_l \in [0, 2]$ is chosen such that $J_l(\bar{u}_l^\nu(\omega_l)) \leq J_l(\bar{u}_l^\nu)$.

Remark. In view of (2.16) the coarse grid correction on level $l-1$ is equivalent to an algebraic inclusion of the same kind as that one initially given on level l.

Finally, we complete the two-grid cycle by performing a certain number κ_2 of post-smoothing steps using again symmetric nonlinear Gauss–Seidel iteration as a smoother

$$u_l^{\nu+1} = S_l^{\kappa_2}(\bar{u}_l^\nu(\omega_l); b_l). \tag{2.21}$$

In case of more than two levels the solution of (2.21) is replaced by an additional two-grid cycle involving the levels $k = l-1$ and $k = l-2$. This process will then be repeated until the lowest level $k = 0$ is reached. Symmetric nonlinear Gauss–Seidel iteration will also be used as an iterative solver of the correction problem on the lowest level, since by Elliott's result it is known to yield a globally convergent minimizing sequence for the associated nonsmooth minimization problem.

Note that the coarse grid correction problems on levels $0 \leq k < l$ are equivalent to the unconstrained minimization of functionals which are different from those given by (2.10). Therefore, in the following we will refer to $\bar{J}_k$, $0 \leq k \leq l$, as the functionals given by $\bar{J}_l = J_l$ while $\bar{J}_k$, $0 \leq k \leq l-1$, is defined as in (2.10) with b_k replaced by $\bar{b}_k = A_k r_{k+1}^k \bar{u}_{k+1}^\nu - r_{k+1}^k(A_{k+1}\bar{u}_{k+1}^\nu - \bar{b}_{k+1})$, $\bar{b}_l = b_l$. We will further refer to $u_k^* \in R^{n_k}$, $0 \leq k \leq l$, as the unique solutions to the associated minimization problems.

For finite element discretizations of second order elliptic boundary value problems restrictions r_k^{k-1} and prolongations p_{k-1}^k, $1 \leq k \leq l$, are usually chosen in a canonical way according to

$$r_k^{k-1} I^k = I^{k-1}, \qquad I_k p_{k-1}^k = I_{k-1} \tag{2.22}$$

where I_k and I^k are the maps defined by means of (2.7) and (2.9), respectively.

Remark. In case of triangulations T_k with triangles $\{(x, y), (x + h_k, y), (x + h_k, y + h_k)\}$ and $\{(x, y), (x, y + h_k), (x + h_k, y + h_k)\}$, $(x, y) = (ih_k, jh_k)$, $i, j \in \mathbb{Z}$, $h_k > 0$, the restrictions and prolongations as given by (2.22) coincide with the standard seven-point restrictions and seven-point prolongations (cf. e.g. Hackbusch (1985)).

However, in the present situation we cannot use such weighted restrictions globally due to the occurrence of discrete free boundaries. To make this point more transparent, we subdivide the set N_k of interior nodal points c_i^k, $1 \leq i \leq n_k$, into three mutually disjoint subsets with respect to the actual values of $\bar{u}_{k,i}^\nu = (I_k \bar{u}_k^\nu)(c_i^k)$:

$$N_k^\alpha(\bar{u}_k^\nu) = \{c_i^k \in N_k \mid (-1)^\alpha \bar{u}_{k,i}^\nu > 0\}, \qquad 1 \leq \alpha \leq 2, \tag{2.23a}$$

$$N_k^3(\bar{u}_k^\nu) = \{c_i^k \in N_k \mid \bar{u}_{k,i}^\nu = 0\}. \tag{2.23b}$$

We further denote by $N_k^r(c_i^k) \subset N_k$ the set consisting of c_i^k and its maximal six nearest neighbours in N_k. Then, if we consider a nodal point $c_i^{k-1} \in N_k^\alpha(\bar{u}_k^\nu)$, $\alpha \in \{1, 2, 3\}$, with a neighbouring grid point representing a different phase, i.e., $c_j^k \in N_k^r(c_i^{k-1}) \cap N_k^\beta(\bar{u}_k^\nu)$, $\beta \in \{1, 2, 3\} \backslash \{\alpha\}$, weighted restriction cannot be used, since the defect $d_{k,j}^\nu$ in c_j^k is not a reliable indicator for the accuracy of the approximation in c_i^{k-1}. In other words, performing weighted restriction globally, the solution u_l^* to (2.11) on level l is no longer a fixed point of the multi-grid iteration. This problem can be circumvented by using pointwise restriction in a vicinity of the discrete free boundaries and weighted restriction elsewhere. To be more precise, a nodal point c_i^k will be called regular, if all nearest neighbours in N_k represent the same phase, and irregular otherwise, i.e.,

$$N_k^{\text{reg}}(\bar{u}_k^\nu) = \{c_i^k \in N_k \mid N_k^r(c_i^k) \cap N_k \subset N_k^\alpha(\bar{u}_k^\nu), \quad \alpha \in \{1, 2, 3\}\}, \tag{2.24a}$$

$$N_k^{\text{irr}}(\bar{u}_k^\nu) = N_k \backslash N_k^{\text{reg}}(\bar{u}_k^\nu). \tag{2.24b}$$

Denoting by $\hat{r}_k^{k-1}$ the weighted restriction as given by (2.22) and by $\mathring{r}_k^{k-1}$ the pointwise restriction, we define r_k^{k-1}, $1 \leq k \leq l$, locally for $1 \leq i \leq n_{k-1}$ according to

$$(r_k^{k-1} v_k)_i = \begin{cases} (\hat{r}_k^{k-1} v_k)_i, & \text{if} \quad c_i^{k-1} \in N_k^{\text{reg}}(\bar{u}_k^\nu) \\ (\mathring{r}_k^{k-1} v_k)_i, & \text{if} \quad c_i^{k-1} \in N_k^{\text{irr}}(\bar{u}_k^\nu). \end{cases} \tag{2.25}$$

As far as the prolongations are concerned we will use the strategy that a change of the discrete free boundaries should not be caused by the prolongated coarse grid correction. Therefore, we have to make sure that $\bar{u}_k^\nu(\omega_k)$ does not change sign over the whole range of possible values of the damping parameter and we do not prolongate, if the weighted prolongation involves nodal points on level $k-1$ representing a different phase. In particular, we define $N_{k-1}^\alpha(u_{k-1}^{\nu+1})$ and $N_k^\alpha(\bar{u}_k^\nu(\omega_k))$, $1 \leq \alpha \leq 3$, according to (2.23a–b) and we refer to $N_{k-1}^p(c_i^k)$ as the set consisting either of the single element c_i^k, if $c_i^k \in N_{k-1}$, or of the adjacent nodal points in N_{k-1}, if $c_i^k \notin N_{k-1}$. Then a nodal point $c_i^k \in N_k$ will be called regular with respect to $\bar{u}_k^\nu(\omega_k)$, if the following condition holds true:

$$\begin{aligned} &c_i^k \in N_k^\alpha(\bar{u}_k^\nu(\omega_k)) \quad \text{for all } \omega_k \in [0, 2] \quad \text{and} \\ &N_{k-1}^p(c_i^k) \subset N_{k-1}^\alpha(u_{k-1}^{\nu+1}), \qquad \alpha \in \{1, 2, 3\}. \end{aligned} \tag{2.26}$$

Accordingly we set

$$N_k^{\text{reg}}(\bar{u}_k^\nu(\omega_k)) = \{c_i^k \in N_k \mid (2.26) \text{ is satisfied}\}, \tag{2.27a}$$

$$N_k^{\text{irr}}(\bar{u}_k^\nu(\omega_k)) = N_k \backslash N_k^{\text{reg}}(\bar{u}_k^\nu(\omega_k)). \tag{2.27b}$$

Then, denoting by $\hat{p}_{k-1}^k$ the weighted prolongation as in (2.22), we specify p_{k-1}^k, $1 \leq k \leq l$, locally for $1 \leq i \leq n_k$ as follows

$$(p_{k-1}^k v_{k-1})_i = \begin{cases} (\hat{p}_{k-1}^k v_{k-1})_i, & \text{if} \quad c_i^k \in N_k^{\text{reg}}(\bar{u}_k^\nu(\omega_k)) \\ 0, & \text{if} \quad c_i^k \in N_k^{\text{irr}}(\bar{u}_k^\nu(\omega_k)). \end{cases} \tag{2.28}$$

Although the algorithm is based on a fixed domain formulation of the problem, due to the choice of restrictions and prolongations by (2.25) and (2.28) the two-level iteration has the flavour of a combined approach of fixed domain and

front tracking techniques. The smoothing procedure obviously is a fixed domain method which allows the *a posteriori* specification of the discrete free boundaries while the coarse grid correction can be seen as an approximation to the respective heat equations describing the temperature in the two different phases. Moreover, in the next section we will see that with the above adaptive choice of prolongations and restrictions the prolongated coarse grid correction $\omega_k p_{k-1}^k(r_k^{k-1}\bar{u}_k^\nu - u_{k-1}^{\nu+1})$ yields a descent direction of the associated functional for all $0 \leq \omega_k \leq \bar{\omega}_k$. It will be further shown that an optimal $\omega_k^* \in [0, \bar{\omega}_k]$ can be cheaply computed by means of easily accessible data.

Finally, it should be mentioned that a suitable startiterate u_l^0 on the highest level can be efficiently determined by nested iteration taking into account the values at the previous time t_{m-1} on all levels $0 \leq k \leq l$. Note that an appropriate choice of $H^{m-1} \in H(u_k^{m-1})$ is given by $H_i^{m-1} = H(u_{k,i}^{m-1})$ for $u_{k,i}^{m-1} \neq 0$ and $H_i^{m-1} = (\bar{b}_k - A_k u_k^{m-1})_i$ for $u_{k,i}^{m-1} = 0$, $1 \leq i \leq n_k$. Since the process of nested iteration is fairly standard and has also been used in Hoppe & Kornhuber (1988), the reader is referred to that paper for more details.

3. Convergence results

In this section we will first prove that a suitable choice of the damping parameter ω_k on levels $1 \leq k \leq l$ results in global convergence of the multi-grid algorithm, provided that at least one pre-smoothing or post-smoothing step is performed on each of these levels. It should be mentioned that the techniques used by Hackbusch & Reusken (1989) do not apply here, since the design of the multi-grid algorithm under consideration involves several non-standard features that take into account the special nature of the moving boundary problem.

The basic step in the global convergence proof is to show that on each level $1 \leq k \leq l$ both components of the multi-grid cycle, namely the smoother and the coarse grid correction, do provide a descent direction for the functional $\bar{J}_k$ to be minimized. As far as the smoothing process is concerned, this result is well known (cf. Elliott (1981)) but will be stated for the sake of completeness.

LEMMA 3.1 For $1 \leq k \leq l$ and $v_k \in \mathbb{R}^{n_k}$ let $u_k = S_k^\kappa(v_k; \bar{b}_k)$, $\kappa > 0$. Then, there exists a positive constant $c_k^{(1)} = c_k^{(1)}(\kappa, A_k)$ such that

$$\bar{J}_k(v_k) - \bar{J}_k(u_k) \geq c_k^{(1)} |v_k - u_k|_k^2. \tag{3.1}$$

Proof. It is sufficient to prove (3.1) for $\kappa = 1$ and the first substep of symmetric nonlinear Gauss–Seidel iteration, since the general result can be easily deduced from that special case. We start by decomposing the left-hand side in (3.1) into a telescoping sum according to

$$\bar{J}_k(v_k) - \bar{J}_k(u_k) = \sum_{i=1}^{n_k} \gamma_i^k [\bar{J}_{k,i}(v_{k,i}) - \bar{J}_{k,i}(u_{k,i})],$$

$$\bar{J}_{k,i}(\lambda) = \tfrac{1}{2} a_{ii}^k \lambda^2 - d_{k,i}\lambda + \Phi(\lambda), \qquad 1 \leq i \leq n_k,$$

where $d_{k,i}$ is given as in (2.13) with l, b_l, $z_l^{\mu+\frac{1}{2}}$, z_l^μ replaced by k, $\bar{b}_k$, u_k, v_k,

respectively. Using the pointwise relations

$$d_{k,i} - a_{ii}^k u_{k,i} \in \partial\Phi(u_{k,i}),$$

$$\Phi(v_{k,i}) - \Phi(u_{k,i}) + \partial\Phi(u_{k,i})(v_{k,i} - u_{k,i}) \geq 0,$$

we find

$$\bar{J}_{k,i}(v_{k,i}) - \bar{J}_{k,i}(u_{k,i}) \geq \tfrac{1}{2} a_{ii}^k (v_{k,i} - u_{k,i})^2$$

which immediately yields the assertion.

In order to prove the descent property for the coarse grid correction, i.e., $\bar{J}_k(\bar{u}_k^\nu(\omega_k)) \leq \bar{J}_k(\bar{u}_k^\nu)$, $1 \leq k \leq l$, we have to estimate $\Phi_k(\bar{u}_k^\nu) - \Phi_k(\bar{u}_k^\nu(\omega_k))$ from below and to evaluate $\Phi_{k-1}(r_k^{k-1}\bar{u}_k^\nu) - \Phi_{k-1}(u_{k-1}^{\nu+1})$ in a proper way. This will be done in the following technical lemma which is easy to prove but involves some tedious computations due to the fact that the vectors $r_k^{k-1}\bar{u}_k^\nu$ and $u_{k-1}^{\nu+1}$ may have components of different sign. For notational convenience, given $v_k \in \mathbb{R}^{n_k}$, we introduce vectors $a_k(v_k) \in \mathbb{R}^{n_k}$ and $s_k(v_k) \in \mathbb{R}^{n_k}$ by

$$a_{k,i}(v_k) = \begin{cases} a_1, & \text{if } v_{k,i} < 0 \\ a_2, & \text{if } v_{k,i} \geq 0 \end{cases} \qquad s_{k,i}(v_k) = \begin{cases} s_1, & \text{if } v_{k,i} < 0 \\ -s_2, & \text{if } v_{k,i} \geq 0 \end{cases}$$

Further, we refer to $u_k * v_k \in R^{n_k}$ as the vector with components $(u_k * v_k)_i = u_{k,i} v_{k,i}$, $1 \leq i \leq n_k$. Then, denoting by $w_{k-1} = r_k^{k-1}\bar{u}_k^\nu - u_{k-1}^{\nu+1}$ the coarse grid correction and using the preceding notations, for $1 \leq k \leq l$ we define

$$\delta_{k-1}^{(1)} = \langle (r_k^{k-1} - (p_{k-1}^k)^*)(a_k(\bar{u}_k^\nu) * \bar{u}_k^\nu - s_k(\bar{u}_k^\nu)),\ w_{k-1} \rangle_{k-1}, \tag{3.2}$$

$$\delta_{k-1}^{(2)} = \langle \eta_{k-1}^a * u_{k-1}^{\nu+1} - \eta_{k-1}^s,\ u_{k-1}^{\nu+1} \rangle_{k-1}, \qquad 2 \leq k \leq l, \tag{3.3a}$$

$$\delta_0^{(2)} = \langle 2\eta_0^a * u_0^{\nu+1} - \eta_0^s,\ w_0 \rangle_0 \tag{3.3b}$$

where $\eta_{k-1}^a = \frac{1}{2}(a_{k-1}(u_{k-1}^{\nu+1}) - a_{k-1}(r_k^{k-1}\bar{u}_k^\nu))$ and $\eta_{k-1}^s = s_{k-1}(u_{k-1}^{\nu+1}) - s_{k-1}(r_k^{k-1}\bar{u}_k^\nu)$, $1 \leq k \leq l$. Note that $\eta_{k-1,i}^a = \eta_{k-1,i}^s = 0$, if $c_i^{k-1} \in N_{k-1}^\alpha(u_{k-1}^{\nu+1}) \cap N_{k-1}^\alpha(r_k^{k-1}\bar{u}_k^\nu)$, $\alpha \in \{1, 2, 3\}$, $1 \leq i \leq n_{k-1}$.

LEMMA 3.2 For $1 \leq k \leq l$ there holds

$$\Phi_k(\bar{u}_k^\nu) - \Phi_k(\bar{u}_k^\nu(\omega_k)) \geq \omega_k[\langle a_{k-1}(r_k^{k-1}\bar{u}_k^\nu) * r_k^{k-1}\bar{u}_k^\nu - s_{k-1}(r_k^{k-1}\bar{u}_k^\nu),\ w_{k-1}\rangle_{k-1} - \delta_{k-1}^{(1)}] - \tfrac{1}{2}\omega_k^2 \langle a_{k-1}(r_k^{k-1}\bar{u}_k^\nu) * w_{k-1},\ w_{k-1}\rangle_{k-1}. \tag{3.4}$$

Moreover, for $2 \leq k \leq l$

$$\Phi_{k-1}(r_k^{k-1}\bar{u}_k^\nu) - \Phi_{k-1}(u_{k-1}^{\nu+1}) = \langle a_{k-1}(r_k^{k-1}\bar{u}_k^\nu) * u_{k-1}^{\nu+1} - s_{k-1}(r_k^{k-1}\bar{u}_k^\nu),\ w_{k-1}\rangle_{k-1} + \tfrac{1}{2}\langle a_{k-1}(r_k^{k-1}\bar{u}_k^\nu) * w_{k-1},\ w_{k-1}\rangle_{k-1} + \delta_{k-1}^{(2)}. \tag{3.5}$$

Proof. Since by definition of the prolongations it is guaranteed that $\bar{u}_k^\nu$ and $\bar{u}_k^\nu(\omega_k)$ are of the same sign, we find by elementary calculations

$$\Phi_k(\bar{u}_k^\nu) - \Phi_k(\bar{u}_k^\nu(\omega_k)) = \omega_k[\langle r_k^{k-1}(a_k(\bar{u}_k^\nu) * \bar{u}_k^\nu - s_k(\bar{u}_k^\nu)),\ w_{k-1}\rangle_{k-1} + \delta_{k-1}^{(1)}] - \tfrac{1}{2}\omega_k^2 \langle a_k(\bar{u}_k^\nu) * p_{k-1}^k w_{k-1},\ p_{k-1}^k w_{k-1}\rangle_k. \tag{3.6}$$

In view of the fact that the restrictions are sign preserving, it follows that

$$r_k^{k-1}\big(a_k(\bar{u}_k^\nu) * \bar{u}_k^\nu - s_k(\bar{u}_k^\nu)\big) = a_{k-1}(r_k^{k-1}\bar{u}_k^\nu) * r_k^{k-1}\bar{u}_k^\nu - s_{k-1}(r_k^{k-1}\bar{u}_k^\nu). \tag{3.7}$$

Moreover, denoting by $a_k^{1/2}(v_k)$ the vector with components $(a_{k,i}(v_k))^{1/2}$, $1 \leq i \leq n_k$, we have

$$\begin{aligned}\langle a_k(\bar{u}_k^\nu) * p_{k-1}^k w_{k-1}, p_{k-1}^k w_{k-1}\rangle_k &= |a_k^{1/2}(\bar{u}_k^\nu) * p_{k-1}^k w_{k-1}|_k^2 \\ &\leq |a_{k-1}^{1/2}(r_k^{k-1}\bar{u}_k^\nu) * w_{k-1}|_{k-1}^2 = \langle a_{k-1}(r_k^{k-1}\bar{u}_k^\nu) * w_{k-1}, w_{k-1}\rangle_{k-1}. \end{aligned}\tag{3.8}$$

Using (3.7) and (3.8) in (3.6) immediately gives (3.4). The second assertion (3.5) can be derived by straightforward evaluation of the left-hand side.

Now we are in the position to establish the desired descent property for the coarse grid correction:

THEOREM 3.3 *For all $1 \leq k \leq l$ there exists $\bar{\omega}_k \in [0, 2]$ such that for all $\omega_k \in [0, \bar{\omega}_k]$ we can find a constant $c_k^{(2)} = c_k^{(2)}(\omega_k) \geq 0$ such that*

$$\bar{J}_k(\bar{u}_k^\nu) - \bar{J}_k(\bar{u}_k^\nu(\omega_k)) \geq c_k^{(2)}\, |p_{k-1}^k w_{k-1}|_k^2. \tag{3.9}$$

Proof. We may assume $w_{k-1} \neq 0$, since otherwise (3.9) becomes trivial. Then a straightforward evaluation of the left-hand side in (3.9) gives

$$\begin{aligned}\bar{J}_k(\bar{u}_k^\nu) - \bar{J}_k(\bar{u}_k^\nu(\omega_k)) &= \omega_k \langle d_k^\nu, p_{k-1}^k w_{k-1}\rangle_k \\ &\quad - \tfrac{1}{2}\omega_k^2 \langle A_k p_{k-1}^k w_{k-1}, p_{k-1}^k w_{k-1}\rangle_k + \Phi_k(\bar{u}_k^\nu) - \Phi_k(\bar{u}_k^\nu(\omega_k)). \end{aligned}\tag{3.10}$$

In order to prove the assertion we now proceed by induction on k.

For $k = 1$ we know that the solution $u_0^{\nu+1}$ to the coarse grid problem on level 0 satisfies

$$\langle r_1^0 d_1^\nu, w_0\rangle_0 + \langle \partial\Phi_0(u_0^{\nu+1}), w_0\rangle_0 = \langle A_0 w_0, w_0\rangle_0. \tag{3.11}$$

Then, using (3.2), (3.3b) and (3.11) in (3.10), we find

$$\begin{aligned}\bar{J}_1(\bar{u}_1^\nu) - \bar{J}_1(\bar{u}_1^\nu(\omega_1)) &\geq \tfrac{1}{2}\omega_1[2(1 - \varepsilon_0^{(1)}) - \omega_1(1 + \varepsilon_0^{(2)})]\langle A_0 w_0, w_0\rangle_0 \\ &\quad + \tfrac{1}{2}\omega_1[2(1 - \varepsilon_0^{(3)}) - \omega_1]\langle a_0(r_1^0 \bar{u}_1) * w_0, w_0\rangle_0 \end{aligned}\tag{3.12}$$

where

$$\begin{aligned}\varepsilon_0^{(1)} &= |\langle (r_1^0 - (p_0^1)^*) d_1^\nu, w_0\rangle_0| / \langle A_0 w_0, w_0\rangle_0, \\ \varepsilon_0^{(2)} &= |\langle ((p_0^1)^* A_1 p_0^1 - A_0) w_0, w_0\rangle_0| / \langle A_0 w_0, w_0\rangle_0, \\ \varepsilon_0^{(3)} &= |\delta_0^{(1)} + \delta_0^{(2)}| / \langle a_0(r_1^0 \bar{u}_1^\nu) * w_0, w_0\rangle_0. \end{aligned}$$

Consequently, choosing

$$\bar{\omega}_1 = \max\{0, \min\{2(1 - \varepsilon_0^{(1)})/(1 + \varepsilon_0^{(2)}), 2(1 - \varepsilon_0^{(3)})\}\} \tag{3.13}$$

the assertion holds true by observing the ellipticity of A_0 and $|p_0^1 w_0|_1^2 \leq |w_0|_0^2$. Now, assuming (3.9) to hold true for some $1 \leq k - 1 \leq l - 1$ and observing Lemma 3.1 we have

$$\bar{J}_{k-1}(u_{k-1}^\nu) = \bar{J}_{k-1}(r_k^{k-1}\bar{u}_k^\nu) \geq \bar{J}_{k-1}(\bar{u}_{k-1}^\nu) \geq \bar{J}_{k-1}(\bar{u}_{k-1}^\nu(\omega_{k-1})) \geq \bar{J}_{k-1}(u_{k-1}^{\nu+1}). \tag{3.14}$$

Using (3.14) and taking into account the symmetry of A_{k-1}, by straightforward calculations it follows that

$$\langle r_k^{k-1} d_k^\nu, w_{k-1}\rangle_{k-1} + \Phi_{k-1}(r_k^{k-1}\bar{u}_k^\nu) - \Phi_{k-1}(u_{k-1}^{\nu+1}) \geq \tfrac{1}{2}\langle A_{k-1}w_{k-1}, w_{k-1}\rangle_{k-1}. \quad (3.15)$$

Then, if we use (3.2), (3.3a), (3.4), (3.5) and (3.15) in (3.10) in the same way as we did for $k = 1$, we get

$$\bar{J}_k(\bar{u}_k^\nu) - \bar{J}_k(\bar{u}_k^\nu(\omega_k)) \geq \tfrac{1}{2}\omega_k[(1-\varepsilon_{k-1}^{(1)}) - \omega_k(1+\varepsilon_{k-1}^{(2)})]\langle A_{k-1}w_{k-1}, w_{k-1}\rangle_{k-1} + \tfrac{1}{2}\omega_k[(1-\varepsilon_{k-1}^{(3)}) - \omega_k]\langle a_{k-1}(r_k^{k-1}\bar{u}_k^\nu) * w_{k-1}, w_{k-1}\rangle_{k-1} \quad (3.16)$$

where

$$\varepsilon_{k-1}^{(1)} = |\langle (r_k^{k-1} - (p_{k-1}^k)^*)d_k^\nu, w_{k-1}\rangle| / [\langle r_k^{k-1} d_k^\nu, w_{k-1}\rangle_{k-1} + \Phi_{k-1}(r_k^{k-1}\bar{u}_k^\nu) - \Phi_{k-1}(u_{k-1}^{\nu+1})],$$

$$\varepsilon_{k-1}^{(2)} = |\langle ((p_{k-1}^k)^* A_k p_{k-1}^k - A_{k-1})w_{k-1}, w_{k-1}\rangle_{k-1}| / \langle A_{k-1}w_{k-1}, w_{k-1}\rangle_{k-1},$$

$$\varepsilon_{k-1}^{(3)} = |\delta_{k-1}^{(1)} + \delta_{k-1}^{(2)}| / \langle a_{k-1}(r_k^{k-1}\bar{u}_k^\nu) * w_{k-1}, w_{k-1}\rangle_{k-1}.$$

Hence, if we choose

$$\bar{\omega}_k = \max\{0, \min\{(1-\varepsilon_{k-1}^{(1)})/(1+\varepsilon_{k-1}^{(2)}), 1-\varepsilon_{k-1}^{(3)}\}\}, \quad (3.17)$$

it follows from (3.16) that the assertion holds true on level k.

Remark. If we assume convergence of the discrete free boundaries to the continuous ones, we can expect the quantities $\varepsilon_k^{(\alpha)}$, $1 \leq \alpha \leq 3$, in (3.13) and (3.17) to become small such that $\bar{\omega}_1 \simeq 2$ whereas $\bar{\omega}_k \simeq 1$, $2 \leq k \leq l$. Apparently, the bound $\bar{\omega}_k$, $2 \leq k \leq l$, is too pessimistic, since in the proof we have only used $\bar{J}_{k-1}(r_k^{k-1}\bar{u}_k^\nu) - \bar{J}_{k-1}(u_{k-1}^{\nu+1}) \geq 0$. A more detailed analysis would have revealed

$$\bar{J}_{k-1}(r_k^{k-1}\bar{u}_k^\nu) - \bar{J}_{k-1}(u_{k-1}^{\nu+1}) \geq c_{k-1}^{(3)}\langle A_{k-1}w_{k-1}, w_{k-1}\rangle_{k-1} + c_{k-1}^{(4)}\langle a_{k-1}(r_k^{k-1}\bar{u}_k^\nu) * w_{k-1}, w_{k-1}\rangle_{k-1}$$

with positive $c_{k-1}^{(\alpha)}$, $3 \leq \alpha \leq 4$, thus yielding more realistic bounds $\bar{\omega}_k \geq 1$, $2 \leq k \leq l$. Using the preceding result we can easily deduce global convergence of the damped multi-grid algorithm:

THEOREM 3.4. Let us assume $\kappa = \kappa_1 + \kappa_2 > 0$ and $\omega_k \in [0, \bar{\omega}_k]$, $1 \leq k \leq l$, with $\bar{\omega}_k$ given by (3.13), (3.17), respectively. Then, for any initial value $u_l^0 \in \mathbb{R}^{n_l}$, the sequence $(u_l^\nu)_{\mathbb{N}}$ of multi-grid iterates converges to the unique solution u_l^* of (2.11) on level l.

Proof. In view of Lemma 3.1 and Theorem 3.3 there exists a positive constant c such that for all $\nu \geq 0$

$$\bar{J}_l(u_l^\nu) - \bar{J}(\bar{u}_l^\nu) \geq c\,|u_l^\nu - \bar{u}_l^\nu|_l^2, \quad (3.18a)$$

$$\bar{J}_l(\bar{u}_l^\nu) - \bar{J}_l(\bar{u}_l^\nu(\omega_l)) \geq c|\bar{u}_l^\nu - \bar{u}_l^\nu(\omega_l)|_l^2, \quad (3.18b)$$

$$\bar{J}_l(\bar{u}_l^\nu(\omega_l)) - \bar{J}_l(u_l^{\nu+1}) \geq c\,|\bar{u}_l^\nu(\omega_l) - u_l^{\nu+1}|_l^2. \quad (3.18c)$$

Due to the fact that A_l is positive definite and $\Phi(\lambda) \geq 0$, $\lambda \in \mathbb{R}$, the sequence $(u_l^\nu)_\mathbb{N}$ is bounded, and hence there exist a subsequence $\mathbb{N}' \subset \mathbb{N}$ and a vector $u_l^{**} \in \mathbb{R}^{n_l}$ such that $u_l^\nu \to u_l^{**}$ $(\nu \in \mathbb{N}')$. By (3.18a–c) it follows that

$$\bar{u}_l^\nu \to u_l^{**}, \qquad \bar{u}_l^\nu(\omega_l) \to u_l^{**}, \qquad u_l^{\nu+1} \to u_l^{**} \quad (\nu \in \mathbb{N}').$$

To fix the ideas let us suppose $\kappa = \kappa_1 > 0$. As in the proof of Lemma 3.1 it is sufficient to consider the case $\kappa_1 = 1$ and the first substep of symmetric nonlinear Gauss–Seidel iteration. For $1 \leq i \leq n_l$ we then have

$$\partial\Phi^*(d_{l,i} - a_{ii}^l \bar{u}_{l,i}^\nu) = \bar{u}_{l,i}^\nu, \qquad \nu \in \mathbb{N}' \tag{3.19}$$

where $d_{l,i}$ is as in (2.13) with $z_l^{\mu+1/2}$, z_l^μ replaced by $\bar{u}_l^\nu$, u_l^ν, respectively. Passing to the limit $\nu \to \infty$ in (3.19) by using the continuity of $\partial\Phi^*$ gives

$$\partial\Phi^*(b_{l,i} - (A_l u_l^{**})_i) = u_{l,i}^{**}, \qquad 1 \leq i \leq n_l.$$

Thus u_l^{**} solves (2.11) on level l and hence, $u_l^{**} = u_l^*$ and $u_l^\nu \to u_l^* (\nu \in \mathbb{N})$ by uniqueness.

The computation of an optimal steplength ω_k^* in the descent direction on level $1 \leq k \leq l$ requires the solution of the one-dimensional nonsmooth minimization problem

$$J_k(\bar{u}_k^\nu(\omega_k^*)) = \min_{\omega_k \in [0, \bar{\omega}_k]} J_k(\bar{u}_k^\nu(\omega_k))$$

which is equivalent to

$$\langle \bar{b}_k - A_k(\bar{u}_k^\nu - \omega_k^* p_{k-1}^k w_{k-1}), p_{k-1}^k w_{k-1} \rangle_k = \langle \partial\Phi_k(\bar{u}_k^\nu - \omega_k^* p_{k-1}^k w_{k-1}), p_{k-1}^k w_{k-1} \rangle_k.$$

Due to the definition of the prolongations we have that $\bar{u}_k^\nu$ and $\bar{u}_k^\nu(\omega_k^*)$ are of the same sign and $(p_{k-1}^k w_{k-1})_i = 0$ iff $\bar{u}_{k,i}^\nu = \bar{u}_{k,i}^\nu(\omega_k^*) = 0$, $1 \leq i \leq n_k$. Consequently, we do not have to resort to special nonsmooth minimization algorithms such as bundle methods but can determine ω_k^* explicitly according to

$$\omega_k^* = \min(\hat{\omega}_k, \bar{\omega}_k) \tag{3.20}$$

$$\hat{\omega}_k = \frac{\langle d_k^\nu, p_{k-1}^k w_{k-1} \rangle_k + \langle \partial\Phi_k(\bar{u}_k^\nu), p_{k-1}^k w_{k-1} \rangle_k}{\langle A_k p_{k-1}^k w_{k-1}, p_{k-1}^k w_{k-1} \rangle_k + \langle \partial\Phi_k(p_{k-1}^k w_{k-1}), p_{k-1}^k w_{k-1} \rangle_k} \tag{3.21}$$

By arguments similar to those used in Hoppe & Kornhuber (1988) we will now establish grid-size independent local convergence of W-cycles. This will be done under some requirements concerning the regularity of the continuous free boundaries (1.3) and the approximation by their discrete counterparts (2.6). In particular, we assume the following.

The projections $\Pi\Sigma^\alpha|_{t_m}$ of the continuous free boundaries $\Sigma^\alpha|_{t_m}$, $1 \leq \alpha \leq 2$, $0 \leq m \leq M$, onto the Ω-plane admit Lipschitzian parametrizations. The discrete free boundaries $\Sigma_k^\alpha|_{t_m}$, $0 \leq k \leq l$, approximate $\Pi\Sigma^\alpha|_{t_m}$ according to

$$\sup_{x \in \Sigma_k^\alpha|_{t_m}} \operatorname{dist}(x, \Pi\Sigma^\alpha|_{t_m}) = O(h_k). \tag{3.22}$$

Furthermore, we assume the following discrete nondegeneracy condition with respect to the solutions u_k^* of the minimization problems on levels $0 \leq k \leq l$ within a multi-grid cycle

$$u_{k,i}^* = 0 \Leftrightarrow \partial\Phi(u_{k,i}^*) \in (-s_1, s_2), \qquad 1 \leq i \leq n_k. \tag{3.23}$$

Remarks. (i) Error estimates for finite element approximations of free boundaries based on L^p-error estimates for the solutions and a nondegeneracy condition for the continuous solution have been derived by Nochetto (1986) and Nochetto & Verdi (1988b). In particular, if there is an L^2-error estimate of order $O(h_k^\beta)$ for some $\beta > 0$, then (3.22) can be expected to hold true for the same order. In the papers cited above the authors were only able to verify $\beta = \frac{1}{2}$ (see also Elliott (1987)). However, there is numerical evidence that (3.22) is satisfied, i.e., $\beta = 1$ (cf. e.g. Hoppe & Kornhuber (1988)).

(ii) In view of $u_k^* = r_{k+1}^k u_{k+1}^*$, $0 \leq k \leq l-1$, and the definition of the restriction operators by (2.25) it is sufficient to require (3.23) on the highest level $k = l$, because this implies nondegeneracy on all lower levels.

The nonlinear mappings F_k and $S_k(\cdot; \bar{b}_k)$, $0 \leq k \leq l$, as given by (2.20) and (2.15), respectively, are not differentiable everywhere, but as locally Lipschitzian maps admit generalized Jacobians in the sense of Clarke (1983). However, as an immediate consequence of the nondegeneracy condition (3.23), both F_k and $S_k(\cdot; \bar{b}_k)$ are differentiable at least in a suitable neighbourhood $U_k(u_k^*)$ of the solutions u_k^*. In particular, denoting by $M_{k,i}$, $1 \leq i \leq n_k$, the i-th row of an (n_k, n_k)-matrix M_k, the Jacobians $L_k = (JF_k)(u_k^*)$, $0 \leq k \leq l$, are given by

$$L_{k,i} = \begin{cases} I_{k,i} + a_1^{-1} A_{k,i}, & \text{if } (\bar{b}_k - A_k u_k^*)_i < -s_1 \\ I_{k,i}, & \text{if } -s_1 < (\bar{b}_k - A_k u_k^*)_i < s_2 \\ I_{k,i} + a_2^{-1} A_{k,i}, & \text{if } (\bar{b}_k - A_k u_k)_i > s_2 \end{cases} \tag{3.24}$$

Concerning the Jacobians $G_k = (JS_k)(u_k^*; \bar{b}_k)$, $0 \leq k \leq l$, we obtain

$$G_k = I_k - \hat{L}_k^{-1} L_k \tag{3.25}$$

where

$$\hat{L}_k = (D_k - B_k) D_k^{-1} (D_k - C_k)$$

and $L_k = D_k - B_k - C_k$ pertains to the decomposition of L_k into its diagonal, subdiagonal and superdiagonal part, respectively.

As for all nonlinear iterative methods local convergence can be achieved, if the Jacobian of the nonlinear iteration map can be bounded by a constant strictly less than one with respect to a suitable matrix norm, we will now introduce some appropriate norms. In view of the fact that the finite element discretizations A_k of the elliptic operator $A = -\Delta t \Delta$ are symmetric, positive definite, setting $\Lambda_k = A_k^{\frac{1}{2}}$, for $s \in \mathbb{R}$ we define discrete Sobolev norms $\|\cdot\|_s$ on $\mathbb{R}^{n_k}$ by $\|v_k\|_s = \|\Lambda_k^s v_k\|_0$ where $\|\cdot\|_0$ refers to the discrete L^2-norm $|\cdot|_k$ which has been defined following (2.8). The corresponding matrix norms are then given by $\|M_k\|_{p,q} = \sup\{\|M_k v_k\|_q / \|v_k\|_p,\ v_k \neq 0\}$.

Since multi-grid convergence in case of more than two grids can be deduced from the two-grid situation (cf. Hackbusch (1981, 1983)), we analyze the two-grid case and obtain:

LEMMA 3.5 Consider the damped multi-grid algorithm in case of two levels l and $l-1$ with $\kappa = \kappa_1 > 0$ and ω_l^* chosen according to (3.20) with $\bar{\omega}_l \geq 1$. Then there holds

$$u_l^{\nu+1} - u_l^* = (M_1^{l-1} + Z_1)(u_l^\nu - u_l^*), \qquad \nu \geq 0 \tag{3.26}$$

where

$$M_l^{l-1} = [L_l^{-1} - p_{l-1}^l L_{l-1}^{-1} r_l^{l-1}][L_l G_l^\kappa] \tag{3.27}$$

and $\|Z_l\|_{s,s} \leq C(\kappa)\eta(\nu)$ for some $s \in (0, 1]$ with $C(\kappa) > 0$ and $\eta(\nu) \to 0$ as $\|u_l^\nu - u_l^*\|_s \to 0$.

Proof. Using elementary subdifferential calculus, the assertion can be verified by straightforward calculations following the lines of Lemma 3.4 and Lemma 3.5 in Hoppe & Kornhuber (1988) and observing that

$$\omega_l^* \to 1 \quad \text{as} \quad u_l^\nu \to u_l^*. \tag{3.28}$$

The proof of (3.28) follows by taking into account that both the nominator and denominator in (3.21) can be rewritten as

$$\langle r_l^{l-1} d_l^\nu, w_{l-1} \rangle_{l-1} + \langle \partial \Phi_{l-1}(r_l^{l-1} \bar{u}_l^\nu), w_{l-1} \rangle_{l-1} + \tau_{l-1}^{(1)}$$
$$\langle A_{l-1} w_{l-1}, w_{l-1} \rangle_{l-1} + \langle \partial \Phi_{l-1}(w_{l-1}), w_{l-1} \rangle_{l-1} + \tau_{l-1}^{(2)},$$

with $\tau_{l-1}^{(\alpha)} \to 0$, $1 \leq \alpha \leq 2$, as $u_l^\nu \to u_l^*$. But the coarse grid solution satisfies $A_{l-1} w_{l-1} - r_l^{l-1} d_l^\nu \in \partial \Phi_{l-1}(u_{l-1}^{\nu+1})$ and hence, (3.28) can be easily deduced.

Using the preceding result, two-grid convergence results by verifying an appropriate approximation and smoothing property.

LEMMA 3.6 There exists a function $C(\kappa)$ satisfying $C(\kappa) \to 0$ as $\kappa \to \infty$ such that for some $s \in (\frac{1}{2}, 1)$

$$\|M_l^{l-1}\|_{s,s} \leq C(\kappa). \tag{3.29}$$

Proof. In view of the representation (3.27) of the two-grid iteration operator the assertion holds true, if we can establish the approximation and the smoothing property

$$\|L_l^{-1} - p_{l-1}^l L_{l-1}^{-1} r_l^{l-1}\|_{-s,s} \leq C h_l^{\alpha_1}, \tag{3.30}$$

$$\|L_l G_l^\kappa\|_{s,-s} \leq C(\kappa) h_l^{-\alpha_2}, \qquad 0 \leq \kappa \leq \kappa_{\max}(h_l) \tag{3.31}$$

for some suitable $\alpha_1 \geq \alpha_2 \geq 0$ and a function $\kappa_{\max}(h)$ satisfying either $\kappa_{\max}(h) = \infty$ or $\kappa_{\max}(h) \to \infty$ as $h \to 0$. Now, setting $V_l = \{v_l \in \mathbb{R}^{n_l} \mid v_{l,i} = 0,\ c_i^l \in N_l^3(u_l^*)\}$, we have $M_l^{l-1} v_l \in V_l$, $v_l \in \mathbb{R}^{n_l}$, and hence, it is sufficient to prove (3.30), (3.31) for $\hat{M}_l^{l-1} = M_l^{l-1}|_{V_l}$. But $\hat{M}_l^{l-1}$ admits the decomposition $\hat{M}_l^{l-1} = \operatorname{diag}(\hat{M}_{l,1}^{l-1}, \hat{M}_{l,2}^{l-1})$ where the operators $\hat{M}_{l,\mu}^{l-1}$, $1 \leq \mu \leq 2$, pertain to two-grid iterations involving symmetric finite element discretizations L_k^μ, $l-1 \leq k \leq l$, of elliptic boundary value problems with homogeneous Dirichlet boundary data for the operators

$A^\mu = I - a_\mu^{-1}\,\Delta t\,\Delta$ considered on the projections $\Pi Q^\mu|_{t_m}$ of the domains $Q^\mu|_{t_m}$ onto the Ω-plane. Then, in view of the results established by Hackbusch (1985) for the smoothing property of symmetric Gauss–Seidel iteration, for L_l^μ and the correspondingly defined G_l^μ (3.30) can be shown to hold true with $\alpha_2 = 0$ and $\kappa_{\max}(h) = \infty$. On the other hand, since the free boundary of $\Pi Q^\mu|_{t_m}$, $1 \leqslant \mu \leqslant 2$, is assumed to be Lipschitzian, in the standard case $r_l^{l-1} = \hat{r}_l^{l-1}$ and $p_{l-1}^l = \hat{p}_{l-1}^l$, where $L_{l-1}^\mu = \hat{r}_l^{l-1} L_l \hat{p}_{l-1}^l$, the approximation property (3.30) holds true for some $s \in (\frac{1}{2}, 1)$ and $\alpha_1 = 2(1-s)$. But in view of (2.25) and (2.28) the restrictions r_l^{l-1} and prolongations p_{l-1}^l only differ from $\hat{r}_l^{l-1}$ and $\hat{p}_{l-1}^l$ in irregular nodal points which, by assumption (3.22), are located within an $O(h_k)$-neighbourhood of $\Pi\Sigma^\mu|_{t_m}$ so that (3.31) can be shown to remain true by similar arguments as used in Hackbusch (1980).

Remark. In Lemma 3.5 and Lemma 3.6 the case $\kappa_2 > 0$ can be treated analogously involving only slight modifications.

The multi-grid iteration operator for more than two grids can be recursively defined by means of the corresponding two-grid operators on levels $1 \leqslant k \leqslant l$ and step size independent local convergence of W-cycles can be shown along the lines of Hackbusch (1981, 1985):

THEOREM 3.7 Under the assumptions (3.22) and (3.23) there exist a neighbourhood $U_\delta(u_l^*)$, a positive integer $\kappa_{\min}$ and a positive real number $\xi < 1$, independent of h_l, such that for any $u_l^0 \in U_\delta(u_l^*)$ the iterates u_l^ν, $\nu \geqslant 1$, obtained by the execution of W-cycles of the damped multi-grid algorithm with $\kappa > \kappa_{\min}$ smoothing iterations satisfy

$$\|u_l^\nu - u_l^*\|_s \leqslant \xi\,\|u_l^{\nu-1} - u_l^*\|_s. \tag{3.32}$$

4. Numerical results

We have compared the performance of the damped multi-grid Stefan solver (DMGSTEF) with the (undamped) multi-grid algorithm MGSTEF2 from Hoppe & Kornhuber (1988) and Elliott's single-grid SOR algorithm in its symmetric version (cf. Elliott (1981)) for the following model two-phase Stefan problem from Ciavaldini (1975).

The space-time domain $Q = \Omega \times (0, T)$ is specified by $\Omega = (0, 1)^2$ and $T = 0{\cdot}5$, while the physical data are $c_1 = 2$, $\kappa_1 = 1$, $s_1 = 0$ and $c_2 = 6$, $\kappa_2 = 2$ and $s_2 = 1$. The right-hand side f in (1.1a) is chosen according to

$$f(x_1, x_2, t) = 4\kappa_\mu - c_\mu \exp(-4t), \qquad (x_1, x_2, t) \in Q^\mu, \quad \mu = 1, 2$$

so that the explicit solution in terms of the temperature $\theta = \theta(x_1, x_2, t)$ turns out to be

$$\theta(x_1, x_2, t) = (x_1 - 0{\cdot}5)^2 + (x_2 - 0.5)^2 - \exp(-4t)/4, \qquad (x_1, x_2, t) \in Q.$$

Initial and boundary conditions are taken from the exact solution. We have discretized Q with respect to uniform time steps $\Delta t > 0$ and hierarchies $(T_k)_{k=0}^l$ of triangulations obtained by regular refinements from an initial uniform triangula-

tion T_0 with the center of Ω as interior nodal point. Consequently, setting $M_k = 2^{k+1}$, $0 \leq k \leq l$, on level k we have $n_k = (M_k - 1)^2$ interior nodal points and 2^{M_k+1} triangles.

In the actual execution of a multi-grid cycle, starting from an iterate u_l^ν, $\nu \geq 0$, on level l, we may encounter a level $1 \leq k^* \leq l$ with $N_{k^*}^{\mathrm{reg}}(\bar{u}_k^*(\omega_k^*)) = 0$ which means that, in view of definition (2.28) of the prolongations, the computations on levels $0 \leq k < k^*$ do not provide an improved iterate on level k^*. Therefore, we skip all levels below k^*, specify $k_{\min} = k^*$ as lowest level and solve the coarse grid correction problem on level $k_{\min}$ iteratively by repeated symmetric Gauss–Seidel iterations.

In order to provide an adequate comparison between the single-grid SSOR scheme and the multi-grid algorithms, the computational work is measured in work units where one work unit (WU) corresponds to one symmetric Gauss–Seidel iteration on the highest level l. We denote by $\Delta_l^\nu = u_l^\nu - u_l^{\nu-1}$, $\nu \geq 1$, the difference of two subsequent multi-grid iterates and refer to $N_{WU}(\nu)$ as the total number of work units for the multi-grid cycle which computes u_l^ν from $u_l^{\nu-1}$. Then an asymptotic efficiency rate q_l can be determined according to

$$q_l = (\|\Delta_l^{\nu^*}\|_0 / \|\Delta_l^1\|_0) ** \left(1 \Big/ \sum_{\nu=1}^{\nu^*} N_{WU}(\nu)\right)$$

where ν^* indicates the iterate for which $\|\Delta_l^\nu\|_0 < \varepsilon_l$ with respect to a prespecified accuracy bound ε_l.

Despite the theoretical convergence result in Theorem 3.7 (cf. also Theorem 3.6 in Hoppe & Kornhuber (1988)), referring only to W-cycles, we found step size independent multi-grid convergence both for V-cycles and W-cycles. Actually, for DMGSTEF and MGSTEF2 we got best asymptotic efficiency rates for V-cycles with one pre-smoothing step ($\kappa_1 = 1$) and one post-smoothing step ($\kappa_2 = 1$), but post-smoothing only applied to irregular nodal points $c_i^k \in N_k^{\mathrm{irr}}(\bar{u}_k^\nu(\omega_k))$, $1 \leq k \leq l$. (Note that such a post-smoothing step only involves n_k^{irr}/n_l instead of the standard n_k/n_l WU's where $n_k^{\mathrm{irr}} = \#N_k^{\mathrm{irr}}(\bar{u}_k^\nu(\omega_k))$ and $n_k^{\mathrm{irr}} \ll n_k$, especially on higher levels in the chosen hierarchy). For the example considered here we did achieve full multi-grid efficiency for a hierarchy $(T_k)_{k=0}^l$ with $l = 5$. Choosing $\Delta t = 1{\cdot}25\mathrm{E}-2$ and $\varepsilon_5 = 1{\cdot}0\mathrm{E}-8$, Table 1 below displays the asymptotic efficiency rates q_5 at $t_j = j \cdot 0{\cdot}05$, $1 \leq j \leq 10$, for DMGSTEF and MGSTEF2 as well as the convergence rates for the symmetric version of Elliott's single-grid SOR algorithm (SSOR) on level $l = 5$ with suboptimal relaxation parameter $\omega = 1{\cdot}7$. The results clearly demonstrate a considerable increase in

TABLE 1
Asymptotic efficiency rates

	0·05	0·10	0·15	0·20	0·25	0·30	0·35	0·40	0·45	0·50
DMGSTEF	0·35	0·34	0·32	0·31	0·32	0·33	0·32	0·30	0·30	0·29
MGSTEF2	0·60	0·50	0·50	0·45	0·49	0·50	0·47	0·44	0·45	0·43
SSOR	0·79	0·77	0·77	0·76	0·75	0·74	0·74	0·73	0·71	0·70

efficiency for the damped multi-grid Stefan solver DMGSTEF compared to MGSTEF2. It can also be seen that DMGSTEF apparently is more robust than MGSTEF2 in so far as for MGSTEF2 the asymptotic efficiency rate q_l differs at subsequent time steps within a margin up to 0·1 (depending on the actual shape of the free boundary) which is not so for DMGSTEF.

Finally, we remark that we also applied DMGSTEF to more complicated moving boundary problems such as the coupled system of Stefan type equations arising in induction heating of steel slabs (cf. Hoppe & Kornhuber (1989, 1990)) and observed the same increase in efficiency as in the test example reported here.

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