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ON THE NUMERICAL SOLUTION OF VARIATIONAL INEQUALITIES BY MULTI-GRID TECHNIQUES

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Abstract. Multi-grid techniques are by now well established tools for the numerical solution of large systems of equations arising in the discretization of boundary or initial-boundary value problems for P.D.E.'s (cf. e.g. [1], [15], [33]). Recently, several multi-grid algorithms have been developed for the fast and efficient solution of variational inequalities (cf. [2], [16], [18], [19], [20], [21], [27]). This paper attempts to give a survey on these schemes by clarifying the underlying concepts and discussing their mutual relationships. The performance of the algorithms is illustrated by numerical results for problems in elasto-plasticity and heat conduction with a change of phase.

1. INTRODUCTION

We want to report on some recent results in the efficient numerical solution of variational inequalities by multi-grid methods. Since the underlying algorithms are based on the affinity between variational inequalities and extremum problems resp. complementarity problems, it seems appropriate to begin with a short review of these relationships.

In convex analysis variational inequalities are well known as necessary and also sufficient optimality conditions for constrained extremum problems. In particular, let us consider the minimization of a convex functional $J : K \subset V \to (-\infty, +\infty]$ over a closed convex set of a reflexive Banach space V

$$J(u) = \inf \{ J(v) \mid v \in K \} \quad . \tag{1.1}$$

If the functional J is proper, lower semi-continuous and coercive, then the constrained minimization problem (1.1) admits a solution $u \in K$ which is unique for strictly convex J (cf. e.g. [9;Prop. 1.2]).

If J is Gateaux differentiable on K with Gateaux derivative $J'(u) \in V'$, $u \in K$, then a necessary and sufficient condition for $u \in K$ to be a solution of (1.1) is that u satisfies the variational inequality

$$< J'(u), v - u > \geq 0 \ , \ v \in K \tag{1.2}$$

where $< \cdot, \cdot >$ denotes the dual pairing between V' and V (cf. e.g. [9;Prop. 2.1]).
In applications, a typical example is the determination of the equilibrium of a state constrained mechanical system in the stationary case where the equilibrium is characterized as the state for which the potential energy of the system attains its minimum. An example modeling elastic-plastic phenomena will be discussed in detail in § 4.
Variational inequalities also appear as optimality conditions in unconstrained extremum problems

$$J(u) = inf \{ J(v) \mid v \in V \} \tag{1.3}$$

if the functional J is only subdifferentiable.
Denoting by $\partial J(\cdot)$ the subdifferential of J , a function $u \in V$ solves (1.3) if and only if the inclusion

$$0 \in \partial J \tag{1.4}$$

is satisfied which, by definition of the subdifferential, is equivalent to the inequality

$$J(v) - J(u) \geq 0 \ , \ v \in V \ . \tag{1.5}$$

In applications one often encounters the situation where the functional to be minimized consists of a Gateaux differentiable part J and a subdifferentiable part ϕ . In this case the associated variational inequality reads

$$< J'(u), v - u > + \phi(v) - \phi(u) \geq 0 \ , \ v \in V \tag{1.6}$$

which is commonly referred to as a variational inequality of the second kind (cf. e.g. [9 ; Chap. II.3]).
In § 4 we will be concerned with such an inequality arising from an implicit time discretization of the enthalpy equation for a two-phase Stefan problem.

An important special case is that where V is a dense subspace and sublattice of a Hilbert lattice H and, given elements $\psi^1, \psi^2 \in H$, the set K of constraints is given by either

$$K^i = \{ v \in V \mid (-1)^i v \leq \psi^i \} \ , \ 1 \leq i \leq 2 \tag{1.7a}$$

or

$$K^3 = \{ v \in V \mid \psi^1 \leq v \leq \psi^2 \} \ . \tag{1.7b}$$

The corresponding minimization problem is called an obstacle problem, namely a one-sided obstacle problem if $K = K^i$, $1 \le i \le 2$, and a two-sided obstacle problem if $K = K^3$.
Let us consider a one-sided obstacle problem with upper obstacle ψ and an associated functional J of the form

$$J(v) = \frac{1}{2} < Av, v > - < f, v > , \quad v \in V \tag{1.8}$$

where A represents an operator from V into V' and f is a given element in H.
Then, if the obstacle ψ is admissible in (1.8) and if the solution $u \in K$ to the upper obstacle problem under consideration is sufficiently regular such that $Au \in H$, it can be shown that u satisfies the inequalities

$$Au \le f \ , \quad u \le \psi \tag{1.9a}$$

which are complementary to each other in the sense that

$$< Au - f, u - \psi > = 0 \ . \tag{1.9b}$$

Therefore, the problem to find $u \in V$ such that (1.9a),(1.9b) hold true is called a complementarity problem.
A simple example is the determination of the stationary equilibrium of a clamped membrane whose deflection, caused by an exterior force f, is limited by a fixed rigid body with surface ψ. If Ω is the two-dimensional domain covered by the membrane in the unloaded state, the mathematical model is given by $V = H^1_0(\Omega)$, $H = L^2(\Omega)$ equipped with the canonical ordering, and $A = -\Delta$ thus leading to a linear complementarcity problem. For the same choice of V, H a nonlinear counterpart is $Au = -\nabla\cdot((1 + |\nabla u|^2)^{-1/2}\nabla u)$, $f \equiv 0$ and $\psi < 0$ representing a minimal surface problem with obstacle.

To summarize we state that in the present context variational inequalities do appear as necessary and sufficient optimality conditions for constrained extremum problems with differentiable objective functional resp. unconstrained problems with subdifferentiable functional and that under sufficient regularity assumptions variational inequalities are equivalent to complementarity problems. Since the numerical solution of both extremum problems and complementarity problems has a long history and is still a subject of current research interest, it seems natural to solve variational inequalities by such methods. In particular, in § 2 we will present a minimization algorithm based on an active set strategy and a special complementarity problem solver. Then, in § 3 it will be shown how to incorporate multi-grid techniques in order to

obtain fast, efficient solution methods. Also, the relationships to the multi-grid schemes of Brandt, Cryer [2], Hackbusch, Mittelmann [16] and Mandel [27] will be outlined. In § 4 some numerical results will be given for an elastic-plastic torsion problem and a minimal surface problem with obstacle. Finally, § 5 concludes with a multi-grid scheme for variational inequalities of the second kind arising in the numerical solution of two-phase Stefan problems.

2. TWO BASIC ITERATIVE SCHEMES

Throughout the following we will restrict ourselves to obstacle problems, in particular unilateral problems with upper obstacle ψ where the state space V is a closed subspace of the Sobolev space $H^1(\Omega)$, Ω being a bounded domain in Euclidean space $\mathbf{R}^d$ with Lipschitzian boundary $\Gamma = \partial\Omega$. We start from a discretization J_h of the functional J to be minimized, obtained by the application of finite difference techniques with respect to a grid-point set Ω_h. Denoting by V_h the finite dimensional state space of grid functions and by ψ_h the discrete upper obstacle, which we assume to approximate ψ in an appropriate sense, the constraint set K_h is given by

$$K_h = \{ v_h \in V_h \mid v_h \leq \psi_h \} . \tag{2.1}$$

Hence, the discrete minimization problem reads as follows

$$J_h(u_h) = \min \{ J_h(v_h) \mid v_h \in K_h \} . \tag{2.2}$$

Assuming J_h to be twice Fréchet-differentiable with uniformly positive definite second Fréchet derivative, the above problem represents a finite dimensional convex minimization problem with constraints in the form of linear inequalities. Standard numerical schemes for its approximate solution are projected gradient methods (cf. e.g. [31], [32]) and projected SOR-techniques (cf. e.g. [12]).

On the other hand, it is easily seen that (2.2) is equivalent to the complementarity problem

$$J_h'(u_h) \leq 0 \quad , \quad u_h \leq \psi_h \tag{2.3a}$$

$$J_h'(u_h) \cdot (u_h - \psi_h) = 0 \tag{2.3b}$$

In the sequel we will present a special class of projected gradient methods and a complementarity problem solver. Both methods are iterative schemes which have in common that at each iteration step a reduced algebraic system has to be solved and it is that reduced system to which multi-grid techniques will be applied.

2.1 Active set strategies

A characteristic feature of projected gradient methods is the application of a so-called active set stategy which, at each iteration step, selects a certain subset $\Omega^a_h \subset \Omega_h$ of active constraints. These active constraints are then treated as equations and a descent direction will be computed by minimizing J_h over the corresponding subspace $V^a_h = \{ v_h \in V_h \mid v_h(x) = \psi_h(x) , x \in \Omega^a_h \}$. To be more precise, a typical iteration step consists of the following substeps :

Step 1 : *Identification of active constraints*

Starting from an iterate $u^j_h \in K_h$, the first step is to identify the set of active constraints resp. active grid-points as the set of all grid-points where u^j_h is in contact with the obstacle ψ_h

$$\Omega^a_h(u^j_h) = \{ x \in \Omega_h \mid u^j_h(x) = \psi_h(x) \} . \tag{2.4a}$$

The elements of the complementary set

$$\Omega^i_h(u^j_h) = \Omega_h \setminus \Omega^a_h(u^j_h) \tag{2.4b}$$

will be referred to as inactive grid-points.

Since in the active grid-points the Kuhn-Tucker conditions require non positive components of the gradient of J_h, the next step consists in a possible inactivation of one or several active constraints where that condition is violated.

Step 2: *Inactivation*

According to a certain inactivation strategy a set

$$Z_h(u^j_h) \subset \{ x \in \Omega^a_h(u^j_h) \mid J'_h(u^j_h)(x) > 0 \}$$

of active grid-points is specified. Eliminating these grid-points from $\Omega^a_h(u^j_h)$, new sets of active/inactive grid-points are determined by

$$\tilde{\Omega}^a_h(u^j_h) = \Omega^a_h(u^j_h) \setminus Z_h(u^j_h) , \tag{2.5a}$$

$$\tilde{\Omega}^i_h(u^j_h) = \Omega^i_h(u^j_h) \cup Z_h(u^j_h) . \tag{2.5b}$$

There are different active set logics for choosing the active constraints to be inactivated, among them a most-constrained rule where only one active constraint is dropped, namely that one which corresponds to the largest positive component of the gradient of J_h (for an overview see e.g. [29]). A general problem is the "zig-zag" or "cycling" phenomenon: Inactivated grid-points may become active again in the following iteration step and then alternate between active and inactive status (cf. e.g. [8]).

Step 3: *Computation of a descent direction*

Treating the active constraints associated with $x \in \tilde{\Omega}^a{}_h(u^j{}_h)$ as equalities and minimizing J_h over the corresponding subspace leads to the computation of a solution $\bar{u}^j{}_h$ to

$$J'_h(\bar{u}^j_h)(x) = 0 \ , \ x \in \tilde{\Omega}^i_h(u^j_h) \tag{2.6a}$$

$$\bar{u}^j_h(x) = \psi_h(x) \ , \ x \in \tilde{\Omega}^a_h(u^j_h) \ . \tag{2.6b}$$

Then $p^j{}_h = \bar{u}^j{}_h - u^j{}_h$ is a descent direction for J_h.

Step 4: *Computation of a new iterate*

Computing α_j as maximal admissible step-length in direction p^j_h, a new iterate $u_h{}^{j+1}$ is obtained by

$$u^{j+1}_h = u^j_h + \min(1, \alpha_j)\, p^j_h \ . \tag{2.7}$$

The auxiliary problem (2.6) which has to be solved in Step 3 of the algorithm requires the solution of the difference equations (2.6a) in the $N^i{}_h = \operatorname{card} \tilde{\Omega}^i{}_h(u^j{}_h)$ unknowns corresponding to inactive grid-points while the remaining $N^a{}_h = \operatorname{card} \tilde{\Omega}^a{}_h(u^j{}_h)$ components are prescribed by the values of the upper obstacle ψ_h in the corresponding active grid-points. In general, $N^i{}_h < N_h = \operatorname{card} \Omega_h$ and therefore, (2.6) may be referred to as a "reduced" algebraic system.

In applications one often encounters the situation where J_h is of the form

$$J_h(v_h) = \frac{1}{2} \langle A_h v_h, v_h \rangle - \langle f_h, v_h \rangle \tag{2.8}$$

involving a linear difference operator A_h which represents a nonsingular M-matrix. In this case, if the startiterate $u^0{}_h \in K_h$ is chosen as a subsolution in the sense that $A_h u^0{}_h \le f_h$, the inactivation step can be dispensed with, since all components of the gradient of J_h corresponding

to activated grid-points will be non positive. We thus obtain monotone convergence both of the sequence $\{u^j_h\}$ of iterates and the sequence $\{\Omega^a{}_h(u^j_h)\}$ of active grid-point sets (cf. [19]):

THEOREM 2.1. *Under the previous assumptions let* $u^*_h \in K_h$ *be the unique solution to* (2.2). *Then the sequence of iterates* u^j_h *and the corresponding sequence of active grid-point sets* $\Omega^a{}_h(u^j_h)$ *are monotonely increasing sequences that converge after a finite number of steps to* u^*_h *resp. the discrete coincidence set* $\Omega^a{}_h(u^*_h)$.

Remarks: (i) An appropriate choice of the startiterate is the solution of $A_h u^0_h = \min(f_h, A_h\psi_h)$. (ii) In case of a lower obstacle, under the same hypotheses and starting from a supersolution $u^0_h \in K_h$ (i.e. $A_h u^0_h \geq f_h$) the algorithm generates a monotonely decreasing, convergent sequence of iterates (cf. [19], [24]).
(iii) For bilateral problems and a nonlinear operator A_h monotonicity can't be expected any longer. In this case convergence results have been established in [16] for some kind of the most-constrained rule mentioned above as well as in [18] assuming A_h to be T-monotone and using a least-constrained active set logic.

2.2 A complementarity problem solver

If the functional J_h is given by (2.8), then the complementarity problem (2.3a),(2.3b) takes the form

$$A_h u_h \leq f_h \ , \ u_h \leq \psi_h \tag{2.9a}$$

$$(A_h u_h - f_h) \cdot (u_h - \psi_h) = 0 \ . \tag{2.9b}$$

Note that (2.9a),(2.9b) can be equivalently written as the nonlinear system

$$F_h u_h = max(A_h u_h - f_h \ , \ u_h - \psi_h) = 0 \ . \tag{2.10}$$

In the sequel we will assume A_h to be a continuous, surjective M-function. We recall that an M-function is a mapping which is off-diagonally antitone and inverse isotone, i.e. an M-function can be viewed as the nonlinear counterpart of an M-matrix (cf. e.g. [30]).
The following algorithm, which has been proposed by Lions, Mercier [26] in the more general case of Hamilton-Jacobi-Bellman equations of the form $\max\{A^l{}_h u_h - f^l_h \mid 1 \leq l \leq m\} = 0$ (cf. also [17]), consists of two steps:

Step 1: *Specification of active/inactive grid-points*

Given an iterate $u_h^j \in \mathbb{R}^{N_h}$, $j \geq 0$, we first compute the defects of u_h^j with respect to the competitive equations $A_h u_h = f_h$ and $u_h = \psi_h$

$$d_h^1 = A_h u_h^j - f_h \quad , \quad d_h^2 = u_h^j - \psi_h \tag{2.11}$$

Then, the sets $\Omega_h^a(u_h^j)$ and $\Omega_h^i(u_h^j)$ of active resp. inactive grid-points are determined by

$$\Omega_h^a(u_h^j) = \{x \in \Omega_h \mid d_h^2(x) \geq d_h^1(x)\} \tag{2.12a}$$

$$\Omega_h^i(u_h^j) = \{x \in \Omega_h \mid d_h^2(x) < d_h^1(x)\} . \tag{2.12b}$$

Step 2: *Computation of a new iterate*

The $(j+1)$-st iterate u_h^{j+1} is obtained as the solution of the reduced system

$$A_h u_h^{j+1}(x) = f_h(x) \quad , \quad x \in \Omega_h^i(u_h^j) \tag{2.13a}$$

$$u_h^{j+1}(x) = \psi_h(x) \quad , \quad x \in \Omega_h^a(u_h^j) . \tag{2.13b}$$

Note that the reduced system (2.13a),(2.13b) can be written as

$$A_h^j u_h^{j+1}(x) = f_h^j(x) \quad , \quad x \in \Omega_h$$

where A_h^j is the principal subfunction of A_h of order $N_h^i = \text{card } \Omega_h^i(u_h^j)$ while f_h^j is correspondingly given by $f_h^j(x) = f_h(x)$, if $x \in \Omega_h^i(u_h^j)$, and $f_h^j(x) = \psi_h(x)$, if $x \in \Omega_h^a(u_h^j)$. The principal subfunction A_h^j inherits the properties of A_h to be a continuous, surjective M-function (cf. e.g. [28]).

The following convergence results can be shown (cf. [18], [19]):

THEOREM 2.2. *Let u_h^* be the unique solution to* (2.9a),(2.9b) *and suppose that a startiterate u_h^0 is chosen as a supersolution in the sense that $F_h u_h^0 \geq 0$. Then, under the preceding hypotheses we have:*

(i) *The sequence of iterates u_h^j is a monotonely decreasing sequence converging after a finite number of steps to u_h^*.*

(ii) *If additionally strict complementarity is assumed (i.e.* $A_h u^*_h(x) < f_h(x)$, $x \in \Omega^a_h(u^*_h)$ *), then the same holds true for the sequence of active grid-point sets, i.e.* $\{\Omega^a_h(u^j_h)\}$ *is monotonely decreasing and converges after a finite number of steps to the discrete coincidence set* $\Omega^a_h(u^*_h)$.

Remarks.: (i) An appropriate supersolution is given by the solution of $A_h u^0_h = f_h$ or simply by $u^0_h = \psi_h$.

(ii) For lower obstacle problems, choosing u^0_h as a subsolution (i.e. $F_h u^0_h \leq 0$), we get a monotonely increasing sequence of iterates .

(iii) The condition to choose the startiterate u^0_h as a supersolution can be dropped, since no matter how u^0_h is chosen it is guaranteed that after one iteration step $F_h u^1_h \geq 0$ is satisfied. In other words, the complementarity problem solver is globally convergent.

(iv) In view of its convergence properties, in case of a linear complementarity problem, the above algorithm can be used together with the active set strategy in order to obtain a two-sided approximation of the given obstacle problem (cf. [19]) .

3. MULTI-GRID SOLVERS FOR VARIATIONAL INEQUALITIES

For discretized elliptic boundary-value problems multi-grid methods are known as fast, efficient solvers due to the fact that the computational work is directly proportional to the number of unknowns in contrast to e.g. direct methods while the convergence rate does not depend on the step-length used in the discretizations in contrast to standard iterative schemes (cf. e.g. [1] , [15] and [33]) .

For variational inequalities multi-grid methods based on active set strategies like those discussed in § 2.1 have been considered by Hackbusch, Mittelmann [16] and the author [19] while the application of multi-grid techniques based on the complementarity problem solver presented in § 2.2 has been investigated by the author in [18] , [19] and [20] . The basic feature of these methods is that it is the reduced algebraic system (2.4a),(2.4b) resp. (2.13a),(2.13b) which is solved by multi-grid techniques in such a way that the structure of the defect equations on all coarser grids is prespecified by the structure of the reduced system on the finest grid. This will be discussed in more detail in § 3.1 where also the relationship to Newton multi-grid methods will be outlined.

On the other hand, using projected SOR-techniques as smoothing procedures and formulating the defect correction processes on the coarser grids as complementarity problems of the same structure, one is led to multi-grid algorithms which have been proposed by Brandt, Cryer [2] in the linear and by Hackbusch, Mittelmann [16] in the nonlinear case. These schemes, for which rigorous convergence proofs have not yet been obtained, will be presented in § 3.2 and it will be

indicated how local convergence can be shown for a slightly modified version, the proof relying on elementary subdifferential calculus and nonlinear multi-grid convergence theory.

3.1 Multi-grid algorithms . I .

In the following we will consider variational inequality solvers which result when the two basic algorithms of § 2 are combined with multi-grid techniques.

For notational simplicity we restrict ourselves to two-dimensional problems, i.e. we assume $\Omega \subset \mathbb{R}^2$. We start from a hierarchy of grids

$$\Omega_0 \subseteq \Omega_1 \subseteq \cdot \quad \cdot \quad \cdot \subseteq \Omega_l \tag{3.1}$$

with step-length $h_k = h_{k-1}/2$, $1 \le k \le l$, given some $h_0 > 0$, and we denote by A_k , f_k and ψ_k , $0 \le k \le l$, analogously constructed finite difference operators, right-hand sides and discrete upper obstacles, respectively . We assume that an iterate u_l^j , $j \ge 0$, is given on the finest grid Ω_l which determines a corresponding reduced system of type (2.4a),(2.4b) resp. (2.13a),(2.13b) . Then, in contrast to standard multi-grid methods for discretized elliptic equations the problem occurs how to mimic the special structure of the reduced system on the lower levels or, in other words, how to specify the active and inactive grid-points on the coarser grids. A natural strategy would be to specify a grid-point $x \in \Omega_k$ on a lower level $k < l$ as inactive if that grid-point is also an inactive one on the finer grid Ω_{k+1} . However, when using that strategy, discrete free boundaries on lower levels could remain undetected and therefore, it is reasonable to perform the specification of inactive grid-points on lower levels in a more restrictive way. Namely, we will call a grid-point $x \in \Omega_k$, $k<l$, inactive if and only if that grid-point is inactive on Ω_{k+1} together with all its eight neighbours. Denoting by

$$N_k(x) = \{ x, x \pm h_k e_1, x \pm h_k e_2, x \pm h_k e_3, x \pm h_k e_4 \} \quad , \quad x \in \Omega_k \tag{3.2}$$

where e_1 , e_2 are the unit vectors in $\mathbb{R}^2$ and $e_3 = e_1 + e_2$, $e_4 = e_1 - e_2$, the corresponding set consisting of $x \in \Omega_k$ and its eight neighbours, we can thus recursively define the sets $\Omega^i_k(u_l^j)$, $\Omega^a_k(u_l^j)$ of inactive resp. active grid-points on all lower levels $k<l$ as follows

$$\Omega^i_k(u_l^j) = \{ x \in \Omega_k \mid N_{k+1}(x) \subseteq \Omega^i_{k+1}(u_l^j) \} \tag{3.3a}$$

$$\Omega^a_k(u_l^j) = \Omega_k \setminus \Omega^i_k(u_l^j) \tag{3.3b}$$

Since in case $\Omega^i_k(u_l^j) = \emptyset$ there is no difference equation to be solved, we define as lowest level k_{min} that level with at least one inactive grid-point, i.e.

$$k_{min} = min \{ 0 \le k \le l \mid \Omega_k^i(u_l^j) \neq \emptyset \} . \tag{3.4}$$

A related problem is that in the fine-to-coarse and coarse-to-fine transfers during a multi-grid cycle the prespecified values in the active grid-points should remain unchanged. This means that restrictions and prolongations have to be defined appropriately. If we denote by p^k_{k-1} resp. r_k^{k-1}, $1 \le k \le l$, the standard prolongations based on bilinear interpolation resp. the corresponding full weighted restrictions (cf. e.g. [15]), a convenient choice of prolongations $\tilde{p}^k_{k-1}$ resp. restrictions $\tilde{r}_k^{k-1}$ fulfilling the above requirement is as follows

$$(\tilde{p}^k_{k-1}u_{k-1})(x) = \begin{cases} (p^k_{k-1}u_{k-1})(x) & , \ if \ x \in \Omega_k^i(u_l^j) \\ 0 & , \ otherwise \end{cases} \tag{3.5a}$$

$$(\tilde{r}_k^{k-1}u_k)(x) = \begin{cases} (r_k^{k-1}u_k)(x) & , \ if \ x \in \Omega_{k-1}^i(u_l^j) \\ 0 & , \ otherwise \end{cases} \tag{3.5b}$$

Further, we denote by $G_k(u_k ; g_k)$ a suitable smoothing process, e.g. Gauss-Seidel iteration, applied to a reduced system on level k with startiterate u_k and right-hand side g_k. We assume that $G_k(\cdot ; g_k)$ can also be used as an iterative solver on the lowest level k_{min}.
If u_k is a smoothed iterate on level k, then an appropriate startiterate on level k-1 is u^0_{k-1} given by

$$u^0_{k-1}(x) = \begin{cases} (r_k^{k-1}u_k)(x) & , \ x \in \Omega_{k-1}^i(u_l^j) \\ \psi_{k-1}(x) & , \ x \in \Omega_{k-1}^a(u_l^j) \end{cases} \tag{3.6}$$

Finally, a complete multi-grid cycle can be described by the following procedure MGV11 (l,u_l,g_l) with $g_l = f_l$ and $u_l = u^j_l$ before resp. $u_l = u_l^{j+1}$ after the execution of the algorithm :

```
procedure MGV11 (l,u_l,g_l) ; integer i , l ; array u_l , g_l ;
if l = k_min then
   for i := 1 step 1 until κ_3 do u_{k_min} := G_{k_min}(u_{k_min} ; g_{k_min}) else
begin array u_{l-1} , g_{l-1} ;
```

for $i := 1$ **step** 1 **until** κ_1 **do** $u_l := G_l(u_l ; g_l)$;
$u_{l-1} := u^0_{l-1}$;
$g_{l-1} := \Lambda_{l-1} u^0_{l-1} - \tilde{r}^{l-1}_l (\Lambda_l u_l - g_l)$;
for $i := 1$ **step** 1 **until** γ_{l-1} **do** MGVII $(l-1, u_{l-1}, g_{l-1})$;
$u_l := u_l + \tilde{p}^l_{l-1} (u_{l-1} - \tilde{r}^{l-1}_l u_l)$;
for $i := 1$ **step** 1 **until** κ_2 **do** $u_l := G_l(u_l ; g_l)$;
end MGVII .

The nonnegative integers κ_1 resp. κ_2 denote the number of smoothing steps before resp. after the defect correction, κ_3 stands for the number of iterations for solving the defect equation on the lowest level and γ_k , $1 \le k \le l-1$, is the number of cycles performed on the intermediate levels. Typical values are $\kappa_1 = \kappa_2 = 2$ and $\gamma_k = 1$ ("V-cycle") resp. $\gamma_k = 2$ ("W-cycle").

Another important feature of multi-grid methods, besides the interplay between smoothing and defect correction, is the computation of an appropriate startiterate u^0_l on the finest grid Ω_l . This is usually done by a process called nested iteration (cf. e.g. [15]). In the present situation, choosing suitable prolongations $\hat{p}^k_{k-1}$, $1 \le k \le l$, not necessarily the same as in MGVII, a startiterate on level l is computed by $u^0_l = \hat{p}^l_{l-1} u^0_{l-1}$, where, given an approximation u^0_0 on the coarsest grid Ω^0_0 , on all intermediate levels $1 \le k \le l-1$ approximations u^0_k are obtained by executing a few steps with the underlying basic iterative scheme of §2, using $\hat{p}^k_{k-1} u^0_{k-1}$ as a startiterate and solving the reduced algebraic systems by MGVII with respect to the grid hierarchy $\Omega_0 \subseteq \cdots \subseteq \Omega_k$. Note that in case of the active set strategy some modifications of that nested iteration process are necessary in order to retain monotonicity of the iterates (for details see [19]).

When solving the reduced systems (2.4a) , (2.4b) resp. (2.13a) , (2.13b) by the multi-grid algorithm MGVII, the resulting schemes consist of "outer" and "inner" iterations. Here, an "outer" iteration means that one prescribed by the basic algorithm of §2 while an "inner" iteration is the execution of a multi-grid cycle for the approximate solution of the corresponding reduced system. This reminds us of Newton multi-grid methods where an "outer" iteration is a Newton step requiring the solution of a linear system and an "inner" iteration is a multi-grid cycle for computing an approximation to that linear system. Thus, a natural question is whether there is a relationship between the multi-grid schemes discussed above and Newton multi-grid techniques. As we shall instantly see, the answer to that question is affirmative for the multi-grid complementarity problem solver in the linear case : It has already been pointed out that a complementarity problem of type (2.9a) , (2.9b) is equivalent to a nonlinear system of the form (2.10). Now, the nonlinear map $F_h : \mathbb{R}^{N_h} \to \mathbb{R}^{N_h}$, defined by means of (2.10), admits a generalized Jacobian $\partial F_h(u_h)$, $u_h \in \mathbb{R}^{N_h}$, in the sense of Clarke (cf. e.g. [5]) which satisfies

$$\partial F_h(u_h) \subseteq \partial F_{h,1}(u_h) \times \cdot \cdot \cdot \times \partial F_{h,N_h}(u_h) \quad . \tag{3.7}$$

The right-hand side in (3.7) stands for the set of all matrices whose i-th row consists of the generalized gradient of the i-th component $F_{h,i}$ of F_h. The generalized gradients are easily computed giving

$$\partial F_{h,i}(u_h) = \begin{cases} A_{h,i} & , \quad if\ (A_h u_h - f_h)_i > (u_h - \psi_h)_i \\ e^i_h & , \quad if\ (A_h u_h - f_h)_i < (u_h - \psi_h)_i \\ co\ (e^i_h, A_{h,i}) & , \quad if\ (A_h u_h - f_h)_i = (u_h - \psi_h)_i \end{cases} \tag{3.8}$$

where $A_{h,i}$ denotes the i-th row of the matrix representing the linear difference operator A_h, e^i_h is the i-th unit vector in R^{N_h} and $co\,(e^i_h, A_{h,i})$ stands for the set of all convex combinations of the vectors e^i_h and $A_{h,i}$. Note that in general the generalized gradients $\partial F_{h,i}(u_h)$, $1 \le i \le N_h$, are multi-valued. However, if strict complementarity is assumed, there exists a neighbourhood $U_h(u^*_h)$ of the solution u^*_h to (2.9a), (2.9b) such that for each $u_h \in U_h(u^*_h)$ the generalized gradients $\partial F_{h,i}(u_h)$ are single-valued and hence, regarding (3.7), the same holds true for the generalized Jacobian $\partial F_h(u_h)$. Then, given an iterate $u^j_h \in U_h(u^*_h)$, $j \ge 0$, a Newton step for the iterative solution of (2.10) is given by

$$-\partial F_h(u^j_h)(u^{j+1}_h - u^j_h) = F_h(u^j_h) \quad . \tag{3.9}$$

In view of (3.7), (3.8) it is easily verified that the linear system (3.9) exactly coincides with (2.13a), (2.13b) obtained in Step 2 of the complementarity problem solver.

3.2 Multi-grid algorithms. II.

In this section we will be concerned with multi-grid variational inequality solvers which can be obtained by the application of nonlinear multi-grid techniques to the complementarity problem (2.9a), (2.9b).

Again, given a hierarchy of grids as in (3.1) and starting from an iterate u^j_l, $j \ge 0$, on the finest grid Ω_l, an alternative to the procedures discussed in § 3.1 is to use nonlinear Gauss-Seidel iteration applied to the nonlinear system (2.10) as smoothing process. This amounts to the successive solution of the scalar nonlinear equations

$$max\ ((A_l{}^i w_l^{q+1} - f_l)_i\ ,\ ({}^i w_l^{q+1} - \psi_l)_i) = 0\ ,\ 1 \le i \le N_l\ ,\ q \ge 0 \tag{3.10}$$

where

$$ {}^{i}w_l^{q+1} = (w_{l,1}^{q+1}, \cdots, w_{l,i}^{q+1}, w_{l,i+1}^{q}, \cdots, w_{l,N}^{q}) , \; w_l^0 = u_l^j . $$

In case of linear A_l the solution of (3.10) exactly corresponds to projected Gauss-Seidel iteration which is known as a standard single-grid solver for linear complementarity problems (cf. e.g. [7]). In the nonlinear case a related procedure is projected Newton Gauss-Seidel iteration where an approximation to the solution of (3.10) is obtained by performing a Newton step for the solution of $(A_l {}^{i}w_l^{q+1} - f_l)_i = 0$ and then projecting onto the constraint set $\{ z \in R \mid z \le \psi_{l,i} \}$. The formal application of such a smoothing step will again be denoted by $w_l^{q+1} = G_l(w_l^q ; f_l)$.

If $\bar{u}_l^j$ is the iterate resulting from the execution of a certain number of smoothing steps, it can be easily shown that the error

$$ e_l^j = u_l^* - \bar{u}_l^j $$

solves the complementarity problem

$$ \bar{F}_l e_l^j = max(A_l e_l^j - d_l^j , e_l^j - (\psi_l - \bar{u}_l^j)) = 0 $$

where d_l^j is the defect $d_l^j = f_l - A_l \bar{u}_l^j$.

Hence, an appropriate approximation on the coarser grid Ω_{l-1} can be obtained by the defect equation

$$ \bar{F}_{l-1} u_{l-1} = max(A_{l-1} u_{l-1} - A_{l-1} r_l^{l-1} \bar{u}_l^j - r_l^{l-1} d_l^j , \; u_{l-1} - r_l^{l-1} \psi_l) = 0 \qquad (3.11) $$

Then, interpolating u_{l-1} onto Ω_l an improved iterate $\bar{u}_l^{j,new}$ is computed by

$$ \bar{u}_l^{j,new} = min(\bar{u}_l^j + p_{l-1}^l (u_{l-1} - r_l^{l-1} \bar{u}_l^j) , \psi_l) , \qquad (3.12) $$

i.e. the result of the correction process is again projected onto the constraint set.

Finally, performing several post-smoothing iterations yields the $(j+1)$-st iterate u_l^{j+1}.

So far we have described a two-grid iteration. In the multi-grid case the solution of the defect equation (3.11) will be replaced by a corresponding two-grid iteration involving the grids $\Omega_{l-1}, \Omega_{l-2}$ and this process will be recursively continued until the coarsest grid Ω_0 is reached.

If the restrictions r_k^{k-1}, $1 \le k \le l$, are chosen as pointwise restrictions, it is guaranteed that the solution u_l^* to the complementarity problem on the finest grid Ω_l is a fixed point of the multi-grid iteration.

The above multi-grid algorithm is that considered by Brandt, Cryer in [2] for linear complementarity problems while its nonlinear counterpart corresponds to the multi-grid scheme used by Hackbusch, Mittelmann [16] in phase I of their two-phase multi-grid algorithm for variational inequalities.

Neither in [2] nor in [16] a convergence proof is given. Note however, that for linear complementarity problems with symmetric, positive definite A_h, arising from finite element discretizations of obstacle problems, Mandel in [27] has proved convergence for any feasible startiterate of a formally related multi-grid scheme with canonical choice of prolongations and restrictions. The idea of proof is to show that the sequence of iterates is a minimizing sequence for the corresponding constrained quadratic optimization problem.

In the sequel we will consider a modified version of Brandt, Cryer's resp. Hackbusch, Mittelmann's multi-grid schemes and we will indicate how to obtain local convergence by using subdifferential calculus and nonlinear multi-grid convergence theory as basic tools. The modifications are thus that we choose full weighted restrictions except there where problems might occur, namely in a certain neighbourhood of the discrete free boundary, where pointwise restriction is used and that we do not interpolate onto grid-points in this very neighbourhood. In other words, a change of status of a grid-point should not be caused by the defect correction process. To be more precise, denoting by $\bar{u}_k^j$ the smoothed j-th iterate on level k, we define

$$\tilde{\Omega}_k^{reg}(\bar{u}_k^j) = \tilde{\Omega}_k^i(\bar{u}_k^j) \cup \tilde{\Omega}_k^a(\bar{u}_k^j) \tag{3.13}$$

where

$$\tilde{\Omega}_k^i(\bar{u}_k^j) = \{ x \in \Omega_k \mid N_k(x) \cap \Omega_k \subseteq \Omega_k^i(\bar{u}_k^j) \} \tag{3.14a}$$

$$\tilde{\Omega}_k^a(\bar{u}_k^j) = \{ x \in \Omega_k \mid N_k(x) \cap \Omega_k \subseteq \Omega_k^a(\bar{u}_k^j) \} \tag{3.14b}$$

as the set of regular grid-points while

$$\tilde{\Omega}_k^{irr}(\bar{u}_k^j) = \Omega_k \setminus \tilde{\Omega}_k^{reg}(\bar{u}_k^j) \tag{3.15}$$

is referred to as the set of irregular grid-ponts.

Then, denoting by p^k_{k-1}, $1 \le k \le l$, the prolongations based on bilinear interpolation and by $\tilde{r}_k^{k-1}$ resp. r_k^{k-1}, $1 \le k \le l$, the pointwise resp. full weighted restrictions, we define prolongations $\tilde{p}^k_{k-1}$ and restrictions $\tilde{r}_k^{k-1}$ according to

$$(\tilde{p}^k_{k-1} u_{k-1})(x) = \begin{cases} (p^k_{k-1} u_{k-1})(x) & , \ if\ x \in \tilde{\Omega}^{reg}_k(\bar{u}^j_k) \\ 0 & , \ if\ x \in \tilde{\Omega}^{irr}_k(\bar{u}^j_k) \end{cases} \tag{3.16a}$$

$$(\tilde{r}^{k-1}_k u_k)(x) = \begin{cases} (r^{k-1}_k u_k)(x) & , \ if\ x \in \tilde{\Omega}^{reg}_k(\bar{u}^j_k) \\ (\overset{*}{r}{}^{k-1}_k u_k)(x) & , \ if\ x \in \tilde{\Omega}^{irr}_k(\bar{u}^j_k) \ . \end{cases} \tag{3.16b}$$

Then, a full multi-grid cycle, starting from the j-th iterate u_l^j, can be described by the following procedure MGVI2 (l,u_l,ψ_l,g_l) with $g_l = f_l$ and $u_l = u_l^j$ before resp. $u_l = u_l^{j+1}$ after the execution of the algorithm:

```
procedure MGVI2 (l,u_l,ψ_l,g_l) ; integer i , l ; array u_l , ψ_l , g_l ;
if l = 0 then
   for i := 1 step 1 until κ_3 do u_0 := G_0 (u_0 ; g_0) else
begin array u_{l-1} , ψ_{l-1} , g_{l-1} ;
   for i := 1 step 1 until κ_1 do u_l := G_l (u_l ; g_l) ;
   u_{l-1} := r̃_l^{l-1} u_l ;
   ψ_{l-1} := r̃_l^{l-1} ψ_l ;
   g_{l-1} := A_{l-1} u_{l-1} - r̃_l^{l-1} (A_l u_l - g_l) ;
   for i := 1 step 1 until γ_{l-1} do MGVI2 (l-1,u_{l-1},ψ_{l-1},g_{l-1}) ;
   u_l := u_l + p̃_{l-1}^l (u_{l-1} - r̃_l^{l-1} u_l) ;
   for i := 1 step 1 until κ_2 do u_l := G_l (u_l ; g_l) ;
end MGVI2 .
```

In order to prove convergence of the multi-grid algorithm MGVI2 we assume that the free boundary Γ^* of the infinite dimensional complementarity problem (1.9a) , (1.9b) admits a Lipschitzian parametrization and that the discrete free boundaries $\Gamma^*_k = \partial\, \tilde{\Omega}^i_k(u^*_k)$ of the discrete complementarity problems (2.9a) , (2.9b) on levels $0 \le k \le l$ are situated in a $O(h_k)$ - neighbourhood of Γ^*, i.e.

$$max\ \{\, dist\,(x,\Gamma^*) \mid x \in \Gamma^*_k \,\} = O(h_k) \qquad (h_k \to 0) \tag{3.17}$$

The first condition is a regularity assumption while, in view of recent results by Brezzi, Caffarelli [4] , the second one can be expected to hold true if the solutions u^*_k to the discrete complementarity problems do converge in L^∞ of order $O(h^p_k)$, $p \geq 1$, to the solution u^* of the infinite dimensional complementarity problem.

Further assumptions include uniform estimates for the Jacobians $JA_k(v_k)$ of the maps $\Lambda_k : R^{N_k} \to R^{N_k}$ in $v_k \in R^{N_k}$, $0 \leq k \leq 1$, and for their inverses as well as the approximation of $JA_{k-1}(\tilde{r}_k^{k-1} v_k)$ by $\tilde{r}_k^{k-1} JA_k(v_k) \tilde{p}^k_{k-1}$ with respect to suitably chosen discrete Sobolev norms. These assumptions are fairly standard for multi-grid methods applied to nonlinear finite difference equations arising from elliptic boundary value problems and therefore will be omitted here (the reader is referred to e.g. [13] , [14]).

In the following we will sketch the basic ingredients of the convergence proof (details will be published elsewhere [21]):

We consider the case of two grids Ω_l and Ω_{l-1} with $\kappa_1 = \kappa$ pre-smoothings and $\kappa_2 = 0$ post-smoothings (other smoothing strategies can be treated similarly). Then, using the generalized mean-value theorem (cf. [5;Prop. 2.6.5])

$$F_k u_k - F_k v_k \in co\, \partial F_k([u_k, v_k])$$

where the right-hand side denotes the convex hull of all vectors of the form $DF_k (u_k - v_k)$, $DF_k \in \partial F_k (w_k)$, $w_k \in [u_k, v_k] = \{ z_k \mid z_k = tu_k + (1-t)v_k , t \in [0,1] \}$, and taking advantage of the upper semicontinuity of the map $\partial F_k (\cdot)$ (cf. [5;Prop. 2.6.2]) , in case of strict complementarity it can be shown that

$$u_l^{j+1} - u_l^* = (M_l^{l-1} + Z_l)(u_l^j - u_l^*) \, . \tag{3.18}$$

Here, M_l^{l-1} is given by

$$M_l^{l-1} = [(\partial F_l(u_l^*))^{-1} - \tilde{p}^l_{l-1} (\partial F_{l-1}(\tilde{r}_l^{l-1} u_l^*))^{-1} \tilde{r}_l^{l-1}] \cdot \tag{3.19}$$

$$[\partial F_l(u_l^*)(\partial G_l(u_l^*))^\kappa]$$

while Z_l satisfies

$$\| Z_l \| \leq C_\kappa \eta^{(j)} \tag{3.20}$$

where $\|Z_l\| = \sup\{\|Z_l v_l\|_0 \mid \|v_l\|_0 \le 1\}$, $\|\cdot\|_0$ is the discrete L^2-norm, C_κ stands for a positive constant depending on κ and $\eta^{(j)}$ is a function such that $\eta^{(j)} \to 0$ as $\|u_l^j - u_l^*\|_0 \to 0$.
Denoting by V_l^a the subspace of all vectors $v_l \in R^{N_l}$ whose components corresponding to grid-points within the coincidence set $\Omega_l^a(u_l^*)$ are zero, it is easily seen that $M_l^{l-1} v_l \in V_{l-1}^a$, $v_l \in R^{N_l}$, and hence, it is sufficient to consider $M_l^{l-1}|_{V_l^a}$. Taking into account $\partial F_l(u_l^*)|_{V_l^a} = J\Lambda_l(u_l^*)|_{V_l^a}$, the assumed regularity of Γ^* and the approximation property (3.17) as well as the fact that pointwise restriction is only used in irregular grid-points, it follows from Hackbusch' results in [13] that

$$\|M_l^{l-1}\| \le C(\kappa) \tag{3.21}$$

where $C(\kappa) \downarrow 0$ as $\kappa \to \infty$.
Using (3.20),(3.21) in (3.18) implies convergence of the two-grid iteration from which convergence in the multi-grid case can be deduced by standard means (see e.g. [14]). Altogether, we obtain

THEOREM 3.1. *Let* u_l^j, $j \ge 0$, *be the iterates generated by the multi-grid algorithm* MGV12 *in case of* $l+1$ *grids* Ω_k, $0 \le k \le l$, *with* $\kappa = \kappa_1 + \kappa_2 > 0$ *and* $\gamma_k = 2$, $1 \le k \le l-1$. *Then, under the previous hypotheses there exist a constant* $\kappa_{min} \ge 1$ *and a function* $\kappa_{max}(h)$ *with* $\kappa_{max}(h) \to \infty$ *as* $h \to 0$ *such that for all* $\kappa_{min} \le \kappa \le \kappa_{max}(h_l)$ *and sufficient large* κ_3 *there holds*

$$\|u_l^{j+1} - u_l^*\|_0 \le (C(\kappa) + C_{\kappa_3}\eta^{(j)})\,\|u_l^j - u_l^*\|_0 \quad . \tag{3.22}$$

4. NUMERICAL RESULTS

As an example for a linear obstacle problem we consider the torsion of an elastic, perfectly plastic cylindrical bar $Q := \Omega \times (0,l]$ of cross section $\Omega \subset R^2$ and length $l > 0$ with cylindrical cavities $Q_i := \Omega_i \times (0,l]$, $1 \le i \le m$, which have the same direction of generatrices and cross sections $\Omega_i \subset \Omega$ being mutually disjoint, i.e. $\Omega_i \cap \Omega_j = \emptyset$, $i \ne j$. At the upper end $\partial Q_1 := \Omega \times \{l\}$ the bar is supposed to be twisted around its longitudinal axis by an angle $\theta > 0$ in such a way that the lateral surface $\partial Q_s := \Gamma \times (0,l]$, $\Gamma = \partial\Omega$, remains stress-free. In this case, using Hencky's law and modelling the plastic region by the von Mises yield criterion, it can be shown that the only nonzero components of the stress tensor $\{\sigma_{ij}\}$ are $\sigma_{i3} = \sigma_{3i}$, $1 \le i \le 2$, which can be computed by means of a stress potential u_c according to $\sigma_{13} = \partial u_c / \partial x_2$, $\sigma_{23} = -\partial u_c / \partial x_1$. Normalizing physical constants, the stress potential u_c turns out to be the unique solution of the constrained minimization problem

$$J_c(u_c) = \inf\{J_c(v) \mid v \in K\} \tag{4.1}$$

where

$$J_c(v) = \frac{1}{2}\int_\Omega |\nabla v|^2 dx - 2C\int_\Omega v\,dx\ ,\ C=\theta/l \tag{4.2}$$

and the constraint set K is given by

$$K = \{ v \in H_0^1(\Omega) \mid v|_{\overline{\Omega}_i} = c_i = const.\ , 1\le i\le m\ , |\nabla v| \le 1\ a.e. \}\ . \tag{4.3}$$

In order to show that (4.1) is intimately connected to an obstacle problem we denote by Λ_i, $0\le i\le m$, the set of directed paths from $\Gamma_i = \partial\Omega_i$ to $\Gamma_0 = \partial\Omega_0$, where Ω_0 is the exterior of Ω, a path consisting of directed edges $P_{i_j,i_{j+1}}$, $0\le j\le n-1$, $n\in N$, of length dist $(\Gamma_{i_j}, \Gamma_{i_{j+1}})$ with $i_0 = i$ and $i_n = 0$. Then, we define

$$\psi(x) = inf\{ dist\,(x,\Omega_i) + d_i \mid 0\le i\le m \} \tag{4.4}$$

as a generalized distance function with d_i denoting the length of the shortest path within Λ_i. It has been shown in [25] that for $C\to\infty$ the family $\{u_c\}$ of solutions to (4.7) converges in $H_0^1(\Omega)$, uniformly in C, to $u_\infty = \psi$. This gives rise to consider the related obstacle problem

$$J_c(u_c) = inf\{ J_c(v) \mid v\in K' \} \tag{4.5}$$

with

$$K' = \{ v\in H_0^1(\Omega) \mid v|_{\overline{\Omega}_i} = c_i\ , 1\le i\le m\ , |v|\le\psi\ a.e. \}\ . \tag{4.6}$$

The equivalence of (4.1) and (4.5) has been conjectured in [11] while a rigorous proof has been given in [3] for the case of a simply connected domain, i.e. m=0.
Assuming positive torsion $C>0$, (4.5) reduces to an upper obstacle problem which in view of Lanchon's regularity results [25] is equivalent to the linear complementarity problem

$$-\Delta u_c(x) \le 2C\ ,\quad u_c(x)\le\psi(x)\ ,\quad x\in\Omega^* \tag{4.7a}$$

$$(\Delta u_c(x) + 2C)\cdot(u_c(x) - \psi(x)) = 0\ ,\quad x\in\Omega^* \tag{4.7b}$$

where $\Omega^* = \Omega \setminus \bigcup_{i=1}^{m} \bar{\Omega}_i$ denotes the region effectively occupied by the elastic-plastic material.

We have solved (4.5) resp. (4.7a),(4.7b) by the active set strategy resp. the complementarity problem solver of § 2 combined with the multi-grid scheme MGV11 using a hierarchy of grids $\Omega_k = \Omega \cap R^2{}_k$, $0 \le k \le l$, where $\{ R^2{}_k \}^l{}_{k=0}$, $l \ge 5$, is a sequence of equidistant grids with step sizes $h_{k+1} = h_k/2$, $h_0 = 1/2$. All results reported in this section are based on computations performed on the Cyber 175 of ZRZ, TU Berlin.

Fig. 1a and Fig. 1b represent the plastification in dependence of the applied torsion for a bar with circular cross section and no cavities (Fig. 1a) resp. a bar whose cross section resembles a perforated disk (Fig. 1b). Grid-points belonging to the discrete coincidence set and thus representing the plastified region are marked by a dot. The numerical results reflect the regularity of the free boundary. In particular, in Fig. 1b cusp-like singularities are clearly visible.

	r_3	r_4	r_5
3	1.9E-2		
4	1.6E-3	7.3E-4	
5	1.3E-4	1.5E-4	6.6E-4
6	1.0E-5	3.2E-5	4.5E-4
7	8.3E-7	6.8E-6	3.7E-4
8	6.7E-8	1.4E-6	7.0E-5
9	9.7E-9	2.9E-7	1.4E-5
10	2.4E-9	6.2E-8	3.1E-6

Table 1a

For a bar with rectangular cross section $\Omega = (0,1)^2$ Table 1a shows the residues computed with respect to the inactive grid-points

$$r_l = (\Sigma_{x \in \Omega_l^i} |(A_l(u_l^j) - f_l)(x)|^2 / N_l^i)^{1/2} \tag{4.8}$$

for $l = 3,4,5$ using W-cycles with 2 pre- and post-smoothings.

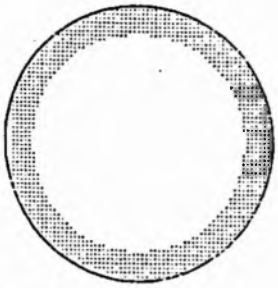
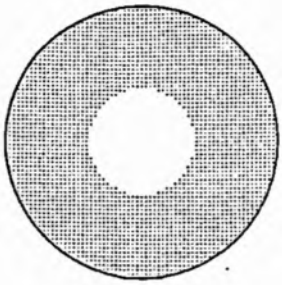
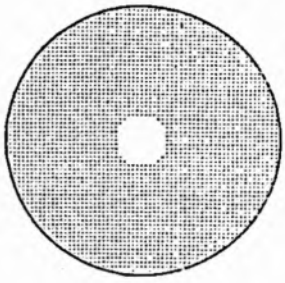


Fig. 1a C = 2.5



C = 5.0



C = 10.0

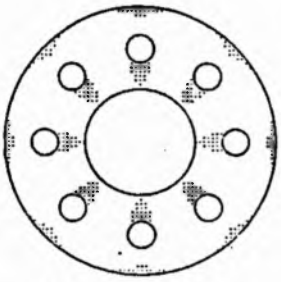
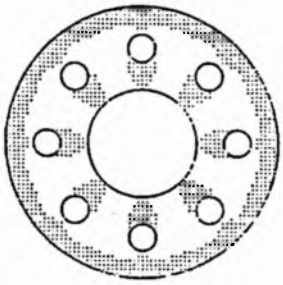
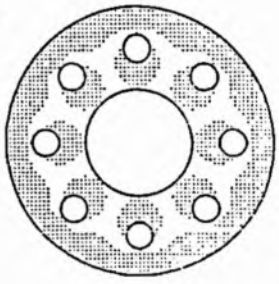


Fig. 1b C = 2.5



C = 5.0



C = 10.0

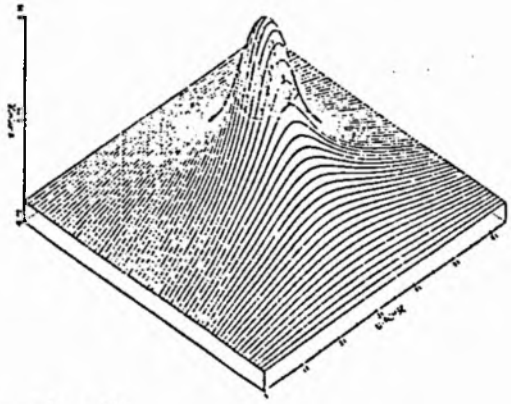


Fig. 2

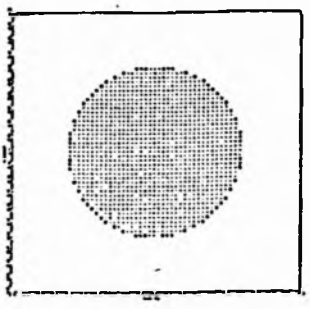


Fig. 3a

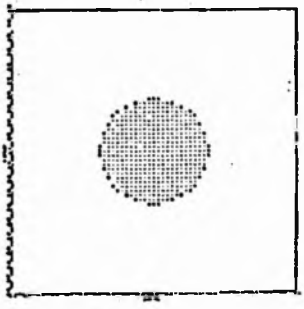


Fig. 3b

	3	4	5
MGCPS	0.35	1.55	4.98
MGASS	0.46	2.00	7.58
PSOR	1.10	3.99	17.36

Table 1b

Finally, Table 1b gives the execution times for the multi-grid complementarity problem (MGCPS), the multi-grid active set strategy (MGASS) and the single-grid projected SOR iteration with suboptimal relaxation parameter $\omega = 1.7$ (PSOR) where $\varepsilon = 10^{-5}$ has served as termination criterion for the iterations. Note that MGCPS is considerably faster than MGASS which can be explained by the fact that when using active set strategies the iterates must stay within the constraint set while this is not required for the complementarity problem solver (for further results the reader is referred to [18], [19] and [20]).

As an example for an obstacle problem leading to a nonlinear variational inequality we consider the following minimal surface over an obstacle:
Minimize the functional

$$J(v) = \int_\Omega (1 + |\nabla v|^2)^{1/2} dx \tag{4.9}$$

over

$$K = \{ v \in H_0^1(\Omega) \mid v(x) \geq \psi(x) \ a.e. \} \tag{4.10}$$

where $\Omega = (0,1)^2$ and

$$\psi(x) = max\,(0, 0.2 - 8|x - w|^2), \quad w = (7/16, 7/16). \tag{4.11}$$

Choosing the same grid hierarchy as in the example before and following Concus [6] we have discretized the minimal surface operator $Au = -\nabla\cdot(1 + |\nabla u|^2)^{-1/2}\nabla u)$ by

$$A_k u_k = -\nabla_k^+ \cdot a(\nabla_k^- u_k) \tag{4.12}$$

where

$$\nabla_k^+ = (D_{k,1}^+, D_{k,2}^+)^T, \quad a(\nabla_k^- u_k) = (a_1(\nabla_k^- u_k), a_2(\nabla_k^- u_k))^T,$$

$$a_1(\nabla_k^- u_k) = \frac{1}{2}[\gamma(|\nabla_k^2 u_k|^2_{(\eta_1,\eta_2)}) + \gamma(|\nabla_k^2 u_k|^2_{(\eta_1,\eta_2+1)})]\cdot D^-_{k,1} u_k(x_\eta) ,$$

$$a_2(\nabla_k^- u_k) = \frac{1}{2}[\gamma(|\nabla_k^2 u_k|^2_{(\eta_1,\eta_2)}) + \gamma(|\nabla_k^2 u_k|^2_{(\eta_1+1,\eta_2)})]\cdot D^-_{k,2} u_k(x_\eta) ,$$

where $x_\eta = (x_{\eta 1}, x_{\eta 2})$, $\gamma(r) = (1+r)^{-1/2}$, $r \geq 0$, and

$$|\nabla_k^2 u_k|_\eta = \frac{1}{2}|(D^-_{k,1} u_k)^2(x_{\eta_1}, x_{\eta_2}) + (D^-_{k,1} u_k)^2(x_{\eta_1}, x_{\eta_2} - h_k)$$

$$+ (D^-_{k,2} u_k)^2(x_{\eta_1}, x_{\eta_2}) + (D^-_{k,2} u_k)^2(x_{\eta_1} - h_k, x_{\eta_2})| ,$$

$D_{k,\mu}$ denoting the forward resp. backward difference operator with respect to the μ-th argument.

	MGCPS		MGTPS	
	r_3	r_4	r_3	r_4
2			1.9E-2	
3	2.4E-4		1.3E-3	1.1E-3
4	2.3E-5	1.1E-3	9.4E-5	3.6E-4
5	2.2E-6	4.2E-4	7.2E-6	1.4E-4
6	2.2E-7	1.5E-4	5.9E-7	5.6E-5
7	2.0E-8	5.3E-5	5.3E-8	2.3E-5
8	5.0E-9	1.9E-5		
9	1.3E-9	6.7E-6		
10	3.2E-10	2.4E-6		

Table 2

Table 2 gives the residues for $l=3$ and $l=4$ both for the multi-grid complementarity problem solver (MGCPS), using W-cycles with 2 pre-smoothings, and for the two-phase multi-grid solver of [16] (MGTPS) while Fig. 2 is a graphical display of the minimal surface, the hatched region representing the coincidence set (for more details see [18]).

5. MULTI-GRID SOLUTION OF TWO-PHASE STEFAN PROBLEMS

Two-phase Stefan problems describe the temperature distribution $\theta(x,t)$, $(x,t) \in Q := \Omega \times (0,T)$ of a heat-conducting substance undergoing a change of phase at a certain temperature θ_c. For simplicity we assume the heat capacity c and the thermal conductivity k to be constant in each phase and we suppose $\theta_c = 0$. Then the temperature satisfies the heat equations

$$c_i \frac{\partial}{\partial t} \theta(x,t) - k_i \Delta \theta(x,t) + f(x,t) = 0 \quad , \quad 1 \le i \le 2 \tag{5.1a}$$

$$\theta(x,0) = \theta_0(x) \ , \ x \in \Omega \ , \quad \theta(x,t) = 0 \ , \ x \in \Gamma = \partial\Omega \tag{5.1b}$$

$$(x,t) \in Q^i = \{ (x,t) \in Q \mid (-1)^i \theta(x,t) > 0 \}$$

where the function f denotes sink/source terms.

When a change of phase occurs, at the free boundary a jump condition relates the intensity of change of phase to the absorption rate of heat energy

$$k_2 \nabla\theta(x,t) \cdot n\nu|_{\Sigma^2} - k_1 \nabla\theta(x,t) \cdot n\nu|_{\Sigma^1} = s \cos(\nu, 1_t) \tag{5.2}$$

where $\Sigma^i = \mathrm{cl}\, Q^i \cap \Sigma$, $\Sigma = \{(x,t) \in Q \mid \theta(x,t) = 0\}$, ν is the normal to Σ^1 resp. Σ^2, outward for $\{\theta > 0\}$ and inward for $\{\theta < 0\}$, $n\nu$ is its projection into the Ω-plane and s stands for the latent heat.

Introducing a generalized temperature via the standard Kirchhoff transformation

$$u_i(x,t) = k_i \theta(x,t) \ , \ 1 \le i \le 2 \ ,$$

one is led to the so-called enthalpy formulation of the two-phase Stefan problem

$$\frac{\partial}{\partial t} H(u) - \Delta u + f = 0 \tag{5.3}$$

where $H(\cdot)$ denotes the generalized enthalpy given by

$$H(\lambda) = \begin{cases} a_1 \lambda & , \ \lambda < 0 \\ [0,s] & , \ \lambda = 0 \\ a_2 \lambda + s & , \ \lambda > 0 \end{cases} \tag{5.4}$$

where $a_i = c_i / k_i$, $1 \le i \le 2$.

Of course, the enthalpy equation (5.3) has to be understood in an appropriate weak sense (cf. e.g. [23]).

Formally discretizing (5.3) implicitly in time yields the boundary value problem

$$H(u^{m+1}) - \Delta t\, \Delta u^{m+1} + \Delta t\, f^{m+1} = H(u^m) \quad in\ \Omega \tag{5.5a}$$

$$u^{m+1} = 0 \quad on\ \Gamma = \partial\Omega \tag{5.5b}$$

where u^m is an approximation to u at $t_m = m\,\Delta t$, $\Delta t = T / M$, $M \in \mathbb{N}$. Again, (5.5a) has to be interpreted appropriately due to the fact that the enthalpy function is multi-valued.

If at time level t_m an enthalpy $H^m \in H(u^m)$ is selected, the discrete-time problem (5.5a),(5.5b) can be written as the differential inclusion

$$-L\,u^{m+1} + b^{m+1} \in H(u^{m+1}) \quad in\ \Omega \tag{5.6a}$$

$$u^{m+1} = 0 \quad on\ \Gamma = \partial\Omega \tag{5.6b}$$

where $L = -\Delta t\,\Delta$ and $b^{m+1} = H^m - \Delta t\, f^{m+1}$.

Since H is the subgradient $\partial\Phi$ of the piecewise quadratic function

$$\Phi(\lambda) = \frac{1}{2} a_2 \lambda_+^2 + \frac{1}{2} a_1 \lambda_-^2 + s\lambda_+ \quad , \quad \lambda \in \mathbb{R} \tag{5.7}$$

the inclusion (5.6a) is equivalent to the variational inequality of the second kind

$$a(u^{m+1}, v - u^{m+1}) + \phi(v) - \phi(u^{m+1}) + \langle b^{m+1}, v - u^{m+1} \rangle \ge 0 \ , \ v \in H_0^1(\Omega) \tag{5.8}$$

where $a(u,v) = \Delta t \int_\Omega \nabla u \cdot \nabla v\, dx$ and $\phi(v) = \int_\Omega \Phi(v(x))\, dx$.

Discretization of (5.6a),(5.6b) in the space variables with respect to a grid-point set Ω_h results in the difference inclusion

$$-L_h u_h^{m+1} + b_h^{m+1} \in \partial\Phi(u_h^{m+1}) \quad in\ \Omega_h \tag{5.9a}$$

$$u_h^{m+1} = 0 \quad on\ \Gamma_h = \partial\Omega_h \ . \tag{5.9b}$$

Here, $L_h = -\Delta t\,\Delta_h$, Δ_h denoting the standard five-point approximation of the Laplacian. By incorporating the boundary conditions, (5.9a),(5.9b) can be written algebraically as

$$-A_h u_h^{m+1} + b_h^{m+1} \in \partial\Phi(u_h^{m+1}) \ . \tag{5.10}$$

Now, from convex analysis it is well known that (5.10) is equivalent to (cf. e.g. [9])

$$u_h^{m+1} \in \partial\Phi^*(-A_h u_h^{m+1} + b_h^{m+1}) \tag{5.11}$$

where Φ^* is the Fenchel conjugate to Φ with subgradient $\partial\Phi^*$ given by the piecewise linear continuous function

$$\partial\Phi^*(\lambda) = \begin{cases} a_1^{-1}\lambda & , \ \lambda < 0 \\ 0 & , \ \lambda \in [0,s] \\ a_2^{-1}(\lambda - s) & , \ \lambda > s \end{cases} \tag{5.12}$$

The fact that $\partial\Phi^*$ is single-valued allows to write (5.11) as the nonlinear system

$$F_h(u_h^{m+1}) = u_h^{m+1} - \partial\Phi^*(-A_h u_h^{m+1} + b_h^{m+1}) = 0 \tag{5.13}$$

which is the key to the following multi-grid algorithm :

While nonlinear Gauss-Seidel iteration applied to (5.13) is an easily implementable smoothing process, the problem is how to perform an appropriate defect correction process. Restricting ourselves to the two-grid case $\Omega_{l-1} \subseteq \Omega_l$ and assuming $\bar{u}_l^{m+1}$ to be a smoothed iterate on level l, a correction w_l is sought such that

$$\bar{u}_l^{m+1} + w_l = \partial\Phi^*(-A_l w_l - (A_l \bar{u}_l^{m+1} - b_l^{m+1})) \ .$$

Consequently, a suitable approximation on level $l-1$ can be obtained by

$$u_{l-1}^{m+1} = \partial\Phi^*(-A_{l-1} u_{l-1}^{m+1} + A_{l-1} r_l^{l-1} \bar{u}_l^{m+1} - r_l^{l-1}(A_l \bar{u}_l^{m+1} - b_l^{m+1})) \tag{5.14}$$

thus leading to the improved iterate

$$\bar{u}_l^{m+1} + p_{l-1}^{l}(u_{l-1}^{m+1} - r_l^{l-1}\bar{u}_l^{m+1}) \quad .$$

Note that (5.14) is formally equivalent to the inclusion

$$-A_{l-1}u_{l-1}^{m+1} + b_{l-1}^{m+1} \in H(u_{l-1}^{m+1})$$

where $b_{l-1} = A_{l-1}r_l^{l-1}\bar{u}_l^{m+1} - r_l^{l-1}(A_l\bar{u}_l^{m+1} - b_l^{m+1})$.

If the restrictions and prolongations are chosen according to a strategy analogous to that used in MGVI2 before, convergence of the multi-grid algorithm can be proved by similar techniques as used in the proof of Theorem 3.1 (for details see [22]).

For a model problem with domain $\Omega = (0,1)^2$, time-interval [0,0.5] and physical data $c_1 = 2$, $c_2 = 6$, $k_1 = 1$, $k_2 = 2$, $s = 1$ and $f(x,y,t) = 4k_i - c_i \exp(-4t)$, $(x,y,t) \in Q^i$, $1 \le i \le 2$, we have used a grid hierarchy $(\Omega_k)_{k=0}^{l}$ with $h_k = 2^{-(k+1)}$, $0 \le k \le 1$.

The numerical temperature history of the process is illustrated by Figs. 3a and 3b showing the numerical temperature pattern at times $t = 0.25$ and $t = 0.50$ where positive/negative and zero temperatures at grid-points on level $l = 5$ are marked by a dot/blank and "0", respectively.

In order to compare the performance of the multi-grid algorithm described above (MGSTEF) with Elliott's related single-grid SOR algorithm [10] we have computed the asymptotic convergence rate

$$q^l(t_m) = (\|\Delta_l^{\nu^*}\|_0 / \|\Delta_l^1\|_0)^{**}(1/[(\nu^* - 1)*N_{WU}])$$

where $\Delta_l^{\nu}(t_m) = 0_l^{\nu}(t_m) - 0_l^{\nu-1}(t_m)$, $0_l^{\nu^*}(t_m)$ is the iterate at which the accuracy bound 10^{-8} is reached and N_{WU} is the number of work units used for one iteration step. Since at each step of the single-grid solver we have used two SOR-iterations on Ω_l (the first with respect to an ordering of grid-points from south-west to north-east and the second one in reverse order), a work unit consists of two Gauss-Seidel iterations on the highest level l.

Table 3 below contains the asymptotic convergence rates for MGSTEF (V-cycle, 1 pre- and post-smoothing) and the convergence rates for the single-grid solver (with suboptimal relaxation parameter $\omega = 1.7$) at times $t_m = m \cdot 0.05$, $1 \le m \le 10$, for $l = 4$, $\Delta t = 1/40$ and $l = 5$, $\Delta t = 1/80$.

The results, which illustrate the superiority of the multi-grid solver, are based on computations which have been performed on the CRAY XMP/24 at Konrad Zuse Institut für Informationstechnik, Berlin.

t_m	l=4 , Δt = 1/40		l=5 , Δt = 1/80	
	MGSTEF	SOR	MGSTEF	SOR
0.05	0.57	0.66	0.51	0.78
0.10	0.62	0.67	0.65	0.78
0.15	0.42	0.68	0.54	0.77
0.20	0.57	0.67	0.60	0.78
0.25	0.52	0.68	0.51	0.77
0.30	0.50	0.68	0.50	0.76
0.35	0.52	0.68	0.50	0.76
0.40	0.54	0.69	0.49	0.75
0.45	0.42	0.68	0.49	0.74
0.50	0.52	0.67	0.59	0.73

Table 3

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REFERENCES

[1] A. Brandt, *Guide to multigrid development.* In: Multigrid Methods, Proc. Conf. Köln-Porz, November 23-27, 1981 (eds.: W. Hackbusch, U. Trottenberg), pp. 220-312, Lect. Notes in Math. 960, Springer, Berlin-Heidelberg-New York (1982)

[2] A. Brandt and C W. Cryer, *Multi-grid algorithms for the solution of linear complementarity problems arising from free boundary problems.* SIAM J. Sci. Stat. Comput. 4, 655-684 (1983)

[3] H. Brezis et M. Sibony, *Équivalence de deux inéquations variationnelles et applications.* Arch. Rat. Mech. Anal. 41, 254-265 (1971)

[4] F. Brezzi and L. A. Caffarelli, *Convergence of the discrete free boundaries for finite element approximations.* R.A.I.R.O. Analyse numérique / Numerical analysis 17, 385-395 (1983)

[5] F. H. Clarke, *Optimization and nonsmooth analysis.* Wiley, New York (1983)

[6] P. Concus, *Numerical solution of the minimal surface equation.* Math. Comput. 21, 340-350 (1967)

[7] C. W. Cryer, *The solution of quadratic programming problems using systematic overrelaxation.* SIAM J. Control Optimization 9, 385-392 (1971)

[8] A. Das, E. M. Cliff and H. J. Kelley, *An active-constraint logic for nonlinear programming.* Optim. Control Appl. Methods 5, 221-234 (1984)

[9] I. Ekeland and R. Temam, *Convex analysis and variational problems.* North-Holland, Amsterdam (1976)

[10] C. M. Elliott, *On the finite element approximation of an elliptic variational inequality arising from an implicit time discretization of the Stefan problem.* I.M.A. J. Numer. Anal. 1, 115-125 (1981)

[11] R. Glowinski et H. Lanchon, *Torsion élastoplastique d'une barre cylindrique de section multiconnexe*. J. Mec. Theor. Appl. 12, 151-171 (1973)
[12] R. Glowinski, J. L. Lions and R. Trémolières, *Numerical analysis of variational inequalities*. North-Holland, Amsterdam (1981)
[13] W. Hackbusch, *Convergence of multi-grid iterations applied to difference equations*. Math. Comput. 34, 425-440 (1980)
[14] W. Hackbusch, *On the convergence of multi-grid iterations*. Beitr. Numer. Math. 9, 47-62 (1981)
[15] W. Hackbusch, *Multi-grid methods and applications*. Springer, Berlin-Heidelberg-New York (1985)
[16] W. Hackbusch and H. D. Mittelmann, *On multi-grid methods for variational inequalities*. Numer. Math. 42, 65-76 (1983)
[17] R. H. W. Hoppe, *Multi-grid methods for Hamilton-Jacobi-Bellman equations*. Numer. Math. 49, 239-254 (1986)
[18] R. H. W. Hoppe, *Multi-grid algorithms for variational inequalities*. to appear in SIAM J. Numer. Anal. 24, No. 5 (1987)
[19] R. H. W. Hoppe, *Two-sided approximations for unilateral variational inequalities by multi-grid methods*. to appear in Optimization 18, No. 5/6 (1987)
[20] R. H. W. Hoppe, *Multi-grid solutions to the elastic plastic torsion problem in multiply connected domains*. to appear in Int. J. Numer. Methods Eng.
[21] R. H. W. Hoppe, *A multi-grid algorithm for nonlinear complementarity problems* (to appear)
[22] R. H. W. Hoppe and R. Kornhuber, *Multi-grid methods for the two-phase Stefan problem*. to appear in Proc. Conf. 3rd Copper Mountain Conf. on Multigrid Methods, Copper Mountain (Colorado), April 6-10, 1987 (ed.: St. McCormick), Marcel Dekker, New York (1987)
[23] J. W. Jerome, *Approximation of nonlinear evolution systems*. Academic Press, New York (1983)
[24] H. Kirsten and R. Tichatschke, *On a method of feasible directions for solving variational inequalities*. Optimization 16, 535-546 (1985)
[25] H. Lanchon, *Sur la solution du problème de torsion élastoplastique d'une barre cylindrique de section multiconnexe*. C. R. Acad. Sci. Paris, Ser. I 271, 1137-1140 (1970)
[26] P. L. Lions et B. Mercier, *Approximation numérique des équations de Hamilton-Jacobi-Bellman*. R.A.I.R.O. Analyse numérique / Numerical analysis 14, 369-393 (1980)
[27] J. Mandel, *A multilevel iterative method for symmetric, positive definite linear complementarity problems*. Appl. Math. Optimization 11, 77-95 (1984)
[28] J. J. Moré and W. C. Rheinboldt, *On P- and S-functions and related classes of n-dimensional nonlinear mappings*. Linear Algebra Appl. 6, 45-68 (1973)
[29] D. Rew, H. J. Kelley and E. M. Cliff, *A computational study of active-set logics for nonlinear programming*. In: Proc. Conf. IFAC Control Applications of Nonlinear Programming and Optimization, Capri, Italy, pp. 157-170
[30] W C. Rheinboldt, *On M-functions and their application to nonlinear Gauss-Seidel iterations and to network flows*. J. Math. Anal. Appl. 32, 274-307 (1970)
[31] J. B. Rosen, *The gradient projection method for nonlinear programming. Part I: Linear constraints*. J. Soc. Indust. Appl. Math. 8, 181-217 (1960)
[32] J. B. Rosen, *The gradient projection method for nonlinear programming. Part II: Nonlinear constraints*. J. Soc. Indust. Appl. Math. 9, 514-531 (1961)
[33] K. Stüben and U. Trottenberg, *Multigrid methods: Fundamental algorithms, model problem analysis and applications*. In: Multigrid Methods, Proc Conf. Köln-Porz, November 23-27, 1981 (eds.: W. Hackbusch, U. Trottenberg), pp. 1-176, Lect. Notes in Math. 960, Springer, Berlin-Heidelberg-New York (1982)