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ON THE RELATIONSHIP BETWEEN THE INVESTIGATION OF NONLINEAR DIFFERENCE SCHEMES AND THE PROBLEM OF MINIMIZATION

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Abstract. This paper is devoted to the investigation of difference schemes for the solution of an important free-surface problem: modelling of a liquid-metal contact. The existence of a solution and the convergence of proposed iterative processes are investigated in a weak sense, using the alternative form of the problem as a nonlinear constrained minimization problem.

Key words: nonlinear difference schemes, nonlinear constrained optimization, free-surface problem.

Introduction. The paper is devoted to the investigation of the connection between the method used to investigate nonlinear difference schemes and the problems of constrained optimization. The problem of determination of the liquid-metal contact free-surface is used as the sample problem. Such a connection is well-known, especially for linear boundary value problems. Variational methods (as the Galerkin method, the least squares method and others) are founded on the alternative formulation as an optimization problem (see Fletcher, 1984; Marchuk and Agoshkov, 1981). Two important features of such a methodology may be outlined. First, the constructed difference schemes are conservative, i.e., a discrete analogue of the conservation law is satisfied exactly (for exact definition of conservative difference schemes see

Samarskij, 1983); second, the usage of the alternative variation formulation naturally enables us to define a generalized (weak) solution of a boundary value problem. The solution of nonlinear differential problems is a considerably more difficult task, because there is no general theory for the investigation of nonlinear difference schemes (in the linear case such a theory is developed and based on the connection between the approximation, the stability, and the convergence of the difference scheme solution, as well as on the necessary and sufficient conditions for the solution's stability, given by Samarskij (1983)).

This work is a continuation of a series of our papers (see Čiegis and Čiupaila, 1990a, 1990b, 1991), devoted to the theoretical investigation of numerical methods, used for computational simulation of liquid-metal contact evolution processes. The main interests of this paper are the construction of a conservative difference scheme, investigation of the existence of its generalized (weak) solution, and the iterative methods for finding the solution. A comparison of the methods, used in the theory of nonlinear difference schemes, with that of the constrained nonlinear optimization is one of our main goals, too.

1. Equations. We consider a physical model of a connected drop of electroconductive nonviscous liquid of the prescribed volume V_0, which is compressed by two parallel planes and fixed to a specially treated disks of radius R. The remaining part of the contact surface is considered free and depends only on a vertical gravity field and the surface tension. We restricted our attention to the case, when the electromagnetic forces can be neglected. Using the symmetricity of the problem it is sufficient to investigate only $1D$ case. A more complete physical model is given by Čiegis and Čiupaila (1990a); Kairytė et.al. (1986). The mathematical differential model follows from the constrained minimization problem of total energy (see also Čiegis and Čiupaila, 1990a).

$$\inf_{u\in U} E(u) = E(u^*), \quad E(u) = E_p(u) + E_s(u), \tag{1.1}$$

$$U = \{u(x) \geqslant 0,\ u(0) = R,\ u(H) = R,\ g(u) = 0\},$$

where $E_p(u)$, $E_s(u)$ are the gravitational energy and free surface energy, respectively,

$$E_s(u) = 2\pi\sigma \int_0^H u(x)\sqrt{1+u_x^2}\,dx, \quad E_p(u) = \pi\rho g \int_0^H x u^2(x)\,dx. \tag{1.2}$$

The constancy of volume of the fluid is a constraint that must be respected, when the minimum of total energy is determined

$$g(u) \equiv \pi \int_0^H u^2(x)\,dx - V_0 = 0. \tag{1.3}$$

The variational formulation of the free surface problem is a general method for the solution of such problems (see Concus and Finn, 1974; Huisken, 1983; Giusti, 1984). Introducing a Lagrange parameter λ and using the necessary conditions of the minimum, we get the differential boundary value problem with an additional nonlocal condition, from which the solution $u(x)$ is obtained.

$$-\frac{d}{dx}\Big(\frac{\sigma u(x)}{\sqrt{1+u_x^2}}\frac{du}{dx}\Big) + (\rho g x + \lambda)u(x) = -\sigma\sqrt{1+u_x^2}, \tag{1.4}$$

$$u(0) = R, \quad u(H) = R, \tag{1.5}$$

$$g(u) = 0. \tag{1.6}$$

The numerical methods for the solution of some problems with nonlocal conditions are investigated by Čiegis (1991).

For the sake of simplicity we take a uniform mesh $\omega_h = \{x_i : x_i = ih, i = 0,1,\dots,N, x_N = H\}$. We propose the following method to construct a conservative difference scheme. At first we directly approximate the energy integrals (1.2) and the volume constraint condition (1.3)

$$E_h(y) = E_{hp}(y) + E_{hs}(y), \quad g_h(y) = \pi \sum_{i=0}^{N-1} \frac{y_i^2 + y_{i+1}^2}{2} h - V_0,$$

$$E_{hp}(y) = \pi\rho g \sum_{i=0}^{N-1} x_{i+0,5} \frac{y_i^2 + y_{i+1}^2}{2} h,$$

$$E_{hs}(y) = 2\pi\sigma \sum_{i=0}^{N-1} x_{i+0,5}\sqrt{1+y_x^2}\, h.$$

Then problem (1.1) is replaced by the approximate constrained minimization problem

$$\inf_{y\in U_h} E_h(y) = E_h(y^*), \tag{1.7}$$
$$U_h = \{y_i : y_i \geqslant 0,\ y_0 = R,\ y_N = R,\ g_h(y) = 0\}.$$

We get the conservative difference scheme with the additional nonlocal condition from the necessary minimum conditions for the function $E_{h\mu}(y) = E_h(y) + \mu g_h(y)$

$$-\left(\frac{\sigma \bar{y}}{\sqrt{1+y_x^2}}\, y_x\right)_{\bar{x}} + (\rho g x_i + \mu) y_i = -\frac{\sigma}{2}\left(\sqrt{1+y_x^2} + \sqrt{1+y_{\bar{x}}^2}\right), \tag{1.8}$$
$$y_0 = R, \qquad y_N = R, \tag{1.9}$$
$$g_h(y) = 0. \tag{1.10}$$

The notation and conventions adopted here are as that introduced by Samarskij (1983)

$$y_x = \frac{y_{i+1} - y_i}{h}, \quad y_{\bar{x}} = \frac{y_i - y_{i-1}}{h}, \quad \bar{y} = \frac{y_i + y_{i+1}}{2}.$$

A simple Taylor expansion reveals that the approximation error of the difference scheme (1.8) - (1.10) is of order $O(h^2)$, i.e., of the same order as the approximation accuracy of the integrals (1.2), (1.3) by discrete sums.

2. Existence and convergence. In this section we investigate the methods, that can be used to prove the existence of solutions to the above problems (1.7) and (1.8) - (1.10), and their convergence to the exact solution of problem (1.1). We start from the difference scheme (1.8) - (1.10) solution. It can be called a strong solution, as compared to the weak solution (generalized solution) of the constrained minimization problem (1.7). We may write the scheme (1.8) - (1.10) in the form

$$L(y,\mu) = 0, \qquad g_h(y) = 0. \tag{2.1}$$

By substituting $y_i = u_i + z_i$, $\mu = \lambda + \omega$ into problem (2.1) where (u_i, λ) is the exact solution of the differential boundary value problem (1.4) – (1.6), (z_i, ω) is the error function of the difference scheme (1.8) – (1.10) solution, we get equations (2.2)

$$L(u, \lambda) = \psi_1, \qquad g_h(u) = \psi_2. \tag{2.2}$$

Functions ψ_j are the approximation errors and as stated above, they can be bounded by $|\psi_j| \leqslant Ch^2$. Subtracting equations (2.2) from equations (2.1) and using the Taylor expansion for the error (z_i, ω) we get a linear boundary value problem with the additional nonlocal condition

$$\frac{\partial L}{\partial y} z + \frac{\partial L}{\partial \mu} \omega = \psi_1, \quad \frac{\partial g_h}{\partial y} z = \psi_2, \tag{2.3}$$

or if to use the operator notation

$$AY = \Psi, \quad Y = (z_i, \omega), \quad \Psi = (\psi_1, \psi_2).$$

It is well-known that the condition of strong monotonicity of the operator A ($A \geqslant \gamma E$, where E is the unity operator)

$$(AY, Y) \geqslant \gamma(Y, Y), \quad \gamma > 0 \tag{2.4}$$

is the sufficient condition for the stability of difference scheme (2.3) (see Samarskij, Nikolayev, 1978). Condition (2.4) gives us the convergence of the difference scheme (1.8) – (1.10) solution to the exact solution of the boundary value problem with additional nonlocal condition (1.4) – (1.6)

$$\|Y\| \leqslant \frac{1}{\gamma}\|\Psi\| \leqslant Ch^2, \quad \|Y\|^2 = \|z\|^2 + |\omega|^2. \tag{2.5}$$

The existence of the unique difference scheme (1.8) – (1.10) solution follows from the fixed point theorem too, if condition (2.4) is satisfied.

It is interesting to compare condition (2.4) with the conditions that guarantee the existence of the constrained optimization problem (1.7) solution. The well-known sufficient conditions for the existence of the global minimum are (see Vasilyev, 1988):

a) $E_h(y)$ is a strongly convex functional,

b) $U_h(y)$ is a closed and convex set of permissible functions.

It is easy to prove that in this case the weak solution of problem (1.7) coincides with the classical (strong) solution of the difference scheme (1.8) – (1.10). Simple calculations reveal to us that the set $U_h(y)$ is not convex. Using the Lagrangian function we obtain the equivalent form of problem (1.7)

$$\inf_{v\in V_h} L_h(v) = L_h(v^*), \quad L_h(v) = E_h(y) + \mu g_h(y), \tag{2.6}$$

$$V_h = \{v: \ v = (y,\mu), \quad y_i \geqslant 0\}.$$

For this case the set of the permissible functions V_h is convex and closed. The necessary and sufficient condition for the function $L_h(v) \in C^2(V_h)$ to be strongly convex functional is the existence of the positive constant $\gamma > 0$, such that (Vasilyev, 1988)

$$(L_h''(v)w, w) \geqslant \mu(w,w), \quad w \in V_h. \tag{2.7}$$

It is easy to see that condition (2.7) coincides with condition (2.4), obtained when investigated the difference scheme (1.8) – (1.10). If we restrict the problem only to local minimum of (1.7) then the sufficient condition for the existence of such a solution if $L_h(v) \in C^2(V_h)$ (we have the strong solution again) is positivity of the quadratic form

$$\Big(\frac{\partial^2 L_h(v)}{\partial y^2} z, z\Big) > 0, \quad (g_h'(y)z, z) = 0, \tag{2.8}$$

i.e., only nonzero vectors z that are orthogonal to the constraint gradient $g_h'(y)$ are investigated. A comparison of expressions (2.7) and (2.8) suggests that condition (2.8) is weaker than condition (2.7), it suffices to expand the quadratic form (2.7) to see that

$$(L_h''(v)w, w) = \Big(\frac{\partial^2 L_h(v)}{\partial y^2} z, z\Big) + 2\omega(g_h'(y)z, z).$$

Considering this fact, we investigated only condition (2.8). It follows after simple calculations that

$$\left(\frac{\partial^2 L_h(v)}{\partial y^2} z, z\right) = \left(\frac{\sigma \bar{y}}{(1+y_{\bar{x}}^2)^{1.5}} z_{\bar{x}}, z_{\bar{x}}\right] + \rho g(xz, z) + \mu(z,z) - \left(\left(\frac{\sigma}{(1+y_{\bar{x}}^2)^{0.5}}\right)_x z, z\right). \tag{2.9}$$

The positive definitness of the two last terms can not be guaranteed, so the validity of condition (2.8) can't be proved. The existence of the solution (maybe not unique) can be investigated directly using the weak formulation of problem (1.7), as a nonlinear constrained minimization problem. But the convergence of the discrete solution y_i to the exact solution of the boundary value problem with additional nonlocal condition (1.4) – (1.6) must be assumed as a generalized convergence of total energy integrals only.

Theorem 1. *The following statements are true for the constrained minimization problem* (1.7)

a) $E_h(y^*) = \inf_{y \in U_h} E_h(y) > -\infty$,

b) the set $U_h^* = \{y : \ y \in U_h, \ E_h(y) = E_h(y^*)\}$ is non-empty and compact,

c) each minimizing sequence y^l converges to U_h^*.

Proof. As it follows from the Veierstras's theorem (see Vasilyev, 1988), it suffices to prove that U_h is a compact set and the function $E_h(y)$ is bounded and lower semicontinuous in U_h. The set U_h is closed, this follows from the continuity of the function $g_h(y)$. From the definition of the function $g_h(y)$ we get the boundedness of U_h $\|y\|_c \leqslant \max(R, (V_0/h)^{0.5})$, i.e., the set U_h is compact. The function $E_h(y)$ is bounded from below by zero and belongs to the space of functions $E_h(y) \in C^{1,1}(U_h)$ ($E_h'(y)$ is the Lipschitz function in U_h), so it is lower semicontinuous with respect to the maximum norm convergence. The theorem is proved.

REMARK 1. If the objective $E_h(y)$ and constraint $g_h(y)$ functions are smooth (have the first derivatives), then the local minimum can be achieved only if $\partial L_h'(v)/\partial v = 0$, i.e., if (y, μ) is the solution of the difference scheme (1.8) – (1.10). So Theorem 1 guarantees the existence of the difference scheme (1.8) – (1.10) solution, too.

3. Iterative methods. The difference scheme (1.8) – (1.10) is nonlinear, therefore some iterative method is needed to find the solution, existence of which is guaranteed by Theorem 1. Some iterative processes are given and investigated by Čiegis, Čiupaila (1990a). At first we introduce some helpful notation

$$\begin{aligned} E_h'(y) =& L_1(y)y + \varphi(y), \\ L_1(y)v \equiv& -\Big(\frac{\sigma \bar{y}}{(1+y_x^2)^{0.5}} v_x\Big)_{\bar{x}} + \rho g x_i v_i, \\ \varphi(y) =& 0.5\sigma\big((1+y_x^2)^{0.5} + (1+y_{\bar{x}}^2)^{0.5}\big). \end{aligned}$$

We start from the two-stage iterative process, which perfectly illustrates the main idea, used in this paper to construct iterative processes

$$L_1(y^k)y^{k+1} + \mu y^{k+1} = -\varphi(y^k), \quad g_h(y^{k+1}) = 0. \tag{3.1}$$

It is necessary to solve the linear boundary problem with the nonlinear nonlocal additional condition (3.1) in order to find the iteration y^{k+1}. For this purpose the inner iterative process is proposed

$$\mu_{k+1} = G(\mu_k, y^k). \tag{3.2}$$

The bisection method may be used as such a process. The convergence of the inner iterative process (bisection method) follows from the lemma (the proof is given by Čiegis, Čiupaila, 1990a).

Lemma 1. *The solution of problem* (3.1) *monotonously depends on the parameter* μ *and* $\partial g_h(y^{k+1})/\partial\mu < 0$.

The proof of the outer iterative process convergence is more complicated. Obviously, it is directly connected with the violence of condition (2.4). The weak formulation of the difference scheme (2.8) – (2.10) must be used again as the problem of constrained optimization (2.7). It is easy to prove that iterative process (3.1) is equivalent to the variational problem

$$\inf_{y \in U_h} E_k(y) = E_k(y^{k+1}), \tag{3.3}$$

where the objective function is defined as

$$E_k(y) = E_h(y^k) + E_h'(y^k)(y - y^k) + \frac{1}{2}(y - y^k)L_1(y^k)(y - y^k). \quad (3.4)$$

The quadratic approximation $E_k(y)$ coincides with the Taylor expansion of $E_h(y)$, only the second derivative matrix $E_h''(y)$ is replaced by its part $L_1(y)$. In order to achieve the convergence from poor starting approximations the change $y^{k+1} - y^k$ may be additionally imposed to depend on a merit function $\Phi(y)$ (the objective function $E_h(y)$ may serve as an example of such a function). A new iteration y^{k+1} is proved as a new vector only if $\Phi(y^{k+1}) < \Phi(y^k)$. If the matrix $L_1(y)$ does not provide sufficient proper second derivative information for some parameters of problem, then the Newton method is used

$$\inf_{y\in U_h} E_{k,N}(y) = E_{k,N}(y^{k+1}),$$

$$E_{k,N}(y) = E_h(y^k) + E_h'(y^k)(y - y^k) + 0.5(y - y^k)E_h''(y^k)(y - y^k).$$

Such a variational problem is equivalent to the iterative process

$$E_h''(y^k)(y^{k+1} - y^k) + \mu y^{k+1} = -(L_1(y^k)y^k + \varphi(y^k)), \quad g_h(y^{k+1}) = 0. \quad (3.4)$$

A modified iterative process may be constructed, if it is necessary to obtain the convergence of the iteration process

$$(\delta E_h''(y^k) + I)\frac{y^{k+1} - y^k}{\tau} + \mu y^{k+1} = -(L_1(y^k)y^k + \varphi(y^k)), \quad (3.5)$$
$$g_h(y^{k+1}) = 0.$$

In the limit case $\delta \to 0$ we have a variant of the gradient method (see Powell, 1982). An obvious defect of the proposed iterative processes (3.1), (3.2) is their noneconomical realization, because one must use additional inner iterative process (3.2) to find the iteration y^{k+1}. In order to overcome this difficulty the linearization of constraints is implemented in the following two iterative processes. The simplest way is to assume the vector y^{k+1} as the one minimizing the quadratic function

$$\inf_{y\in U_h} E_{k,N}(y) = E_{k,N}(y^{k+1}), \quad (3.6)$$

subject to the linear constrains

$$U_k = \{y : y_i \geqslant 0,\ y_0 = R,\ g_h(y^k) + g_h'(y^k)(y - y^k) = 0\}.$$

The solution y^{k+1} of variational problem (3.6) can be found from the linear boundary value problem with the additional nonlocal linear condition

$$\begin{aligned} &E_h''(y^k)(y^{k+1} - y^k) + \mu y^k = -(L_1(y^k)y^k + \varphi(y^k)), \\ &g_h(y^k) + g_h'(y^k)(y^{k+1} - y^k) = 0. \end{aligned} \tag{3.7}$$

The iterative process is economically realized by a modified factorization algorithm (see Čiegis, Čiupaila, 1990a, Samarskij, 1983). The iterative process (3.7) converges only linearly, while the two-stage iterative process (3.4), (3.2) converges quadratically. It is necessary to correct the objective function of (3.6) to get the quadratic convergence

$$\inf_{y \in U_k} E_{k,N} + 0.5\mu_k(y - y^k)g_h''(y^k)(y - y^k). \tag{3.8}$$

It is easy to prove that the iterative process generated by variational problem (3.8) coincides with the classical Newton method, applied directly to the nonlinear difference scheme (1.8) – (1.10)

$$\begin{aligned} &(E_h''(y^k) + \mu_k)(y^{k+1} - y^k) + (\mu_{k+1} - \mu_k)y^k \\ &\quad = -(L_1(y^k)y^k + \mu_k y^k + \varphi(y^k)), \\ &g_h(y^k) + g_h'(y^k)(y^{k+1} - y^k) = 0. \end{aligned} \tag{3.9}$$

The computer simulation data, presented by Čiegis, Čiupaila (1990a), show the efficiency of the proposed difference scheme (1.8) – (1.10) and iterative processes (3.1) – (3.9).

4. The parametric difference scheme. The difference scheme, constructed in Section 1 and, consequently, the iterative processes proposed in Section 3 are the problems of specific kind. They consist of a boundary value problem and additional discrete nonlocal condition. The nonlocal condition causes serious troubles both in the course of investigation of the difference scheme and during the construction of economical iterative processes. We propose a new different method for the solution of such problems (we follow here the methodology given in the paper of Čiegis, Čiupaila (1991)). The method is based on some appropriate parametrization of integrals (1.2), (1.3). At first the parametrization of the region is introduced

$$x = x(\alpha), \qquad u = u(x(\alpha)) = u(\alpha), \qquad \alpha \in [0,1].$$

Then the integrals (1.2), (1.3) must be rewritten in the form

$$\begin{aligned} E_s(u) &= 2\pi\sigma \int_0^1 u(\alpha)\left(\left(\frac{\partial x}{\partial\alpha}\right)^2 + \left(\frac{\partial u}{\partial\alpha}\right)^2\right)^{0.5} d\alpha, \\ E_p(u) &= \pi\rho g \int_0^1 x(\alpha)u^2(\alpha)\frac{\partial x}{\partial\alpha} d\alpha, \end{aligned} \tag{4.1}$$

$$g(u) = \int_0^1 u^2(\alpha)\frac{\partial x}{\partial\alpha} d\alpha. \tag{4.2}$$

Only the difference case of problem (1.1) is investigated in our paper. Two difference grids are constructed in the interval [0,1]

$$\begin{aligned} \omega_1 &= \{\alpha_i = ih,\ i = 0,1,\ldots,N,\ \alpha_N = 1\}, \\ \omega_2 &= \{\alpha_{i-0.5},\ i = 0,1,\ldots,N+1\}. \end{aligned}$$

The function $u(\alpha)$ is approximated on the grid ω_1 and the function $x(\alpha)$ – on the grid ω_2. The volume constraint (4.2) is approximated by the sum

$$g_h(w) = \sum_{i=0}^{N-1} \frac{w_i + w_{i+1}}{2} h - V_0, \quad w_i = \pi y_i^2 \frac{x_{i+0.5} - x_{i-0.5}}{h}. \tag{4.3}$$

The parametrization is introduced so that the following condition be valid

$$g_h(w) = 0, \qquad w_i \geqslant \varepsilon > 0, \qquad i = 0,1,\ldots,N. \tag{4.4}$$

Obviously, the definition of parametrization is not unique, the simplest case is $w_i = w^*$. Then from equation (4.4) we have

$$\sum_{i=0}^{N-1} w^* h = V_0, \qquad w^* = V_0.$$

For a given function w_i, the function y_i may be attained from equation (4.3)

$$y_i = \Big(\frac{w_i h}{\pi(x_{i+0.5} - x_{i-0.5})}\Big)^{0.5},$$

therefore the unknown function is only $x_{i-0.5}$, $i = 0, 1, \dots, N+1$. Then integrals (4.1) are approximated by discrete sums

$$E_{h,s} = 2\pi \sum_{i=0}^{N-1} \bar{y}_i \big(y_\alpha^2 + 0.5(x^2_{\alpha,i-0.5} + x^2_{\alpha,i+0.5})\big)^{0.5} h,$$
$$E_{h,p} = 0.5\rho g \sum_{i=0}^{N-1} w_i (x_{i+0.5} + x_{i-0.5}).$$

The form of the contact free surface is determined by the minimization problem

$$\inf_{x\in X} \big(E_{h,s}(x) + E_{h,p}(x)\big) = E_{h,s}(x^*) + E_{h,p}(x^*), \tag{4.5}$$
$$X = \Big\{x_{i-0.5} : x_{0.5} + x_{-0.5} = 0,\ \frac{x_{0.5} - x_{-0.5}}{h} = \frac{w^*}{\pi R^2},$$
$$\frac{x_{N-0.5} + x_{N+0.5}}{2} = H,\ \frac{x_{N+0.5} - x_{N-0.5}}{h} = \frac{w^*}{\pi R^2}\Big\}.$$

The difference scheme for the function $x_{i-0.5}$, $i = 0, 1, \dots, N+1$ follows from the necessary minimum condition

$$\frac{\partial E_h}{\partial x_{i+0.5}} = \frac{\partial E_{h,p}}{\partial x_{i+0.5}} + \frac{\partial E_{h,s}}{\partial x_{i+0.5}} + \frac{\partial E_{h,s}}{\partial y_i}\frac{\partial y_i}{\partial x_{i+0.5}} + \frac{\partial E_{h,s}}{\partial y_{i+1}}\frac{\partial y_{i+1}}{\partial x_{i+0.5}}, \tag{4.6}$$

with the corresponding boundary conditions. The existence theorem, analogous to Theorem 1 from Section 2, can be proved for problem (4.5), (4.6). The nonlinear difference scheme is solved by the Newton iterative method, each iteration x^k being the solution of the linear equation system with the fivediagonal matrix.

We have got the boundary value problem without the additional nonlocal condition. Such a method is especially useful for the evolution free-surface problems (see Čiegis, Čiupaila, 1991).

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