pp. 1–14 (2022)

Mesh scheme for a phase transition problem with time-fractional derivative

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Abstract — The time-fractional phase transition problem, formulated in enthalpy form, is studied. This nonlinear problem with an unknown moving boundary includes, as an example, a mathematical model of one-phase Stefan problem with the latent heat accumulation memory. The posed problem is approximated by the backward Euler mesh scheme. The unique solvability of the mesh scheme is proved and a priori estimates for the solution are obtained. The properties of the mesh problem are studied, in particular, an estimate of movement rate for the mesh phase transition boundary is established. The proved estimate make it possible to localize the phase transition boundary and split the mesh scheme into the sum of a nonlinear problem of small algebraic dimension and a larger linear problem. This information can be used for further construction of efficient algorithms for implementing the mesh scheme. Several algorithms for implementing mesh scheme are briefly discussed.

Keywords: Phase transition problem, time-fractional derivative, finite difference scheme, a priori estimates, domain decomposition, iterative solution method

MSC 2010: 65M06, 65M12, 65M22

1. Introduction

Nonlinear problems with a moving boundary are one of the most important areas in partial differential equations. Boundary value problems of this type describe the process of a solid–liquid phase transition (problems of the Stefan type), transport of dissolved substances, molecular diffusion, and other phenomena.

The classical one-phase Stefan problem establishes that the temperature u is described by the heat equation and the movement of phase transition boundary $x = s(t)$ is characterized by the Stefan condition:

$$\begin{aligned} \rho c\,\frac{\partial u}{\partial t}(x,t) &= k\,\frac{\partial^2 u}{\partial x^2}(x,t), \quad 0 < x < s(t), \quad t > 0 \\ \rho L\frac{\mathrm{d}s}{\mathrm{d}t} &= -k\frac{\partial u}{\partial x}(s(t)^-,t), \quad t > 0. \end{aligned} \tag{1.1}$$

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This research was supported by the Russian Science Foundation, project No. 20-61-46017.

The constant parameters ρ, k, c, and L represent the material density, the thermal conductivity, the specific heat, and the latent heat in the liquid phase.

It has been experimentally noted that in many systems thermal conductivity does not obey the Fourier law underlying the classical model. Recently, fractional derivatives have been used to model such problems. Various mathematical models with fractional Caputo or Riemann–Liouville derivatives of order $\alpha \in (0,1)$ have been proposed (see [5, 4]), and their analytical solutions have been constructed. For example, a fractional-order problem with a time-fractional Caputo derivative $\mathscr{D}_t^\alpha$ was formulated as follows:

$$\begin{aligned} \rho c\,\mathscr{D}_t^\alpha u(x,t) &= k\frac{\partial^2 u}{\partial x^2}(x,t), \quad 0 < x < s(t), \quad t > 0 \\ \rho L \mathscr{D}_t^\alpha s &= -k\frac{\partial u}{\partial x}(s(t)^-,t), \quad t > 0 \end{aligned} \tag{1.2}$$

where

$$\mathscr{D}_t^\alpha v(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t (t-z)^{-\alpha}\frac{\partial v}{\partial z}(z)\,\mathrm{d}z$$

is Caputo derivative, $\Gamma(x)$ is gamma-function.

The problems (1.1) and (1.2) are so-called sharp interface models of classical and time-fractional one-phase Stefan problems, respectively. Within the framework of these models, the enthalpy (the sum of latent and sensible heat) at any point in the domain is determined by the expression

$$H(x,t) = \{\rho c u \ \text{ if } \ x > c; \ \ \rho c u + L \ \text{ if } \ x \leqslant s\}.$$

To correctly reflect the physical properties of a material, the diffusion interface model is used, which contains a 'regularized' enthalpy function $H_\varepsilon(x,t)$. The diffusion interface model for fractional problem is formulated in a fixed domain $(0,X)\times(0,T]$:

$$\mathscr{D}_t^\alpha H_\varepsilon = \frac{\partial^2 T}{\partial x^2}, \quad 0 < x < X, \quad t > 0. \tag{1.3}$$

Function $H_\varepsilon(x,t)$ is continuous and tends to $H(x,t)$ at $\varepsilon \to 0$. Note that in the case of the classical Stefan problem, the solutions of the diffusion interface model converge to the solutions of the sharp interface model when $\varepsilon \to 0$, but this is generally not true for the fractional diffusion model (1.3) and sharp model (1.2). A review of time-fractional Stefan problems, which were considered for modelling anomalous phase transitions, is given in [4].

The numerical solution of time-fractional one-phase and two-phase Stefan problems is the subject of [1] and [2], respectively. In these researches, the one-dimensional problems in sharp interface formulations are solved by the front tracking method.

In the present article, we use a problem statement containing a multivalued enthalpy function H, although all results can be easily adapted to the case of a regularized function. It should also be noted that the mesh approximations of H and H_ε practically coincide when ε is much smaller than the mesh steps.

We consider a two-dimensional nonlinear problem containing the Laplace operator in space variables and an integro-differential operator in time. This problem includes the enthalpy formulation of the one-phase Stefan problem with fractional time derivative. The posed nonlinear problem with unknown moving (phase transition) boundary is approximated by backward Euler mesh scheme. The unique solvability of the mesh problem is proved and a priori estimates for the solutions are obtained. An estimate of movement rate for the mesh phase transition boundary is given. Thanks to this estimate, at each computational time layer, it is possible to single out a ‘narrow’ strip from the mesh domain containing an unknown moving boundary, i.e. actually containing a nonlinear term of the problem. This allows us to split the finite difference scheme into a non-linear problem of small algebraic dimension and a larger linear problem with further use of domain decomposition methods for the numerical implementation of the finite difference scheme. The results on the estimation of of movement rate for the mesh phase transition boundary are largely based on and develop the results of the papers [6, 7, 8], in particular, [6], where the finite-difference approximation of the classical one-phase Stefan problem with integer time derivative was studied.

2. Formulation of the problem

Define a first-order fractional derivative of an absolutely continuous function $y(t):(0,T)\to\mathbb{R}$ in such a way

$$\mathscr{D}_t y(t) = \int_0^t G(t-s)\frac{\partial y}{\partial s}(s)\,\mathrm{d}s \tag{2.1}$$

$$\begin{gathered} G(t):(0,+\infty)\to\mathbb{R}^+ \text{ is continuous, } \int_0^\tau G(t)\,\mathrm{d}t<\infty \quad \forall\tau>0 \\ G(t) \text{ decreases and strictly decreases at the point } t=0. \end{gathered} \tag{2.2}$$

Examples of derivatives that satisfy the above conditions are, for example, the classical and generalized Caputo derivatives, the multiterm derivative, the Caputo–Fabrizio derivative, etc.

Next, define the multivalued function

$$H(t)=\big\{0 \text{ for } t<0;\ [0,L] \text{ for } t=0;\ t+L \text{ for } t>0\big\} \tag{2.3}$$

that is used to determine the enthalpy function in a one-phase Stefan-type problem.

Let $\Omega=(0,1)\times(0,1)$ with the boundary $\partial\Omega=\sum_{i=1}^3\Gamma_i$, where $\Gamma_1=\{x\in\partial\Omega: x_1=0\}$ and $\Gamma_3=\{x\in\partial\Omega: x_1=1\}$, and let $\bar{n}$ be the outward normal vector to the boundary, Δ means Laplace operator.

Consider the following differential problem:

$$\begin{cases} \mathscr{D}_t \xi - \Delta u = 0, \quad \xi \in H(u), \quad (x,t) \in \Omega \times (0,T] \\ u = \vartheta(x_2) \geqslant 0, \quad (x,t) \in \Gamma_1 \times (0,T] \\ u = 0, \quad (x,t) \in \Gamma_3 \times (0,T] \\ \dfrac{\partial u}{\partial n} = 0, \quad (x,t) \in \Gamma_2 \times (0,T] \\ \xi = 0, \quad (x,t) \in \Omega \times \{t = 0\}. \end{cases} \tag{2.4}$$

The formulated problem can be interpreted as a mathematical model corresponding to the process of melting a substance with a solid initial state, phase transition temperature $u = 0$ and initial value of the enthalpy function $H(u) = 0$. A positive temperature $\vartheta(x_2)$ is specified on a part Γ_1 of the boundary, there are no internal heat sources, and the thermal insulation conditions are satisfied at the boundary Γ_2. If instead of the fractional derivative $\mathscr{D}_t$ in the differential equation we put an integer derivative $\partial \xi / \partial t$, then we get the enthalpy formulation of the classical one-phase Stefan problem.

We do not discuss the question of the existence of a solution to problem (2.4), which seems to be an open problem, paying attention only to the construction of its mesh approximation, the study of the properties of this discrete problem and approaches to its numerical implementation.

3. Mesh scheme and properties of its solution

We approximate problem (2.4) by an implicit (backward Euler) finite difference scheme on a uniform mesh.

To approximate the time-fractional derivative, the well-known $L1$-approximation is used. Namely, a function $y(t) : [0,T] \to \mathbb{R}$ is replaced by the continuous and piecewise linear function with nodal values $y^k = y(t_k)$ at $t_k \in \omega_\tau = \{t_k = k\tau, k = 0,1,\dots,N_t\}$, whence

$$\mathscr{D}_t y(t_k) \approx \partial_t \bar{y}^k = \sum_{j=1}^{k} d_{k+1-j}(y^j - y^{j-1}) = d_1 y^k + \sum_{j=1}^{k-1} (d_{j+1} - d_j) y^{k-j} - d_k y^0 \tag{3.1}$$

with $\bar{y}^k = (y^0, y^1, \dots, y^k)$ and the coefficients

$$d_j = d_j(\tau) = \frac{1}{\tau} \int_{t_{k-j}}^{t_{k-j+1}} G(t_k - s)\, \mathrm{d}s = \frac{1}{\tau} \int_{(j-1)\tau}^{j\tau} G(s)\, \mathrm{d}s.$$

The properties (2.2) imply the inequalities

$$d_1 > d_2 \geqslant d_3 \geqslant \dots \geqslant d_{N_t} \geqslant 0. \tag{3.2}$$

It should be noted that in the case of approximation of the classical derivative $\partial y/\partial t$, the coefficients equal $d_1 = 1/\tau$ and $d_2 = \cdots = d_{N_t} = 0$, while in the case of Caputo derivative $\mathscr{D}_t^{\alpha} y(t)$ the coefficients are

$$d_j = \frac{1}{\tau^{\alpha}\Gamma(2-\alpha)} \left(j^{1-\alpha} - (j-1)^{1-\alpha} \right)$$

so, $d_1 > d_2 > \cdots > d_{N_t}$.

To approximate the elliptic part of the problem we construct on $\bar{\Omega} = \Omega \cup \Gamma$ a uniform mesh $\bar{\omega}$ with step $h > 0$. Let $\omega = \bar{\omega} \cap \Omega$ be the set of the internal mesh points, and the mesh boundary $\partial\omega \cap \Gamma$ consists of three parts:

$$\gamma_1 = \partial\omega \cap \{x_1 = 0\}, \quad \gamma_3 = \partial\omega \cap \{x_1 = 1\}, \quad \gamma_2 = \partial\omega \setminus (\gamma_1 \cup \gamma_3).$$

We introduce the difference quotients $\partial_i u(x) = h^{-1}\big(u(x+e_i h) - u(x)\big)$ and $\bar{\partial}_i u(x) = h^{-1}\big(u(x) - u(x-e_i h)\big)$, where $e_1 = (1,0)$, $e_2 = (0,1)$. For the points $x \in \omega \cup \gamma_2$ and mesh functions $u(x)$ vanishing at the points $x \in \gamma_1 \cup \gamma_3$ we define finite difference expression

$$Au(x) = \begin{cases} -\partial_1\bar{\partial}_1 u(x) - \partial_2\bar{\partial}_2 u(x), & x \in \omega \\ -\partial_1\bar{\partial}_1 u(x) - \dfrac{2}{h}\partial_2 u(x), & x \in \gamma_2 \cap \{x_2 = 0\} \\ -\partial_1\bar{\partial}_1 u(x) + \dfrac{2}{h}\bar{\partial}_2 u(x), & x \in \gamma_2 \cap \{x_2 = 1\}. \end{cases}$$

Let also $f(x) = h^{-2}\vartheta(x - he_1)$ at the mesh points x, adjacent to γ_1 in the sense that $x - he_1 \in \gamma_1$, and $f(x) = 0$ at all other mesh points.

Let us assign a one-to-one correspondence to the mesh function defined at the nodes $\omega \cup \gamma_2$ with the vector of its nodal values. We denote by n the dimension of the corresponding vector space and use the same notation for mesh functions and vectors from $\mathbb{R}^n$ of their nodal values, as well as for linear mesh operators and $n \times n$ matrices.

In accordance with this convention, we can write a finite difference scheme that approximates the (2.4) problem as the following nonlinear problem in $\mathbb{R}^n$: Given vector $\xi^0 = 0$, for $k = 1, 2, \ldots N_t$ find $(u^k, \xi^k) \in \mathbb{R}^n \times \mathbb{R}^n$ such that

$$\partial_t \bar{\xi}^k + Au^k = f, \quad \xi^k \in H(u^k). \tag{3.3}$$

Before examing the mesh scheme (3.3) we present some auxiliary results. Define the norms $\|u\|_\infty = \max_{1\leqslant i\leqslant n} |u_i|$, $\|u\|_1 = \sum_{i=1}^n |u_i|$ on the space $\mathbb{R}^n$. We use the notation $u \ll v$ for the vectors u and v, when $u_i \leqslant v_i$ for all i. Let also f^+ be the vectors with positive parts of the coordinates of vector f. We call an operator B a diagonal maximal monotone operator if $Bu = \mathrm{diag}(b_1(u_1), b_2(u_2), \ldots, b_n(u_n))$ and each $b_i(u_i)$ is maximal monotone (multivalued) operator in $\mathbb{R}^1$ (on the theory of maximal monotone operators, see, e.g., [3], Chap. II).

In what follows, we will make essential use of the following lemmas.

Lemma 3.1. *Let C be an $n \times n$ M-matrix and $B : \mathbb{R}^n \to \mathbb{R}^n$ be a diagonal maximal monotone operator, i.e., $Bu = \mathrm{diag}(b_1(u_1), b_2(u_2), \ldots, b_n(u_n)$ and $b_i(u_i)$ is a maximal monotone in $\mathbb{R}^1$.*

Then for any $f \in \mathbb{R}^n$ there exists a unique solution of the equation (inclusion)

$$Cu + Bu \ni f. \tag{3.4}$$

If u_1 and u_2 are the solutions of equation (3.4) *with the right-hand sides f_1 and f_2, then*

$$u_1 - u_2 \ll C^{-1}(f_1 - f_2)^+. \tag{3.5}$$

The proof of the formulated results follows from Theorem 6.1 in [9].

Lemma 3.2. *Let $C \in \mathbb{R}^{n\times n}$ be a diagonally dominant in columns M-matrix and $\psi_i(t), i = 1, 2, \ldots, n$, be non-decreasing Lipschitz functions.*

Then problem

$$\xi + Cu = f, \quad u_i = \psi_i(\xi_i) \tag{3.6}$$

has a unique solution $\xi \in \mathbb{R}^n$ for all $f \in \mathbb{R}^n$.

If ξ_1 and ξ_2 are the solutions of (3.6) *with right-hand sides f_1 and f_2, respectively, then*

$$\|\xi_1 - \xi_2\|_1 \leqslant \|f_1 - f_2\|_1. \tag{3.7}$$

Proof. The inverse to ψ_i functions ψ_i^{-1} are maximal monotone in $\mathbb{R}^1$ due to the properties of ψ_i. Define a diagonal maximal monotone operator

$$Bu = \mathrm{diag}(\psi_1^{-1}(u_1), \psi_2^{-1}(u_2), \ldots, \psi_n^{-1}(u_n)).$$

Then equation (3.6) can be written in the equivalent form of inclusion $Cu + Bu \ni f$. Applying Lemma 3.1 proves the existence of a unique solution u of this inclusion, and $\xi = f - Cu$ is the unique solution of (3.6).

Let us take the right-hand sides in (3.6) such that $f_1 \gg f_2$. By virtue of Lemma 3.1 and the connection between the problems (3.6) and (3.4) noted above, the inequality $\xi_1 \gg \xi_2$ holds. Define the vector $\nabla u = \nabla u(\xi_1, \xi_2)$ with coordinates

$$\nabla u_i = \begin{cases} \dfrac{\psi_i(\xi_{1i}) - \psi_i(\xi_{2i})}{\xi_{1i} - \xi_{2i}}, & \text{if } \xi_{1i} \neq \xi_{2i} \\ 0, & \text{otherwise} \end{cases}$$

and the diagonal matrix $D \gg 0$ with elements $d_{ii} = \nabla u_i \geqslant 0$. The vector $\xi_1 - \xi_2$ satisfies the equation

$$\xi_1 - \xi_2 + AD(\xi_1 - \xi_2) = f_1 - f_2.$$

Let us denote the elements of the matrix A as a_{ij} , then the elements c_{ij} of $I+AD$ equal

$$c_{ii}=1+a_{ii}\nabla u_i,\quad c_{ji}=a_{ji}\nabla u_i,\quad \text{where } a_{ii}>0,\quad a_{ji}\leqslant 0,\quad a_{ii}+\sum_{j\neq i}a_{ji}\geqslant 0. \tag{3.8}$$

The properties (3.8) provide the inequality $\|(I+AD)^{-T}\|_\infty\leqslant 1$. Indeed, let us denote by x the solution of the equation $(I+AD)^T x=y$ with $\|y\|_\infty=1$ and prove that $\|x\|_\infty\leqslant 1$. Let $|x_i|=\max_j|x_j|$, then

$$1\geqslant|y_i|\geqslant(1+a_{ii}\nabla u_i)\big|x_i\big|-\sum_{j\neq i}\big|a_{ji}\nabla u_i\big|\cdot\big|x_j\big|\geqslant\Big(1+a_{ii}\nabla u_i+\sum_{j\neq i}a_{ji}\nabla u_i\Big)\big|x_i\big|\geqslant|x_i|.$$

Now, by duality of the norms $\|\cdot\|_\infty$ and $\|\cdot\|_1$, the inequality $\|(I+AD)^{-T}\|_\infty\leqslant 1$ implies $\|(I+AD)^{-1}\|_1\leqslant 1$. Therefore,

$$\|\xi_1-\xi_2\|_1\leqslant\|f_1-f_2\|_1 \ \text{ in case of } \ f_1\gg f_2.$$

Let now f_1 and f_2 be arbitrary vectors. Define the vector f with the coordinates $f_i=\max\{f_{1i},f_{2i}\}$ and let ξ be the solution of (3.6) with this right-hand side. Since $f\gg f_1$ and $f\gg f_2$, it is proved that

$$\|\xi-\xi_1\|_1\leqslant\|f-f_1\|_1,\quad \|\xi-\xi_2\|_1\leqslant\|f-f_2\|_1$$

so, $|\xi_1-\xi_2\|_1\leqslant\|f-f_1\|_1+\|f-f_2\|_1=\sum_{i=1}^n(f_i-f_{1i}+f_i-f_{2i})$. But $f_i-f_{1i}+f_i-f_{2i}=|f_i^1-f_i^2|$, and inequality (3.7) is proved.

Let us return to the consideration of problem (3.3). Using the definition of $\partial_t\bar{\xi}^k$ we can rewrite the finite difference scheme (3.3) in the form of the following system: Given $\xi^0=0$, for $k=1,2,\dots N_t$ find (u^k,ξ^k) such that

$$d_1\xi^k+Au^k=\sum_{j=1}^{k-1}(d_{j+1}-d_j)\xi^{k-j}+f,\quad \xi^k\in H(u^k). \tag{3.9}$$

By construction, matrix A and operator H satisfy the following properties:

$$\begin{gathered} A \ \text{ is symmetric diagonally dominant } M\text{-matrix} \\ \text{with positive diagonal and nonpositive off-diagonal elements;} \end{gathered} \tag{3.10}$$

$$H \ \text{ is a maximal monotone and diagonal operator.} \tag{3.11}$$

Theorem 3.1. *Mesh scheme* (3.3) *has a unique solution or, equivalently, system* (3.9) *has a unique solution* (u^k,ξ^k) *for any* $k=1,2,\dots N_t$.

Let (u_1^k,ξ_1^k) *and* (u_2^k,ξ_2^k) *be the non-negative solutions to problem* (3.9) *with the right-hand sides* f_1^k *and* f_2^k. *Then for all* $k\geqslant 1$

$$\|\xi_1^k-\xi_2^k\|_1\leqslant d_1^{-1}\sum_{i=1}^k\|f_1^i-f_2^i\|_1,\qquad \|u_1^k-u_2^k\|_1\leqslant d_1^{-1}\sum_{i=1}^k\|f_1^i-f_2^i\|_1. \tag{3.12}$$

Proof. The unique solvability of (3.9) follows from the properties (3.10), (3.11) of the matrix A and the operator H, as well as from Lemma 3.1.

Now, let us prove the a priori estimates (3.12). In case of the non-negative solutions the function $H(t)$ in the formulation of problem (3.9) can be formally replaced with the function

$$\widetilde{H}(t) = \{(-\infty, L] \text{ if } t = 0;\ t + L \text{ if } t > 0\}.$$

The inverse of $\widetilde{H}$ is the non-decreasing and Lipschitz function $\psi(t)$. So, (u_1^k, ξ_1^k) and (u_2^k, ξ_2^k) are the solutions of the problem

$$\xi^k + d_1^{-1} A u^k = d_1^{-1} \sum_{j=1}^{k-1} (d_j - d_{j+1}) \xi^{k-j} + d_1^{-1} f^k, \quad u_i^k = \psi(\xi_i^k) \tag{3.13}$$

with right-hand sides $f^k = f_1^k$ and $f^k = f_2^k$. The matrix $d_1^{-1}A$ and the function $\psi(t)$ satisfy the assumptions of Lemma 3.2, and we can apply the estimate (3.7). For $k = 1$ we immediately obtain

$$\|\xi_1^1 - \xi_2^1\|_1 \leqslant d_1^{-1} \|f_1^1 - f_2^1\|_1 = F^1.$$

Let now the inequality

$$\|\xi_1^j - \xi_2^j\|_1 \leqslant d_1^{-1} \sum_{i=1}^{j} \|f_1^i - f_2^i\|_1 = \sum_{i=1}^{j} F^i$$

is proved for all $j \leqslant k-1$ and prove it for k. Using the assumption of induction and the properties (3.2) of the coefficients d_j, we get

$$\begin{aligned}\|\xi_1^k - \xi_2^k\|_1 &\leqslant d_1^{-1} \sum_{j=1}^{k-1} (d_j - d_{j+1}) \|\xi_1^{k-j} - \xi_2^{k-j}\|_1 + d_1^{-1} \|f_1^k - f_2^k\|_1 \\ &\leqslant d_k^{-1} \sum_{j=1}^{k-1} \sum_{i=1}^{k-j} (d_j - d_{j+1}) F^i + F^k = d_k^{-1} \sum_{i=1}^{k-1} F^i \sum_{j=1}^{k-i} (d_j - d_{j+1}) + F^k \leqslant \sum_{i=1}^{k} F^i.\end{aligned}$$

Thus, the first estimate (3.12) is proved. It remains to use the Lipschitz continuity of $\psi(t)$ with constant 1 to derive from this estimate an estimate for $\|u_1^k - u_2^k\|_1$.

Remark 3.1. Introduce the mesh norms

$$\|y\|_{L^1(\omega_\tau; L^1(\bar{\omega}))} = \sum_{k=1}^{N_t} \tau \|y^k\|_1, \qquad \|y\|_{L^\infty(\omega_\tau; L^1(\bar{\omega}))} = \max_{1 \leqslant k \leqslant N_t} \|y^k\|_1.$$

Then the estimates (3.12) can be written as follows:

$$\|\xi_1 - \xi_2\|_{L^\infty(\omega_\tau; L^1(\bar{\omega}))} \leqslant (d_1 \tau)^{-1} \|f_1 - f_2\|_{L^1(\omega_\tau; L^1(\bar{\omega}))}$$

$$\|u_1 - u_2\|_{L^\infty(\omega_\tau;L^1(\bar\omega))} \leqslant (d_1\tau)^{-1}\|f_1 - f_2\|_{L^1(\omega_\tau;L^1(\bar\omega))}.$$

In case of problem with integer time derivative the constant in these estimates equals $(d_1\tau)^{-1} = 1$, while in case of problem with Caputo time derivative of order $\alpha \in (0,1)$ it is $(d_1\tau)^{-1} = \text{const}\,\tau^{\alpha-1}$. This is the usual deterioration of the stability estimate as the order α decreases.

4. Estimate of the movement rate of the mesh phase transition boundary

Lemma 4.1. *The following inequalities take place:*

$$u^k \gg u^{k-1} \gg 0, \quad \xi^k \gg \xi^{k-1} \gg 0 \quad \forall k \geqslant 1. \tag{4.1}$$

Proof. We prove the statement by induction. Since for $k = 1$ equation (3.9) becomes $d_1\xi^1 + Au^1 = f \gg 0$ and the pair $(0,0)$ is the solution of the equation $d_1\xi + Au = 0$, then $u^1 \gg 0$ by (3.5) and $\xi^1 \gg 0$ by its definition. Suppose the inequalities (4.1) are true for all $j \leqslant k-1$, $k > 1$, and prove them for k. From (3.9) we have

$$d_1H(u^k) + Au^k \ni \Phi^k = \sum_{j=1}^{k-1}(d_j - d_{j+1})\xi^{k-j} + f$$

where $d_j - d_{j+1} \geqslant 0$ by (3.2) and $\xi^{k-j} \gg 0$ by the induction hypothesis. Then $\Phi^k \gg \Phi^{k-1}$ whence the inequality $u^k \gg u^{k-1}$ due to (3.5).

It remains to prove inequality $\xi^k \gg \xi^{k-1}$, which we will do using the contradiction method. Let there exists i such that $\xi_i^k - \xi_i^{k-1} < 0$. Since $u_i^k \geqslant u_i^{k-1} \geqslant 0$ and the function $H(t)$ is strictly increasing for $t \geqslant 0$, then the inequality $\xi_i^k - \xi_i^{k-1} < 0$ can take place only at the point $t = 0$ of its multivaluedness, whence, $u_i^k = u_i^{k-1} = 0$. Then $A(u^k - u^{k-1})_i \leqslant 0$ due to the properties of the matrix A, and together with the inequalities $d_1(\xi^k - \xi^{k-1})_i < 0$, $\Phi_i^k - \Phi_i^{k-1} \geqslant 0$ this contradicts to the equality $d_1(\xi^k - \xi^{k-1})_i + A(u^k - u^{k-1})_i = \Phi_i^k - \Phi_i^{k-1}$.

Define the mesh neighbourhood of the point $x^* \in \bar\omega$ as the set $\eta(x*) = \{x \in \bar\omega : x = x^* \pm e_ih\}$. A set $D \subset \bar\omega$ is called connected if for any two points $x', x'' \in D$ there exists a sequence of the mesh nodes $x_i \in D$ such that

$$x' \in \eta(x_1),\ x_1 \in \eta(x_2), \dots, x_n \in \eta(x'')$$

and $\partial D = \{x \in \bar\omega \setminus D : \eta(x) \cap D \neq \varnothing\}$ is the boundary of the set $D \subseteq \omega \cup \gamma_2$.

The properties of A imply the validity of the maximum principle: if $D \subset \omega \cup \gamma_2$ is a connected mesh set with the boundary ∂D and internal nodes int$D$, then

$$Au(x) \leqslant 0\ \ \forall x \in D \ \Rightarrow\ \max_{x\in D} u(x) \leqslant \max_{x\in\partial D} u(x) \tag{4.2}$$

$$Au(x) \geqslant 0\ \ \forall x \in D \ \Rightarrow\ \min_{x\in D} u(x) \geqslant \min_{x\in\partial D} u(x). \tag{4.3}$$

Let (u^k, ξ^k) be the solution of problem (3.9) at the time layer t_k. Define the sets $\omega_0(t_k) = \{x \in \omega \cup \gamma_2 : u^k = 0\}$ and $\omega_+(t_k) = \{x \in \omega \cup \gamma_2 : u^k > 0\}$, and let $S(t_k) = \{x \in \omega_0(t_k) : \eta(x) \cap \omega_+(t_k) \neq \varnothing\}$ be the mesh boundary of the phase transition at a time t_k (mesh 'curve', separating $\omega_0(t_k)$ and $\omega_+(t_k)$.) Since $\omega_+(0) = \varnothing$, we can assume that $S(t_0)$ coincides with γ_1 at time $t = 0$.

The main result of this paragraph is given by the following theorem:

Theorem 4.1. *For the mesh problem* (3.9) *we have:*

1. *The sets $\omega_0(t_k)$ and $\omega_+(t_k)$ are connected and*

$$\omega_+(t_{k-1}) \subseteq \omega_+(t_k). \tag{4.4}$$

2. *The distance between $S(t_{k-1})$ and $S(t_k)$ is estimated as*

$$\rho(x, S(t_{k-1})) \leqslant \max\{Cd_1^{-1}, h\} \quad \forall x \in S(t_k) \tag{4.5}$$

where the constant C is determined by an explicit formula through the input data of the problem.

Proof. 1. The set-theoretic inclusion (4.4) follows from the inequalities (4.1).

Next we prove that for all k the mesh function $\xi^k = 0$ at the internal points of $\omega_0(t_k)$. First, let $k = 1$. The right side $f(x)$ is positive at the nodes of γ_1^+ adjacent to the boundary γ_1, whence these points lie in $\omega_+(t_1)$. Let x^* is an internal point of $\omega_0(t_1)$, then $\eta(x^*) \cap \gamma_1^+ = \varnothing$. At the point x^*, the right side $f(x^*) = 0$, $\xi^0(x^*) = 0$ and $Au^1(x^*) = 0$ since the stencil of the mesh operator A coincides with $\eta(x^*)$. As a consequence,

$$d_1 \xi_i^1(x^*) + Au^1(x^*) - f(x^*) = d_1 \xi_i^1(x^*) = 0 \;\Rightarrow\; \xi_i^1(x^*) = 0.$$

Further we proceed by induction. For $k > 1$ let x^* is an internal point of $\omega_0(t_k)$, then

$$d_1 \xi^k(x^*) - \sum_{j=1}^{k-1} (d_j - d_{j+1}) \xi^{k-j}(x^*) + Au^k(x^*) - f(x^*) = 0.$$

But $Au^k(x^*) = f(x^*) = 0$, and for all $i < k$ the inclusion $\omega_+(t_i) \subseteq \omega_+(t_k)$ is true, whence $\xi^i(x^*) = 0$. Therefore, $\xi^k(x^*) = 0$ by virtue of the previous equality.

Suppose that the set $\omega_0(t_k)$ is disconnected, so there exists its subset D lying inside $\omega_+(t_k)$. Then by the previous results it follows that $\xi^i(x) = 0$ for all $i \leqslant k$ at the points of D. In addition $f(x) = 0$ because the points of D do not belong to γ_1^+. Thus, $Au^k(x) = 0$ at all $x \in D$ and $u^k(x) > 0$ at all points of ∂D. This contradicts (4.3).

Suppose now that the set $\omega_+(t_k)$ is disconnected, so there exists its subset D lying inside $\omega_0(t_k)$. Due to (4.1) $\xi^k \gg \xi^i$ for all $i < k$, so,

$$Au^k(x) = -d_1\xi^k(x) + \sum_{j=1}^{k-1}(d_j - d_{j+1})\xi^{k-j}(x) \leqslant 0$$

at all points $x \in D$ and $u^k(x) = 0$ on ∂D. This contradicts (4.2).

Thus, we have proved that the sets $\omega_0(t_k)$ and $\omega_+(t_k)$ are connected.

2. Let us prove the second assertion of the theorem by comparing, at a fixed time layer t_k, the solutions of problem (3.9) and the auxiliary problem, which can be considered as a finite-difference approximation of the classical one-phase Stefan problem with a time step d_1^{-1}.

   Using, as before, the nonnegativity of the solutions of problem (3.9), we replace the function $H(t)$ (2.3) in the formulation of the mesh problem with the function

$$G(t) + t + L, \text{ where } G(t) = \{-\infty, 0) \text{ if } t = 0; \ 0 \text{ if } t > 0\}$$

   which coincides with $H(t)$ for $t > 0$, and which non-negative part at $t = 0$ coincides with the range of $H(t)$. Thus, if (u^k, ξ^k) is a solution to (3.9), then u^k is also the solution of the problem

$$d_1u^k + Au^k + d_1(\widetilde{\xi}^k - \xi^{k-1}) = \sum_{j=1}^{k-1} d_{j+1}(\xi^{k-j} - \xi^{k-j-1}) + f - d_1L, \quad \widetilde{\xi}^k \in G(u^k). \tag{4.6}$$

   Consider along with problem (4.6) the following one:

$$d_1y^k + Ay^k + d_1(\zeta^k - \xi^{k-1}) = f - d_1L, \ \zeta^k \in G(y^k). \tag{4.7}$$

Since $\sum_{j=1}^{k-1} d_{j+1}(\xi^{k-j} - \xi^{k-j-1}) \geqslant 0$, then similarly to the previous part of the proof, we have

$$u^k \ll y^k, \quad \xi^k \ll \zeta^k.$$

This inequality means (taking into account (4.4)) that

$$\omega_+(t_{k-1}) \subseteq \omega_+(t_k) \subset \widetilde{\omega}_+(t_k), \quad \text{where } \widetilde{\omega}_+(t_k) = \{x \in \omega_h : y^k > 0\}. \tag{4.8}$$

But $G(y)$ is the subdifferential of the indicator function of the set $K = \{y \in \mathbb{R}^n : y \gg 0\}$, and problem (4.7) is a mesh approximation with the time step d_1^{-1} of the one-phase Stefan problem with integer time derivative on a fixed interval $[t_{k-1}, t_k]$, written in enthalpy form. This problem was thoroughly investigated in [6], in particular, the following estimate was obtained for the proximity of the phase transition boundaries $S(t_{k-1})$ and $\widetilde{S}(t_k) = \{x \in \omega_0(t_k) : \eta(x) \cap \widetilde{\omega}_+(t_k) \neq \varnothing\}$ on neighboring time layers:

$$\rho(x, S(t_{k-1})) \leqslant \max\{Cd_1^{-1}, h\} \quad \forall x \in \widetilde{S}(t_k). \tag{4.9}$$

The estimates (4.8) and (4.9) lead to (4.5).

5. Notes on the implementation of the mesh scheme

5.1. SOR method

The implementation of mesh scheme (3.9) for a fixed time layer k consists of the solution of the inclusion

$$d_1 H(u^k) + Au^k \ni \Phi^k, \quad \Phi^k = \sum_{j=1}^{k-1} (d_j - d_{j+1}) \xi^{k-j} + f \tag{5.1}$$

with symmetric and positive definite matrix A and maximal monotone and diagonal operator H. Taking these properties into account, a possible method for solving (5.1) is the SOR method (point or block variants). It converges for any relaxation parameter $\sigma \in (0,2)$ (see proof in [9]). The implementation of the point version of the SOR method is reduced to the sequential solution of one-dimensional inclusions of the form

$$h(t) + at \in b$$

with known b, $a > 0$, and multivalued function $h(t) = \{0 \text{ if } t < 0; [0,L] \text{ if } t = 0; L + t \text{ if } t > 0\}$. The inverse function $\psi = (h(t) + at)^{-1}$ is Lipschitz-continuous, and the solution $t = \psi(b)$ can be find directly. Thus, the implementation of the SOR method is very simple. The optimal relaxation parameter σ is unknown for the nonlinear problems, and we know from computational practice that it is close to the parameter of the corresponding linear problem. It is also known from the theory of the method for linear problems that the rate of convergence essentially depends on the accuracy of determining the optimal parameter and on the algebraic dimension of the problem.

5.2. Domain decomposition methods

The proved estimate (4.5) allows us to single out a rather small mesh subdomain $D_k \subset \bar{\omega}$ on the current time layer t_k, which contains an unknown moving boundary. Using this a priori information, various methods of domain decomposition can be constructed that allow solving a nonlinear problem only in D_k and a linear problem in the remaining, larger mesh subdomain. Therefore, applying an efficient method for solving linear algebraic equations and the SOR method only to a nonlinear problem of small algebraic dimension can lead to an efficient algorithm. In particular, in [6, 7, 8], the iteration-free domain decomposition methods for the mesh scheme approximating Stefan problems with integer time derivative were proposed and justified. A similar iteration-free domain decomposition method can be used for implementation of the mesh scheme for problem with a fractional time derivative. We will not describe this method, referring the interested reader to the cited papers.

5.3. A direct method for the mesh scheme approximating 1D problem

Consider the one-dimensional case of problem (2.4):

$$\begin{cases} \mathscr{D}_t \xi - \dfrac{\partial^2 u}{\partial x^2} = 0, \;\; \xi \in H(u), \quad (x,t) \in (0,1) \times (0,T] \\ u = \vartheta > 0 \text{ for } x = 0, t \in (0,T]; \;\; u = 0 \text{ for } x = 1, t \in (0,T] \\ \xi = 0, \quad t = 0. \end{cases} \tag{5.2}$$

Mesh scheme (5.1) for this problem contains tridiagonal matrix A and the function $H(t)$ given by (2.3).

It was established that the phase transition boundary moves to the right. Its position $S(t_{k-1})$ on the layer t_{k-1} is known and let it be a mesh node z_{k-1}, so that $u_i^{k-1} > 0$ for $i < z_{k-1}$ and $u_i^{k-1} = 0$ for $i \geqslant z_{k-1}$. The mesh function $\xi_i^{k-1} = u_i^{k-1} + L$ for $i < z_{k-1}$, ξ^{k-1} is in the range from zero to L at the node z_{k-1}, and $\xi_i^{k-1} = 0$ for $i > z_{k-1}$.

We are trying to find the mesh node, in which the phase transition boundary $S(t_k)$ is located, choosing a node z_k to the right of z_{k-1}. The criterion for determining the reliability of the selected point is as follows. If the selected node is to the right of the true point, then u^k to the left of z_k will be negative. If it is to the left of the true point, then ξ^k will be greater than L.

We can use the sweep method to solve systems of linear equations with tridiagonal matrix. On the direct sweep, we calculate the coefficients α_i and β_i for all $i = 1, 2, \dots, n$. Then we perform the search for the current boundary point $S(t_k)$, moving one step to the right along the mesh from the known $S(t_{k-1})$. It suffices to compute the values of u^k at only three grid points, including our hypothetical boundary point $\widetilde{z}$, by backsweep to determine the value of $\xi^k(\widetilde{z})$ at that point. Then, based on the analysis described above, we conclude that the true boundary point is found or it needs to be moved one step. After the true point $S(t_k)$ is found, we do a backward sweep and find u^k and ξ^k at all grid points. It is clear that in any case the execution of this algorithm requires $O(n)$ operations.

So, the proposed method has the same complexity as the sweep method for solving a system of linear algebraic equations with tridiagonal matrices.

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