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CONSERVATIVE METHOD FOR A MOVING BOUNDARY PROBLEM WITH KINETIC CONDITION

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1. Moving boundary problem with a kinetic condition

Non-equilibrium melting of a material can be described by a Stefan-like problem. Here, the classical Stefan condition of local thermodynamic equilibrium is replaced by a condition describing the kinetics of the phase interface movement.

Let $T \in R^+$ and put $\Omega =]0,1[$, $\Omega_T = \Omega \times]0,T[$. Now we formulate the problem under consideration in a classical way as introduced in [4].

Problem formulation. Let $c_l, c_s, k_l, k_s, L \in R^+$, $q_1(t), q_2(t) :]0,T[\mapsto \mathrm{R}$, $u_0(x) : \Omega \mapsto \mathrm{R}$, $s_0 \in \Omega$, and $\beta(u) : \mathrm{R} \mapsto \mathrm{R}$ are given data. Find a pair of functions $\{s(t), u(x,t)\}$, $u : \Omega_T \mapsto \mathrm{R}$, $s : [0,T] \mapsto \Omega$, where $s(t)$ defines the domains $\Omega_T^+ = \{(x,t) \in \Omega_T; x < s(t)\}$ and $\Omega_T^- = \{(x,t) \in \Omega_T; x > s(t)\}$, such that

$$c_l \frac{\partial u}{\partial t} - k_l \frac{\partial^2 u}{\partial x^2} = 0, \quad (x,t) \in \Omega_T^+, \tag{1}$$

$$c_s \frac{\partial u}{\partial t} - k_s \frac{\partial^2 u}{\partial x^2} = 0, \quad (x,t) \in \Omega_T^-, \tag{2}$$

$$k_l \frac{\partial u}{\partial x}(0,t) = q_1(t), \quad 0 < t < T, \tag{3}$$

$$k_s \frac{\partial u}{\partial x}(1,t) = q_2(t), \quad 0 < t < T, \tag{4}$$

$$u(x,0) = u_0(x), \quad x \in \Omega, \tag{5}$$

$$k_s \frac{\partial u}{\partial x}(s(t)+0) - k_l \frac{\partial u}{\partial x}(s(t)-0) = L \frac{\mathrm{d}s}{\mathrm{d}t}, \quad 0 < t < T, \tag{6}$$

$$\frac{\mathrm{d}s}{\mathrm{d}t} = \beta\left(u\left(s(t),t\right)\right), \tag{7}$$

$$s(0) = s_0. \tag{8}$$

The symbols $\frac{\partial u}{\partial x}(s(t) \pm 0)$ stand for corresponding one-side limits when $x \to s(t)_\pm$ and the subscripts l, s denote the liquid and solid phase, respectively.

Variational problem. Let us turn to the variational formulation of the above moving boundary problem. For this purpose, we introduce the spaces $V = H^1(\Omega)$, $W = L^2(\Omega)$ and suppose that $\beta \in C^0(\mathrm{R})$, $u_0 \in V'$, $0 < s_0 < 1$.

The variational problem is to find $u(x,t) \in L^2(0,T;V)$ and $s \in W^{1,1}(0,T)$ such that the following identities hold:

$$\int_0^1 c\,\frac{\partial u}{\partial t}\,v\,\mathrm{d}x + \int_0^1 k\frac{\partial u}{\partial x}\frac{\partial v}{\partial x}\,\mathrm{d}x + L\frac{\mathrm{d}s}{\mathrm{d}t}v(s) = q_2 v(1) - q_1 v(0) \quad \forall v \in V, \tag{9}$$

$$\text{a. e. in }]0,T[,$$

$$\left[\frac{\mathrm{d}s}{\mathrm{d}t} - \beta\left(u(s(t),t)\right)\right](\xi - s(t)) \geq 0, \quad 0 \leq \xi \leq 1, 0 \leq s(t) \leq 1, \tag{10}$$

$$\text{a. e. in, }]0,T[,$$

$$u(x,0) = u_0(x) \qquad \text{in } V', \tag{11}$$

$$s(0) = s_0. \tag{12}$$

The symbols c, k mean c_l, k_l in the liquid phase and c_s, k_s in the solid one. The existence of a solution to the above variational problem is proved in [4] assuming $c_l = c_s$, $k_l = k_s$ and $|\beta(\xi)| \leq C_1|\xi| + C_2$ for all real ξ.

2. Numerical method

The basis of the method we are going to present is the identity (9) and the Faedo–Galerkin approximation. A similar approach was also applied in the existence proof of [4] and used in [3] to solve the classical Stefan problem numerically.

We discretize Ω by a set of points $\mathcal{M} = \{x_0, x_1, \ldots, x_N\}$ that remain fixed for all the time. Upon the mesh we set up the piecewise linear basis functions and denote them by $\phi_0(x), \phi_1(x), \ldots, \phi_N(x)$. The unknown function $U(x,t)$ which is the approximation to the true solution $u(x,t)$ of (9)–(12) is then searched in the form

$$U(x,t) = \sum_{k=0}^{N} U_k(t)\phi_k(x). \tag{13}$$

Substituting (13) into (9)–(12) and approximating the space V of the test functions with $V_h = \text{span}\,\{\phi_0(x), \phi_1(x), \ldots, \phi_N(x)\}$ we obtain a system of ordinary differential equations for $\{U_0(t), U_1(t), \ldots, U_N(t)\}$ and the function $S(t)$ that approximates $s(t)$ in the form

$$\sum_{j=0}^{N}\int_0^1 c\phi_i\phi_j\,\mathrm{d}x\,\frac{\mathrm{d}U_j}{\mathrm{d}t}t = -\sum_{j=0}^{N}\int_0^1 k\frac{\partial\phi_i}{\partial x}x\frac{\partial\phi_j}{\partial x}x\,\mathrm{d}x\,U_j - L\frac{\mathrm{d}S}{\mathrm{d}t}\phi_i(S) + \tag{14}$$

$$+ q_2\,\phi_i(1) - q_1\,\phi_i(0), \quad i = 0,1,\ldots,N,$$

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \beta(U(S,t)), \tag{15}$$

$$U_i(0) = u_0(x_i), \quad i = 0,1,\ldots,N, \tag{16}$$

$$S(0) = s_0. \tag{17}$$

Here, the symbols c, k stand for c_l, k_l when $x < S(t)$ and for c_s, k_s when $x > S(t)$. The system (14)–(17) is then solved with some ODE stiff system solver. This algorithm will be called Algorithm 1 in what follows.

Note that the computed values of $S(t)$ generally do not coincide with the mesh points. Lynch and Sullivan [3], however, use a moving mesh which is deformed in such a way that at each time t their moving boundary $S(t)$ coincides with some mesh point.

Energy conservation. The phase change temperature is constant in the classical Stefan problem. However, it varies in case of a kinetic condition. Each point of the sample can melt at a different melting temperature and different points can have different specific internal energy consequently. Alexiades et al. in [1], assuming constant thermophysical properties, showed that the change of the total energy E of the sample can be expressed as

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \int_0^{s(t)} c_l \frac{\partial u}{\partial t}\,\mathrm{d}x + L\frac{\mathrm{d}s}{\mathrm{d}t} + \int_{s(t)}^1 c_s \frac{\partial u}{\partial t}\,\mathrm{d}x. \tag{18}$$

The amount of the total energy can be shown [1] to be

$$\begin{aligned} E \;=\; & \int_0^{s(T)} c_l\, u(\xi,T)\,\mathrm{d}\xi + \int_{s(T)}^1 c_s\, u(\xi,T)\,\mathrm{d}\xi - \int_0^{s(0)} c_l\, u(\xi,0)\,\mathrm{d}\xi - \\ & - \int_{s(0)}^1 c_s\, u(\xi,0)\,\mathrm{d}\xi + \int_0^T (c_s - c_l) u(s(\tau),\tau)\frac{\partial s}{\partial \tau}(\tau)\,\mathrm{d}\tau + L(s(T) - s(0)). \end{aligned} \tag{19}$$

The space V in (9) contains constant functions. Choosing $v \equiv 1$ in the identity (9) we find that the change of total energy equals to the net heat flow rate, as follows from (18). In Algorithm 1, we approximate the space V with V_h. If V_h also contains the constants, then it can be easily shown that the total energy conservation property holds for the approximate solution as well.

3. Experiments

We compare the above introduced Algorithm 1 to Algorithm 2 resulting from a front-fixing finite difference method in space [2] using the Landau transformation. The space-discretized problem is integrated in time by a standard stiff ODE solver.

Front-fixing finite difference method. We now describe Algorithm 2 in more detail. The Landau transformation changes the variables $x \to \xi = xs^{-1}(t)$ for $0 < x < s(t)$ and $x \to \eta = (x - s\,(t))\,(1 - s(t))^{-1}$ for $s(t) < x < 1$. The true solution

$u(x,t)$ is then decomposed into functions $\tilde{u}^l(\xi,t)$ and $\tilde{u}^s(\eta,t)$. The system (1)–(8) transforms into

$$c_l\tilde{u}^l_t - c_l\frac{\xi}{s}\frac{\mathrm{d}s}{\mathrm{d}t}\frac{\partial\tilde{u}^l}{\partial x} - \frac{k_l}{s^2}\frac{\partial^2\tilde{u}^l}{\partial x^2} = 0, \tag{20}$$

with the fixed boundary condition

$$k_l s^{-1}\frac{\partial\tilde{u}^l}{\partial x}|_{\xi=0} = q_1$$

and

$$c_s\tilde{u}^s_t - c_s\frac{1-\eta}{1-s}\frac{\mathrm{d}s}{\mathrm{d}t}\tilde{u}^s_\eta - \frac{k_s}{(1-s)^2}\tilde{u}^s_{\eta\eta} = 0, \tag{21}$$

with the fixed boundary condition

$$(k_s)(1-s)^{-1}\tilde{u}^s_\eta|_{\eta=1} = q_2.$$

On the moving boundary, we have the kinetic condition $\mathrm{d}s/\mathrm{d}t = \beta\left(\tilde{u}^l(1,t)\right)$, continuity condition $\tilde{u}^l(1,t) = \tilde{u}^s(0,t)$ and Stefan condition $k_s(1-s)^{-1}\tilde{u}^s_\eta - k_l s^{-1}\tilde{u}^l_\xi = L\mathrm{d}s/\mathrm{d}t$. The initial conditions are processed in a obvious way.

We create two meshes. One in the ξ-domain and the other in the η-domain. The meshes we use in Algorithm 2 are identical and equidistant. The number of nodes of each of the meshes will be $N/2+1$ for some even N. Hence, the degree of the ODE system resulting from Algorithm 2 is $N+2$, which is equal to that of Algorithm 1.

Results. We will solve two problems with known exact solutions numerically. For the purpose of comparison, we restrict ourselves to problems with the value of $u(s(t),t)$ equal to zero identically. This is achieved by a proper choice of β. We compute $S(t)$ and $U(S(t),t)$ and estimate the norms of the approximation errors $e_s(t) = S(t) - s(t)$, $e_u(t) = U(S(t),t) - 0$, namely $\|e_s\|_{C^0]0,T[}$ and $\|e_u\|_{C^0]0,T[}$. Moreover, we compute the relative disproportion in the energy

$$\delta E = \left| E\left(\int_{t_0}^{T} q_2(\tau) - q_1(\tau)\,\mathrm{d}\tau\right)^{-1} - 1\right|, \tag{22}$$

where E is defined by (19).

Experiment 1. We solve the problem (1)–(8) with the parameters given below:

$$\begin{aligned} q_1(t) &= -\mathrm{e}^{t+t_0}, \quad q_2(t) = 0, \quad 0 < t < T, \\ \beta(u) &= u + 1, \\ u_0(x) &= \begin{cases} \mathrm{e}^{t_0-x} - 1, & 0 < x < s_0, \\ 0, & s_0 < x < 1, \end{cases} \end{aligned}$$

where $T = 0.98$ and $s_0 = t_0 = 0.01$. All of the material constants c_l, c_s, k_l, k_s and L are equal to one.

The analytical solution to the above problem is the pair $\{s(t), u(x,t)\}$ where $s(t) = t_0 + t$ and

$$u(x,t) = \begin{cases} \mathrm{e}^{t+t_0-x} - 1, & 0 < x < s(t), \\ 0, & s(t) < x < 1. \end{cases} \tag{23}$$

The results are summarized in Table 1. The abbreviations "Alg 1" and "Alg 2" mean the Algorithm 1 or Algorithm 2, respectively. The value of N is the number of elements. In Algorithm 2, the number of subintervals in each of the ξ- and η-domains equals to $N/2$. Symbol e means the decadic order.

	δE		$\|e_s\|_{C]0,T[}$		$\|e_u\|_{C]0,T[}$	
N	Alg 2	Alg 1	Alg 2	Alg 1	Alg 2	Alg 1
12	1.5e-3	1.1e-6	1.1e-3	5.8e-3	4.4e-3	1.7e-2
24	3.3e-4	3.7e-7	2.5e-4	3.0e-3	1.0e-3	9.3e-3
50	4.6e-5	2.1e-7	4.8e-5	1.4e-3	2.4e-4	5.0e-3
100	3.8e-5	2.3e-7	2.3e-5	7.0e-4	8.6e-5	1.6e-3

Tab. 1: *Results of Experiment 1.*

Experiment 2 In this experiment, we modify the parameters of Experiment 1 in the following way:

$$\begin{aligned} q_1(t) &= -6\mathrm{e}^{2(t+t_0)}, \quad q_2(t) = -\mathrm{e}^{t+t_0-1}, \quad 0 < t < T, \\ u_0(x) &= \begin{cases} \mathrm{e}^{2(t_0-x)} - 1, & 0 < x < s_0, \\ \mathrm{e}^{t_0-x} - 1, & s_0 < x < 1. \end{cases} \\ \beta(u) &= u + 1. \end{aligned}$$

The values of T, s_0 and t_0 remain unchanged, the material constants are set to $c_l = 6$, $c_s = 1$, $k_l = 3$, $k_s = 1$, $L = 5$.

It can be easily verified that the solution is now the pair

$$\begin{aligned} u(x,t) &= \begin{cases} \mathrm{e}^{2(t+t_0-x)} - 1, & 0 < x < s(t), \\ \mathrm{e}^{t+t_0-x} - 1, & s(t) < x < 1, \end{cases} \\ s(t) &= t + t_0. \end{aligned}$$

The results are contained in Table 2. The meaning of the symbols is the same as in the previous experiment.

	δE		$\|e_s\|_{C]0,T[}$		$\|e_u\|_{C]0,T[}$	
N	Alg 2	Alg 1	Alg 2	Alg 1	Alg 2	Alg 1
12	3.7e-3	5.7e-6	5.8e-3	3.0e-3	2.2e-2	2.0e-2
24	5.9e-4	9.1e-6	1.3e-3	1.7e-3	4.8e-3	1.1e-2
50	5.1e-5	3.8e-7	2.6e-4	8.4e-4	1.1e-3	5.1e-3
100	7.2e-6	3.0e-6	4.6e-5	4.2e-4	2.7e-4	7.1e-4

Tab. 2: *Results of Experiment 2.*

4. Conclusion

Before we compare the results of the experiments we have to point out that since the principles of the discretization are completely different, the same amount of mesh points in both algorithms does not mean the same conditions.

The main advantage of Algorithm 1 is the property of the energy conservation. As can be seen in Table 1, the decadic order of the relative energy disproportion is two less than that of Algorithm 2. This holds also in Table 2 with the exception of $N = 100$. In that case, the relative energy disproportion in Algorithm 1 is still one half of that of Algorithm 2 approximately.

As for the approximation errors, it seems that Algorithm 2 provides us with more accurate results, since both of its approximation errors are less than the corresponding ones of Algorithm 1. This is true in both the experiments with the only exception of $N = 6$ in case of Experiment 2.

On the other hand, Algorithm 1 has an advantage if mesh adaptation is used. As can be seen in Sec. 2., the mesh $\mathcal{M}$ is completely independent of the moving boundary position $s(t)$. Then, refining the mesh can be done very easily.

References

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