On a special integro-differential problem occurring in diffusional phase transformation *

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Abstract

Nonlocal analysis in continuum mechanics typically require numerical treatment of integro-differential problems. This paper demonstrates a model stationary problem of this type, taken (after a sequence of simplifications) from the physical thick-interface model for diffusive and massive phase transformation in substitutional alloys. For certain sufficiently small nonlinear terms both the existence of solution and the convergence of a simple iterative algorithm can be verified using the finite difference method. Some practical applications, based on the original software code for numerical simulations and on the extensive experimental work, are available.

1 Introduction

Most problems from continuum mechanics, from the mathematical point of view, are formulated as boundary and/or initial problems for certain special classes of (ordinary or partial) differential equations. However, some considerations, typically those incorporating the thermal behaviour of material at high temperature, insert non-local (integral) terms into such equations, which brings complication both to the existence theory and to the design of effective algorithms for numerical simulations. Such one-dimensional stationary model problem, taken from [5], includes the physical analysis of diffusive and massive phase transformation in substitutional alloys for an arbitrary finite number $r+1$ of components where $r \in \{1, 2, \ldots\}$ under the assumption of the finite positive thickness h of the interface between two different material phases. It is needed to find a vector

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of molar fractions c of all components, in practice of all except the last one which are allowed to be completed a posteriori. Consequently $c(x)$ have values in the r-dimensional Euclidean space R^r where $0 \leq x \leq H$; $H > h$ is some positive length. We have to know all initial values c_0 as the values of c for $x = 0$ (where the phase transformation starts) and consider the interface for $x \leq h$ and the final phase for $x > h$.

The proper mathematical theory of diffusional phase transformation has been published only for very special cases, as in [4]. The general case with a non-negligible interface thickness and with $r > 1$ seems to be uncovered by any available mathematical literature. The aim of this paper is to demonstrate, at least for sufficiently small nonlinear terms, how the effective algorithm for numerical simulations can be suggested and how its mathematical correctness can be verified. An original MATLAB- (and partially also MAPLE-) supported software solver has been created; some numerical results have been presented in [5], a more extensive study (covering non-stationary analysis, interstitial components, etc.) is being prepared. All equations, discretization schemes, etc. (unlike those implemented in the software procedures), are simplified as much as possible to be transparent enough, but not to avoid substantial phenomena. Some (more or less standard) parts of proofs are only sketched or left to the reader's phantasy (or maybe to his better ideas); the author believes that this is justifiable for the workshop presentation (not for the scientific article).

2 Formulation of a model problem

The basic simplified differential equation for stationary phase transformation, in various forms repeated several times in [5], defined for $0 \leq x \leq H$, is

$$B(c)c' + K(c)c + vN(x)c = vN(x)c_0\,; \tag{1}$$

c' is the brief notation for $\mathrm{d}c/\mathrm{d}x$ and

$$v = \int_0^h \mu(c)\,\mathrm{d}x\,. \tag{2}$$

In this equation c has to be found from a subspace V of Sobolev space $W^{1,2}((0,H),R^r)$ satisfying $c(0) = c_0$; consequently c' belongs to the Lebesque space $L^2((0,H),R^r)$ and, by the Sobolev imbedding theorem, discussed in [1], p. 134, c is even absolutely continuous on $(0,H)$. The values of $\mu(c)$ are real numbers, supposed to be non-negative and lesser than M/h where M is a positive constant. Let us notice that consequently $0 \leq v \leq M$. Some additional assumptions must be accepted also for $B(c)$, $K(c)$ and $N(x)$, whose values are real square matrices of order r: B and K map V to the Lebesgue space $L^\infty((0,H),R^{r\times r})$, N can be taken from $L^\infty((0,H),R^{r\times r})$ directly.

Let $(.,.)$ denote a scalar product and (later) $\|.\|$ a norm in $L^2((0,H),R^r)$. Clearly (1) can be converted into its weak form

$$(\varphi, Bc') + (\varphi, Kc) + v(\varphi, N(c - c_0)) = 0 \tag{3}$$

for $\varphi \in W^{1,2}((0,H),R^r)$; the arguments c and x are omitted for brevity. For an arbitrary $s \in \{1,\dots,m\}$ let B_{s-1} denote the value of B for c_{s-1}, K_{s-1} the value of K for c_{s-1} and L_s the value of L for $s\delta$ where for simplicity the equidistant decomposition of $(0,H)$ into m subintervals is considered, $\delta = H/m$ and h coincides with some $s\delta$. Let us remark that such simplifying assumptions are not very realistic (because in practice h is much smaller than H), but could be removed easily in all following considerations. We can define, for $m \to \infty$, a sequence c^m with values $c_{s-1} + (c_s - c_{s-1})(x - x_{s-1})/\delta$ if $(s-1)\delta < x \le s\delta$, similarly a sequence $\tilde{c}^m$ with values c_{s-1} and a sequence $\bar{c}^m$ with values c_s.

Extending the notation in the natural way, we obtain (3) in general in a discretized form

$$\left(\varphi, \tilde{B}^m c'^m\right) + \left(\varphi, \tilde{K}^m \bar{c}^m\right) + v\left(\varphi, \bar{N}^m(\bar{c}^m - c_0)\right) = 0 \tag{4}$$

and for $(s-1)\delta < x \le s\delta$ only

$$\left(\varphi, B_{s-1}\frac{c_s - c_{s-1}}{\delta}\right) + (\varphi, K_{s-1}c_s) + v\left(\varphi, N_s(c_s - c_0)\right) = 0\,. \tag{5}$$

For a fixed v, ignoring (2), then it is easy to verify the solvability of each system (5): for every s we have only a system of linear algebraic equations and it is sufficient to suppose that $(\psi, B\varphi)$ are positive for each value of $B(.)$, $(\psi, K\varphi)$ are non-negative for each value of $K(.)$ and $(\psi, N\varphi)$ are non-negative for each value of $N(.)$ with every $\varphi, \psi \in W^{1,2}((0,H),R^r)$. Then the following analysis can contain two steps: i) the verification of convergence of c^m, etc., to c in corresponding function spaces for an arbitrary fixed v (in other words: the admissibility of the discretization scheme (4)), ii) the study of certain iteration algorithm taking (2) into account.

3 Calculation with a fixed integral term

Let us choose $\varphi = (c_s - c_{s-1})/\delta$ in (5). In the following text φ, ψ will denote arbitrary elements of $W^{1,2}((0,H),R^r)$. We know that there exists such positive β that $(\varphi, B(.)\varphi) \ge \beta\|\varphi\|^2$. In practice all values (as results of laboratory measurements) of $K(.)$ and $N(.)$ are bounded; this yields $(\psi, K(.)\varphi) \le \kappa\|\psi\|\|\varphi\|$ and $(\psi, N(.)\varphi) \le \nu\|\psi\|\|\varphi\|$ for some positive constants κ and ν. Thus we have

$$\beta\left\|\frac{c_s - c_{s-1}}{\delta}\right\|^2 \le \kappa\left\|\frac{c_s - c_{s-1}}{\delta}\right\|\|c_s\| + v\nu\left\|\frac{c_s - c_{s-1}}{\delta}\right\|\|c_s - c_0\|$$

and with respect to the obvious identity

$$c_s = c_0 + (c_1 - c_0) + \ldots + (c_s - c_{s-1})$$

consequently

$$\left\| \frac{c_s - c_{s-1}}{\delta} \right\| \leq \kappa \left\| c_0 \right\| + \delta(\kappa + M\nu) \sum_{q=1}^{s} \left\| \frac{c_q - c_{q-1}}{\delta} \right\| .$$

The discrete Gronwall-Bellman lemma, derived in [2], p. 719, guarantees the existence of a positive constant C, independent of m and s, for the estimate

$$\| \frac{c_s - c_{s-1}}{\delta} \| \leq C ;$$

this yields the boundedness of $c^{m\prime}$ and also of c^m in $L^2((0,H),R^r)$. We have moreover

$$\|c_s\| \leq \|c_0\| + \|c_1 - c_0\| + \ldots + \|c_s - c_{s-1}\| \leq \|c_0\| + s\delta C \leq C_*$$

where $C_* = \|c_0\| + HC$. Similar results can be thus received for $\tilde{c}^m$ and $\bar{c}^m$, too. Then the Eberlein-Shmul'yan theorem by [1], p. 197, implies that c^m convergs weakly to some $c \in V$; thanks to the continuity properties the same c is the strong limit of c^m, $\bar{c}^m$ and $\tilde{c}^m$ in $L^2((0,H),R^r)$ and (4) tends to (5).

4 Convergence of iterations

As the first estimate of c, denoted by c^0, we can (if no better information is available) extend c_0 to the whole interval $(0,H)$. Then we are allowed to apply some discrete version of (2), here that based on the Simpson rule for sufficiently large even $m = 2n$, to evaluate

$$v = \frac{\delta}{3} \left(\mu(c_0) + \mu(c_m) + 2 \sum_{q=1}^{m-1} \mu(c_q) + 2 \sum_{q=1}^{n} \mu(c_{2q-1}) \right) ; \qquad (6)$$

the upper indices 0 are omitted for simplicity, the resulting v has to be denoted by v^0. Consequently (5) is applicable to generate (for sufficiently large m by (4) again) c^1 satisfying the modified version of (3)

$$(\varphi, B^0 c^{1\prime}) + (\varphi, K^0 c^1) + v(\varphi, N(c^1 - c_0)) = 0 ; \qquad (7)$$

here we have briefly $B^0 = B(c_0)$, $K^0 = K(c_0)$. The recurrent use of this approach gives

$$(\varphi, B^1 c^{2\prime}) + (\varphi, K^1 c^2) + v(\varphi, N(c^2 - c_0)) = 0 , \qquad (8)$$

etc. We shall work formally with such two first equations only; the generalization is trivial.

We wish to expect that, at least for some appopriate B, K, N and μ, the above sketched approach based on (7), (8), etc., supported by evaluations of type (6), generates the sequences $c^0, c^1, c^2, \ldots$ and $v^0, v^1, v^2, \ldots$, whose limits are c and v from (3). However, it is not difficult to find (using the software support) rather simple counter-examples of divergence; evidently more additional assumptions are needed. We shall have arbitrary φ, ψ from $W^{1,2}((0,H),R^r)$ again and also any η, ζ from V. Let $\|.\|_\infty$ denote the norm in the Lebesgue space $L^\infty((0,H),R^r)$. We shall suppose

$$(\psi,(B(\eta)-B(\zeta))\varphi') \leq \beta_*\|\psi\|\|\varphi'\|\|\eta-\zeta\|_\infty\,, \qquad (\psi,(K(\eta)-K(\zeta))\varphi) \leq \kappa_*\|\psi\|\|\varphi\|\|\eta-\zeta\|_\infty$$

and also

$$|\mu(\eta)-\mu(\zeta)| \leq \mu_*|\eta-\zeta|$$

on $(0,h)$ with a simple consequence

$$\int_0^h |\mu(\eta)-\mu(\zeta)|\,\mathrm{d}x \leq \mu_* h\|\eta-\zeta\|_\infty\,. \tag{9}$$

Other group of useful assumptions is

$$(\varphi,B(.)\varphi') \geq \beta_0\left(|\varphi(h)|^2-|\varphi(0)|^2\right)-\beta_1\|\varphi\|^2\,, \qquad (\varphi,K(.)\varphi)\geq 0\,, \qquad (\varphi,N(.)\varphi)\geq 0\,.$$

The symbols β_*, κ_*, μ_*, β_0 and β_1 refer to some positive constants.

Let us set $\varphi = c^2-c^1$ and subtract (7) from (8). We receive

$$(c^2-c^1,B^1c^{2\prime}-B^0c^{1\prime})+(c^2-c^1,K^1c^2-K^0c^1)+(c^2-c^1,v^1Nc^2-v^0Nc^1)$$

$$=(v^1-v^0)(c^2-c^1,Nc_0)$$

and in a slightly rearranged form (seemingly more complicated, by useful for convergence estimates)

$$(c^2-c^1,B^1(c^{2\prime}-c^{1\prime}))+(c^2-c^1,K^1(c^2-c^1))+v^1(c^2-c^1,N(c^2-c^1))=$$

$$(v^1-v^0)(c^2-c^1,N(c_0-c^1))-(c^2-c^1,(B^1-B^0)c^{1\prime})-(c^2-c^1,(K^1-K^0)c^1)\,.$$

Applying, step by step, the above formulated assumptions, respecting that $c^1(0)=c^2(0)=c_0$, we obtain

$$\beta_0|c^2(H)-c^1(H)|^2 \leq \beta_1\|c^2-c^1\|^2$$

$$+\beta_*C\|c^2-c^1\|\|c^1-c^0\|_\infty+\kappa_*C_*\|c^2-c^1\|\|c^1-c^0\|_\infty+\mu_*h\nu C_*\|c^2-c^1\|\|c^1-c^0\|_\infty\,.$$

Using simple algebraic manipulations, namely $ab \leq (a^2 + b^2)/2$ for real a and b, we come to the result

$$|c^2(H) - c^1(H)|^2 \leq A_0 \int_0^h \|c^2 - c^1\|^2 \, \mathrm{d}x + A_1 \sup_{0 \leq x \leq H} |c^1(x) - c^0(x)|^2 \tag{10}$$

with

$$A_0 = \frac{\beta_1 + \varepsilon(\beta_* C + \kappa_* C_* + \mu_* h \nu C_*)}{\beta_0}, \qquad A_1 = \frac{4(\beta_* C + \kappa_* C_* + \mu_* h \nu C_*)}{\varepsilon \beta_0}$$

and any positive ε. Then the classical Gronwall lemma by [3], p. 52, gives

$$|c^2(H) - c^1(H)|^2 \leq A_1 \exp(A_0 H) \sup_{0 \leq x \leq H} |c^1(x) - c^0(x)|^2 .$$

The same can be repeated for $c^2(x) - c^1(x)$ instead of $c^2(H) - c^1(H)$. By (9) we have also

$$|v^1 - v^0| \leq \mu_* h \|c^1 - c^0\|_\infty ,$$

etc. One can see immediatelly that for sufficiently large β_0 and sufficiently small other above introduced constants the iteration process converges.

5 Conclusions and applications

Our convergence result needs relatively strong assumptions on small values of some coefficients or their parts. It could be even criticized not to cover any reasonable practicle problem. But, fortunately, the first rough (linear in certain sense) estimate of B is a unit matrix, K can be removed and h tends to zero, too: the interface thickness is much smaller than the size of the whole specimen. However, the whole physical problem was reduced dramatically in this paper; a lot of directions for generalizations is needed, their overview can be found in [6].

The results of [5] show that even relatively simple equations, as those presented in this paper, can give new both qualitative and quantitative results. Nevertheless, the validity of such results needs not only proper physical and mathematical analysis and development of effective software procedures, but also extensive experimental work. The characteristics B, K and μ, in fact very complicated functions of c, prepared automatically by symbolic software manipulations, are derived from chemical potentials, whose identification is rather difficult; the same is true for the interface mobility hidden in μ and diffusive characteristics contained in N. The still open questions are now intensively studied in the collaboration of the Montan University of Leoben (Austria), of the Institute of Physics of Materials (Czech Academy of Sciences, Brno), and of the Brno University of Technology.

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