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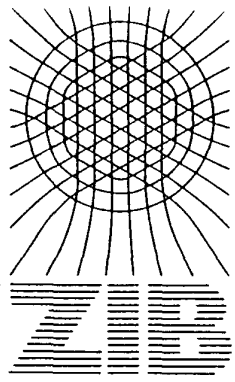

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Numerical Solution of Multicomponent Alloy Solidification by Multi-Grid Techniques

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Contents

Abstract

The solidification of an N–component alloy is described by an initial boundary value problem for a system of degenerate parabolic equations modelling heat conduction and mass diffusion. Discretizing implicitly in time and by piecewise linear finite elements in the space variables, at each time step the solution of a system of quasivariational inequalities is required. For the numerical solution of that system, a multi–grid algorithm is developed by making use of game theoretic concepts and duality arguments from convex analysis. Finally, the efficiency of the algorithm is demonstrated by displaying numerical results for a ternary alloy.

1. Introduction

The computation of the temperature distribution and the concentration profiles in the solidification of a multicomponent alloy plays a decisive role in the metallurgical industry, because the spatial distribution of the alloy components strongly affects the structural behaviour of the fully solidified workpiece. In this paper, we will be concerned with the numerical solution of a mathematical model taking into account heat conduction and mass diffusion. Since the occurrence of mushy regions, i.e., regions where we do have coexistence of liquid and solid regime, is a typical phenomenon in alloy solidification, that model is not based on the classical formulation of the process which assumes a sharp interface between the liquid and solid phase, but relies on a weak formulation in terms of an initial boundary value problem for a coupled system of degenerate parabolic equations (cf. e.g. BERMUDEZ, SAGUEZ [5], CROWLEY, OCKENDON [8] and FIX [11]). Note, however, that the weak formulation does not allow for a determination of the microstructure within the mushy region (see e.g. LACEY, OCKENDON, TAYLER [21] and the recent work of RAPPAZ [24] for microscopic modelling).

In existing work, in particular in the engineering literature, the difficulty to deal with degenerate parabolic equations is often circumvented by introducing the liquid fraction of the solution as an additional unknown to model the temporal evaluation of the latent heat (cf. e.g. TACKE ET AL. [26], VOLLER ET AL. [27], WHITE [28]). We do not follow this approach, but rather take the system as it is and discretize it implicitly in time and by piecewise linear finite elements in the space variables. At each time step, this leads to a coupled system of algebraic inclusions being equivalent to a system of quasivariational inequalities which, however, is not uniquely solvable but possesses a partially ordered set of solutions. The minimum and maximum element of that set can be computed by an iterative procedure based on fixed point arguments, which is typical for the solution of quasivariational inequalities (cf. e.g. [5]).

The novelty of the approach presented in this paper is twofold:

- First, we will make use of game theoretic concepts to determine a unique and physical reasonable solution. This is motivated by the intrinsic relationship between solutions to systems of quasivariational inequalities and Nash equilibria of noncooperative N–person games (cf. e.g. AUBIN [1], MOSCO [22]). In particular, within the set of Nash equilibria we aim to determine a weak Pareto minimum for which the sum of the loss functionals is minimal. From a physical point of view, such a Pareto minimum characterizes a collectively stable equilibrium configuration on the lowest energy level and hence appears to be the most appropriate selection from the set of Nash equilibria, which are known as being only individually stable. However, that Pareto minimum

will not be computed globally, but in a decentralized way by using a symmetric nonlinear block Gauss–Seidel iterative scheme requiring the successive solution of local noncooperative N–person games. As it turns out, by means of the easily accessible local data, we can instantly decide whether a nodal point is situated within the liquid, solid or mushy region. In particular, we do have uniqueness of a Nash equilibrium for a "liquid" and "solid" nodal point while for a "mushy" nodal point the computation of a unique Pareto minimum on the lowest energy level can be done inexpensively. An additional feature of this procedure is that, after having computed the unique local multistrategy, we can assign to each nodal point a liquid fraction which varies between 0 and 1 for a "mushy" nodal point and, expectedly, turns out to be 1 and 0 for a "liquid" and "solid" nodal point, respectively. As mentioned before, in contrast to other work the liquid fraction can be cheaply obtained as a by–product of the calculations, but is not an integral part of the mathematical model.

- The second novelty is that the above described symmetric nonlinear block Gauss–Seidel iteration will be used as a smoothing procedure within a multi–grid framework involving a hierarchy of triangulations. Besides the special smoother, the multi–grid algorithm has two distinctive features:

  a) The first one is the choice of the coarse grid correction. Following the approach by HOPPE/KORNHUBER [16], [17], [18] for the multi–grid solution of two–phase Stefan problems, by well–known results from convex analysis it can be shown that the system of algebraic inclusions is equivalent to a system of nonlinear algebraic equations and it is that system to which a modification of Brandt's FAS scheme [7], [13] will be applied.

  b) As in previous work on the multi–grid solution of free and moving boundary problems (cf. e.g. [6], [15], [16], [17], [18], [19]), the second characteristic of the algorithm is an adaptive choice of restrictions and prolongations in the fine–to–coarse and coarse–to–fine parts of the multi–grid cycle to allow for monitoring of an appropriate transfer of data.

The paper is organized as follows:

- Following this introduction, in section 2, we will introduce the system of degenerate parabolic equations modelling the solidification process, discuss its semi–discretization in time and outline the basic relationship between the resulting system of quasivariational inequalities and noncooperative N–person games.

- Section 3 is entirely devoted to the presentation of the multi–grid algorithm including a detailed description of its basic ingredients, i.e., the special smoother, the coarse grid correction process and the special realization of the fine–to–coarse and coarse–to–fine transfers.
- Finally, in section 4, we will present some numerical results for a ternary *Fe-C-Mn* alloy.

2. The mathematical model

We consider an alloy with $N \geq 2$ components occupying a bounded domain $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$, with piecewise smooth boundary $\Gamma = \partial\Omega$. We denote by $u(x,t)$, $(x,t) \in Q := \Omega \times (0,T)$, $T > 0$, the temperature and by $c_\nu(x,t)$, $(x,t) \in Q$, $1 \leq \nu \leq N-1$, the concentrations of the $N-1$ impurities. Then denoting by $u_m(x,t)$, $(x,t) \in Q$, the unknown melting temperature, the sets

$$Q_L = \left\{(x,t) \in Q \,|\, u(x,t) > u_m(x,t)\right\} \tag{2.1.a}$$

$$Q_S = \left\{(x,t) \in Q \,|\, u(x,t) < u_m(x,t)\right\} \tag{2.1.b}$$

will be called liquid and solid region, respectively. Moreover, setting

$$\Sigma = \left\{(x,t) \in Q \,|\, u(x,t) = u_m(x,t)\right\},$$

we define

$$\Sigma_L = \overline{Q}_L \cap \Sigma\,, \quad \Sigma_S = \overline{Q}_S \cap \Sigma \tag{2.1.c}$$

$$\Sigma_M = \Sigma \setminus \left(\Sigma_L \cup \Sigma_S\right) \tag{2.1.d}$$

where Σ_M refers to the so–called mushy zone while Σ_L, Σ_S are the free boundaries between the liquid and mushy region ("liquidus") and between the solid and mushy region ("solidus"), respectively. The mushy zone represents a region where we do have coexistence of solid and liquid regime.
We set $u_L = u|_{\Sigma_L}$, $u_S = u|_{\Sigma_S}$, $c_{L,\nu} = c_L|_{\Sigma_L}$ and $c_{S,\nu} = c_\nu|_{\Sigma_S}$, $1 \leq \nu \leq N-1$, and we assume that in the mushy region, the liquid fraction (solid fraction) is in chemical equilibrium with the solid (liquid) such that the formation of liquid (solid) is coupled with the temperature at the liquidus (solidus) surface of the phase diagram according to

$$u_L = u_d - \sum_{\nu=1}^{N-1} \gamma_{L,\nu} c_{L,\nu} \tag{2.2.a}$$

$$u_S = u_d - \sum_{\nu=1}^{N-1} \gamma_{S,\nu} c_{S,\nu} \tag{2.2.b}$$

where $\gamma_{S,\nu} > \gamma_{L,\nu}$ and u_d denotes the melting temperature of the pure material (no impurities). From the above, we then get the following constitutive equation for the unknown melting temperature

$$u_m = u_L = u_S\,. \tag{2.3}$$

In order to complete our notations of relevant physical quantities, the function $\rho = \rho(x)$, $x \in \Omega$, refers to the density, $\alpha(u) = \int_{u_d}^{u} \sigma(\xi) d\xi$ denotes the heat content with respect to the melting temperature of the pure material where σ stands for the heat capacity, $s = s(u)$ is the latent energy content, $\kappa = \kappa(u)$ the thermal conductivity and $\beta_\nu = \beta_\nu(u)$, $1 \leq \nu \leq N-1$, the molecular diffusion coefficient of the ν–th component of the alloy.
In the sequel, for simplicity, we assume the density ρ and the heat capacity to be constant while the functions s, κ and β_ν are assumed to be piecewise constant, in particular $s(u) = 0$ for $u < u_m$, $s(u) = \rho L$ for $u > u_m$, $L \neq 0$ denoting the latent heat, $\kappa(u) = \kappa_S$ for $u < u_m$, $\kappa(u) = \kappa_L$ for $u > u_m$ and $\beta_\nu(u) = \beta_{S,\nu}$ for $u < u_m$, $\beta_\nu(u) = \beta_{L,\nu}$ for $u > u_m$, $1 \leq \nu \leq N-1$.
It is further assumed that the alloy will be cooled only at the boundary Γ, i.e., there are no internal sinks. Then, under the hypothesis that $\Sigma_M = \emptyset$ and $\Sigma = \Sigma_L = \Sigma_S$ is a sufficiently smoothly oriented hypersurface, from the heat– and mass–balance relations in integral form it may be deduced that in Q_L and Q_S we do have the pointwise equations

$$\rho\sigma \frac{\partial u}{\partial t} - \nabla \cdot (\kappa \nabla u) = 0 \tag{2.4.a}$$

$$\frac{\partial c_\nu}{\partial t} - \nabla \cdot (\beta_\nu \nabla c_\nu) = 0 \,, \quad 1 \leq \nu \leq N-1 \tag{2.4.b}$$

while the following pointwise jump conditions hold true at the change–of–phase boundary

$$\kappa_L \nabla u|_{\Sigma_L} \cdot \pi\nu_\tau|_{\Sigma_L} - \kappa_S \nabla u|_{\Sigma_S} \cdot \pi\nu_\tau|_{\Sigma_S} = \rho L \cos(\nu_\tau, 1_t) \,, \tag{2.5.a}$$

$$\begin{aligned} &\beta_{L,\nu} \nabla c_\nu|_{\Sigma_L} \cdot \pi\nu_\tau|_{\Sigma_L} - \beta_{S,\nu} \nabla c_\nu|_{\Sigma_S} \cdot \pi\nu_\tau|_{\Sigma_S} \\ &= (c_{L,\nu} - c_{S,\nu}) \cos(\nu_\tau, 1_t) \,, \quad 1 \leq \nu \leq N-1 \,. \end{aligned} \tag{2.5.b}$$

Here ν_τ is the normal to Σ, outward for Q_L and inward for Q_S, respectively. $\pi\nu_\tau$ is its projection onto the Ω–plane and $1_t \in \mathbb{R}^{d+1}$ denotes the unit vector in t–direction.
The preceding equations have to be completed by the Neumann–type boundary conditions

$$\kappa \frac{\partial u}{\partial n} = q \text{ on } \quad \Gamma \times (0,T) \tag{2.6.a}$$

$$\beta_\nu \frac{\partial c_\nu}{\partial n} = 0 \text{ on } \quad \Gamma \times (0,T) \,, \quad 1 \leq \nu \leq N-1 \tag{2.6.b}$$

where $q = q(x,t)$, $(x,t) \in \Gamma \times (0,T)$ denotes the thermal flux through the boundary.

The equations (2.4.a), (2.4.b), (2.5.a), (2.5.b) and (2.6.a), (2.6.b) constitute the classical multicomponent alloy solidification problem. However, there is both experimental and mathematical evidence (cf. eg. [23], [26]) that the classical formulation, which excludes the existence of mushy regions, is a less suitable physical model for alloy solidification than those models which allow the coexistence of liquid and solid regime. In pure heat transfer problems with a change of phase, it is well known that the enthalpy formulation does provide a framework for a weak solution concept including the existence of mushy regions (cf. e.g. [10], [20] and the references therein). As far as alloy solidification problems are concerned for binary alloys, i.e., $N = 2$, a related weak solution concept has been developed by CROWLEY, OCKENDON [8] and FIX [11] and has been extended to the case of more than one impurity ($N > 2$) by BERMUDEZ and SAGUEZ [5] (cf. also work done by TACKE ET AL. [26]). This basic idea is to introduce new variables according to

$$w_\nu = \begin{cases} -\gamma_{L,\nu} c_\nu & \text{in } Q_L \\ -\gamma_{S,\nu} c_\nu & \text{in } Q_S \end{cases} . \tag{2.7}$$

Then, setting

$$w = \sum_{\nu=1}^{N-1} w_\nu \ , \quad u_\nu = u - \sum_{\substack{\mu=1 \\ \mu \neq \nu}}^{N-1} w_\mu \ , \quad 1 \leq \nu \leq N-1 \tag{2.8}$$

in view of (2.2.a), (2.2.b), the transformed constitutive equation for the unknown melting temperature u_m can be given the equivalent forms

$$u_m - u_d = w \tag{2.9.a}$$

$$u_\nu - u_d = w_\nu \ , \quad 1 \leq \nu \leq N-1 \ . \tag{2.9.b}$$

In particular, in terms of the new variables u, w_ν, $1 \leq \nu \leq N-1$, the liquid and solid region as well as the change–of–phase zone can be expressed by

$$\begin{aligned} Q_L &= \Big\{(x,t) \in Q | u(x,t) - u_d > w(x,t)\Big\} = \\ &= \Big\{(x,t) \in Q | w_\nu(x,t) < u_d + u_\nu(x,t) \ , \ 1 \leq \nu \leq N-1\Big\} \ , \end{aligned} \tag{2.10.a}$$

$$\begin{aligned} Q_S &= \Big\{(x,t) \in Q | u(x,t) - u_d < w(x,t)\Big\} = \\ &= \Big\{(x,t) \in Q | w_\nu(x,t) > u_d + u_\nu(x,t) \ , \ 1 \leq \nu \leq N-1\Big\} \ , \end{aligned} \tag{2.10.b}$$

$$\begin{aligned} \Sigma &= \Big\{(x,t) \in Q | u(x,t) - u_d = w(x,t)\Big\} = \\ &= \Big\{(x,t) \in Q | w_\nu(x,t) = u_d + u_\nu(x,t) \ , \ 1 \leq \nu \leq 1\Big\} \ . \end{aligned} \tag{2.10.c}$$

For the sake of simplicity, in the sequel we will assume $u_d = 0$, which can always be achieved by a suitable transformation.

Introducing the multivalued mappings $H_r : \mathbb{R} \to \mathbb{R}$ and $G_r^\nu : \mathbb{R} \to \mathbb{R}$, $1 \le \nu \le N-1$, where $r \in \mathbb{R}^-$, by

$$H_r(\lambda) = \begin{cases} \rho\sigma\lambda & \text{if } \lambda < r \\ [\rho\sigma r,\ \rho\sigma r + \rho L] & \text{if } \lambda = r \\ \rho\sigma\lambda + \rho L & \text{if } \lambda > r \end{cases} \tag{2.11.a}$$

$$G_r^\nu(\lambda) = \begin{cases} \lambda/\gamma_{L,\nu} & \text{if } \lambda < r \\ [r/\gamma_{L,\nu}, r/\gamma_{S,\nu}] & \text{if } \lambda = r \\ \lambda/\gamma_{S,\nu} & \text{if } \lambda > r \end{cases} \tag{2.11.b}$$

and setting

$$\kappa(u,w) = \begin{cases} \kappa_L & \text{if } u > w \\ \kappa_S & \text{if } u < w \end{cases} \tag{2.12.a}$$

$$\beta_\nu(u_\nu, w_\nu) = \begin{cases} \beta_{L,\nu}/\gamma_{L,\nu} & \text{if } u_\nu > w_\nu \\ \beta_{S,\nu}/\gamma_{S,\nu} & \text{if } u_\nu < w_\nu \end{cases} \quad 1 \le \nu \le N-1\,, \tag{2.12.b}$$

then the system (2.4.a) – (2.6.b) can be written in conservation form by means of the following system of degenerate parabolic equations

$$\frac{\partial H_w(u)}{\partial t} - \nabla \cdot \Big(\kappa(u,w)\nabla n\Big) = 0 \text{ in } Q\,, \tag{2.13.a}$$

$$\frac{\partial G_{u_\nu}(w_\nu)}{\partial t} - \nabla \cdot \Big(\beta_\nu(u_\nu, w_\nu)\nabla w_\nu\Big) = 0 \text{ in } Q\,,\ 1 \le \nu \le N-1 \tag{2.13.b}$$

$$\kappa\frac{\partial u}{\partial n} = q\,,\ \ \frac{\partial w_\nu}{\partial n} = 0 \text{ on } \Gamma \times (0,T)\,,\ \ 1 \le \nu \le N-1\,. \tag{2.13.c}$$

Evidently, the above system has to be understood in a suitable weak sense. Namely, an N–tuple $(u, w_1, \cdots, w_{N-1})$ of functions

$$u, w_\nu \in L^\infty\Big((0,T);\ H^1(\Omega)\Big) \cap H^1\Big([0,T];\ L^2(\Omega)\Big) \cap L^\infty(Q)$$

is said to be a weak solution to the alloy solidification problem, if the equations

$$\begin{aligned} \int_Q \left[H_w(u)\frac{\partial\phi}{\partial t} - \kappa(u,w)\nabla u \cdot \nabla\phi\right] dx\,dt - \int_{\Omega\times\{T\}} H_w(u)\phi\,dx + \\ + \int_{\Omega\times\{0\}} H^0\phi\,dx = \int_{\Gamma\times(0,T)} q\phi\,d\sigma\,dt \end{aligned} \tag{2.14.a}$$

$$\int_Q \left[G^\nu_{u_\nu}(w_\nu) \frac{\partial \phi}{\partial t} - \beta_\nu(u_\nu, w_\nu) \nabla w_\nu \cdot \nabla \phi \right] dx\, dt - \int_{\Omega \times \{T\}} G^\nu_{u_\nu}(w_\nu) \phi dx + \\ + \int_{\Omega \times \{0\}} G^{\nu,0} \phi \, dx = 0 \,, \quad 1 \le \nu \le N-1 \tag{2.14.b}$$

hold true for all test functions

$$\phi \in C\big([0,T],\, H^1(\Omega)\big) \cap H^1\big([0,T],\, L^2(\Omega)\big)$$

where $H^0 \in H_{w^0}(u^0)$ and $G^{\nu,0} \in G^\nu_{u^0_\nu}(w^0_\nu)$, $1 \le \nu \le N-1$, are appropriately given initial data at time $t = 0$.

In case of pure heat transfer with a change of phase at a fixed temperature u_m, the existence of a weak solution can be shown in a constructive way by discretizing the corresponding degenerate parabolic equation (enthalpy formulation of the two–phase Stefan problem) implicitly in time with respect to a uniform partition $t_m = m\Delta t$, $0 \le m \le M$, $\Delta t = T/M$, $M \in \mathbb{N}$, of the time interval $[0,t]$. At time levels t_m, $m \ge 1$, this semi–discretization requires the solution of elliptic differential inclusions being equivalent to elliptic variational inequalities of the second kind which admit unique solutions whose piecewise linear prolongations can be shown to converge for $\Delta t \to 0$ in the L^2–sense to a weak solution of the problem [20].

For multicomponent alloy solidification problems, a closely related approach has been used by BERMUDEZ and SAGUEZ [5]: Denoting by u^m, w^m_ν approximations to u, w_ν, $1 \le \nu \le N-1$, at time t_m, linearizing the nonlinear elliptic part in (2.14.a), (2.14.b) by evaluating the coefficient functions κ and β_ν at the preceding time level t_{m-1}, averaging the time–dependent Neumann data q on $[t_{m-1}, t_m]$ and finally, selecting some $H^{m-1} \in H_{w^{m-1}}(u^{m-1})$, $G^{\nu,m-1} \in G^\nu_{u^{m-1}_\nu}(w^{m-1}_\nu)$, $1 \le \nu \le N-1$, we arrive at the following system of elliptic differential inclusions

$$H^{m-1} - \Delta t L^m_0 u^m \in H_{w^m}(u^m) \text{ in } \Omega \,, \tag{2.15.a}$$

$$G^{\nu,m-1} - \Delta t L^m_\nu w^m_\nu \in G^\nu_{u^m_\nu}(w^m_\nu) \text{ in } \Omega \,, \quad 1 \le \nu \le N-1 \,, \tag{2.15.b}$$

$$\kappa^{m-1} \frac{\partial u^m}{\partial n} = \overline{q}^{\,m} \,, \quad \frac{\partial w^m_\nu}{\partial n} = 0 \text{ on } \Gamma \,, \quad 1 \le \nu \le N-1 \tag{2.15.c}$$

where

$$L^m_0 u^m = -\nabla \cdot (\kappa^{m-1} \nabla u^m) \,, \quad \kappa^{m-1} = \kappa(u^{m-1}, w^{m-1}) \,, \tag{2.16.a}$$

$$L_\nu w_\nu^m = -\nabla \cdot (\beta_\nu^{m-1} \nabla w_\nu^m) \ , \ \ \beta_\nu^{m-1} = \beta_\nu(u_\nu^{m-1}, w_\nu^{m-1}) \ , \tag{2.16.b}$$

$$\overline{q}^m = (\Delta t)^{-1} \int_{(m-1)\Delta t}^{m\Delta t} q(t)dt \ . \tag{2.16.c}$$

Now, for fixed $r \in \mathbb{R}^-$ the multivalued functions $H_r(\cdot)$ and $G_r^\nu(\cdot)$, $1 \leq \nu \leq N-1$, as given by (2.12.a), (2.12.b), respectively, turn out to be the subdifferentials $\partial\Phi_r(\cdot)$ and $\partial\Psi_r^\nu(\cdot)$ of the piecewise quadratic functions

$$\Phi_r(\lambda) = \begin{cases} \frac{1}{2}\rho\sigma\lambda^2 + \rho L r & \text{if } \lambda \neq r \\ \frac{1}{2}\rho\sigma\lambda^2 + \rho L\lambda & \text{if } \lambda \geq r \end{cases} \tag{2.17.a}$$

$$\Psi_r^\nu(\lambda) = \begin{cases} \frac{1}{2}\gamma_{L,\nu}^{-1}\lambda^2 - \frac{1}{2}r^2\left(\gamma_{L,\nu}^{-1} - \gamma_{S,\nu}^{-1}\right) & \text{if } \lambda \leq r \\ \frac{1}{2}\gamma_{S,\nu}^{-1}\lambda^L & \text{if } \lambda \geq r \end{cases} \tag{2.17.b}$$

where the integration constants have been chosen such that $\Phi_r(0) = 0$, $\Psi_r^\nu(0) = 0$, $1 \leq \nu \leq N-1$.
By means of (2.17.a), (2.17.b), we define functionals $\phi : L^2(\Omega) \times L^2(\Omega) \to \mathbb{R}$ and $\psi^\nu : L^2(\Omega) \times L^2(\Omega) \to \mathbb{R}$, $1 \leq \nu \leq N-1$, according to

$$\phi(u,v) = \int_\Omega \Phi_{u(x)}\big(v(x)\big)dx \ , \ \ u, v \in L^2(\Omega) \ , \tag{2.18.a}$$

$$\psi^\nu(u,v) = \int_\Omega \Psi_{u(x)}^\nu\big(v(x)\big)dx \ , \ \ u, v \in L^2(\Omega) \ . \tag{2.18.b}$$

Then, for fixed $u \in L^2(\Omega)$ we consider the functionals $\phi_u : L^2(\Omega) \to \mathbb{R}$ and $\psi_u^\nu : L^2(\Omega) \to \mathbb{R}$ as given by

$$\psi_u(v) = \phi(u,v) \ , v \in L^2(\Omega) \ , \tag{2.19.a}$$

$$\psi_u^\nu(v) = \psi^\nu(u,v) \ , v \in L^2(\Omega) \ . \tag{2.19.b}$$

Furthermore, we denote by $a_0^m(\cdot,\cdot)$ and $a_\nu^m(\cdot,\cdot)$, $1 \leq \nu \leq N-1$, the bilinear forms on $H^1(\Omega) \times H^1(\Omega)$ associated with the second order elliptic differential operators L_0^m, L_ν^m, respectively, i.e.:

$$a_0^m(v,z) = \int_\Omega \kappa^{m-1} \nabla v \cdot \nabla z \, dx \ , \ \ v, z \in H^1(\Omega) \ , \tag{2.20.a}$$

$$a_\nu^m(v,z) = \int_\Omega \beta_\nu^{m-1} \nabla v \cdot \nabla z \, dx \ , \quad v, z \in H^1(\Omega) \ . \tag{2.20.b}$$

Then, it is easily shown that (2.15.a) – (2.15.c) is equivalent to the following system of quasivariational inequalities of the second kind

$$\begin{gathered} \Delta t a_0^m(u^m, v - u^m) + \phi_{w^m}(v) - \phi_{w^m}(u^m) \geq l_o^m(v - u^m) \ , \\ v \in H^1(\Omega) \end{gathered} \tag{2.21.a}$$

$$\begin{gathered} \Delta t a_\nu^m(w_\nu^m, v - w_\nu^m) + \psi_{u_\nu^m}^\nu(v) - \psi_{u_\nu^m}^\nu(w_\nu^m) \geq l_\nu^m(v - w_\nu^m) \ , \\ v \in H^1(\Omega) \ , \ \ 1 \leq \nu \leq N-1 \end{gathered} \tag{2.21.b}$$

where

$$\begin{aligned} l_0^m(z) &= (H^{m-1}, z)_0 + \Delta t < \overline{q}^m \ , \ z >_0 \ , \ \ z \in H^1(\Omega) \\ l_\nu^m(z) &= (G^{\nu,m-1}, z)_0 \ , \ \ z \in H^1(\Omega) \ , \ \ 1 \leq \nu \leq N-1 \ , \end{aligned} \tag{2.22}$$

$(\cdot,\cdot)_0$ and $\langle \cdot, \cdot \rangle_0$ denoting the usual L^2–inner products with respect to Ω and Γ, respectively.

Let us define functionals $J_\nu^m : \left(H^1(\Omega)\right)^N \to \mathbb{R}$, $0 \leq \nu \leq N-1$, by

$$J_0^m(u^m, w_1^m, \cdots, w_{N-1}^m) = \tfrac{1}{2} \Delta t a_0^m(u^m, u^m) + \phi_{w^m}(u^m) - l_0^m(u^m) \ , \tag{2.23.a}$$

$$\begin{gathered} J_\nu^m(u^m, w_1^m, \cdots, w_{N-1}^m) = \tfrac{1}{2} \Delta t a_\nu^m(w_\nu^m, w_\nu^m) + \psi_{u_\nu^m}^\nu(w_\nu^m) - l_\nu^m(w_\nu^m) \ , \\ 1 \leq \nu \leq N-1 \ . \end{gathered} \tag{2.23.b}$$

Then, setting $v^m = (v_0^m, v_1^m, \cdots, v_{N_1}^m)$ with $v_0^m = u^m$, $v_\nu^m = w_\nu^m$, $1 \leq \nu \leq N-1$, and using the fact that $J_\nu^m(v_0^m, \cdots, v_{\nu-1}^m, \cdot\ , v_{\nu+1}^m, \cdots, v_{N-1}^m)$ are subdifferentiable convex functionals on $H^1(\Omega)$, it is easily verified (cf. e.g. [1]) that any $v \in \left(H^1(\Omega)\right)^N$ is a solution to (2.21.a), (2.21.b) if and only if v is a Nash equilibrium of the following noncooperative N–person game:
Find $v \in \left(H^1(\Omega)\right)^N$ such that

$$\begin{gathered} J_\nu^m\left(v_0^m, \cdots, v_{N-1}^m\right) = \inf_{z \in H^1(\Omega)} J_\nu^m\left(v_0^m, \cdots, v_{\nu-1}^m, z, v_{\nu+1}^m, \cdots, v_{N-1}^m\right) \ , \\ 0 \leq \nu \leq N-1 \ . \end{gathered} \tag{2.24}$$

Both from a theoretical and — as we shall see in the subsequent chapter — from a numerical point of view, it can be advantageous to use duality methods in

the treatment of the semi–discretized alloy equations.
We remind the well known fact from convex analysis (cf. e.g [9]) that for any convex lower semicontinuous functional Θ the equivalence

$$v \in \partial\Theta(u) \Longleftrightarrow u \in \partial\Theta^*(v) \tag{2.25}$$

holds true where Θ^* denotes the Fenchel conjugate of Θ. Taking (2.25) into account, the system of elliptic differential inclusions (2.15.a), (2.15.b) is equivalent to

$$u^m \in \partial\Phi^*_{w^m}\left(H^{m-1} - \Delta t L_0^m u^m\right) \quad \text{in } \Omega \tag{2.26.a}$$

$$w_\nu^m \in \partial\Psi^{\nu,*}_{u_\nu^m}\left(G^{\nu,m-1} - \Delta t L_\nu^m w_\nu^m\right) \quad \text{in } \Omega\,, \quad 1 \le \nu \le N-1\,. \tag{2.26.b}$$

In view of (2.17.a), (2.17.b), the Fenchel conjugates Φ_r^*, $\Psi_r^{\nu,*}$ and their subdifferentials $\partial\Phi_r^*$, $\partial\Psi_r^{\nu,*}$ can be easily computed. In particular, we obtain

$$\partial\Phi_r^*(\lambda) = \begin{cases} \lambda/\rho\sigma & \text{if } \lambda < \rho\sigma r \\ r & \text{if } \lambda \in [\rho\sigma r,\ \rho\sigma r + \rho L] \\ (\lambda - \rho L)/\rho\sigma & \text{if } \lambda > \rho\sigma r + \rho L \end{cases} \tag{2.27.a}$$

$$\partial\Phi_r^{\nu,*}(\lambda) = \begin{cases} \gamma_{L,\nu}\lambda & \text{if } \lambda < r/\gamma_{L,\nu} \\ r & \text{if } \lambda \in [r/\gamma_{L,\nu}\,,\ r/\gamma_{S,\nu}] \\ \gamma_{S,\nu}\lambda & \text{if } \lambda > r/\gamma_{S,\nu}\,. \end{cases} \tag{2.27.b}$$

It turns out that $\partial\Phi_r^*$ and $\partial\Psi_r^{\nu,*}$, $1 \le \nu \le N-1$, are piecewise linear continuous functions and hence, in contrast to the subdifferentials $\partial\Phi_r$ and $\partial\Psi_r^\nu$, $1 \le \nu \le N-1$, they are single–valued. Consequently, the inclusion "$\in$" in (2.26.a), (2.26.b) can be replaced by the equality "=" or, in other words, the "dual" system (2.26.a), (2.26.b) together with the boundary conditions (2.15.c) represents the weak formulation of a system of nonlinear elliptic boundary value problems.
Note that, in terms of the dual formulation, the liquid and solid region $Q_L(t_m)$, $Q_S(t_m)$ and the mushy zone $\Sigma_M(t_m)$ at time t_m (with respect to the alloy equations discretized implicitly in time) can be equivalently described by means of

$$\begin{aligned} Q_L(t_m) &= \left\{x \in \Omega | u^m > w^m\right\} = \\ &= \left\{x \in \Omega | H^{m-1} - \Delta t L_0^m u^m > \rho\sigma w^m + \rho L\,,\right. \\ &\qquad \left. G^{\nu,m-1} - \Delta t L_\nu^m w_\nu^m < u_\nu^m/\gamma_{L,\nu}\,,\ 1 \le \nu \le N-1\right\}, \end{aligned} \tag{2.28.a}$$

$$
\begin{aligned}
Q_S(t_m) &= \left\{x \in \Omega | u^m < w^m\right\} = \\
&= \left\{x \in \Omega | H^{m-1} - \Delta t L_0^m u^m < \rho\sigma w^m \,, \right. \qquad (2.28.b) \\
&\qquad \left. G^{\nu,m-1} - \Delta t L_0^m w_\nu^m > u_\nu^m/\gamma_{S,\nu} \,, 1 \le \nu \le N-1\right\} \,,
\end{aligned}
$$

$$
\begin{aligned}
\Sigma_m(t_m) &= \left\{x \in \Omega | \rho\Sigma^m < H^{m-1} - \Delta t L_0^m u^m < \rho\sigma w^m + \rho L \,, \right. \\
&\qquad u_\nu^m/\gamma_{L,\nu} < G^{\nu,m-1} - \Delta t L_0^m w_\nu^m < u_\nu^m/\gamma_{S,\nu} \,, \qquad (2.28.c) \\
&\qquad \left. 1 \le \nu \le N-1\right\} .
\end{aligned}
$$

(compare (2.10.a–c), but observe the assumption $u_d = 0$).

As far as the existence of solutions is concerned due to the equivalence of (2.21.a), (2.21.b) and (2.24), we may try to apply known existence results either for systems of quasivariational inequalities or for Nash point equilibria of variational integrals (cf. e.g. [1], [2], [3], [4], [22], [29]). Since some of these results are based on order structures, we recall that $L^2(\Omega)$, equipped with the usual L^2–norm $\|\cdot\|_0$, is a complete Hilbert lattice with respect to the canonical ordering given by $u \le v$, $u, v \in L^2(\Omega)$, iff $u(x) \le v(x)$ f.a.a. $x \in \Omega$. In particular, any two elements u, $v \in L^2(\Omega)$ have a common least upper bound and a common greatest lower bound, denoted by $u \vee v$ and $u \wedge v$, respectively, and every subset $\Sigma \subset L^2(\Omega)$ with an upper bound possesses a least upper bound, denoted by $\vee\Sigma$. The Sobolev space $H^1(\Omega)$ is a sublattice of $L^2(\Omega)$, i.e., for any $u, v \in H^1(\Omega)$ the elements $u \vee v$ and $u \wedge v$, formed with respect to the canonical ordering in $L^2(\Omega)$, also belong to $H^1(\Omega)$. The Sobolev norm $\|\cdot\|_1$ on $H^1(\Omega)$ satisfies $\|u^+\|_1 \le \|u\|_1$ and $\|u^-\|_1 \le \|u\|_1$, $u \in H^1(\Omega)$, where $u^+ = u \vee 0$ and $u^- = -u \wedge 0$ (cf. e.g. [14], [25]). Moreover, denoting by $\Gamma_0\big(L^2(\Omega)\big)$ the set of all proper convex functionals on $L^2(\Omega)$, we may define an order relation on $\Gamma_0\big(L^2(\Omega)\big)$ by $\phi_1 \le \phi_2$, $\phi_1, \phi_2 \in \Gamma_0\big(L^2(\Omega)\big)$ iff either $\phi_2 - \phi_1 = c$ for some $c \in \mathbb{R}^+$ or $\phi_2 - \phi_1 \ne c$ for all $c \in \mathbb{R}$ and $\phi_1(u \wedge v) + \phi_2(u \vee v) \le \phi_1(u) + \phi_2(v)$ for all $u, v \in L^2(\Omega)$ (cf. e.g. [2], [14]).
Preparatory, we will now state some basic results which are easy to verify and thus will be given without proofs.

Lemma 2.1 *The functionals ϕ and ψ^ν, $1 \le \nu \le N-1$, as given by* (2.18.a), (2.18.b) *are continuous on $L^2(\Omega) \times L^2(\Omega)$.*

Lemma 2.2 (i) *For any $u \in L^2(\Omega)$, the functionals ϕ_u and ψ_u^ν, $1 \le \nu \le N-1$ defined by means of* (2.19.a), (2.19.b), *are continuous proper convex functionals on $L^2(\Omega)$.*

(ii) *For any* $u_1, u_2 \in L^2(\Omega)$, *there holds*

$$u_1 \leq u_2 \Longrightarrow \begin{cases} \varphi_{u_1} & \leq & \varphi_{u_2} \\ \psi^\nu_{u_1} & \leq & \psi^\nu_{u_2} \end{cases}, \quad 1 \leq \nu \leq N-1 \ .$$

Lemma 2.3 (i) *The bilinear forms* a^m_ν, $0 \leq \nu \leq N-1$, *given by* (2.20.*a*), (2.20.*b*), *are continuous on* $H^1(\Omega) \times H^1(\Omega)$ *and* $L^2(\Omega)$*-coercive in the sense that there exist constants* $\alpha_\nu > 0$ *and* $\lambda_\nu \in \mathbb{R}$ *such that*

$$a^m_\nu(u,u) + \lambda_\nu \|u\|^2_0 \geq \alpha_\nu \|u\|^2_1 \ , \quad u \in H^1(\Omega) \ .$$

(ii) *The bilinear forms* a^m_ν, $0 \leq \nu \leq N-1$, *are compatible with the lattice structure in the sense that*

$$a^m_\nu(u^+, u^-) = 0 \ , \quad u \in H^1(\Omega) \ .$$

Taking advantage of well–known results for standard variational inequalities (cf. e.g. [2], Theorem 10.2), from Lemma 2.2 (i) and Lemma 2.3 the following conclusions can be immediately drawn:

Proposition 2.4 *For fixed* $w^m \in H^1(\Omega)$, *the variational inequality* (2.21.*a*) *is uniquely solvable. Likewise, for* $\nu \in \{1, \ldots, N-1\}$ *and fixed* $u^m_\nu \in H^1(\Omega)$, *the same holds true for the variational inequalities* (2.21.*b*).

In terms of the noncooperative N–person game (2.24), the preceding result tells us that, given the complementary coalition's choice w^m respectively u^m_ν, $1 \leq \nu \leq N-1$, then for player $\nu \in \{0, 1, \ldots, N-1\}$ there exists a uniquely defined strategy $\tilde{u}^m \in H^1(\Omega)$ respectively $\tilde{w}^m_\nu \in H^1(\Omega)$, $1 \leq \nu \leq N-1$, minimizing his loss function J^m_ν, i.e.,

$$J^m_0(\tilde{u}^m, w_1, \ldots, w^m_{N-1}) = \inf_{v \in H^1(\Omega)} J^m_0(v, w^m_1, \ldots, w^m_{N-1})$$

$$J^m_\nu(u^m, w^m_1, \ldots, w^m_{\nu-1}, \tilde{w}^m_\nu, w^m_{\nu+1}, \ldots, w^m_{N-1}) =$$

$$\inf_{v \in H^1(\Omega)} J^m_\nu(u^m, w^m_1, \ldots, w^m_{\nu-1}, v, w^m_{\nu+1}, \ldots, w^m_{N-1}), \quad 1 \leq \nu \leq N-1 \ .$$

Introducing the operators $T_\nu : H^1(\Omega) \to H^1(\Omega)$, $0 \leq \nu \leq N-1$, uniquely defined by $T_0 w^m = \tilde{u}^m$ and $T_\nu u^m_\nu = \tilde{w}^m_\nu$, $1 \leq \nu \leq N-1$, it is evident that any $v^m = (u^m, w^m_1, \ldots, w^m_{N-1}) \in [H^1(\Omega)]^N$ is a solution to the system of quasivariational inequalities (2.21.a), (2.21.b) and a Nash point equilibrium of (2.24) iff v^m is a fixed point of the operator $T : [H^1(\Omega)]^N \to [H^1(\Omega)]^N$ given by

$$Tv^m = (T_0 w^m, T_1 u^m_1, \ldots, T_{N-1} u^m_{N-1}) \ . \tag{2.29}$$

We will now establish some nice mapping properties of T_ν, $0 \leq \nu \leq N-1$, and T which will enable us to deduce the existence of fixed points:

Lemma 2.5 (cf. [5], Lemme 2.1)
The operators T_ν, $0 \leq \nu \leq N-1$ *are monotonely increasing, i.e., given* $z_i \in H^1(\Omega)$, $i = 1,2$, *there holds*

$$z_1 \leq z_2 \Longrightarrow T_\nu z_1 \leq T_\nu z_2 \,. \tag{2.30}$$

Proof. In view of Lemma 2.2 (ii) and Lemma 2.3, the proof is a direct consequence of the standard comparison theorem for variational inequalities (cf. e.g. [2]; Theorem 19.11, [22]; Theorem 3.1). ∎

Let us now define $\underline{u}, \overline{u} \in H^1(\Omega)$ and $\underline{w}_\nu, \overline{w}_\nu \in H^1(\Omega)$, $1 \leq \nu \leq N-1$, as the unique solutions to the variational equalities

$$(\rho\sigma\underline{u} + \rho L, v)_0 + \Delta t a_0^m(\underline{u}, v) = l_0^m(v) \,, \quad v \in H^1(\Omega) \,, \tag{2.31.a}$$

$$(\rho\sigma\overline{u}, v)_0 + \Delta t a_0^m(\overline{u}, v) = l_0^m(v) \,, \quad v \in H^1(\Omega) \,, \tag{2.31.b}$$

$$(\gamma_{S,\nu}^{-1}\underline{w}_\nu, v)_0 + \Delta t a_\nu^m(\underline{w}_\nu, v) = l_\nu^m(v) \,, \quad v \in H^1(\Omega) \,, \tag{2.31.c}$$

$$(\gamma_{L,\nu}^{-1}\overline{w}_\nu, v)_0 + \Delta t a_\nu^m(\overline{w}_\nu, v) = l_\nu^m(v) \,, \quad v \in H^1(\Omega) \,. \tag{2.31.d}$$

Then there holds:

Lemma 2.6 (cf. [5]; Lemme 2.2)
Let $\underline{v} = (\underline{u}, \underline{w}_1, \ldots, \underline{w}_{N-1})$, $\overline{v} = (\overline{u}, \overline{w}_1, \ldots, \overline{w}_{N-1})$ *and let us denote by* $[\underline{v}, \overline{v}] \subset [H^1(\Omega)]^N$ *the order interval with lower bound* $\underline{v}$ *and upper bound* $\overline{v}$. *Then the operator* T, *given by* (2.29), *satisfies*

$$T : \left[H^1(\Omega)\right]^N \to [\underline{v}, \overline{v}] \,. \tag{2.32}$$

Proof. The proof follows immediately from the preceding Lemma 2.5. ∎

Based on the results obtained so far, we will now constructively prove that the set of fixed points of the operator T is non empty and possesses a minimum element $v^* = (u^*, w_1^*, \ldots, w_{N-1}^*)$ and a maximum element $v^{**} = (u^{**}, w_1^{**}, \ldots, w_{N-1}^*)$. Starting from

$$u^0 = \overline{u} \,, \; w_\nu^0 = \underline{w}_\nu \,, \; 1 \leq \nu \leq N-1 \,, \tag{2.33.a}$$

we define u^μ, w_ν^μ, $\mu \geq 1$, recursively by

$$u^\mu = T_0 w^{\mu-1} \,, \; w_\nu^\mu = T_\nu u_\nu^{\mu-1} \,, \; 1 \leq \nu \leq N-1 \,, \; \mu \geq 1 \,. \tag{2.33.b}$$

Then, setting

$$\begin{aligned} \underline{z}^{\mu} &= \left(u^{2\mu+1}, w_1^{2\mu}, \ldots, w_{N-1}^{2\mu}\right), \\ \overline{z}^{\mu} &= \left(u^{2\mu}, w_1^{2\mu+1}, \ldots, w_{N-1}^{2\mu+2}\right), \end{aligned} \tag{2.34}$$

we get:

Theorem 2.7 (cf. [5]; Proposition 2.1)
The fixed point set $F(T)$ of the operator T is non empty, and the sequence $(\underline{z}^{\mu})_{\mu\geq 0}$ respectively $(\overline{z}^{\mu})_{\mu\geq 0}$ is a monotonely increasing respectively monotonely decreasing sequence converging weakly in $[H^1(\Omega)]^N$ to the minimum element $v^* = \wedge F(T)$ respectively the maximum element $v^{**} = \vee F(T)$.

Proof. Since the u^{μ} and w_{ν}^{μ}, $\mu \geq 1$, are solutions to the variational inequalities (2.22) with fixed $w^{\mu-1}$ and $u_{\nu}^{\mu-1}$, respectively, it is easy to see that both sequences $(\underline{z}^{\mu})_{\mu\geq 0}$ and $(\overline{z}^{\mu})_{\mu\geq 0}$ are bounded in $[H^1(\Omega)]^N$. Combined with the monotonicity properties, which follow directly from Lemma 2.5, this implies the existence of elements $z^* \in [H^1(\Omega)]^N$ and $z^{**} \in [H^1(\Omega)]^N$ such that $(\underline{z}^{\mu})_{\mu\geq 0}$ and $(\overline{z}^{\mu})_{\mu\geq 0}$ converge weakly in $[H^1(\Omega)]^N$ to z^* and z^{**}, respectively. Then, passing to the limit in the variational inequalities satisfied by the elements of $\underline{z}^{\mu}$ respectively in the dual variational inequalities satisfied by the elements of $\overline{z}^{\mu}$ and using the results of Lemmas 2.1, 2.2, and 2.3, it can be shown that z^* and z^{**} are solutions to (2.21.a), (2.21.b), i.e., z^*, $z^{**} \in F(T)$. Finally, the assertions $z^* = \wedge F(T)$ and $z^{**} = \vee F(T)$ follow immediately from Lemmas 2.5 and 2.6. (For details, the reader is referred to [5]; Proposition 2.1). ∎

Remark. If we replace the startvalues u^0 and w_{ν}^0 in (2.33.a) by $u^0 = \underline{u}$ and $w_{\nu}^0 = \overline{w}$, $1 \leq \nu \leq N-1$, and define u^{μ} and w_{ν}^{μ}, $\mu \geq 1$, and in (2.33.b), we get the same results with the only difference that the roles of $(\underline{z}^{\mu})_{\mu\geq 0}$ and $(\overline{z}^{\mu})_{\mu\geq 0}$ have to be mutually exchanged.

In the context of noncooperative N–person games, the iterative scheme given by (2.33.a), (2.33.b) corresponds to a parallel minimization, i.e., each player chooses his strategy u^{μ} respectively w_{ν}^{μ}, $1 \leq \nu \leq N-1$, by minimizing his loss function with respect to the previous complementary coalition's choice $w^{\mu-1}$ repectively $u_{\nu}^{\mu-1}$, $\mu \geq 1$. An alternative would be to use some kind of sequential minimization in the sense that, with respect to a prespecified ordering of the players, each player makes up his current strategy by taking into account the chosen strategies of his predecessors. We will come back to this point in the following section on the numerical solution of the multicomponent alloy solidification problem.

By definition, Nash equilibria only exhibit "individual" stability which means that no player can diminish his loss function when the other players do not change

their strategies. However, there may exist strategies which result in a smaller loss for each player. Such strategies require a certain amount of cooperation among the N players and lead to the concept of weak Pareto strategies, which exhibit a "collectively" stable behaviour (cf. [1]; Chapter 10). In particular, in terms of the loss functionals J_ν^m, $0 \leq \nu \leq N-1$, given by (2.23.a), (2.23.b), a strategy $z = (u, w_1, \ldots, w_{n-1}) \in [H^1(\Omega)]^N$ is said to be a weak Pareto strategy iff there is no $v \in [H^1(\Omega)]^N$ such that $J_\nu^m(v) < J_\nu^m(z)$, $0 \leq \nu \leq N-1$. The corresponding multiloss $J^m(z) = \left(J_0^m(z), \ldots, J_{N-1}^m(z)\right)$ is called a weak Pareto minimum.

Finally, a strong equilibrium is a strategy which is both a Nash equilibrium and a weak Pareto strategy, i.e., it satisfies both "individual" and "collective" stability.
Since, with regards to the alloy solidification process, the loss functionals J_ν^m represent individual "energy contents", from a physical point of view it is natural to ask for the existence of strong equilibria. Using Lemma 2.1 and Lemma 2.3, the existence of a weak Pareto strategy as a "best compromise" within the set of Nash equilibria can be shown by standard arguments (cf. [1], Chapter 10.2.4). However, we still do not have uniqueness of a strong equilibrium. Therefore, arguing again from a physical point of view, we may use the "total energy content" $E^m(v) = \sum_{\nu=0}^{N-1} J_\nu^m(v)$ as a further selection and ask for a strong equilibrium $z \in [H^1(\Omega)]^N$ on the lowest energy level $E^m(z)$. In the next section we will show how to use such a selection process within a multi-grid approach based on a discretization of the system (2.21.a), (2.21.b) by piecewise linear finite elements with respect to a hierarchy of triangulations.

3. The multi–grid method

In this section we will present a multi-grid algorithm for the numerical solution of the multicomponent alloy solidification problem based on a finite element discretization with respect to a hierarchy of triangulations.

For simplicity, we will assume that Ω is a bounded domain in $\mathbb{R}^2$ with polygonal boundary $\Gamma = \partial\Omega$. Starting from an initial regular triangulation $\mathcal{T}_0$ with $\overline{\Omega} = \bigcup_{T\in\mathcal{T}_0} T$, we generate a hierarchy $(\mathcal{T}_k)_{k=0}^{l}$, $l \in \mathbb{N}$, of triangulations by successive refinements realized in the usual way, i.e., $\mathcal{T}_{k+1}$ is obtained from $\mathcal{T}_k$ by subdividing each triangle $T \in \mathcal{T}_k$ into four subtriangles such that the midpoints of the edges of T are the additional vertices. We refer to V_k, $0 \le k \le l$, as the finite dimensional subspace of $H^1(\Omega)$ generated by piecewise linear finite elements, i.e.,

$$V_k = \left\{ v_k \in C(\overline{\Omega}) \,|\, v_k|_T \in P_1(T) \ \text{ for all } \ T \in \mathcal{T}_k \right\}$$

where $P_1(T)$ is the set of polynomials on T of degree less than or equal to 1. Denoting by a_i^T, $1 \le i \le 3$, the vertices of $T \in \mathcal{T}_k$, the set Ω_k of nodal points is given by $\Omega_k = \bigcup_{T\in\mathcal{T}_k} \{a_1^T, a_2^T, a_3^T\}$, and we have $\dim V_k = n_k$, $n_k = \text{card } \Omega_k$. Ordering the nodal points lexicographically, we may write $\Omega_k = \{b_1^k, \ldots, b_{n_k}^k\}$, and a suitable basis $\{\varphi_i^k\}_{i=1}^{n_k}$ ov V_k is given by $\varphi_i^k(b_j^k) = \delta_{ij}$, $1 \le i,j \le n_k$. Then for a function $v \in C(\overline{\Omega})$ its interpolate will be denoted by $\Pi_k v = \sum_{i=1}^{n_k} v(b_i^k)\varphi_i^k$.

In order to discretize the multicomponent alloy solidification problem within the above finite element setting, the functionals $\varphi_u : L^2(\Omega) \to \mathbb{R}$ and $\psi_u^\nu : L^2(\Omega) \to \mathbb{R}$, $1 \le \nu \le N-1$ defined by means of (2.19.a), (2.19.b), will be approximated by functionals $\varphi_{k,u_k} : V_k \to \mathbb{R}$ and $\Psi_{k,u_k}^\nu : V_k \to \mathbb{R}$, $u_k \in V_k$, according to

$$\begin{aligned} \varphi_{k,u_k}(v_k) &= \int_\Omega \Big(\Pi_k \Phi_{u_k}(v_k)\Big)(x)dx = \\ &= \sum_{T\in\mathcal{T}_k} \tfrac{1}{3} \text{ area } (T) \sum_{i=1}^{3} \Phi_{u_k(a_i^T)}\Big(v_k(a_i^T)\Big) \end{aligned} \tag{3.1.a}$$

$$\begin{aligned} \psi_{k,u_k}^\nu(v_k) &= \int_\Omega \Big(\Pi_k \Psi_{u_k}^\nu(v_k)\Big)(x)dx = \\ &= \sum_{T\in\mathcal{T}_k} \tfrac{1}{3} \text{ area}(T) \sum_{i=1}^{3} \Psi_{u_k(a_i^T)}^\nu\Big(v_k(a_i^T)\Big) \,. \end{aligned} \tag{3.1.b}$$

Further, we introduce a discrete L^2 inner product

$$(u_k, v_k)_k = \sum_{T\in\mathcal{T}_k} \tfrac{1}{3} \text{ area } (T) \sum_{i=1}^{3} u_k(a_i^T) v_k(a_i^T), \quad u_k, v_k \in V_k \,. \tag{3.2}$$

Moreover, denoting by $\mathcal{T}_k^\Gamma$ the set of all triangles $T \in \mathcal{T}_k$ such that two vertices $a_{i_\mu}^T$, $i_\mu \in \{1,2,3\}$, $1 \le \mu \le 2$, are situated on Γ and assuming the thermal flux function q to be at least piecewise continuous as a function on Γ, we approximate the boundary integral in (2.23.a) by

$$\gamma_{k,\bar{q}^m}(v_k) = \sum_{T \in \mathcal{T}_k^\Gamma} \tfrac{1}{2} \left| a_{i_1}^T, a_{i_2}^T \right| \sum_{\mu=1}^{2} \bar{q}_{i_\nu}^m v_k(a_{i_\mu}^T) \ , \quad v_k \in V_k \ , \tag{3.3}$$

where $|a_{i_1}^T, a_{i_2}^T|$ stands for the Euclidean distance of $a_{i_1}^T, a_{i_2}^T$ and $\bar{q}_{i_\mu}^m = \lim \bar{q}^m(x)$ for $x \in \partial T \cap \Gamma$, $x \to a_{i_\mu}^T$, $1 \le \mu \le 2$.
Assuming given $H_k^{m-1} \in V_k$ and $G_k^{\nu,m-1} \in V_k$, $1 \le \nu \le N-1$, we set

$$l_{k,0}^m(v_k) = (H_k^{m-1}, v_k)_k + \Delta t \gamma_{k,\bar{q}^m}(v_k) \ , \quad v_k \in V_k \ , \tag{3.4.a}$$

$$l_{k,\nu}^m(v_k) = (G_k^{\nu,m-1}, v_k)_k \ , \quad 1 \le \nu \le N-1 \ , \quad v_k \in V_k \ . \tag{3.4.b}$$

Finally, as discrete counterparts of the functionals given by (2.23.a), (2.23.b), we define

$$\begin{aligned} J_{k,0}^m(u_k^m, w_{k,1}^m, \ldots, w_{k,N-1}^m) \ = \ & \tfrac{1}{2}\Delta t a_0^m(u_k^m, u_k^m) \\ & - l_{k,0}^m(u_k^m) + \varphi_{k,w_k^m}(u_k^m) \end{aligned} \tag{3.5.a}$$

$$\begin{aligned} J_{k,\nu}^m(u_k^m, w_{k,1}^m, \ldots, w_{k,N-1}^m) \ = \ & \tfrac{1}{2}\Delta t a_\nu^m(w_{k_\nu}^m, w_{k,\nu}^m) \\ & - l_{k,\nu}^m(w_{k,\nu}^m) + \psi_{k,u_{k,\nu}^m}^\nu(w_{k,\nu}^m) \ , \end{aligned} \tag{3.5.b}$$

where

$$w_k^m = \sum_{\nu=1}^{N-1} w_{k,\nu}^m \quad \text{and}$$

$$u_{k,\nu}^m = u_k^m - \sum_{\substack{\mu=1 \\ \mu \ne \nu}}^{N-1} w_{k,\mu}^m \ , \quad 1 \le \nu \le N-1 \ .$$

As an approximation to (2.24), we consider the following finite dimensional non-cooperative N-person game:
Find $v_k^m = (v_{k,0}^m, \ldots, v_{k,N-1}^m) \in V_k^N$ with $v_{k,0}^m = u_k^m$ and $v_{k,\nu}^m = w_{k,\nu}^m$, $1 \le \nu \le N-1$, such that

$$\begin{aligned} J_{k,\nu}^m(v_{k,0}^m, \ldots, v_{k,N-1}^m) = \min_{z_k \in V_k} J_{k,\nu}^m(v_k^m, \ldots, v_{k,\nu-1}^m, z_k, v_{k,\nu+1}^m, \ldots, v_{k,N-1}^m) \ , \\ 0 \le \nu \le N-1 \ . \end{aligned} \tag{3.6}$$

As in the continuous case, the computation of a Nash equilibrium of (3.6) is equivalent to the solution of a system of quasivariational inequalities, which is the discrete counterpart of (2.21.a), (2.21.b):

$$\Delta t a_0^m(u_k^m, v_k - u_k^m) + \varphi_{k,w_k^m}(v_k) - \varphi_{k,w_k^m}(u_k^m) \geq l_{k,0}^m(v_k - u_k^m) , \quad v_k \in V_k \tag{3.7.a}$$

$$\Delta t a_\nu^m(w_{k,\nu}^m, v_k - w_{k,\nu}^m) + \psi_{k,u_{k,\nu}^m}^\nu(v_k) - \psi_{k,u_{k,\nu}^m}^\nu(w_{k,\nu}^m) \geq l_{k,\nu}^m(v_k - w_{k,\nu}^m) , \quad v_k \in V_k , \ 1 \leq \nu \leq N-1 . \tag{3.7.b}$$

By identifying functions in V_k with vectors via the bijective map

$$I_k v_k = \sum_{i=1}^{n_k} v_{k,i}\varphi_i^k , \quad v_k \in \mathbb{R}^{n_k} , \tag{3.8}$$

we can state (3.6) and (3.7.a), (3.7.b) in the algebraic form. Indeed, it can be easily seen that (3.7.a) , (3.7.b) is equivalent to a coupled system of N algebraic inclusions

$$-(A_{k,0}^m u_{k,0}^m - f_{k,0}^m) \in \partial\Phi_{k,w_k^m}(u_k^m) , \tag{3.9.a}$$

$$-(A_{k,\nu}^m w_{k,\nu}^m - f_{k,\nu}^m) \in \partial\Psi_{k,u_{k,\nu}^m}^\nu(w_{k,\nu}^m) , \ 1 \leq \nu \leq N-1 , \tag{3.9.b}$$

with $n_k \times n_k$ diagonally dominant Z–matrices $A_{k,\nu}^m$, vectors $f_{k,\nu}^m \in \mathbb{R}^{n_k}$, $0 \leq \nu \leq N-1$, and

$$\Phi_{k,v_k}(u_k) = \sum_{i=1}^{n_k} \Phi_{v_{k,i}}(u_{k,i})$$

($\Psi_{k,v_k}^\nu(u_k)$, $1 \leq \nu \leq N-1$, being defined analogously).
Note that the loss functions $J_{k,\nu}^m$ of the associated noncooperative N–person game (3.6) take the form

$$J_{k,0}^m(v_k) = \tfrac{1}{2}v_k^T A_{k,0}^m v_k - (f_{k,0}^m)^T v_k + \Phi_{k,w_k^m}(v_k) ,$$
$$J_{k,\nu}^m(v_k) = \tfrac{1}{2}v_k^T A_{k,\nu}^m v_k - (f_{k,\nu}^m)^T v_k + \Psi_{k,u_{k,\nu}^m}^\nu(v_k) , \ 1 \leq \nu \leq N-1 .$$

Defining subsolutions $\underline{u}_k$, $\underline{w}_{k,v}$ and supersolutions $\overline{u}_k$, $\overline{w}_{k,\nu}$, $1 \leq \nu \leq N-1$, by the discrete analogues of (2.31.a–d) and setting $\underline{v}_k = (\underline{u}_k, \underline{w}_{k,1}, \ldots, \underline{w}_{k,N-1})$, $\overline{v}_k = (\overline{u}_k, \overline{w}_{k,1}, \ldots, \overline{w}_{k,N-1})$, we may introduce the operator

$$T_k : \mathbb{R}^{n_k} \to [\underline{v}_k, \overline{v}_k] \tag{3.10}$$

in the same way as we did in the continuous case by means of (2.29), (2.32). Again, the set of Nash equilibria of (3.6) turns out to be the fixed point set $F(T_k)$ of the

operator T_k and, arguing as in the preceding section, it can be shown that $F(T_k)$ is non empty and possesses a minimal and maximal element v_k^* and v_k^{**}, respectively. We may compute those elements by the discrete analogue of the iterative scheme (2.33.a), (2.33.b) where at each iteration step we have to solve an uncoupled system of N variational inequalities of the second kind. This can be done by applying multi–grid techniques for such variational inequalities as developed in [17] and [18] which are more efficient than working with the single grid approach in [5] based on the Moreau–Yosida proximal approximation of the subdifferentiable functionals φ_{k,v_k} and ψ_{k,v_k}^{ν}, $1 \leq \nu \leq N-1$. However, the use of algorithm (2.33.a), (2.33.b) has an important drawback: The initial vector $v_k^0 = (\overline{u}_k, \underline{u}_k, \underline{w}_{k,1}, \ldots, \underline{w}_{k,N-1})$ is usually "far away" from v_k^* and v_k^{**} and hence, we need unsatisfactorily many iterations to compute sufficiently accurate approximations. For this reason, we propose a quite different strategy which is not based on decoupling techniques but on some kind of decomposition by using symmetric block nonlinear Gauss–Seidel iteration. As we shall see, at each iteration step, we have to solve a system of N coupled scalar inclusions being equivalent to a noncooperative N–person game with loss functions in N variables. We can explicitly determine the set of Nash equilibria and subsequently compute a unique Pareto minimum within this set. This iteration will then be used within a multi–grid framework both as a smoother and as an iterative solver on the lowest level.

We will describe the $(\mu+1)$–st step of the iteration on level k of the hierarchy of discretizations where for notational convenience we will drop the indices k and m, i.e., we will write u instead of u_k^m, etc. and denote by a_{ij}^{ν}, $1 \leq i, j \leq n_k$, the elements of the matrices $A_{k,\nu}^m$, $0 \leq \nu \leq N-1$.
The block structure is obtained by assembling the unknowns according to

$$\begin{aligned} z &= (z_1, \ldots, z_{n_k}) \in \mathbb{R}^{N \cdot n_k}, \\ z_i &= (u_i, w_{1,i}, \ldots, w_{N-1,i}) \in \mathbb{R}^N, \quad 1 \leq i \leq n_k . \end{aligned} \tag{3.11}$$

As said before, we attempt to solve (3.9.a), (3.9.b) by symmetric nonlinear Gauss–Seidel with respect to that block structure. Hence, given an iterate z^{μ}, $\mu \geq 0$, it is sufficient to describe the first half step in the computation of $z^{\mu+1}$, namely the determination of $z_i^{\mu+1/2}$ for $i = 1, \ldots, n_k$, since afterwards $z_i^{\mu+1}$ will be obtained by the same procedure but in reversed order $i = n_k, n_{k-1}, \ldots, 1$.
The computation of $z_i^{\mu+1/2}$ for $i = 1, \ldots, n_k$ will be accomplished within the following two steps:

Step 1. Determination of Nash equilibria
We compute the set $S_i^{\mu+1/2}$ of solutions $\tilde{z}_i^{\mu+1/2}$ of the system of N scalar inclusions

$$-a_{ii}^0 \tilde{u}_i^{\mu+1/2} + f_{0,i} - d_{0,i} \in \partial \Phi_{\tilde{w}_i^{\mu+1/2}}(\tilde{u}_i^{\mu+1/2}) \tag{3.12.a}$$

$$-a_{ii}^{\nu}\tilde{w}_{\nu,i}^{\mu+1/2} + f_{\nu,i} - d_{\nu,i} \in \partial\Psi^{\nu}_{\tilde{u}_{\nu,i}^{\mu+1/2}}(\tilde{w}_{\nu,i}^{\mu+1/2})$$
$$1 \leq \nu \leq N-1 \,. \tag{3.12.b}$$

where

$$d_{\nu,i} = \sum_{j=1}^{i-1} a_{i_j}^{\nu} z_{j,\nu+1}^{\mu+1/2} + \sum_{j=i+1}^{n_k} a_{i_j}^{\nu} z_{j,\nu+1}^{\mu} \,, \quad 0 \leq \nu \leq N-1 \,. \tag{3.13}$$

Again, introducing loss functions

$$J_{0,i}(u_i, w_{1,i}, \ldots, w_{N-1,i}) = \tfrac{1}{2} a_{ii}^{0} u_i^2 + (d_{0,i} - f_{0,i}) u_i + \Phi_{w_1}(u_i) \,, \tag{3.14.a}$$

$$J_{\nu,i}(u_i, w_{1,i}, \ldots, w_{N-1,i}) = \tfrac{1}{2} a_{ii}^{\nu} w_{\nu,i}^2 + (d_{\nu,i} - f_{\nu,i}) w_{\nu,i} + \Psi^{\nu}_{u_{\nu,1}}(w_{\nu,i}) \tag{3.14.b}$$

and setting $v_i = (v_{i,0}, v_{i,1}, \ldots, v_{i,N-1})$ with $v_{i,0} = \tilde{u}_i^{\mu+1/2}$, $v_{i,\nu} = w_{\nu,i}^{\mu+1/2}$, $1 \leq \nu \leq N-1$, the system (3.12.a), (3.12.b) is equivalent to the noncooperative N–person game

$$J_{\nu,i}(v_{i,0}, \ldots, v_{i,N-1}) = \min_{z \in \mathbb{R}} J_{\nu,i}(v_{i,0}, \ldots, v_{i,\nu-1}, z, v_{i,\nu+1}, \ldots, v_{i,N-1}) \,,$$
$$0 \leq \nu \leq N-1 \,. \tag{3.15}$$

From previous results we have seen that the set $S_i^{\mu+1/2}$ of solutions to (3.12.a), (3.12.b) is non empty and corresponds to the Nash equilibria of (3.15). Knowing that in terms of the solidification problem the vector $v_i \in \mathbb{R}^N$ characterizes either the liquid, solid or mushy region, and using the equivalence of (3.12.a), (3.12.b) with the corresponding dual inclusions (cf. (2.26.a), (2.26.b)), we find that the unknowns satisfy exactly one of the following sets of equations or inequalities, respectively:

(i) Liquid region

$$-a_{ii}^{0}\tilde{u}_i^{\mu+1/2} + b_{0,i} = \rho\sigma\tilde{u}_i^{\mu+1/2} + \rho L \,, \tag{3.16.a}$$

$$-a_{ii}^{\nu}\tilde{w}_{\nu,i}^{\mu+1/2} + b_{\nu,1} = \gamma_{L,\nu}^{-1}\tilde{w}_{\nu,i}^{\mu+1/2} \,, \quad 1 \leq \nu \leq N-1 \,; \tag{3.16.b}$$

(ii) Solid region

$$-a_{ii}^{0}\tilde{u}_i^{\mu+1/2} + b_{0,i} = \rho\sigma\tilde{u}_i^{\mu+1/2} \,, \tag{3.17.a}$$

$$-a_{ii}^{\nu}\tilde{w}_{\nu,i}^{\mu+1/2} + b_{\nu,1} = \gamma_{S,\nu}^{-1}\tilde{w}_{\nu,i}^{\mu+1/2} \,, \quad 1 \leq \nu \leq N-1 \,; \tag{3.17.b}$$

(iii) Mushy region

$$\rho\sigma\tilde{w}_i^{\mu+1/2} \le -a_{ii}^0\tilde{u}_i^{\mu+1/2} + b_{0,i} \le \rho\sigma\tilde{w}_i^{\mu+1/2} + \rho L\ ; \tag{3.18.a}$$

$$\gamma_{L,\nu}^{-1}\tilde{u}_{\nu,i}^{\mu+1/2} \le -a_{ii}^{\nu}\tilde{w}_{\nu,i}^{\mu+1/2} + b_{\nu,i} \le \gamma_{S,\nu}^{-1}\tilde{u}_{\nu,i}^{\mu+1/2}\ ,\ \ 1 \le \nu \le N-1\ ; \tag{3.18.b}$$

where $b_{\nu,i} = f_{\nu,i} - d_{\nu,i}\ ,\ \ 0 \le \nu \le N-1.$

In view of (3.16.a), (3.16.b), (3.17.a), (3.17.b) and (3.18.a) (3.18.b), the following quantities obviously play a central role in the computation of solutions to (3.12.a), (3.12.b):

$$c_i^{\min} = (a_{ii}^0 + \rho\sigma)^{-1}(b_{0,i} - \rho L)\ ;\ \ c_i^{\max} = (a_{ii}^0 + \rho\sigma)^{-1}b_{0,i}\ , \tag{3.19.a}$$

$$d_{\nu,i}^{\min} = (a_{ii}^{\nu} + \gamma_{S,\nu}^{-1})^{-1}b_{\nu,i}\ ,\ \ d_{\nu,i}^{\max} = (a_{ii}^{\nu} + \gamma_{L,\nu}^{-1})^{-1}b_{\nu,i}\ ,\ \ 1 \le \nu \le N-1\ , \tag{3.19.b}$$

$$d_i^{\min} = \sum_{\nu=1}^{N-1} d_{\nu,i}^{\min}\ ,\ \ d_i^{\max} = \sum_{\nu=1}^{N-1} d_{\nu,i}^{\max}\ . \tag{3.19.c}$$

In particular, if v_i represents a liquid or solid state, it follows readily from (3.16.a), (3.16.b), (3.17.a), (3.17.b) that we have a unique solution given by

$$\tilde{u}_i^{\mu+1/2} = c_i^{\min}\ ,\ \ \tilde{w}_{\nu,i}^{\mu+1/2} = d_{\nu,i}^{\max}\ ,\ \ ^1 \le \nu \le N-1 \tag{3.20}$$

in case of a liquid state and

$$\tilde{u}_i^{\mu+1/2} = c_i^{\max}\ ,\ \ \tilde{w}_{\nu,i}^{\mu+1/2} = d_{\nu,i}^{\min}\ ,\ \ 1 \le \nu \le N-1 \tag{3.21}$$

for a solid state.
On the other hand, if v_i characterizes the mushy region, we also have

$$\tilde{u}_i^{\mu+1/2} = \tilde{w}_i^{\mu+1/2}\ ,\ \ \tilde{u}_{\nu,i}^{\mu+1/2} = \tilde{w}_{\nu,i}^{\mu+1/2} \le \nu \le N-1\ . \tag{3.22}$$

Substituting (3.32) into (3.18.a), (3.18.b) reveals

$$c_i^{\min} \le \tilde{u}_i^{\mu+1/2} \le c_i^{\max} \tag{3.23.a}$$

$$d_{\nu,i}^{\min} \le \tilde{w}_{\nu,1}^{\mu+1/2} \le d_{\nu,1}^{\max}\ ,\ \ 1 \le \nu \le N-1\ . \tag{3.23.b}$$

Moreover, observing

$$\tilde{w}_i^{\mu+1/2} = \sum_{\nu=1}^{N-1} \tilde{w}_{\nu,i}^{\mu+1/2} = \tilde{u}_i^{\mu+1/2}$$

for mushy states, (3.23.b) gives

$$d_i^{\min} \leq \tilde{u}_i^{\mu+1/2} \leq d_i^{\max} . \tag{3.24}$$

Hence, setting

$$K_i^{\nu} = \left[d_{\nu,i}^{\min}, d_{\nu,i}^{\max}\right] , \quad 1 \leq \nu \leq N-1 , \tag{3.25.a}$$

$$K_i = \left[c_i^{\min}, c_i^{\max}\right] \cap \left[d_i^{\min}, d_i^{\max}\right] , \tag{3.25.b}$$

we must have $K_i \neq \emptyset$ and consequently, the set of solutions to (3.12.a), (3.12.b) is given by

$$N_i^{\mu+1/2} = \Big\{ v_i \;\Big|\; \tilde{w}_{\nu,i}^{\mu+1/2} \in K_i^{\nu} , \; 1 \leq 1 \leq \nu \leq N-1 \quad \text{and} \quad \tilde{u}_i^{\mu+1/2} = \tilde{w}_i^{\mu+1/2} \in K_i \Big\} . \tag{3.26}$$

Summarizing, the above considerations show that the determination of Nash equilibria can be accomplished by means of the easily available local data and the set K_i as given by (3.19.a–c) and (3.25.b), respectively. In particular, we have to distinguish the following three cases:

(i) $c_i^{\min} > d_i^{\max}$ $(K_i = \emptyset)$
In this case there exists a unique Nash equilibrium, which is given by (3.20) and represents a liquid state.

(ii) $c_i^{\max} < d_i^{\min}$ $(K_i = \emptyset)$
Again, we do have uniqueness of a Nash equilibrium being explicitly given by (3.21) and representing a solid state.

(iii) $K_i \neq \emptyset$
In this case there is a set of Nash equilibria given by (3.26) whose elements characterize a state within the mushy region.

Step 2. Determination of a Pareto minimum on lowest energy level
As we have noticed above, the only situation where we are faced with a continuum of Nash equilibria occurs when $K_i \neq \emptyset$, i.e., in the mushy region. If we make use of the relations $\tilde{w}_i^{\mu+1/2} = \tilde{u}_i^{\mu+1/2}$ and $\tilde{u}_{\nu,i}^{\mu+1/2} = \tilde{w}_{\nu,i}^{\mu+1/2}$, $1 \leq \nu \leq N-1$, in (3.14.a), (3.14.b), it is easily seen that the local loss functions $J_{0,1}$ and $J_{\nu,i}$, $1 \leq \nu \leq N-1$, attain their unique minima in $c_i^{\min}$ and $d_{\nu,i}^{\min}$, respectively. Thus, with regard to the computation of Pareto minima, we will distinguish the following two cases:

(iii)$_1$ $c_i^{\min} \le d_i^{\min} \le d_i^{\max} \le c_i^{\max}$ or
$c_i^{\min} \le d_i^{\min} \le c_i^{\max} \le d_i^{\max}$.

Obviously, a unique Pareto minimum within the set $N_i^{\mu+1/2}$ of Nash equilibria is given by

$$\tilde{u}_i^{\mu+1/2} = d_i^{\min} \ , \quad \tilde{w}_{\nu,i}^{\mu+1/2} = d_{\nu,i}^{\min} \ , \quad 1 \le \nu \le N-1 \ . \tag{3.27}$$

(iii)$_2$ $d_i^{\min} \le c_i^{\min} \le d_i^{\max} \le c_i^{\max}$ or
$d_i^{\min} \le c_i^{\min} \le c_i^{\max} \le d_i^{\max}$.

In this case $\tilde{u}_i^{\mu+1/2}$ is uniquely determined by $c_i^{\min}$. On the other hand, due to the monotonicity of $J_{\nu,i}$, $1 \le \nu \le N-1$, on K_i^ν, we do not have uniqueness of the concentrations. Indeed, each element of the set

$$\begin{aligned} P_i^{\mu+1/2} \ = \ & \Big\{ (c_i^{\min}, \tilde{w}_{1,i}^{\mu+1/2}, \ldots, \tilde{w}_{N-1,i}^{\mu+1/2}) \ \Big| \ \tilde{w}_{\nu,i}^{\mu+1/2} \in K_i^\nu \ , \\ & 1 \le \nu \le N-1 \ , \ \sum_{\nu=1}^{N-1} \tilde{w}_{\nu,i}^{\mu+1/2} = c_i^{\min} \Big\} \end{aligned} \tag{3.28}$$

represents a Pareto minimum within the set $N_i^{\mu+1/2}$ of Nash equilibria.
To each Pareto minimum $v_i \in P_i^{\mu+1/2}$, we may assign the sum ot the individual loss functions or equivalently, in terms of the physical solidification process, the total energy content $E_i(v_i) = \sum_{\nu=0}^{N-1} J_{\nu,i}(v_i)$. Hence, each Pareto minimum v_i represents a well–defined energy level $E_i(v_i)$ Then, from a physical point of view, it is natural to ask for that Pareto minimum which characterizes the lowest energy level, and this amounts to the constrained minimization problem: find $v_i^* \in P_i^{\mu+1/2}$ such that

$$E_i(v_i^*) = \min_{v_i \in P_i^{\mu+1/2}} E_i(v_i) \ . \tag{3.29}$$

Since E_i is quadratic and $P_i^{\mu+1/2}$ is a closed convex set, there exists a unique v_i^* which can be easily computed, e.g. by standard Lagrange multiplier techniques.

The preceding nonlinear block Gauss–Seidel iteration can be interpreted as a local selection procedure in (3.9.a) and (3.9.b), respectively. To be more specific, for $i = 1, \ldots, n_k$ we define $\alpha_{\nu,i}$, $0 \le \nu \le N-1$, by

$$-a_{ii}^0 \tilde{u}_i^{\mu+1/2} + b_{0,1} = \rho\sigma \tilde{u}_i^{\mu+1/2} + \alpha_{0,i}\rho L \ , \tag{3.30.a}$$

$$-a_{ii}^\nu \tilde{w}_{\nu,i}^{\mu+1/2} + b_{\nu,i} = \left(\alpha_{\nu,i}\gamma_{S,\nu}^{-1} + (1-\alpha_{\nu,i})\gamma_{L,\nu}^{-1}\right)\tilde{w}_{\nu,i}^{\mu+1/2} \ . \tag{3.30.b}$$

Then, in view of (3.19.a–c), (3.20), (3.21) and (3.27), (3.28), it follows readily that $\alpha_{0,i} = 1 (\alpha_{0,i} = 0)$, if the i–th nodal point represents a liquid (solid) state, while

$\alpha_{0,i} \in [0,1]$, if it is in the mushy region. Correspondingly, for all $1 \leq \nu \leq N-1$ we have $\alpha_{\nu,i} = 0 (\alpha_{\nu,i} = 1)$, if the i–th nodal point is in the liquid (solid) zone, while again $\alpha_{\nu,i} \in [0,1]$ holds true in the mushy region.

Since ρL stands for the release of latent energy at change of phase, we can interpret $\alpha_{0,i}$ as the liquid fraction of the solute corresponding to the i–th nodal point.

Remark: The computation of the liquid fraction $\alpha_{0,i}$ according to (3.30.a,b) constitutes a distinctive feature of the above iterative scheme: The liquid fraction can be determined as a by–product of the iteration in contrast to other approaches where the liquid fraction is introduced as an additional unknown in the mathematical model to account for the temporal evolution of the latent heat (cf. e.g. [26], [27], [28]).

So far, we have only described one basic ingredient of the multi–grid algorithm, namely the smoothing process. We will now focus our interest to the coarse grid correction including an appropriate realization of the grid interactions in the fine–to–coarse and coarse–to–fine transfers.
As already pointed out in the introductory part of this paper, the coarse grid correction will be done by a modification of Brandt's FAS scheme [7] taking advantage of a duality argument from convex analysis. In particular, the duality result (2.25) tells us that the fully discretized system as given by the inclusions (3.9.a), (3.9.b) is equivalent to the following system of nonlinear algebraic equations

$$u_k = \partial \Phi^*_{k,w_k}(f_{k,0} - A_{k,0} u_k) \tag{3.31.a}$$

$$w_{k,\nu} = \partial \Psi^{\nu,*}_{k,u^\nu_k}(f_{k,\nu} - A_{k,\nu} w_{k,\nu}) \ , \quad 1 \leq \nu \leq N-1 \ . \tag{3.31.b}$$

Adopting the approach in [16], [17] and [18], we then proceed as follows:
Given an iterate $v^\mu_k = (u^\mu_k, w^\mu_{k,1}, \ldots, w^\mu_{k,N-1})$ and denoting by $\overline{v}^\mu_k$ the result after having executed a certain number of smoothing steps, we determine a new iterate $\overline{v}^{\mu,\text{new}}_k$ according to

$$\overline{v}^{\mu,\text{new}}_{k,\nu} = \overline{v}^\mu_{k,\nu} - p^k_{k-1}(r^{k-1}_k \overline{v}^\mu_{k,\nu} - v^{\mu+1}_{k-1,\nu}) \ , \quad 0 \leq \nu \leq N-1 \ . \tag{3.32}$$

Here r^{k-1}_k and p^k_{k-1} are suitably chosen restrictions and prolongations while $v^{\mu+1}_{k-1} = (u^{\mu+1}_{k-1}, w^{\mu+1}_{k-1,1}, \ldots, w^{\mu+1}_{k-1,N-1})$ solves the nonlinear algebraic system

$$u_{k-1} = \partial \Phi^*_{k-1,w_{k-1}}(\tilde{f}_{k-1,0} - A_{k-1,0} u_{k-1}) \tag{3.33.a}$$

$$w_{k-1,\nu} = \partial \Psi^{\nu,*}_{k-1,u_{k-1,\nu}}(\tilde{f}_{k-1,\nu} - A_{k-1,\nu} w_{k-1,\nu}) \ , \quad 1 \leq \nu \leq N-1 \tag{3.33.b}$$

where

$$\tilde{f}_{k-1,\nu} = A_{k-1,\nu} r_k^{k-1} \overline{v}_{k,\nu}^{\mu} + r_k^{k-1}(f_{k,\nu} - A_{k,\nu}\overline{v}_{k,\nu}^{\mu}) \ , \ \ 0 \leq \nu \leq N-1 \ .$$

Remark: Note that in view of (2.25) the system (3.33.a), (3.33.b), constituting the coarse grid correction on level $k-1$, can be equivalently reformulated as a system of algebraic inclusions of the same structure as that which we encountered on level k.

In the multi–grid solution of algebraic equations arising from elliptic problems discretized by piecewise linear finite elements with respect to a hierarchy of triangulations, restrictions and prolongations are usually chosen in a canonical way, namely by the so–called seven–point restrictions and prolongations (c.f. e.g. [12], [13]). If we first analyze the fine–to–coarse transfer, by looking at the fine grid system (3.31.a), (3.31.b) and its coarse grid counterpart (3.33.a), (3.33.b) it is evident that we cannot use the standard seven–point restriction globally. The reason is that for a nodal point on level $k-1$ with a neighbouring nodal point on level k representing a different phase, the defect in that fine nodal point is not a reliable indicator for the accuracy of the approximation in the coarse nodal point. This situation typically occurs within a neighbourhood of the discrete liquidus and the discrete solidus so that we have to distinguish between nodal points close to and off the discrete free boundaries. To make this point more explicit, we define $\Omega_k^R(\overline{v}_k^{\mu})$, $R = L, S, M$, as the set of "liquid", "solid" and "mushy" nodal points in Ω_k with respect to the iterate $\overline{v}_k^{\nu}$, i.e., $\Omega_k^L(\overline{v}_k^{\mu}) = \left\{x_j \in \Omega_k | (\overline{u}_k^{\mu})_j > (\overline{w}_k^{\mu})_j\right\}$ and $\Omega_k^S(\overline{v}_k^{\mu})$, $\Omega_k^M(\overline{v}_k^{\mu})$ being defined analogously. Further, for $x \in \Omega_k$ we denote by $U_k^r(x)$ the set consisting of x and its adjacent nodal points in Ω_k. Then a nodal point $x \in \Omega_k$ will be called regular if $U_k^r(x)$ is a subset of either the set of "liquid", "solid" or "mushy" nodal points and will be said irregular otherwise. In particular, we will refer to

$$\Omega_k^{\mathrm{reg}}(\overline{v}_k^{\mu}) = \left\{x \in \Omega_k | U_k^r(x) \subset \Omega_k^R(\overline{v}_k^{\mu}) \ , \ \ R \in \{L, S, M\}\right\}$$
$$\Omega_k^{\mathrm{irr}}(\overline{v}_i^{\mu}) = \Omega_k \setminus \Omega_k^{\mathrm{reg}}(\overline{v}_k^{\mu})$$

as the sets of regular and irregular nodal points on level k with respect to $\overline{v}_k^{\mu}$. Now, a convenient strategy to overcome the above mentioned difficulty in the fine–to–coarse transfer is to use pointwise restriction $\overset{\circ}{r}_k^{k-1}$ for irregular coarse nodal points while the standard seven–point restriction $\hat{r}_k^{k-1}$ can be chosen in regular coarse nodal points:

$$\left(r_k^{k-1} z_k\right)(x) = \begin{cases} \left(\hat{r}_k^{k-1} z_k\right)(x) \ , & \text{if } x \in \Omega_{k-1} \cap \Omega_k^{\mathrm{reg}}(\overline{v}_k^{\mu}) \\ \left(\overset{\circ}{r}_k^{k-1} z_k\right)(x) \ , & \text{if } x \in \Omega_{k-1} \cap \Omega_k^{\mathrm{irr}}(\overline{v}_k^{\mu}) \ . \end{cases} \tag{3.34}$$

On the other hand, concerning a proper choice of prolongations, it is well known (cf. e.g. [6], [16], [17], [18], [19]) that in the context of free boundary problems the coarse grid information on the discrete free boundary is insufficient for a proper modelling of the discrete free boundary on the finer grid. In particular, for nodal points close to the discrete free boundaries the usual transfer of coarse grid information by the standard seven–point prolongation may result in an oscillatory behaviour of both the liquidus and the solidus. Therefore, we will use the strategy that a change of the discrete free boundaries should not be caused by the coarse grid correction process. This can be easily realized by not prolongating onto irregular nodal points on the higher level. To be more precise, we refer to $\Omega_{k-1}^R(v_{k-1}^{\mu+1})$, $R = L, S, M$, as the set of "liquid", "solid" and "mushy" nodal points in Ω_{k-1} with respect to $v_{k-1}^{\mu+1}$. Further, for $x \in \Omega_k$, we define $U_{k-1}^p(x)$ as the set consisting either of the single element x, if $x \in \Omega_{k-1}$, or of the adjacent nodal points in Ω_{k-1} if $x \notin \Omega_{k-1}$. Then, we set

$$\begin{aligned}
\Omega_k^{\mathrm{reg}}\left(\overline{v}_k^{\mu}; v_{k-1}^{\mu+1}\right) &= \left\{x \in \Omega_k | x \in \Omega_k^R\left(\overline{v}_k^{\mu}\right) \text{ and } \right. \\
&\quad \left. U_{k-1}^p(x) \subset \Omega_{k-1}^R\left(v_{k-1}^{\mu+1}\right) \ , \ R \in \{L, S, M\}\right\} , \\
\Omega_k^{\mathrm{irr}}\left(\overline{v}_k^{\mu}; v_{k-1}^{\mu+1}\right) &= \Omega_k \setminus \Omega_k^{\mathrm{reg}}\left(\overline{v}_k^{\mu}; v_{k-1}^{\mu+1}\right) .
\end{aligned}$$

Finally, denoting by $\widehat{p}_{k-1}^k$ the standard seven–point prolongation, we choose p_{k-1}^k according to

$$\left(p_{k-1}^k, z_{k-1}\right)(x) = \begin{cases} \left(\widehat{p}_{k-1}^k z_{k-1}\right)(x) & , \text{ if } x \in \Omega_k^{\mathrm{reg}}\left(\overline{v}_k^{\mu}; v_{k-1}^{\mu+1}\right) \\ 0 & , \text{ if } x \in \Omega_k^{\mathrm{irr}}\left(\overline{v}_k^{\mu}; v_{k-1}^{\mu+1}\right) . \end{cases} \tag{3.35}$$

4. Numerical Results

We consider macrosegregation of carbon and manganese during continuous casting of an *Fe-C-Mn* ternary alloy in a slab of rectangular cross section $R = (0,a) \times (0,b)$. At the initial time $t = 0$, we assume a uniform distribution of both the temperature $u^0 = u(0)$ and the concentrations of the impurities $c_1^0 = c_1(0)$ and $c_2^0 = c_2(0)$ with u^0 given by the melting temperature u_d of the prime component of the alloy so that initially the alloy is in a completely liquid state. We further assume that the slab is cooled uniformly at its boundary ∂R (cf. Table 1 below which contains the basic physical data).

Data	Units	Values	Data	Units	Values
ρ	kg/m^3	$7.40 \cdot 10^3$	$\beta_{S,2}$	m^2/s	$1.00 \cdot 10^{-11}$
σ	$J/(kg \cdot °C)$	$6.91 \cdot 10^2$	$\gamma_{L,1}$	—	$7.80 \cdot 10^1$
κ_L	$J/(m \cdot s \cdot °C)$	$3.40 \cdot 10^1$	$\gamma_{S,1}$	—	$2.23 \cdot 10^2$
κ_S	$J/(m \cdot s \cdot °C)$	$3.40 \cdot 10^1$	$\gamma_{L,2}$	—	4.90
L	J/kg	$2.72 \cdot 10^5$	$\gamma_{S,2}$	—	6.53
q	$J/(m^2 \cdot °C)$	$-6.25 \cdot 10^5$	u_d	$°C$	$15.36 \cdot 10^2$
$\beta_{L,1}$	m^2/s	$1.00 \cdot 10^{-8}$	u^0	$°C$	$15.36 \cdot 10^2$
$\beta_{S,1}$	m^2/s	$0.50 \cdot 10^{-8}$	c_1^0	%	0.60
$\beta_{L,2}$	m^2/s	$1.00 \cdot 10^{-11}$	c_2^0	%	0.60

Table 1. Physical data

For symmetry reasons it is sufficient to perform the computations on a quadrant of R, i.e., the computational domain can be chosen as $\Omega = (0, a/2) \times (b/2, b)$ with an inhomogeneous Neumann boundary condition on the left and upper part of the boundary $\partial\Omega$, and a homogeneous Neumann boundary condition on the right and lower part.

For $a = b = 0.1\,m$ we have discretized the problem implicitly in time using $\Delta t = 1$ as time step size and by continuous, piecewise linear finite elements in the space variables with respect to a hierarchy $(\mathcal{T}_k)_{k=k_{\min}}^{k_{\max}}$ of regular triangulations of $\overline{\Omega}$ involving 2^{2k+3} triangular elements on each level $k_{\min} \leq k \leq k_{\max}$. Choosing $k_{\min} = 2$ and $k_{\max} = 5$, we have computed approximations of the temperature and the concentrations of the impurities at selected time instants by multi-grid V-cycles. In particular, we have performed one pre- and one post-smoothing step on each level $2 < k \leq 5$ while using the special symmetric nonlinear block Gauss-Seidel scheme also as an iterative solver on the lowest level $k = 2$. Suitable

start iterates on the highest level $k = 5$ have been obtained by nested iteration incorporating the already known values at the previous time step (cf. e.g [16]).

For comparison we have also implemented the algorithm proposed in [5] starting at appropriately chosen super– resp. subsolutions and requiring the solution of three "classical" two–phase Stefan problems at each iteration step. These auxiliary problems have been solved using the multi–grid algorithm MGSTEF2 from [16] (which is already much more efficient than the single–grid approach in [5]). The findings were that in terms of execution times the algorithm presented in this paper was up to 4 times faster (depending on the actual time level).

Concerning temperature and concentration profiles, Figures 1a–c display level curves at time $t = 100s$ while Figures 2a–c represent the related curves at $t = 250s$. In Figures 1a, 2a the first level curve from the right corresponds to a temperature of $u = 1486.26\ ^\circ C$ which is the liquidus temperature of the alloy for concentrations $c_1 = c_2 = 0.6\%$. The following curves are associated with temperatures at levels $u = 1400^\circ C$, $1300\ ^\circ C$, $1200\ ^\circ C$, $\cdots$. In Figures 1b,c and 2b,c the first level curve from the right corresponds to the concentrations $c_1 = 0.6\%$ and $c_2 = 0.6\%$, respectively, while the curves close to the left and upper boundary represent slightly lower and the curves in between slightly higher levels.

The computed concentration profiles are in good agreement with experimental observations and confirm that molecular diffusion has a limited impact on macrosegregation in so far as the concentrations only change within a relatively small margin.

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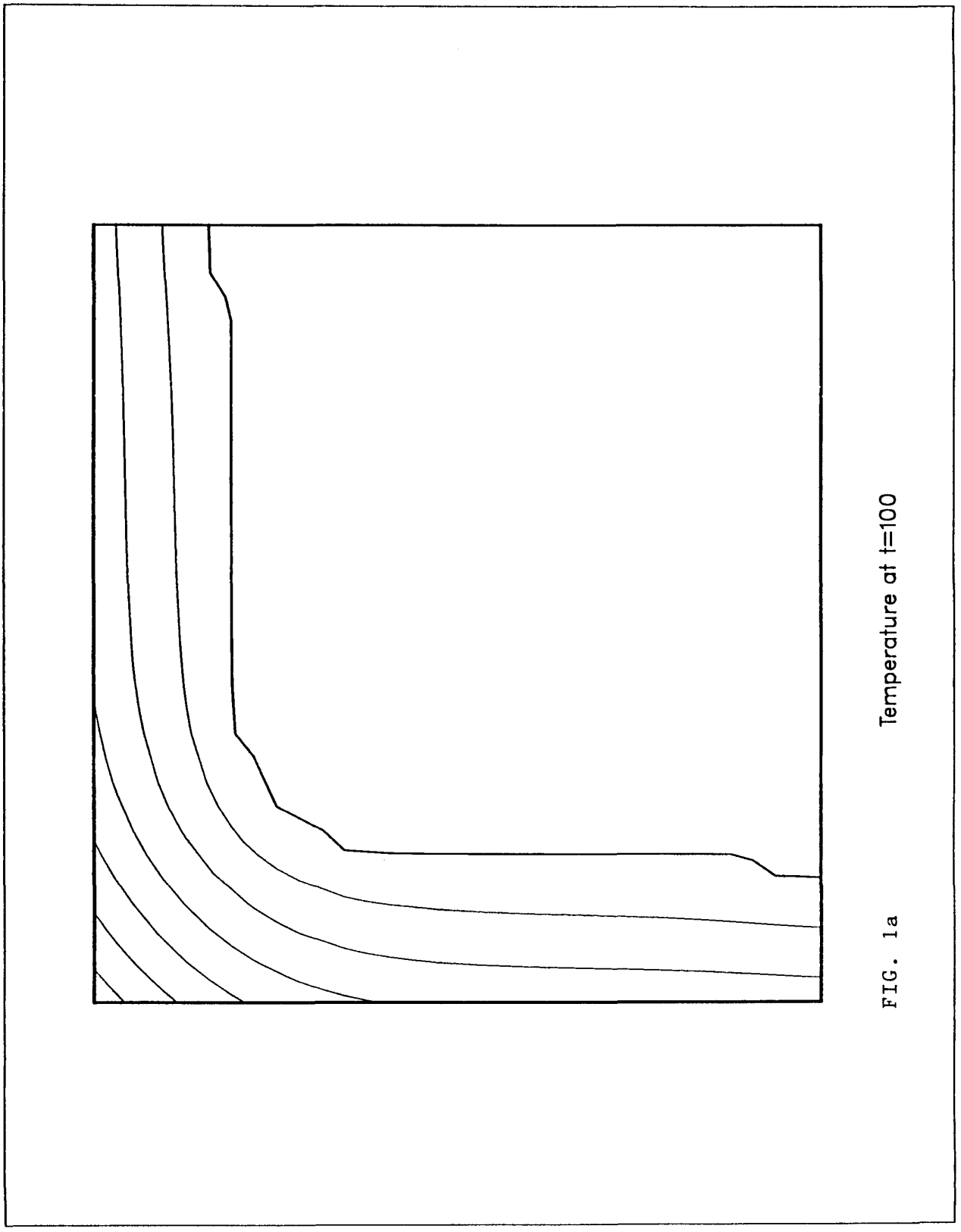

FIG. 1a

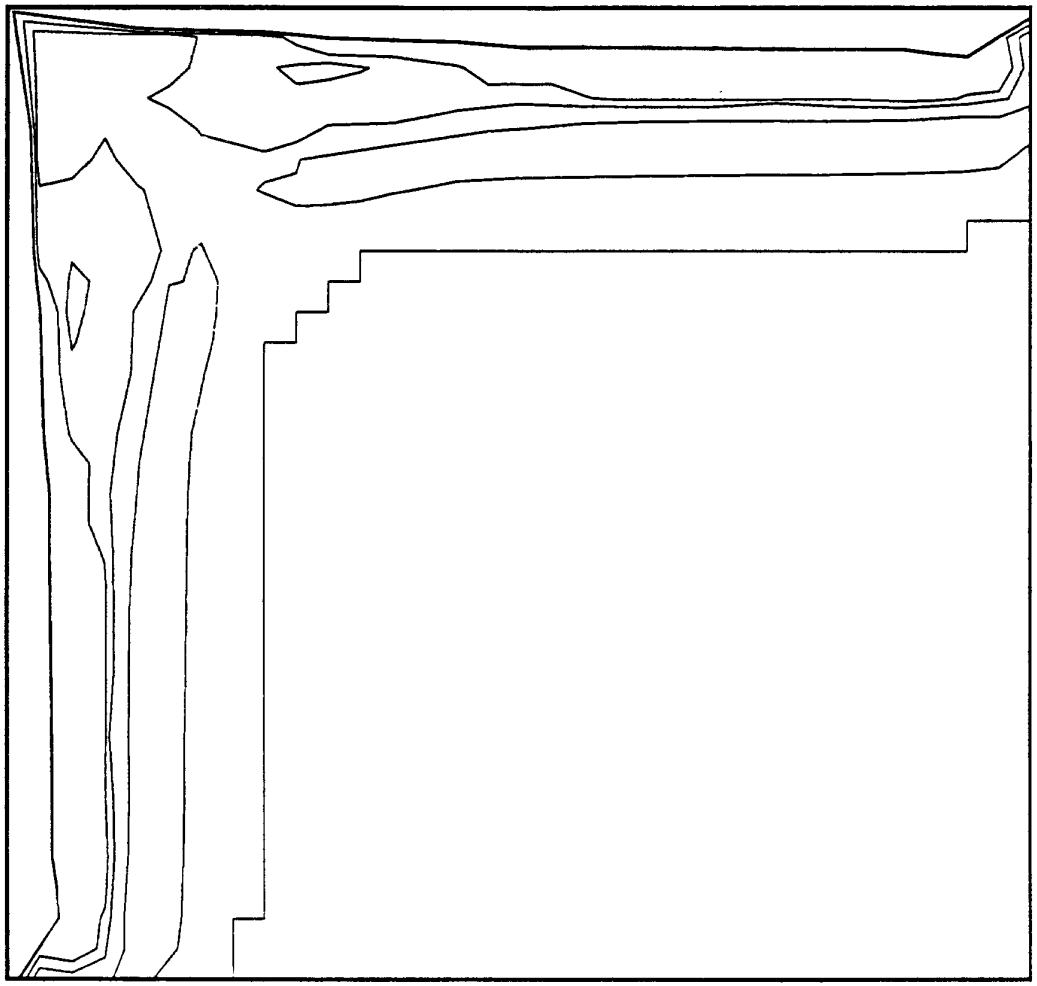

FIG. 1b Carbon Concentration at t=100

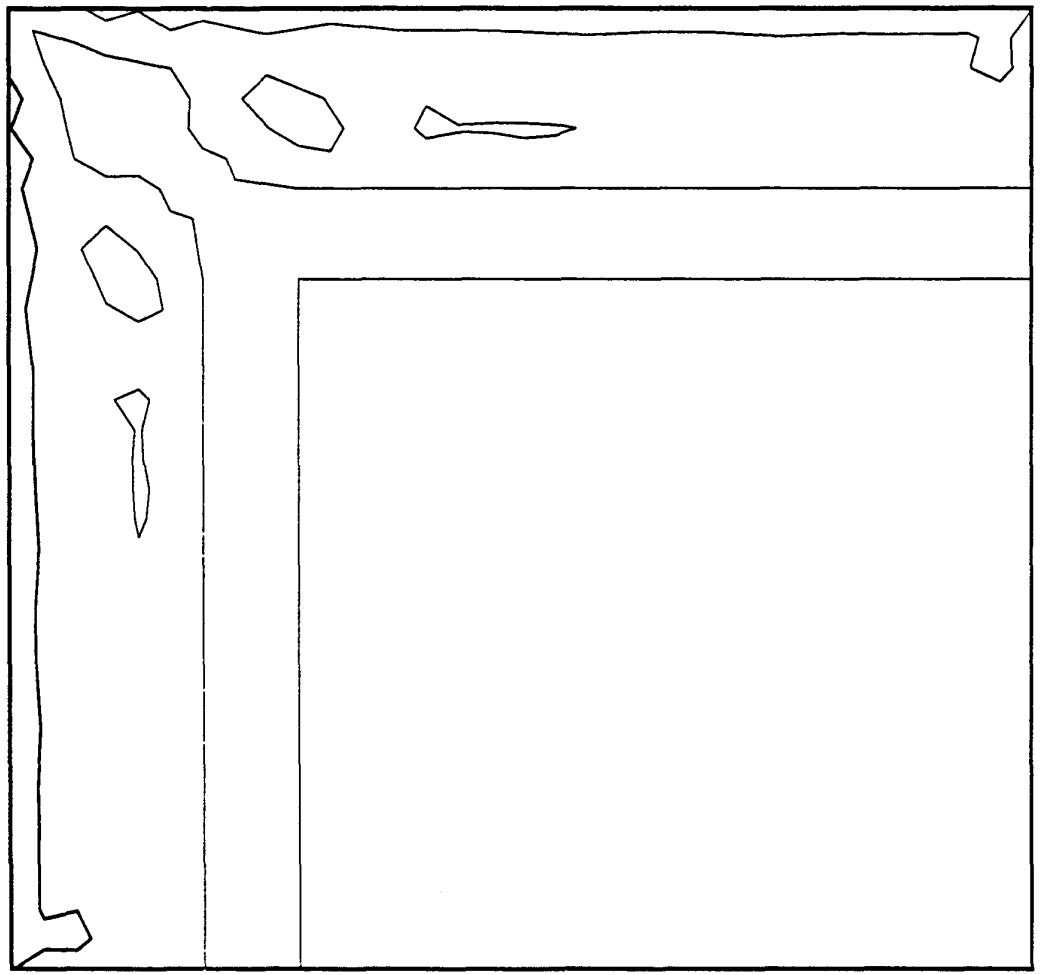

FIG. 1c Manganese Concentration at t=100

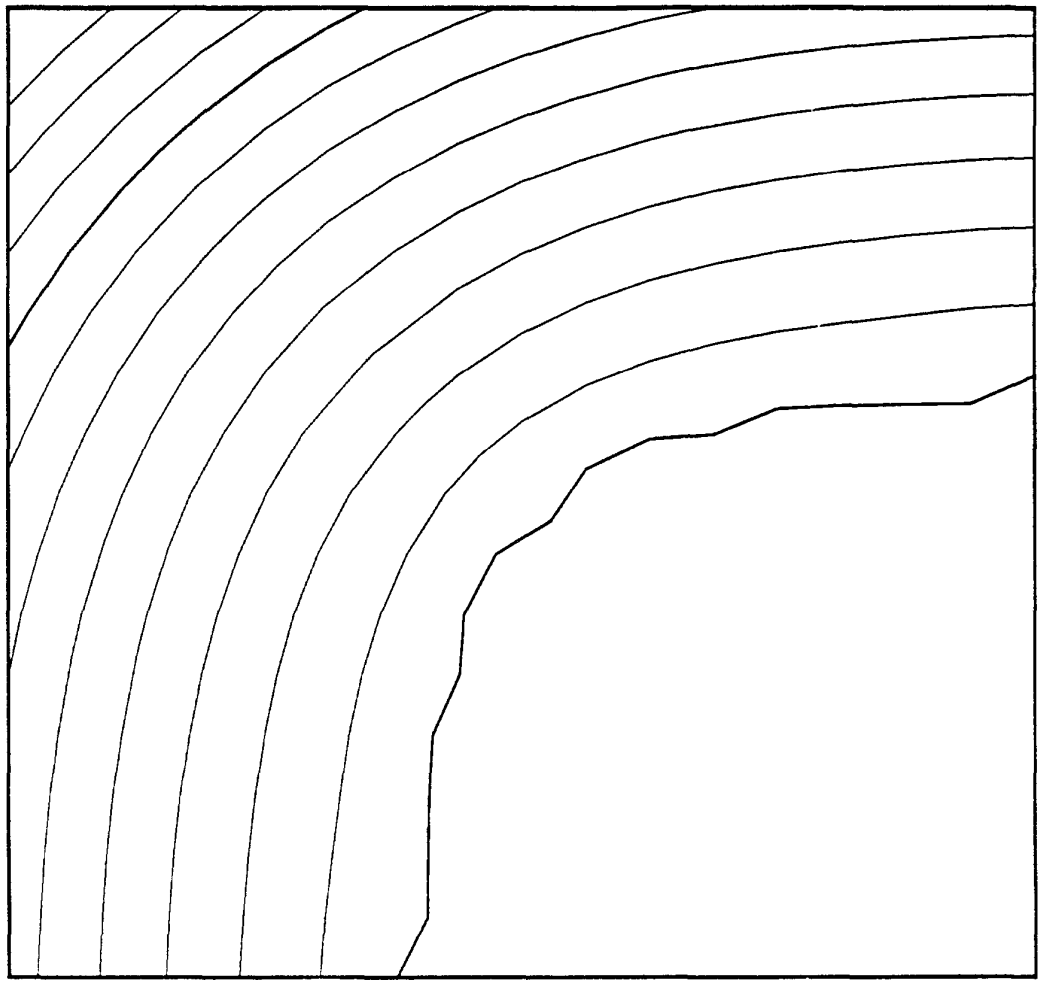

FIG. 2a Temperature at t=250

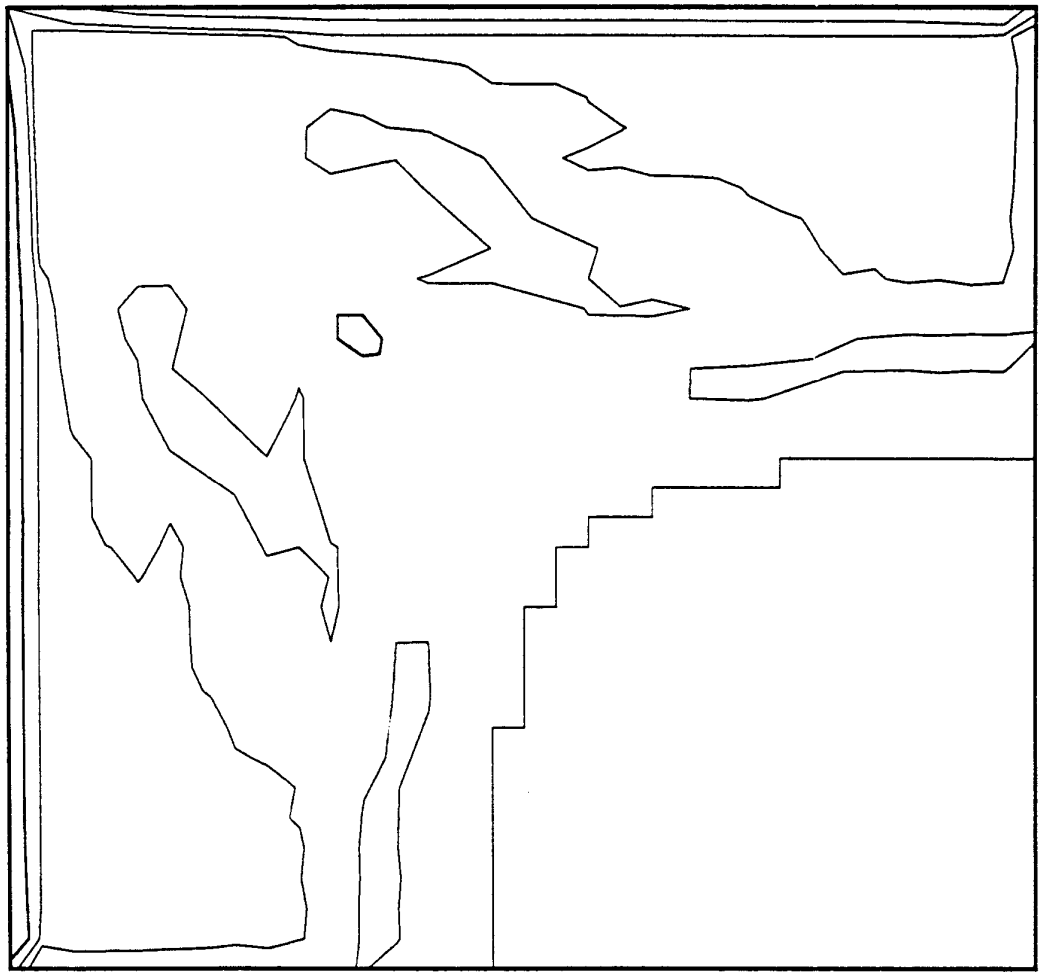

FIG. 2b Carbon Concentration at t=250

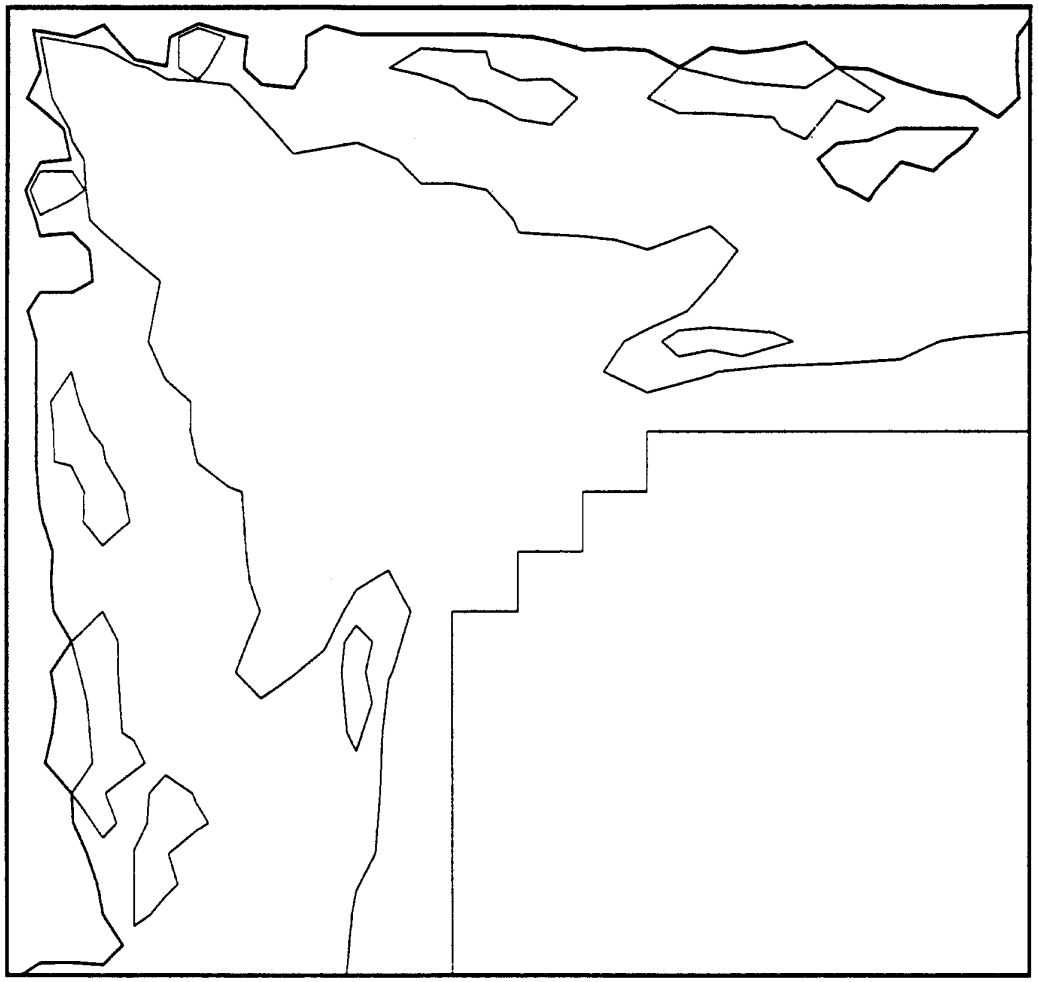

FIG. 2c Manganese Concentration at t=250

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