Numerically Stable Computer Simulation of Solidification: Association Between Eigenvalues of Amplification Matrix and Size of Time Step

Elzbieta Gawronska and Norbert Sczygiol

Abstract The constantly increasing demand for efficient and precise computational solvers becomes the crucial factor deciding about usability of a given domain specific simulation software. The main idea of this article is the use of eigenvalues of amplification matrices to determine the size of time step in modeling of solidification. As far as numerical simulations are concerned it is very important to obtain solutions which are stable and physically correct. It is acquired by fulfilling many assumptions and conditions during the construction a numerical model and carrying out computer simulations. One of the conditions is a proper selection of time step. The size of time step has a great impact on the stability of used time integration schemes (e.g. explicit scheme), or on a proper image of physical phenomena occurring during the simulation (e.g. implicit scheme). The eigenvalues of amplification matrix in governing equations influence on the appropriate selection of size of time step in computer simulations. Hence, it allows to better fit the size of time step and time integration scheme for modeled structure.

Keywords Amplification matrix · Computer simulation · Computer modeling · Eigenvalues · Explicit scheme · Implicit scheme · Solidification process · Stability · Time step

1 Introduction

Modeling and computer simulation is one of the most effective methods of studying of difficult problems in foundry and metallurgical manufacture. Numerical simulations are use for optimization of casting production. In many cases they are a

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unique possible technique for carrying out of the experiments which real statement is complicated. Computer modeling allows defining the major factors for a quality estimation of alloy castings. Simulations help to investigate interaction between solidifying casting and changes of its parameters or initial conditions.

A numerical modeling of solidification is known to be a very time consuming task. The constantly increasing demand for efficient and precise computational solvers becomes the factor that decides about usability of a given solidification simulation software. In many cases practitioners require multiple scenarios to be tested, e.g. for different input parameters, before they make a final decision about the setup of a given technological process. At the same time increasing size of computer memory makes it possible to consider problems with increasing size, which in turn results in increased precision of simulations. There are several possible ways to tackle this kind of problems. For instance, one can use parallel computers or accelerated architectures such as GPUs or FPGAs [1]. However, these solutions require another level of expertise in both, parallel hardware and software, which very often is not easily available. In papers [2–4] we proposed new method, which relies on the application of the technique called mixed time partitioning. Our approach exploits the fact that physical processes inside a mould are of different nature than those in a solidifying casting. As a result different time steps can be used to run computations within both sub-domains. Because processes that are modeled in the casting sub-domain are more dynamic they require very fine-grained time step. On the other hand a heat transfer within the mould sub-domain is less intense, and thus coarse-grained step is sufficient to guarantee desired precision of computations. Obviously, increasing length of a single time step results in decreased computational load, which in turn greatly improves performance of our approach. In this paper we put emphasis on determination of stability criteria for the selected integration method. Mathematical apparatus of the chosen stability analysis method is applied for the homogeneous form of the semi-discretized (after spatial discretization) equation of solidification, as the stability is independent of the inhomogeneous part. The analysis of numerical stability of mixed time partitioning methods for the structural dynamics [5] and for heat conduction problem was adapted to the solidification problem with temperature-dependent material properties.

2 Solidification in Terms of the Finite Element Method

The finite element method facilitates the modeling of many complex problems. Its wide application for founding comes from the fact that it permits an easy adaptation of many existing solutions and technique of solidification modeling.

Computer calculations need to use discrete models, which means problems must be formulated by introducing time-space mesh. These methods convert given physical equations into matrix equations (algebraic equations). This system of

algebraic equations usually contain many thousands of unknowns, that is why the efficiency of method applied to solve them is crucial.

After essential transformations we obtain an ordinary differential equation containing only the time derivative [6] as following:

$$\mathbf{M}(T)\dot{\mathbf{T}} + \mathbf{K}(T)\mathbf{T} = \mathbf{b}(T), \tag{1}$$

where $\mathbf{M}$ is the capacity matrix, $\mathbf{K}$ is the conductivity matrix, $\mathbf{T}$ is temperature vector and $\mathbf{b}$ is right-hand side vector values of which are calculated using boundary conditions. The global form of these matrices is obtained by summing of coefficients for all the finite elements. The matrix components are defined for a single finite element as follows:

$$\mathbf{M} = \sum_e \int_\Omega c^* \mathbf{N}^T \mathbf{N} \, \mathrm{d}\Omega, \tag{2}$$

$$\mathbf{K} = \sum_e \int_\Omega \lambda \nabla^T \mathbf{N} \cdot \nabla \mathbf{N} \, \mathrm{d}\Omega, \tag{3}$$

$$\mathbf{b} = \sum_e \int_\Gamma \mathbf{N}_\Gamma^T \mathbf{q}^T \mathbf{n} \, \mathrm{d}\Gamma, \tag{4}$$

where $\mathbf{N}$ is a shape vector in the area Ω, $\mathbf{N}_\Gamma$ is a shape vector on the boundary Γ, $\mathbf{n}$ is an ordinary vector towards the boundary Γ, and $\mathbf{q}$ is vector of nodal fluxes.

The system of ordinary differential equations (1) containing time derivative was obtained as a result of spatial integration and it may only be solved in approximation. In order to receive an approximate solution it is needed to use the division of time interval $(0, t_{max})$ into sub-intervals (t_k, t_{k+1}) with the length of $\Delta t_k = t_{k+1} - t_k$ and time integration is performed by the use of one step or multisteps methods [7]. We used the one step schemes, so-called Θ schemes, in the following form:

$$\begin{aligned} \mathbf{T}^{n+1} = \mathbf{T}^n &+ (-(\mathbf{M}^{n+\Theta})^{-1}\mathbf{K}^{n+\Theta}\mathbf{T}^n \\ &+ (\mathbf{M}^{n+\Theta})^{-1}\mathbf{b}^n)(1-\Theta)\Delta t \\ &+ (-(\mathbf{M}^{n+\Theta})^{-1}\mathbf{K}^{n+\Theta}\mathbf{T}^{n+1} \\ &+ (\mathbf{M}^{n+\Theta})^{-1}\mathbf{b}^{n+1})\Theta\Delta t. \end{aligned} \tag{5}$$

Due to a possible dependence of materials properties from the temperature, namely $\mathbf{M}$, $\mathbf{K}$ and $\mathbf{b}$ for $\Theta \neq 0$ it is a system of nonlinear equations. To solve this system iterative methods must be used.

The forward Euler scheme:

$$\mathbf{M}^n\mathbf{T}^{n+1} = \mathbf{M}^n\mathbf{T}^n - \Delta t\mathbf{K}^n\mathbf{T}^n + \Delta t\mathbf{b}^n, \tag{6}$$

is obtained for one extreme value $\Theta = 0$ and the backward Euler scheme:

$$\left(\mathbf{M}^{n+1} + \Delta t\mathbf{K}^{n+1}\right)\mathbf{T}^{n+1} = \mathbf{M}^{n+1}\mathbf{T}^n + \Delta t\mathbf{b}^{n+1}, \tag{7}$$

is obtained for the other extreme value $\Theta = 0$. And if the values of matrices coefficients $\mathbf{M}$ i $\mathbf{K}$ in the Eq. (7) are evaluated on the level of previous time step then a modified backward Euler scheme is obtained as follows:

$$(\mathbf{M}^n + \Delta t\mathbf{K}^n)\mathbf{T}^{n+1} = \mathbf{M}^n\mathbf{T}^n + \Delta t\mathbf{b}^{n+1}. \tag{8}$$

3 Basic Equations

In the computer simulations apparent heat formulation (AHC) of solidification is used [8]:

$$\nabla \cdot (\lambda \nabla T) = c^*(T)\frac{\partial T}{\partial t}. \tag{9}$$

The Eq. (9) is solved by mixed time partitioning method considering:

1. semi-discretization,
2. initial-value problem which consists of given functions $\mathbf{T} = \mathbf{T}(t)$ satisfying the Eq. (9) and being the part of initial conditions $\mathbf{T}(t = 0) = \mathbf{T}_0$ for $t \in \langle 0, T\rangle$, $T > 0$,
3. one step Θ time integration scheme.

The finite elements mesh consists of two groups elements (e): connected with a mould (A), where $e \in A$ and connected with a casting (B), where $e \in B$. Each of these can be integrated with the use of different schemes of time integration.

This fact simplifies finding of the critical time step and the stability analysis. If this division is assumed then it may be written as:

$$\begin{aligned} \mathbf{M}_A &= \sum_e \mathbf{M}_e, \mathbf{K}_A = \sum_e \mathbf{K}_e, \mathbf{b}_A = \sum_e \mathbf{b}_e, \\ \mathbf{M}_B &= \sum_e \mathbf{M}_e, \mathbf{K}_B = \sum_e \mathbf{K}_e, \mathbf{b}_B = \sum_e \mathbf{b}_e. \end{aligned} \tag{10}$$

All vectors are also divided into parts according to finite elements mesh division $\mathbf{T} = (\mathbf{T}_A\mathbf{T}_B)^T$, $\dot{\mathbf{T}} = (\dot{\mathbf{T}}_A\dot{\mathbf{T}}_B)^T$, the upper index T represents transportation. As above, vector $\dot{\mathbf{T}}$ may be written as:

$$\begin{aligned}\dot{\mathbf{T}} &= \mathbf{v}_A + \mathbf{v}_B,\\ \mathbf{v}_A &= \mathbf{M}^{-1}(\mathbf{b}_A - \mathbf{K}_A\mathbf{T}),\\ \mathbf{v}_B &= \mathbf{M}^{-1}(\mathbf{b}_B - \mathbf{K}_B\mathbf{T}).\end{aligned} \tag{11}$$

In domain connected with a mould the integration is carried out with a bigger time step ($m\Delta t$, where m is positive integer) whereas in domain connected with a casting with a smaller time step (Δt). This allows to build a system of equations on the basis of Eq. (1) separately for the sub-domain B elements and to carry out calculations more often for it than for the whole mesh with maintaining condition of stability.

4 General Outline of Numerical Stability

Numerical method is stable when a little error in any solution stage moves further with a decreasing amplitude. An error appearing on time level n may be defined as ε^n, on time level $n+1$ as ε^{n+1}, whereas values of this error may be determined with equation:

$$\varepsilon^{n+1} = g\varepsilon^n, \tag{12}$$

where g is amplification factor connected with integral operator $\mathscr{T}(\Delta t, \Delta)$. The amplification factor refers to a method error and is connected with time integration scheme. That is why it is necessary fulfilling one of conditions for stability of the method: the value of an error on time level $n+1$ must not be bigger than value of an error on time level n. That may be written in this formula:

$$|\varepsilon^{n+1}| \leq |\varepsilon^n|, \tag{13}$$

and using the definition of amplification factor (12):

$$|g\varepsilon^n| \leq |\varepsilon^n|. \tag{14}$$

It follows that numerical stability may be achieved if condition:

$$|g| \leq 1 \tag{15}$$

is fulfilled. This condition is limited to issues leading to finite solutions.

For the system N of ordinary differential first-order equations an error vector is defined as ε^n. Each coordinate of this vector is an error connected with an appropriate dependent variable of the system. For each time step an error is multiplied by *amplification matrix* $\mathbf{G}$ in order to obtain an error vector in a new time step:

$$\varepsilon^{n+1} = \mathbf{G}\varepsilon^{n}. \tag{16}$$

Amplification matrix is connected to an integral operator which couples solutions in consecutive time steps. It means that if an error ε^n appeared in a solution $\mathbf{T}^n$ on time level n then after some necessary transformations is obtained:

$$\mathbf{T}^{n+1} + \varepsilon^{n+1} = \mathscr{T}(\mathbf{T}^n + \varepsilon^n). \tag{17}$$

Assuming that an error vector has a small amplitude, the Eq. (17) may be expanded into the Taylor series, taking into account only its two first terms. After some transformations an expression joining together two time levels is obtained:

$$\varepsilon^{n+1} = \left\{ \frac{\partial}{\partial \mathbf{T}} (\mathscr{T}\mathbf{T}) \right\}^{n} \varepsilon^{n}. \tag{18}$$

This expression also defines the amplification matrix in the Eq. (16). The operator $\mathscr{T}$ on the right-hand side of this equation is a linear matrix operator. Using the given integration scheme it is possible to determine an amplification matrix for it. An error vector on a new time level connects with an error vector in a previous step. If in a amplification Eq. (16) a matrix $\mathbf{G}$ is diagonal then the amplitudes of each of the error eigenvectors ε_i connected to each other by appropriate eigenvalues g_i of amplification matrix may be written as:

$$\varepsilon_i^{n+1} = g_i \varepsilon_i^{n}. \tag{19}$$

Stability condition must be used separately for amplitudes of each error eigenvectors:

$$|\varepsilon_i^{n+1}| \leq |\varepsilon_i^{n}|, \tag{20}$$

for all i, that is:

$$|g_i| \leq 1. \tag{21}$$

Stability criterion defined in a given way is limited to a demand that each eigenvalue g_i of an amplification matrix $\mathbf{G}$ was smaller or equal to a unit. In the paper this condition is used for the stability analysis of the mixed time partitioning method of solidification issues.

5 Association Between the Eigenvalues of Amplification Matrix and Size of Time Step

It is essential to find the criterion to determine the size of time step for the explicit scheme [2]. If we assume that $\theta = 0$ the Eq. (33) is reduced to the form:

$$\mathbf{T}^{n+1} = (\mathbf{I} - \Delta t \mathbf{M}^{-1}\mathbf{K})\mathbf{T}^{n}. \tag{22}$$

The Eq. (22) is called the evolution equation, because it gives the possibility to obtain the value of searched size $\mathbf{T}$ at the time level $n + 1$ from appropriate values of nodal quantities at the time level n.

In the evolution equation the capacity matrix $\mathbf{M}$ can be full or diagonal. Depending on the type of matrix in the equation of evolution, numerical stability analysis is combined with carrying out various algebraic operations.

In case of the capacity matrix is diagonal matrix, the calculation of the inverse matrix, namely $\mathbf{M}^{-1}$, is very simple and then finding its eigenvalues, necessary to determine the critical value of time step, is not difficult. However, in case of full capacity matrix which is symmetric and positively definite, in order to determine the inverse matrix we need to use the distribution $\mathbf{M} = \mathbf{L}\mathbf{L}^{T}$ or other transformations which keep the eigenvalues of full matrix. In case of diagonal matrix the inversion process and searching eigenvalue, which decides about the maximum, acceptable value of time step, is less complicated. The evolution Eq. (22) after converting can be written as follows:

$$\mathbf{T}^{n+1} = \mathbf{G}\mathbf{T}^{n}, \tag{23}$$

where amplification matrix $\mathbf{G}$ is given as:

$$\mathbf{G} = \mathbf{I} - \Delta t \mathbf{M}^{-1}\mathbf{K}. \tag{24}$$

The scheme is explicit if the size $\mathbf{T}^{n+1}$ can be received from the Eq. (23), without solving the system of algebraic equations and if updates of searched quantities can be repeated m—times according to the formula [9]:

$$\mathbf{T}^{n+m} = \mathbf{G}^{m}\mathbf{T}^{n}. \tag{25}$$

Finding the maximum eigenvalues of the amplification matrix is a sufficient condition for the numerical stability:

$$\mathbf{G}\mathbf{x} = \lambda \mathbf{x}, \tag{26}$$

where $\mathbf{G}$ is the matrix of N degree, and N is the number of nodes of sub-domain connected with casting or mould domain. The analysis of numerical stability is

conducted separately for each sub-domain on the basis of finite elements inside the sub-domain.

Using the theory of eigenvalues, eigenvectors and algebraic operations on matrices it is known that the size $\mathbf{G}^m\mathbf{T}^n \rightarrow \mathbf{0}$, if $m \rightarrow \infty$ for any $\mathbf{T}^n \in R^N$, if $|\lambda_i| < 1$ for $i = 1...N$, moreover, the size $\mathbf{G}^m\mathbf{T}^n$ is limited, if $m \rightarrow \infty$, if $|\lambda_i| \leq 1$ for $i = 1...N$, if there are linearly independent eigenvectors $\mathbf{x}_i$ for each $|\lambda_i| = 1$, which is satisfied because of symmetry of matrices $\mathbf{G}$.

After substituting $\mathbf{G}$ from the Eq. (24) to the Eq. (26), multiplying this equation by $\mathbf{M}$ and doing transformations the formula for generalized problem of eigenvalues is received:

$$\mathbf{K}\mathbf{x} = \frac{1-\lambda}{\Delta t}\mathbf{M}\mathbf{x}, \tag{27}$$

where $(1-\lambda)/\Delta t$ is an eigenvalue of couple of matrices $\mathbf{K}$ and $\mathbf{M}$. From the Eq. (27) it is known that if λ is equal to the unity then $\mathbf{K}\mathbf{x} = \mathbf{0}$ only if $\mathbf{x} = \mathbf{0}$:

$$\lambda_i = 1 - \Delta t\mu_i. \tag{28}$$

As $|\lambda_i| \leq 1$, the size of time step, which can be used to solve the system of Eq. (33), to be numerical stable and is limited by the inequality:

$$\Delta t \leq \frac{2}{\mu_i}, \tag{29}$$

The most restrictive limitation of the size of time step, which assures the stability is the case in which μ_i is the maximum eigenvalue $\mu_{\max}$ of the matrix of Eq. (37). Taking into account the way of assembly of capacity and conductivity matrices, the Eq. (37) may be written for a definite element e of the given domain:

$$\mathbf{K}^{(e)}\mathbf{x}^{(e)} = \mu^{(e)}\mathbf{M}^{(e)}\mathbf{x}^{(e)}, \tag{30}$$

whereas the limitation of a size of time step may be written as follows:

$$\Delta t \leq \frac{2}{\mu_i^{(e)}}. \tag{31}$$

In order to find a maximum acceptable size of time step for the casting and mould domains it is necessary to determine, for all the elements, their biggest eigenvalues and create from them double inequality. This inequality is limited from the smallest value to the biggest one:

$$\mu_{min}^{(e)} \leq \mu \leq \mu_{max}^{(e)}, \tag{32}$$

where $e = 1...ne$, and ne is the number of elements in the considered domain.

6 The Criterion of Determination of the Critical Time Step

In order to determine the criterion of numerical stability of chosen method, operations converting this equation into general problem of the eigenvalues are conducted. The analysis of stability is carried out to determine the maximum size of time step, which exceeding may be cause of unsteady solutions.

The one step time integration scheme of the equation obtained after spatial discretization is presented by the formula:

$$(\mathbf{M} + \Theta \Delta t \mathbf{K})\mathbf{T}^{n+1} = (\mathbf{M} - (1 - \Theta)\Delta t \mathbf{K})\mathbf{T}^{n}. \tag{33}$$

The right-hand side vector is not taken into consideration because the homogeneous equation is only essential for the numerical stability. If the homogeneous expression is stable so the inhomogeneous one is also stable [7].

The generalised problem of the eigenvalues is connected with casting domain B in sub-cycle and with mould domain A in total cycle [3, 4] and can be written in the universal form:

$$\mathbf{A}\mathbf{x}_i = \lambda_i \mathbf{B}\mathbf{x}_i, \quad i = 1, \ldots, N, \tag{34}$$

where N is a grade of the matrix $\mathbf{A}$ i $\mathbf{B}$ expressed by the formulas:

$$\mathbf{A} = \mathbf{M} - (1 - \Theta^{(e)})\Delta t \mathbf{K}, \tag{35}$$

$$\mathbf{B} = \mathbf{M} + \Theta^{(e)} \Delta t \mathbf{K}, \tag{36}$$

for

$$\Theta^{(e)} = \Theta_A \text{ for } e \in A,$$
$$\Theta^{(e)} = \Theta_B \text{ for } e \in B.$$

After substituting the Eqs. (35) and (36) into the formula (34) and doing the transformations the expression is received:

$$\mathbf{K}\mathbf{x}_i = \mu_i \mathbf{M}\mathbf{x}_i, \tag{37}$$

where μ_i is the eigenvalue of couple matrices of $\mathbf{M}$ i $\mathbf{K}$ form:

$$\mu_i = \frac{1 - \lambda_i}{(1 - \Theta + \Theta\lambda_i)\Delta t}. \tag{38}$$

After transformation the homogeneous Eq. (9) can be written as follows:

$$\dot{\mathbf{T}} + \mathbf{B}\mathbf{T} = \mathbf{0}, \tag{39}$$

where $\mathbf{B} = \mathbf{M}^{-1}\mathbf{K}$. Naturally, such inversion of the matrix $\mathbf{M}$ would cause its asymmetry, therefore Cholesky decomposition is used in this purpose instead of explicit inversions.

The one step Θ method is used in a scalar equation, which comes from the modal decomposition of system of Eq. (39), gives:

$$T^{n+1} = \lambda T^n, \tag{40}$$

where the eigenvalue λ is expressed by the formula:

$$\lambda = \frac{1 - (1 - \Theta)\mu\Delta t}{1 + \Theta\mu\Delta t}. \tag{41}$$

As far as the Eq. (41) and the inequality $|\lambda| \leq 1$ are concerned, the stability of the method is obtained if the following condition is satisfied:

$$2 + (2\Theta - 1)\mu\Delta t \geq 0. \tag{42}$$

It arises from (42) that for $\Theta \geq 1/2$ the condition of the inequality is always satisfied, so the method is stable. Moreover, for $\Theta < 1/2$ the stability of the method depends on the size of quotient $\mu\Delta t$, because of that for the explicit scheme ($\Theta = 0$) the size of maximum and accessible time step is strictly connected with the maximum eigenvalue in a given domain (the casting, the mould).

7 Restrictions Imposed on the Eigenvalues

The solution of N system of Eq. (9) consists of particular integral and complementary function of the solution of the homogeneous equation [9–11]:

$$\mathbf{M}\dot{\mathbf{T}} + \mathbf{K}\mathbf{T} = \mathbf{0}. \tag{43}$$

Substituting $\mathbf{T} = e^{-\lambda t}\mathbf{v}$ to the Eq. (43) is obtained an equivalent system of equations:

$$\lambda\mathbf{M}\mathbf{v} = \mathbf{K}\mathbf{v}. \tag{44}$$

Because of the semi-discretization the Eq. (44) is satisfied for $\lambda = \lambda_i$ and $\mathbf{v} = \mathbf{v}_i$.

The mass matrix $\mathbf{M}$ is diagonal and it helps to reduce the analysis of stability. If this matrix is the full symmetric matrix, the analysis of stability of the equation is conducted in a different way, however, the effect of both operations is the same as the criterion limiting the size of time step in the explicit scheme of the integration.

If the matrix $\mathbf{M}$ is positively definite, Cholesky decomposition can be executed, namely $\mathbf{M} = \mathbf{L}\mathbf{L}^T$, where $\mathbf{L}$ is lower triangular and non singular matrix. Using such

distribution in the Eq. (44) and multiplying both sides of the equation by $\mathbf{L}^{-1}$, it is obtained:

$$\lambda_i \mathbf{L}^T \mathbf{v}_i = \mathbf{L}^{-1}\mathbf{K}(\mathbf{L}^{-1})^T \mathbf{L}^T \mathbf{v}_i, \tag{45}$$

where $\mathbf{L}^T\mathbf{v}_i$ is the eigenvector, and λ_i is the eigenvalue of the symmetric matrix $\mathbf{P} = \mathbf{L}^{-1}\mathbf{K}(\mathbf{L}^{-1})^T$. The matrix $\mathbf{P}$ has the set of linearly independent eigenvalues $\mathbf{v}_i$.

If the matrix $\mathbf{V}$ is composed of $\mathbf{v}_i$, which are the columns of such a matrix and $\mathbf{L}^T\mathbf{V}$ is orthogonal, it can be written:

$$\mathbf{V}^T\mathbf{L}\mathbf{L}^T\mathbf{V} = \mathbf{V}^T\mathbf{M}\mathbf{V} = \mathbf{I}. \tag{46}$$

Moreover, on the basis of the Eq. (44) and the Cholesky decomposition process it can be written:

$$\lambda_i = \lambda_i \mathbf{v}_i^T \mathbf{M}\mathbf{v}_i = \mathbf{v}_i^T \mathbf{K}\mathbf{v}_i. \tag{47}$$

Substituting $\mathbf{T} = \mathbf{V}\mathbf{x}$ into the Eq. (43) and left-multiplying both sides by $\mathbf{V}^T$ it is obtained:

$$\mathbf{V}^T\mathbf{M}\mathbf{V}\dot{\mathbf{x}} + \mathbf{V}^T\mathbf{K}\mathbf{V}\mathbf{x} = \mathbf{0}, \tag{48}$$

and then:

$$\mathbf{I}\dot{\mathbf{x}} + \Lambda\mathbf{x} = \mathbf{0}, \tag{49}$$

where $\Lambda = diag(\lambda_i)$. Such distribution is known as *modal decomposition* and allows to write the system of equations in the scalar form:

$$\dot{x}_i + \lambda_i x_i = 0. \tag{50}$$

The problem of the stability is connected with some restrictions of the eigenvalues. For the problems described by the prime row equations, from the Eq. (44) the eigenvalues and the eigenvectors can be designated. However, the restrictions imposed on the eigenvalues in the Eq. (47) can be derived from Rayleigh quotient:

$$\lambda = \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{M}\mathbf{v}}. \tag{51}$$

Taking into consideration the way of matrix assembling $\mathbf{K}$ i $\mathbf{M}$:

$$\lambda = \frac{\sum_i (\mathbf{v}_i^T \mathbf{K}_i^{(e)} \mathbf{v}_i)}{\sum_i (\mathbf{v}_i^T \mathbf{M}_i^{(e)} \mathbf{v}_i)}, \tag{52}$$

where e is an element, and $\mathbf{v}_i$ is appropriate component of the eigenvector, Rayleigh quotient for an element can be written as follows:

$$\lambda_i^{(e)} = \frac{\mathbf{v}_i^T \mathbf{K}_i^{(e)} \mathbf{v}_i}{\mathbf{v}_i^T \mathbf{M}_i^{(e)} \mathbf{v}_i}. \tag{53}$$

Inserting (53) into (52) and doing certain transformations it is obtained:

$$\lambda = \frac{\sum_i \alpha_i \lambda_i^{(e)}}{\sum_i \alpha_i}, \tag{54}$$

where $\alpha_i = \mathbf{v}_i^T \mathbf{M}_i^{(e)} \mathbf{v}_i > 0$, because the capacity matrix is positively definite. It is resulted from the Eq. (54) that λ is determined as the weighted average from $\lambda_i^{(e)}$ with positively weight, so the restrictions resulting from Rayleigh quotient can be written as follows:

$$\lambda_{\min}^{(e)} \leq \lambda \leq \lambda_{\max}^{(e)}. \tag{55}$$

Estimation of the extreme values is received from the formulas:

$$\lambda_{\min}^{(e)} \leq \frac{\min\{\mathbf{v}_i^T \mathbf{K}_i^{(e)} \mathbf{v}_i\}}{\max\{\mathbf{v}_i^T \mathbf{M}_i^{(e)} \mathbf{v}_i\}}, \tag{56}$$

$$\lambda_{\max}^{(e)} \leq \frac{\max\{\mathbf{v}_i^T \mathbf{K}_i^{(e)} \mathbf{v}_i\}}{\min\{\mathbf{v}_i^T \mathbf{M}_i^{(e)} \mathbf{v}_i\}}. \tag{57}$$

8 Remarks and Conclusion

There are many types of methods used for the integration with respect to time, but two of them are basic: explicit and implicit. Explicit methods usually need few computations per time step, but numerical stability requires small the size of time step. In practice, a time step which is too small results in any unnecessarily long entire simulation time. Implicit methods, on the other hand, need many computations per time step, but allows to use larger the size of time step.

With respect to this problems we proposed to use both explicit and implicit schemes in this study. By using mixed time partitioning methods, computations in different parts of modelled domain were carried out by different integration schemes (*E*—explicit, *I*—implicit) and different the size of time step.

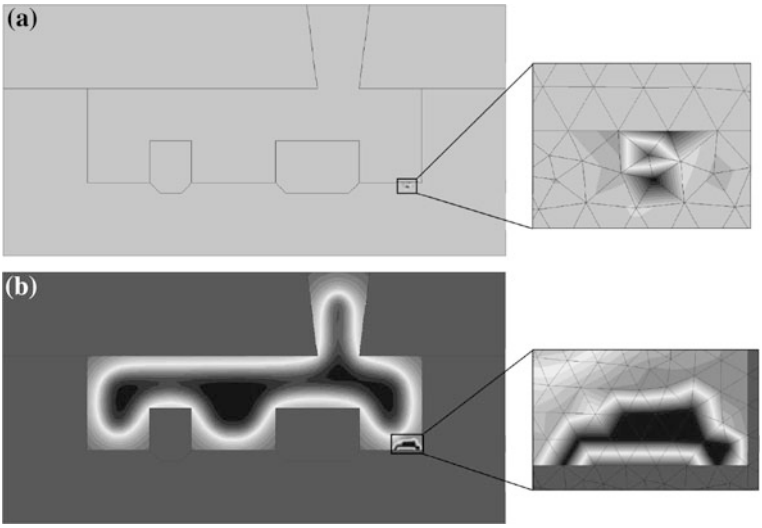

Fig. 1 *Erroneous results*. Errors appearing in computational results for **a** temperature and **b** solid phase fraction are caused by too large time step (e.g. in explicit scheme or when multiplication factor $m > 15$)

If a conditionally stable time integration scheme is used, numerical stability requires less the size of time step than its critical value (Δt_{critic}) calculated on the basis of stability analysis.

Numerical simulation of solidification was carried out for Al–2%Cu alloy casting, solidifying in the metal form [6, 12]. Computations were carried out by using mixed time partitioning methods on the basis of eigenvalues, where $m = 15$ was the largest acceptable value with respect to the numerical stability criterion. The time step equal to 0.0035 s was used in the simulations.

We focused on computational framework to simulate solidification of binary system with casting and mould considered. In our approach, we used a fixed time step in a casting domain and much larger time steps in other parts of mould, while maintaining high accuracy (comparable with case when small time step is used for all domains). We performed series of numerical experiments and noticed the eigenvalues of amplification matrix strongly affect the size of time step. The proper selection of the size of the time step is important for the stability of the method and the accuracy of the results. The simulation results are erroneous and inconsistent with the physics of the phenomenon after crossing the critical time step (see Fig. 1).

The eigenvalues remain with close relation to the stability of numerical method and hence with the size of the time step. For explicit schemes of time integration such a step cannot exceed a certain critical value. For implicit schemes of time integration the size of the time step cannot be unlimited because exceeding certain limit can result in omission of important physical phenomena. The use of the analysis of the relation between the eigenvalues and the size of time step allows to

designate the maximum permissible size of the time step and to conduct the computer simulations correctly. The problem of the eigenvalues of the matrices is a very extensive issue and the works have very deep scientific and practical justification.

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