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finite difference approach

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Abstract

The variable space grid method based on the mixed finite element/finite difference approach is applied on a 1D Stefan problem with time dependent Dirichlet boundary conditions describing a melting process. We obtain the position of the moving boundary between two phases using finite differences, while the finite element method is employed in order to determine temperature distribution. In each time step, the positions of finite element nodes are updated according to the moving boundary, while we map the nodal temperatures with respect to the new mesh using interpolation techniques. We found that that computational results obtained by the proposed approach exhibit good agreement with the exact solution. Moreover, the results for temperature distribution, moving boundary location and moving boundary speed are more accurate than those obtained by variable space grid method based on pure finite differences.

Keywords Stefan problem, finite element method, finite difference variable space grid method, front-tracking.

1 Introduction

Stefan problems involving heat conduction in conjunction with the change of phase are of great interest in numerous important areas of science, engineering, and industry. Such a process covers a wide range of applications in which the phase changes from liquid, solid, or vapor states. The moving boundary problems occur in many areas such as the metal, glass, plastic and oil industries, space vehicle design, preservation of foodstuffs, chemical and diffusion processes, etc. The material is assumed to undergo a phase change with a moving boundary whose position is unknown and has to be determined as a part of the analysis. Across the phase boundary the heat flux is not continuous, and the heat equation is replaced by a flux condition that relates the velocity of the phase boundary and the jump of heat flux across the phase front.

Since moving boundary problems require solving the heat equation in an unknown region that has also to be determined as a part of the solution, they are inherently the non-linear. Hill (1987) reports that due to non-linearity of the moving boundary problems, they can be solved analytically for only a limited number of special cases. Due to difficulties in obtaining analytical solutions, numerical techniques, firstly proposed by Goodman (1958), are far more common. Numerical techniques are specially known to have difficulties with time-dependent boundary conditions, and very small time steps are often needed for accurate solutions. Different numerical methods and their use for different types of problems are systematized by Minkowycz et al. (2006). Esen and Kutluay (2004), Mennig and Özişik (1985), Furzeland (1980), Rizwan-uddin (1999), Savović and Caldwell (2003), Singh et al. (2011), Vitorino et al. (2010), Irawan et al. (2013) and Reutskiy (2011) report various solutions of Stefan problems and include linear, exponential, and periodical variation of the surface temperature or the flux with time.

There are three main approaches to the solution of the Stefan problem. The first is the **front-tracking method**, where the position of the phase boundary is continuously tracked. An example is the heat balance integral method presented by Goodman (1958), which explicitly tracks the motion of isotherms (the phase boundary being one of them). Variable grid methods (variable space grid and variable time step) provide a way to track the phase front explicitly, as in the work of Marshall (1986). Various solutions for heat conduction problems with phase change employ finite elements (Comini et al. (1974), Lewis et al. (1996, 2004), Nithiarasu et al. (2016)), discontinuous Galerkin method in Nguyen et al. (2010), finite volume method in the work of Gloth et al. (2003) etc.

The second approach is **fixed-domain formulation**. An example is the isotherm migration method, which uses the temperature as the independent variable, reported by Churchill and Gupta (1977). A more common method is the enthalpy method, which uses

an enthalpy function together with the temperature as dependent variable, reported by Esen and Kutluay (2004), Voller and Cross (1985), Caldwell and Chan (2000) and Kosec et al. (2011). Level set method introduces a level set function, capturing the interface at its zero level set. The examples of this approach can be found in Vrankar et al. (2010), Reutskiy (2011) and Papac et al. (2013).

The last approach is the **front-fixing formulation**. Using a suitable coordinate transformation, one may immobilize the moving front at the expense of solving a more complicated problem by a numerical scheme. Examples include finite difference schemes as Kutluay et al. (1997), Mitchell and Vynnycky (2012) and Vynnycky and Mitchell (2015) and finite elements in the work of Holmes and Yang (2008).

Comparison of various numerical methods has been carried out by Furzeland (1980), Caldwell and Kwan (2004), and Javierre et al. (2006). [Our approach can be classified as a front-tracking method.](#)

In this paper, we consider one-dimensional Stefan problem with time-dependent boundary conditions describing the melting process, identical to that solved by Savović and Caldwell (2009). Their pure finite difference explicit scheme, although efficient, requires special attention to the choice of the time step in order to retain stability. [The explicit time stepping scheme involving small time step values often leads to the reduced computational efficiency. Also, pure finite difference scheme is not as flexible as finite elements at handling natural boundary conditions.](#) The aim of our paper is to improve the scheme described by Savović and Caldwell (2009) by employing mixed finite element/finite difference scheme including implicit time stepping. The position of the moving boundary between two phases is calculated using finite differences, while we use finite element method for the determination of the temperature distribution. At each time step, the positions of finite element nodes are updated according to the moving boundary, while we map the nodal temperatures with respect to the new mesh using interpolation techniques.

The paper is organized as follows. We formulate the problem in Section 2, while Section 3 defines our mixed MFE/FDMSG scheme. Section 4 gives a brief overview of [the](#) FDMSG method used by Savović and Caldwell (2009). Section 5 presents numerical results and the last section is reserved for conclusions.

2 Formulation of the problem

Stefan problem describes the phenomenon of the phase change. One dimensional phase change problem could be demonstrated by [a](#) semi-infinite solid, like a thin block of ice occupying $0 \leq x < \infty$, on solidification temperature. At the fixed boundary of the thin block of ice ($x = 0$), various types of flux functions could act. In this paper, we used the same boundary condition as Savović and Caldwell (2009), so the temperature at $x = 0$ increases exponentially with time. We also assume that the temperature of the entire solid phase remains at the melting point. Therefore, the problem is to determine temperature distribution in the liquid phase at time t_0 , where $x < s(t_0)$, as well as the location of the free boundary $s(t_0)$. At later time $t_1 > t_0$, the moving boundary $s(t)$ moves to the right and occupies the position $s(t_1) > s(t_0) = s_0$ (Fig. 1). The part of the thin block of ice from position $s(t_0)$ to position $s(t_1)$, has been melted over the time interval (t_0, t_1) .

The temperature distribution $u(x, t)$ in the liquid phase region $0 \leq x \leq s(t)$ is given by the heat equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \quad (1)$$

under [the](#) following boundary conditions:

$$\begin{aligned} u(x, t) &= e^{\alpha t}, & x = 0, & t > 0 \\ u(x, t) &= 1, & x = s(t), & t > 0, \end{aligned} \quad (2)$$

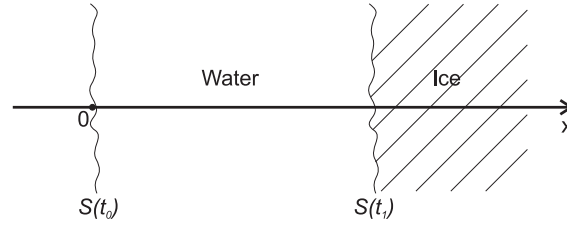


Figure 1: Ice melting.

where α is a physical parameter combining density, specific heat, and thermal conductivity. The location of the moving boundary is given by equation known as Stefan condition:

$$\frac{1}{\alpha} \frac{ds}{dt} = -\frac{\partial u}{\partial x}, \quad x = s(t), \quad t > 0. \quad (3)$$

In the general case, initial condition is given by

$$s(0) = 0. \quad (4)$$

The exact solution for this specific problem is known:

$$\begin{aligned} u(x, t) &= e^{\alpha t - x} \\ s(t) &= \alpha t. \end{aligned} \quad (5)$$

As stated above, in order to determine $s(t)$, we used Finite Difference Variable Space Grid (FDVSG in further text) scheme, and for obtaining $u(x, t)$, we employed the finite element method. It should be noted that we consider a generic solid melting to liquid (depending on the value of α), not only the ice-water case. The following section describes our approach in more detail.

3 Mixed Finite Element/Finite Difference Variable Space Grid Method

The finite element method, as well as the [Finite Difference Variable Space Grid Method \(FDVSG\)](#) proposed by Savović and Caldwell (2009), can be used to estimate temperature distribution in the fixed number of nodes in the liquid phase. Our novel procedure consists of solving Eq. (1) using finite element method, while keeping the FDVSG given by Savović and Caldwell (2009) as a solution to Eq. (3). We designate our combined approach proposed in this paper as Mixed Finite Element/Finite Difference Variable Space Grid (MFE/FDVSG) method.

3.1 Finite element scheme for the temperature distribution

In this subsection, the derivation of the continuous and discrete equations for a single element is briefly presented. Eq. (1) applies Galerkin method, in the way that we multiply both sides of the equation by weighting function v , integrate throughout the volume, and apply Gauss theorem, giving

$$\int_V \alpha \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} dV = - \int_V \frac{\partial u}{\partial t} v dV + \oint_S \alpha \frac{du}{dx} v dS. \quad (6)$$

This is the weak formulation of Eq. (1). The problem is to determine the function u such that Eq. (6) holds for every v . The value of the function can be written as a sum of the

nodal values and the interpolation functions at given point $u = \sum \phi_j u_j$. Furthermore, in place of weighting function introduced in Eq. (6), the interpolation function ϕ_i can be adopted, where $i = \overline{1, K}$, K being the number of finite element nodes. We get

$$C_{i,j} \frac{\partial u_j}{\partial t} + K_{i,j} u_j = F_i, \quad (7)$$

where

$$C_{i,j} = \int_V \phi_i \phi_j dV, \quad (8)$$

$$K_{i,j} = \int_V \alpha \frac{\partial \phi_i}{\partial x} \frac{\partial \phi_j}{\partial x} dV, \quad (9)$$

$$F_i = \oint_S \alpha \frac{du}{dx} \phi_i dS. \quad (10)$$

In the case that the given element is located in the domain interior, due to the orientation of the surface vector, the expression F_i is annulled by the corresponding integral of the adjacent elements. For the boundary elements, according to the conditions, the value of the given integral is also zero. As the model implies fixed values on both ends given by Eq. (2), we pose these Dirichlet boundary conditions by applying standard *penalty* method.

3.2 Boundary update and remeshing

Besides solving system Eq. (7) in each time step, it is necessary to update the position of the moving liquid phase boundary. Also, while boundary is moving, the mesh has to be regenerated, in order to keep constant number of elements with equally distributed nodes throughout the simulation. The temperature gradient at the moving boundary $x = s(t) = N\Delta x$ is given by following finite difference higher three point backward scheme described by Savović and Caldwell (2009):

$$\left. \frac{\partial u}{\partial x} \right|_{x=s(t)} = \frac{3u_N - 4u_{N-1} + u_{N-2}}{2\Delta x} + O(\Delta x^2) \quad (11)$$

According to Eq. (11), the Stefan condition Eq. (3) at $x = s(t)$ can be written as

$$s_{m+1} = s_m - \frac{\Delta t \alpha}{2h_m} [3u(s_m) - 4\bar{u}(s_m - h_m) + \bar{u}(s_m - 2h_m)], \quad (12)$$

$$m = 0, 1, 2, \dots,$$

where m denotes time step count, Δt time step value and $h_m (\equiv \Delta x) = \frac{s(t)}{N}$ nominal space step. The quantities designated as $u(s_m)$, $\bar{u}(s_m - h_m)$ and $\bar{u}(s_m - 2h_m)$ are temperatures at s_m , $s_m - h_m$ and $s_m - 2h_m$, in time step m , respectively. It should be noted that these temperatures usually do not correspond to the nodal values (hence bar notation). The reason for that is the addition of an extra node in the new mesh (in time step $m+1$), exactly at the position of the previous liquid-ice boundary (at s_m). We expect the inclusion of this additional node to improve accuracy. However, an extra node requires interpolation for determining temperatures $\bar{u}(s_m - h_m)$ and $\bar{u}(s_m - 2h_m)$. The interpolation is also required for the transition from the old mesh with nominal step h_m to the new mesh with nominal step $h_{m+1} = \frac{s_{m+1}}{N}$. For both purposes we employed Akima scheme proposed by Franke (1982), which provided a slight improvement over classic cubic spline interpolation defined by McKinley and Levine (1998).

The procedure of the transition between time steps is shown in Fig. 2. It should be noted that mesh consists of N nodes only in the first time step; in all subsequent steps there are actually $N + 1$ nodes. Of course, if the projection of the node to the previous time step falls within ice phase, we take temperature as 1, as shown at the far right side of Fig. 2. Using this approach, we have all necessary building blocks to form Eq. (7) for the time step $m + 1$.

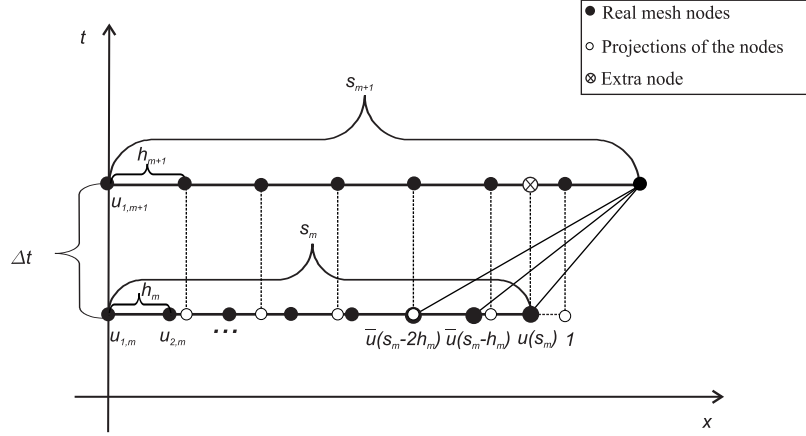


Figure 2: Procedure of updating solution from the previous time step including remeshing

4 Finite Difference Variable Space Grid Method (FDVSG)

In this section, we briefly describe the pure finite difference approach taken by Savović and Caldwell (2009). Taking into account continuous change in the nodal positions due to the boundary movement, the following expression applies at the i -th grid point:

$$\left. \frac{\partial u}{\partial t} \right|_i = \left. \frac{\partial u}{\partial x} \right|_t \frac{\partial x}{\partial t} \Big|_i + \left. \frac{\partial u}{\partial t} \right|_x, \quad (13)$$

while the node x_i moves according to

$$\frac{dx}{dt} = \frac{x_i}{s(t)} \cdot \frac{ds}{dt}, \quad (14)$$

in which suffixes t , i , and x have to be kept constant during differentiation process and omitted for clarity in further text. Upon substituting Eq. (1) and (14) into Eq. (13), we obtain

$$\frac{\partial u}{\partial t} = \frac{x_i}{s} \frac{ds}{dt} \frac{\partial u}{\partial x} + \alpha \frac{\partial^2 u}{\partial x^2}, \quad 0 \leq x \leq s(t), t > 0. \quad (15)$$

Having temperature gradient at the boundary determined by Eq. (11), forward difference approximation for time derivative and central difference approximation for the space derivative, discretization of Eq. (15) can be expressed as

$$u_{i,m+1} = u_{i,m} + \frac{kx_{i,m}\dot{s}_m}{2h_m s_m} (u_{i+1,m} - u_{i-1,m}) + \frac{k\alpha}{h_m^2} (u_{i+1,m} - 2u_{i,m} + u_{i-1,m}), \quad (16)$$

where $u_{i,m} \equiv u(x_{i,m})$, $\dot{s}_m = (s_{m+1} - s_m)/\Delta t$, $x_{i,m} = ih_m$, $t_m = t_0 + mk$, h_m is the space grid size Δx at m^{th} time step, $k \equiv \Delta t$ is the time step, and t_0 is the time at which the numerical process is initialised.

We obtain the position of the moving boundary using identical formula (12), as in the case of MFE/FDVSG method, while updated grid size becomes $h_{m+1} = s_{m+1}/N$. Further details on FDVSG approach can be found in Savović and Caldwell (2009).

5 Results and Discussion

In this section, we present the results obtained using our MFE/FDVSG scheme, applied to one dimensional Stefan problem of ice melting. Our tests aimed at obtaining the following:

1. accuracy of the temperature distribution,
2. time step value sensitivity,
3. accuracy of the location and speed of the moving boundary, and
4. sensitivity regarding mesh density and time step, only for MFE/FDVSG method.

First of all, we compare our computational results for heat distribution with the exact solution for $\alpha = 2$ and $\alpha = 10$, and also with those obtained by Savović and Caldwell (2009), who used pure FDVSG. The parameter values are identical as in Savović and Caldwell (2009). Nominal mesh density is fixed to 10 nodes for both MFE/FDVSG and FDVSG schemes. The initial time is $t_0 = 0.01$, which, according to Eq. (5), corresponds to the initial position of the moving boundary. In the case of $\alpha = 2$, the boundary starts at $s(t_0) = 0.02$, while in the case of $\alpha = 10$, the boundary starts at $s(t_0) = 0.1$. The position of the boundary between ice and water, together with the temperature distribution, is observed in the interval $t_0 = 0.01$ till $t_{max} = 0.5$. We also took identical time step values used by Savović and Caldwell (2009), $\Delta t = 1.0E-06$ for $\alpha = 2$, and $\Delta t = 2.0E-06$ for $\alpha = 10$. This choice of the time step value guarantee stability of differential scheme employed by the pure FDVSG method. In Table 1, we compare temperature distributions for various time points in the case of $\alpha = 10$.

Table 1: Temperature distribution $u(x, t)$ in nodal positions obtained by FDVSG and the MFE/FDVSG, $\alpha = 10$

t	x/s	MFE/FDVSG Error	FDVSG Error
0.1	0	0	0
	0.1	0.00002496	0.00003222
	0.2	0.00003333	0.00003587
	0.3	0.00003602	0.00001741
	0.4	0.00004023	0.00001816
	0.5	0.00005058	0.00006696
	0.6	0.00007064	0.00012614
	0.7	0.00010322	0.00019363
	0.8	0.00015076	0.00026803
	0.9	0.00023918	0.00034846
1	0.00043449	0.00043449	
0.3	0	0	0
	0.1	0.00472279	0.02209676
	0.2	0.00180897	0.02962343
	0.3	0.00279347	0.02938231
	0.4	0.00655247	0.02537378
	0.5	0.00869978	0.01985605
	0.6	0.00910542	0.01402515
	0.7	0.00792414	0.00844575
	0.8	0.00539308	0.00332003
	0.9	0.00119794	0.00134782
1	0.00565342	0.00565343	
0.5	0	0	0
	0.1	0.24347081	0.67711050
	0.2	0.15592026	0.75866250
	0.3	0.02961707	0.63241963
	0.4	0.05352178	0.46327442
	0.5	0.09062042	0.31238079
	0.6	0.09428687	0.19557417
	0.7	0.07782808	0.11096057
	0.8	0.05096659	0.05123940
	0.9	0.01751825	0.00871911
1	0.02299748	0.02299740	

Since Table 1 is insufficient for the exact comparison of the two numerical methods, we considered the root mean square error defined by

$$Error = \sqrt{\frac{1}{N} \sum_{i=1}^N (u_i^{method} - u_i^{exact})^2}, \quad (17)$$

where N is the total number of observed points. Eq. (17) was taken as the *error* function, representing accuracy evaluation of the method. As the error value decreases, a method gives better heat distribution over a given time interval.

Table 2: The accuracy of FDVSG and MFE/FDVSG methods at various times (t)

t	$\alpha = 2$		$\alpha = 10$	
	FDVSG error	MFE/FDVSG error	FDVSG error	MFE/FDVSG error
0.1	5.8152E-06	5.2901E-06	2.0061E-04	1.6277E-04
0.3	3.5864E-05	2.7875E-05	1.8041E-02	5.7222E-03
0.5	1.3531E-04	1.0180E-04	4.0452E-01	1.0177E-01

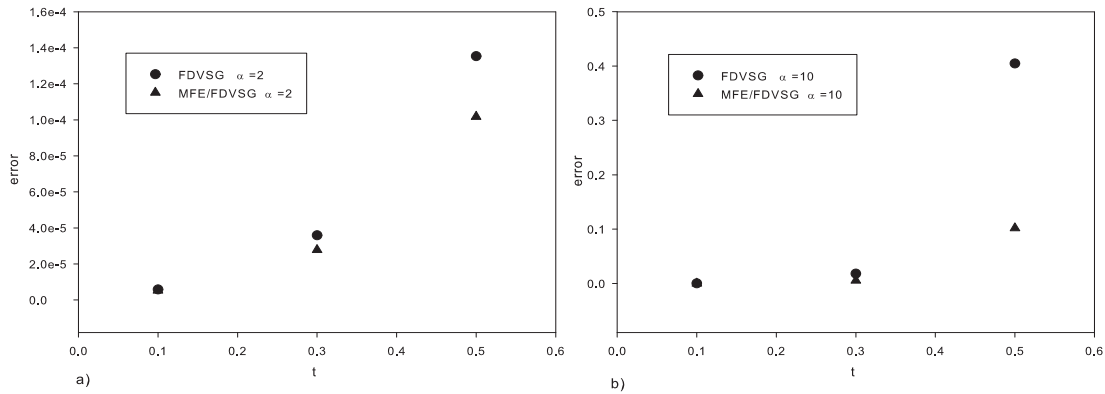


Figure 3: The accuracy of MFE/FDVSG and FDVSG methods for a) $\alpha = 2$ and for b) $\alpha = 10$

Table 2 and Fig. 3 represent accuracy of the two methods for three time instants. It can be noted that for earlier times, the FDVSG method provides solution on par with the MFE/FDVSG, but with increasing time, the MFE/FDVSG gives better stability and better match the exact solution, especially for $\alpha = 10$.

The accuracy of the temperature distribution for the MFE/FDVSG method for $\alpha = 2$ is significantly better than the accuracy of the results achieved for $\alpha = 10$, as shown in Fig. 3. Since α values for almost all technically applicable materials are less than 5, it can be assumed that both methods are sufficiently accurate for most practical applications. Therefore, in all further tests, the value of parameter α will be fixed to the value of 2.

The second accuracy test was the time step value sensitivity. Due to the stability requirements of the FDVSG method, we used value $\Delta t = 1.0E - 06$ for all FDVSG runs. In contrast, as can be seen from Table 3, the MFE/FDVSG method remains stable, even with a significantly higher time step value.

The third test was about determining the location and speed of the moving boundary through time, based on Eq. (3). Although the same equation is used for both numerical schemes, we expect better results than those reported by Savović and Caldwell (2009),

Table 3: Error of MFE/FDVSG and FDVSG method for various time step values at $t = 0.5s$

Δt	Error MFE/FDVSG	Error FDVSG
1.0E-03	1.6189E-04	-
1.0E-04	1.2982E-04	-
1.0E-05	1.3180E-04	-
1.0E-06	1.3228E-04	1.3531E-04

due to a more accurate temperature distribution achieved using finite element method. The results that confirm this assumption are presented in Table 4 and Fig. 4. The MFE/FDVSG is clearly more accurate than the pure FDVSG, which is especially visible considering higher time points, with accumulated errors.

Table 4: Position of moving boundary and its velocity obtained using MFE/FDVSG and FDVSG methods compared to the exact solution for $\alpha = 2$

t	$s(t)$				
	MFE/FDVSG	FDVSG	Error MFE/FDVSG	Error FDVSG	Exact value
0.02	0.0399652	0.0399999	3.480E-05	5.160E-08	0.04
0.05	0.0999859	0.0999991	1.410E-05	8.141E-07	0.1
0.1	0.1999999	0.1999936	1.000E-07	6.377E-06	0.2
0.2	0.3999930	0.3999509	7.000E-06	4.907E-05	0.4
0.3	0.5999228	0.5998399	7.720E-05	1.600E-04	0.6
0.4	0.7999311	0.7996321	6.890E-05	3.679E-04	0.8
0.5	0.9998902	0.9993009	1.098E-04	6.990E-04	1
t	ds/dt				
	MFE/FDVSG	FDVSG	Error MFE/FDVSG	Error FDVSG	Exact value
0.02	2.0017569	1.9999920	1.756E-03	7.967E-06	2.0
0.05	2.0002564	1.99995148	2.564E-04	4.852E-05	
0.1	1.9999762	1.9998113	2.378E-05	1.887E-04	
0.2	1.9996765	1.9992818	3.234E-04	7.182E-04	
0.3	1.9993043	1.9984515	6.956E-04	1.548E-03	
0.4	1.9988485	1.9973471	1.151E-03	2.653E-03	
0.5	1.9983220	1.9959886	1.677E-03	4.011E-03	

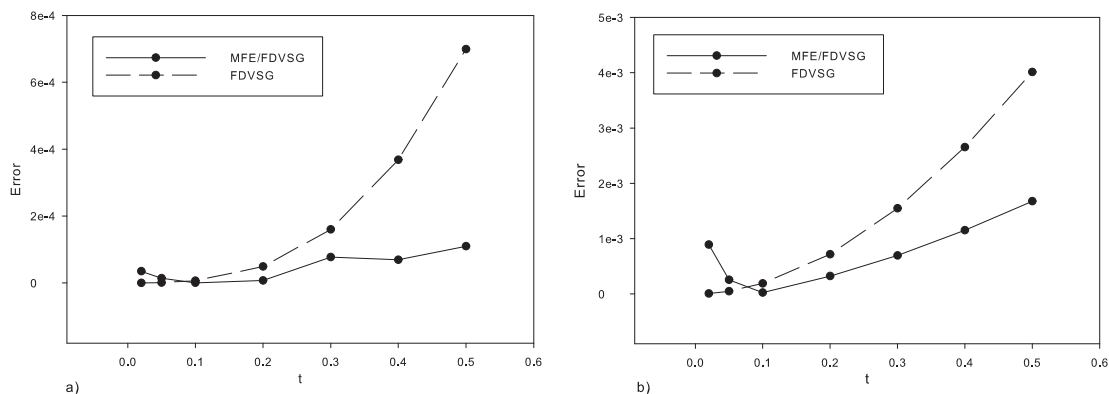


Figure 4: a) The absolute error of the boundary position and b) The absolute error of the boundary speed

Finally, we performed the fourth test, which considers variable time step value and variable finite element mesh density, only for the MFE/FDVSG method. The tests were

carried out with 4 time step values taken as a geometric sequence (Δt) and the nominal number of finite elements 10, 20, 50 and 100 (N), using Eq. (17) as the error descriptor. The obtained results are presented in Table 5 and Fig. 5. It should be noted that in Fig. 5 we single out and show only gray items from Table 5, where the stability for certain N is reached (no significant improvement with further time step decrease). The Fig. 5 also considers the case when no extra node is introduced. It is clear that the addition of the extra node improves the accuracy for over two orders of the magnitude.

Table 5: The accuracy of the MFE/FDVSG method for various time step values and nominal number of elements (extra node present). The gray cells designate points where there's no significant improvement with further time step decrease for certain N .

Δt	1.0E – 03			
N	10	20	50	100
<i>Error</i>	1.6189E-04	1.4839E-04	1.7269E-04	1.9599E-04
Δt	1.0E – 04			
N	10	20	50	100
<i>Error</i>	1.2982E-04	2.3488E-05	1.4841E-05	1.5383E-05
Δt	1.0E – 05			
N	10	20	50	100
<i>Error</i>	1.3180E-04	2.0955E-05	2.7023E-06	1.2072E-06
Δt	1.0E – 06			
N	10	20	50	100
<i>Error</i>	1.3228E-04	2.1220E-05	2.7437E-06	9.4844E-07

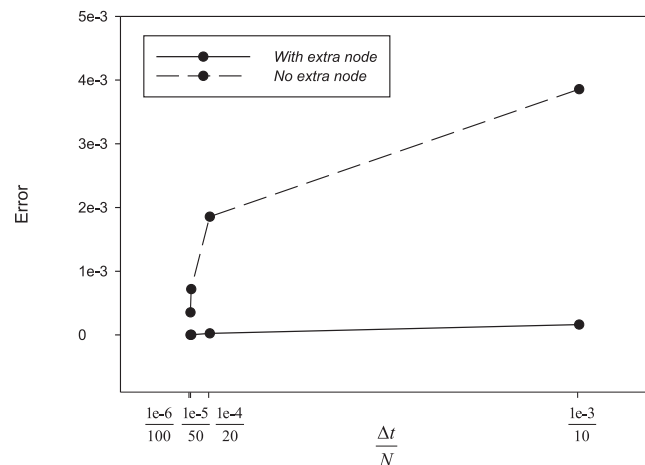


Figure 5: The accuracy of the MFE/FDVSG method for time/space step combinations denoted as $\frac{\Delta t}{N}$ (gray cells in Table 5). For the sake of comparison, we also include the case when no extra node is introduced.

6 Conclusions

We report the implementation of the variable space grid method based on mixed finite element/finite difference approach. The MFE/FDVSG method itself represents a variation of the finite difference FDVSG scheme proposed by Savović and Caldwell (2009). The difference between FDVSG and MFE/FDVSG scheme consists in using the finite element method with remeshing, instead of pure finite difference approach, for the purpose of solving the heat equation. The method is applied to 1D Stefan problem with

the time dependent Dirichlet boundary conditions describing melting process. The novel MFE/FDVSG exhibits very good agreement with exact solution and a clear benefit in terms of accuracy and stability over pure finite difference FDVSG method described in Savović and Caldwell (2009). The benefit is especially visible in the case of $\alpha = 10$. The proposed method is also significantly less sensible to the time step value choice. All presented results encourages us to apply proposed approach to the problems and cases where analytical solutions are not available. Moreover, slightly modified scheme has a potential to be applied for 2D and even 3D Stefan problems, with the inclusion of the automatic mesh generation procedure.

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