

Moving Finite Elements Method for Investigating Stefan Problems

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In this paper we will present a detailed study about a specific algorithm based on the moving finite element method (MFEM) to solve Stefan problems in one dimensional space domain. At each time the MFEM determines both nodal amplitudes and nodal positions. Our formulation of MFEM use different meshes associated to each dependent variable and polynomial approximations of arbitrary degree in each finite element. The algorithm we developed to solve nonlinear moving interface problems is based on a mesh decomposition strategy of the spatial domain. In our moving finite element algorithm the spatial domain decomposition is implemented by the introduction of a moving node describing the position of the internal moving interface. This strategy demands an attentive and accurate choice of initial mesh for the spatial domain with an initial length close to zero. Numerical tests are provided to demonstrate the accuracy and robustness of our formulation of the MFEM to solve moving boundary problems. The algorithm developed enables us to achieve accurate results at acceptable CPU times, showing that MFEM is appropriate to solve these kind of problems.

1. Introduction

A large set of engineering problems require a solution of a time dependent partial differential equation in the presence of several phase transformation. Such problems are usual referred as Stefan problems. The description of different numerical techniques to solve Stefan problems and a useful bibliography can be found in Crank (1981). In this paper a moving finite element method (MFEM) is presented to solve Stefan problems with more than one internal moving boundary, in one dimensional space domain. The MFEM originally proposed by Miller (1981) is a discretization process in two stages: firstly the spatial discretization using finite elements is done allowing the movement of the space nodes and secondly the time integration of the resulting ordinary differential equations (ODE) system. To solve this implicit time-dependent ODE system we use the package LSODI, (Hindmarsh, 1980). We will consider the MFEM with piecewise polynomials of arbitrary degree as basis functions implemented by Sereno (Sereno et al., 1992) and Coimbra (Coimbra et al., 2001, 2004) which generates an adaptive mesh and hence it can be modified in order to be an efficient solver for a class of problems showing one or more internal moving boundary. To modify the moving finite element equations we perform the decomposition of the spatial domain by the introduction of a moving node describing the position of each internal interface. The formulation

presented by Robalo (Robalo et. al., 2005) is expanded in this work to deal with several internal moving boundaries. We study a larger class of problems assuming the existence of linear and nonlinear boundary conditions at each internal moving boundary. The plan of the paper is as follows. In section 2 we present an overview of the proposed algorithm where a concise description of the method is presented. Section 3 is concerned with numerical examples. We apply the computer code resulting from the numerical algorithm implementation to the simulation of an ice-water-ice Stefan problem (Djomehri et al. 1988) and we solve a causticizing reaction model, an important step of the kraft paper process of pulp production (Duarte et al. 1995). We conclude with a short discussion.

2. The moving finite element applied to Stefan problems

In this work we will consider the general mathematical model of k -phases system in one-dimensional fixed space domain, with k internal moving interfaces, defined by a system of n parabolic partial differential equations (PDE) whose m -th equation fill the form

$$\frac{\partial y_m}{\partial t} = f_m\left(x, t, \bar{y}, \frac{\partial \bar{y}}{\partial x}\right) \frac{\partial^2 y_m}{\partial x^2} + g_m\left(x, t, \bar{y}, \frac{\partial \bar{y}}{\partial x}\right), \quad (1)$$

on $a \leq x \leq b$, $t > t_0$. Let us assume some initial conditions and that equation (1) is subject to Dirichlet or Robin boundary conditions at the end points of space domain. We suppose that at initial time, $t = t_0$, it is known the positions of the k internal moving

interfaces, $S = [S_1(t_0), S_2(t_0), \dots, S_k(t_0)]^T$. The discretization of equation (1) by the MFEM is achieved in two stages. Firstly the space domain is discretized by finite element allowing the movement of the spatial nodes. Secondly we must deals with the numerical integration in time of the resulting ordinary differential systems to generate the numerical solution as well the mesh grid where this solution is represented. For this last step we use LSODI integrator described by Hindmarsh (1980). Concerning the discretization of the space domain we consider for each dependent variable a spatial mesh. The solution y_m is approximated by $U_m = \sum_i \phi_i U_{m,j}^k$, where ϕ_i are the

piecewise basis functions at i th node, time dependents through the time dependence of the nodal position, and $U_{m,j}^k$ is the value of U_m at k th interpolation node of the j th element of the mesh. The positions of the mesh points and the solution are predicted by minimizing the square of the norm of the residual of the approximation in the governing partial differential equations with respect to variations in nodal amplitudes and their positions. This procedure originates a nonlinear system of ordinary differential equations. Some of these equations must be overwritten to introduce the boundary conditions. The implementation of the moving finite element method is based on the numerical calculations of all integrals defining the ODE system and the use of penalty functions to prevent the mass-matrix singularities and the grid distortion. These functions do not interfere with the solution and have as an additional effect preventing

the singularities of the mass matrix and the collapse of the spatial mesh. In order to solve Stefan problems the spatial domain is decomposed in $k+1$ subdomains. We also split the space of dependent variable and therefore we have $\bar{\mathbf{y}} = [\bar{\mathbf{y}}^1, \bar{\mathbf{y}}^2, \dots, \bar{\mathbf{y}}^k]^T = [y_1, \dots, y_n]^T$, where $\bar{\mathbf{y}}^i = [y_1^i, \dots, y_{n_i}^i]^T$. Consequently the general Stefan problem to be solved is defined by equation (1), subject to initial conditions and Dirichlet or Robin boundary conditions at the end points of spatial domain. At each internal moving interface the boundary conditions can be expressed by Dirichlet, Robin or implicit conditions in the form

$$h_m \left(S, t, \bar{\mathbf{y}}^j \Big|_{S_j}, \bar{\mathbf{y}}^{j+1} \Big|_{S_j}, \frac{\partial \bar{\mathbf{y}}^j}{\partial x} \Big|_{S_j}, \frac{\partial \bar{\mathbf{y}}^{j+1}}{\partial x} \Big|_{S_j} \right) = 0. \quad (2)$$

To complete the model we assume that on each internal moving interface a well-known condition,

$$\frac{dS}{dt} = w \left(S, t, \bar{\mathbf{y}}^j \Big|_{S_j}, \bar{\mathbf{y}}^{j+1} \Big|_{S_j}, \frac{\partial \bar{\mathbf{y}}^j}{\partial x} \Big|_{S_j}, \frac{\partial \bar{\mathbf{y}}^{j+1}}{\partial x} \Big|_{S_j} \right). \quad (3)$$

is satisfied. Consequently to solve this problem we combine the domain decomposition and the moving finite element method.

3. Numerical examples

3.1 Ice-Water-Ice Stefan Problem

Let us consider the Ice-Water-Ice Stefan Problem that consists in the heat transfer between ice-water-ice interfaces in an ice-water-ice medium occupying a region. The mathematical problem is to find the values of the temperature, $y(t, x) = [y_1(t, x), y_2(t, x), y_3(t, x)]$, in each phase and the position of the liquid/solid and solid/liquid interface. The water is changing phase to ice at both interfaces and initially we suppose and $S_1 = 0.25$ and $S_2 = 0.75$. Initial conditions are $y_1(0, x) = 4x - 1$, $y_2(0, x) = 0$ and $y_3(0, x) = -4x + 3$. The equations defining the internal moving boundaries are

$$\frac{dS_i}{dt} = \frac{\partial y_i}{\partial x}, \quad x = S_i(t) \quad (4)$$

The equations for dimensionless temperature are:

$$\begin{aligned} \frac{\partial y_1}{\partial t} &= \frac{\partial^2 y_1}{\partial x^2}, \quad 0 < x < S_1(t) \quad , \quad t > 0 \\ \frac{\partial y_2}{\partial t} &= 0, \quad S_1(t) < x < S_2(t) \quad , \quad t > 0 \\ \frac{\partial y_3}{\partial t} &= \frac{\partial^2 y_3}{\partial x^2}, \quad S_2(t) < x < 1 \quad , \quad t > 0 \end{aligned} \quad (5)$$

subject to the boundary conditions, $y_1(t,0) = -1$, $y_1(t,S_1(t)) = 0$, $y_2(t,S_1(t)) = 0$, $y_2(t,S_2(t)) = 0$, $y_3(t,S_2(t)) = 0$, $y_3(t,1) = -1$.

The MFEM solutions were obtained using 4 finite elements in each phase and cubic approximations in each element. Figure 1 shows temperature profiles at the interface for time $t=0$ to $t=1.2$. This solution compares favorably to the previous solutions using others techniques. Our results with cubic approximations agree with the results presented by Djomehri (Djomehri et al. 1988) and Robalo (Robalo et al. 2006). The CPU time is 2.8 seconds.

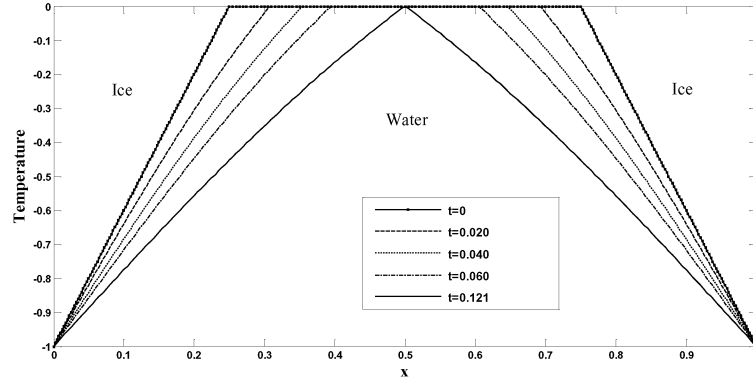


Figure 1: Temperature profiles for ice-water-ice problem.

3.2 Causticizing Reaction

Causticizing reaction is an important step of the kraft pulp production that occurs in a solid / liquid interface which moves to the center of the particles. It is assuming (Duarte et al. 1995) that diffusion controls the process. We want to know the location of the interface and both concentrations of hydroxide ions, y_1 and y_3 , and concentrations of carbonate ions, y_2 and y_4 , on phase 1 and 2 respectively. The initial conditions at $t = 600$, are $y_1 = y_2 = 0$, $y_3 = 2.025$ $y_4 = 0.337$ and $S = 0.8$. D is the diffusion coefficient, ε the porosity, R the length of the particles, K the equilibrium constant, k_L the mass transfer coefficient and C the initial concentration of $Ca(OH)_2$. The normalized equations describing the process are

$$\frac{\partial y_i}{\partial t} = \frac{D}{\varepsilon R^2} \left(\frac{\partial^2 y_i}{\partial x^2} + \frac{2}{x} \frac{\partial y_i}{\partial x} \right), \quad i = 1, 2, 3, 4 \quad (6)$$

subject to the boundary conditions,

$$\begin{aligned} \frac{\partial y_i}{\partial x}(0,t) &= 0, & i &= 1, 2 \\ \frac{\partial y_3}{\partial x} - \frac{\partial y_1}{\partial x} - 2 \frac{\partial y_2}{\partial x} + 2 \frac{\partial y_4}{\partial x} &= 0, & x &= S(t) \\ y_1^2 - K y_2 &= 0, & x &= S(t) \end{aligned} \quad (7)$$

$$\begin{aligned} \frac{\partial y_i}{\partial x}(1,t) &= \frac{Rk_L}{D}(\psi_i(t) - y_i), \quad i=3,4 \\ y_1 - y_3 &= 0, \quad x = S(t) \\ y_2 - y_4 &= 0, \quad x = S(t) \end{aligned} \quad (8)$$

where ψ_i are the concentration around the particles. The reaction front velocity is

$$\frac{dS_i}{dt} = -\frac{D}{CR^2} \left(\frac{\partial y_4}{\partial x} - \frac{\partial y_2}{\partial x} \right), \quad x = S(t) \quad (9)$$

Figure 2 shows the concentrations of hydroxide ions and carbonate ions respectively. The nodes movements for the meshes associated to the concentration of hydroxide ions in phase 1 and 2 are presented in figure 3(a). In figure 3(b) we can see the nodes movements for the meshes associated to the concentration of carbonate ions in phase 1 and 2. In bold we can note the front reaction evolution.

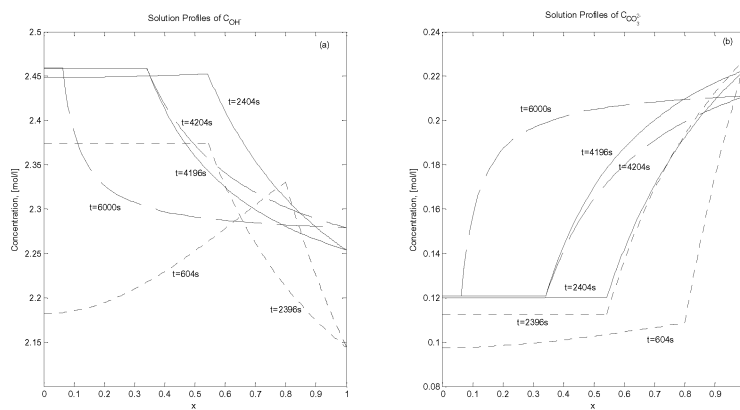


Figure 2: Concentration profiles for hydroxide ions (a) and carbonate (b) ions.

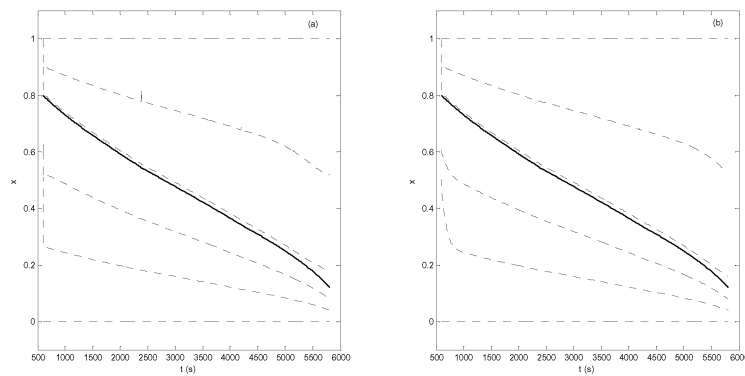


Figure 3: Nodes movements for meshes associated to hydroxide ions concentration (a) and carbonate (b) ions concentration.

The values of all parameters are taken from Duarte (Duarte et al. 1995). For the numerical simulations we consider 3 finite elements for each mesh, cubic approximations on phase 1 and approximations of degree four in phase 2. The CPU time is 24 seconds and the solutions are in good agreement with those obtained by others methods.

4. Conclusions

In this paper we have presented a MFEM for Stefan problems. The main advantages of the method are its simplicity and performance. The numerical results obtained by this formulation of MFEM exhibit very good agreement with those obtained by previous methods so this work establishes the efficiency and applicability of the MFEM to solve moving boundary problems.

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