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The method of approximate fundamental solutions (MAFS) for Stefan problems

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ABSTRACT

The paper presents a new meshless numerical technique for solving one and two-dimensional Stefan problems. The technique presented is based on the use of the delta-shaped functions and the method of approximate fundamental solutions (MAFS) first suggested for solving elliptic problems and heat equations in domains with fixed boundaries. The one-dimensional problems in the plane and cylindrical geometries are considered. The numerical examples are presented and the results are compared with the analytical solutions. The comparison shows that the method presented provides a very high precision in determining the position of the moving boundary even for degenerate and singular problems when a region initially has zero thickness. The same technique was developed for 2D Stefan problems with completely or partially unknown boundary.

1. Introduction

Phase-change, or the Stefan problems in which material melts or solidifies occur in a wide variety of natural and industrial processes. Mathematically, these are special cases of moving-boundary problems, in which the location of the front between the solid and liquid is not known beforehand, but must be determined as a part of the solution [1]. However, apart from a few analytically solvable cases, there is no general solution of this problem. Therefore, a large number of numerical methods have been developed for this goal [2]. Amongst there are the enthalpy method [3,4], the boundary immobilization method [5–8], the variable space grid method [3,8], the finite element numerical method [9], the nodal integral method [10,11]. The comparison of various numerical methods has been made by Furzeland [12], Caldwell et al. [2] and Javierre et al. [13].

There are two main approaches to the solution of the Stefan problem. One is the front-tracing method, where the position of the phase boundary is continuously tracked. Another approach is to use a fixed-domain formulation. The enthalpy method which uses an enthalpy function together with the temperature as a dependent variable may serve as an example. Alternatively, one can use a suitable coordinate transformation to immobilize the moving front [2,8,14].

Very recently, Hon and Li [15] have applied the meshless method of fundamental solutions (MFS), which does not require any domain or boundary discretization, to a boundary determination problem. In [16] this technique was applied to the one-dimensional Stefan problems. It should be noted that [16] presents the classic version of the MFS when the solution of the heat equation

$$\frac{\partial w}{\partial t} = \frac{\partial^2 w}{\partial x^2} \tag{1}$$

is approximated by a linear combination of fundamental solutions in the form

$$w(x,t) \approx w_N(x,t) = \sum_{j=1}^{N} c_j G(x,t\,;y_j,\tau_j),$$

$$G(x,t\,;y,\tau) = \frac{H(t-\tau)}{\sqrt{4\pi(t-\tau)}} \exp\left(-\frac{(x-y)^2}{4(t-\tau)}\right),$$

where H is the Heaviside function, c_j are real coefficients to be determined by imposing the initial and boundary conditions, and the source points y_j,τ_j are located outside the solution domain. As it can be found in the original work, this approximation results in a system of nonlinear equations which is solved by iterations. The coordinates of the moving boundary position are obtained in the framework of the same iteration procedure. The number of the possible positions of the moving boundary is $N_1 = 10$. The movement of the interface is described by its positions at 10 time moments. The whole number of the unknowns reaches 50–90, the typical number of iterations is 150–300.

The goal of the present paper is to describe a new meshless numerical technique for solving problems with moving boundaries. The technique presented is based on the use of the delta-shaped functions [17] and the method of approximate fundamental solutions (MAFS)—a modification of MFS presented in [18–20] for elliptic problems and for heat equations in [21,22].

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Applying the finite difference scheme in time to the heat equation (1), one gets a sequence of equations:

$$\frac{w^{n+1}-w^n}{\Delta t}=\frac{1}{2}\left(\frac{d^2w^{n+1}}{dx^2}+\frac{d^2w^n}{dx^2}\right), \tag{2}$$

or

$$\frac{d^2w^{n+1}}{dx^2}-pw^{n+1}=-\frac{d^2w^n}{dx^2}-pw^n, \quad p=\frac{2}{\Delta t}, \tag{3}$$

when the Crank–Nicholson scheme is used. These equations are solved one from the other beginning with the initial distribution $w^0(x)$. From this point of view the method presented is similar to the finite difference approach. However, contrary to FD techniques we do not use any meshing in space. For this reason the method is characterized as "meshless". The solution of (3) is looked for in the form of the linear combination

$$w^{n+1}(x)=w_p^{n+1}(x)+q_1^{n+1}\Psi(x,\xi_1)+q_2^{n+1}\Psi(x,\xi_2). \tag{4}$$

Here $w_p^{n+1}(x)$ is a particular solution of Eq. (3); the real coefficients q_1^{n+1}, q_2^{n+1} are determined by imposing the boundary conditions; the source points ξ_1, ξ_2 are placed outside the solution domain; the approximate fundamental solution (AFS) $\Psi(x,\xi)$ will be described below. It is important to stress that in the framework of the method presented all the distributions: $w^0(x)$, $w_p^{n+1}(x)$, $\Psi(x,\xi)$ are written in the form of truncated Fourier series over some orthogonal system of functions. So, the solution process consists of some manipulation with coefficients of these expansions. To get the free parameters q_1^{n+1}, q_2^{n+1} we should solve the 2×2 linear system on each time-layer. There is no restriction to the position of the moving boundary. This provides a fast algorithm and high accuracy in determining the position of the moving boundary. In the paper presented a similar technique was developed for 2D Stefan problems.

The organization of this paper is as follows. In Section 2, we introduce briefly the MAFS technique with the use the delta shaped functions and provide three regularization methods for the formulation of the MAFS. We describe the AFSs for 1D equations in the plane and cylindrical geometry and for 2D equation with different boundary conditions. The main results of the paper are presented in Section 3 where we describe the application of the MAFS to the Stefan problems. A finite difference time stepping scheme is employed to reduce the heat equation to a sequence of modified Helmholtz equations. The 1D Stefan problems of two types are considered in the first subsection. There are regular and the degenerated Stefan problems when the solution region initially has zero thickness. Dealing with regular Stefan problems we solve them step by step beginning with the initial distribution $w^0(x)$ and using the AFS for representation of the solution on each time level. The position of the moving boundary is calculated on each time layer using the Euler scheme with correction. In the second part of this section we consider the degenerated Stefan problems when the solution region initially has zero thickness. Then we present the regularizing algorithm to start the boundary movement in the degenerate case. Next, the 1D Stefan problems in the cylindrical geometry are considered. The MAFS algorithm for solving 2D Stefan problems is presented in the second subsection. It is shown that the use of AFS over different basis systems permits to satisfy the boundary conditions on the part of the whole boundary. Finally, in Section 4, we give the conclusion and describe the directions for the future development of the method presented.

2. Delta shaped functions and approximate fundamental solutions

To solve a boundary value problem (BVP)

$$L[w]=f(\mathbf{x}), \quad \mathbf{x}\in\Omega, \tag{5}$$

$$B[w]=g(\mathbf{x}), \quad \mathbf{x}\in\partial\Omega \tag{6}$$

the method of approximate fundamental solution (MAFS) uses as the basis functions the solutions $\Psi(\mathbf{x},\boldsymbol{\xi})$ of the equation

$$L[\Psi(\mathbf{x},\boldsymbol{\xi})]=I(\mathbf{x},\boldsymbol{\xi}). \tag{7}$$

An approximate solution is looked for in the form of the linear combination

$$w(\mathbf{x})\approx w_N(\mathbf{x})=w_p(\mathbf{x})+\sum_{i=1}^{N}q_i\Psi(\mathbf{x},\boldsymbol{\xi}_i).$$

Here w_p is a particular solution of (5); q_i are free parameters which are determined to satisfy the boundary condition (6); $I(\mathbf{x},\boldsymbol{\xi})$ is the delta shaped function (DSF) [20,17] which essentially differs from zero only inside some neighborhood of the source point $\boldsymbol{\xi}$. and which is analogous in some sense to Dirac's functions $\delta(\mathbf{x}-\boldsymbol{\xi})$. The technique of the DSF can be described as follows.

It is well-known that the eigenfunctions

$$\varphi_m(x)=\sin(\lambda_m(x+1)), \quad \lambda_m=0.5m\pi, \ m=1,2,\ldots \tag{8}$$

are the solutions of the following *Sturm–Liouville* problem on the interval $[-1,1]$:

$$\frac{d^2}{dx^2}\varphi=-\lambda^2\varphi, \quad \varphi(-1)=\varphi(1)=0. \tag{9}$$

The eigenfunctions $\varphi_n(x)$ form an orthogonal system on $[-1,1]$ with the scalar product:

$$\int_{-1}^{1}\varphi_n(x)\varphi_m(x)\,dx=\delta_{n,m}=\begin{cases}0, & m\neq n,\\ 1, & m=n.\end{cases}$$

Thus, Dirac's delta function can be formally written as follows:

$$\delta(x-\xi)=\sum_{m=1}^{\infty}\varphi_m(\xi)\varphi_m(x). \tag{10}$$

Note that this series diverges at any point in the interval $[-1,1]$. With various kinds of regularization techniques, a smooth delta-shaped function, $I_{M,\gamma}(x,\xi)$, can be obtained through the formal series expansion (10); i.e., the regularized delta-shaped functions have the form

$$I_{M,\gamma}^{(1)}(x,\xi)=\sum_{m=1}^{M}r_m(M,\gamma)\varphi_m(\xi)\varphi_m(x). \tag{11}$$

Note that $r_m(M,\gamma)$ are the regularization factors which can be obtained using the following regularization techniques:

(1) The Lanczos regularization technique:

$$r_m(M,\gamma)=[\sigma_m(M)]^{\gamma}, \quad \sigma_m(M)=\frac{\sin[v(m,M)]}{v(m,M)}, \quad v(m,M)=\frac{m\pi}{M+1}. \tag{12}$$

$\sigma_m(M)$ are called the Lanczos sigma-factors which are used to overcome the Gibb phenomenon in the Fourier series expansion of non-smooth functions [23]. This technique was employed in [18,20–22] for solving stationary and time-dependent problems. As it is shown in the papers listed above, the parameters M and γ should be taken in coupling. In all the calculations presented for $M=30$, 40, 50, 60 we use $\gamma=8$, 10, 12, 14. This choice of the regularization parameter γ is found to be close to the optimal one.

(2) The Riesz regularization technique:

$$r_m(M,\gamma)=\left(1-\frac{\lambda_m^2}{\lambda_{M+1}^2}\right)^{\gamma}=\left(1-\left(\frac{m}{M+1}\right)^2\right)^{\gamma}. \tag{13}$$

This was proposed in [18,20] for solving elliptic PDEs with scattered data in irregular domains.