International Conference
Nuclear Energy for New Europe 2006
Portorož, Slovenia, September 18-21, 2006
http://www.djs.si/port2006

Solving One-Dimensional Phase Change Problems with Moving Grid Method and Mesh Free Radial Basis Functions

Leopold Vrankar
Slovenian Nuclear Safety Administration
Železna cesta 16, SI-1001 Ljubljana, Slovenia
leopold.vrankar@gov.si

Goran Turk
Faculty of Civil and Geodetic Engineering, University of Ljubljana
Jamova cesta 2, SI-1000 Ljubljana, Slovenia
gturk@fgg.uni-lj.si

Franc Runovc
Faculty of Natural Sciences and Engineering, University of Ljubljana
Aškerčeva cesta 12, SI-1000 Ljubljana, Slovenia
franc.runovc@ntf.uni-lj.si

Edward J. Kansa
Department of Mechanical and Aeronautical Engineering, University of California
Davis 96616-5294 USA
ejkansa@ucdavis.edu

ABSTRACT

Many heat-transfer problems involve a change of phase of material due to solidification or melting. Applications include: the safety studies of nuclear reactors (molten core concrete interaction), the drilling of high ice-content soil, the storage of thermal energy, etc. These problems are often called Stefan's or moving boundary value problems. Mathematically, the interface motion is expressed implicitly in an equation for the conservation of thermal energy at the interface (Stefan's conditions). This introduces a non-linear character to the system which treats each problem somewhat uniquely. The exact solution of phase change problems is limited exclusively to the cases in which e.g. the heat transfer regions are infinite or semi-infinite one dimensional-space. Therefore, solution is obtained either by approximate analytical solution or by numerical methods. Finite-difference methods and finite-element techniques have been used extensively for numerical solution of moving boundary problems. Recently, the numerical methods have focused on the idea of using a mesh-free methodology for the numerical solution of partial differential equations based on radial basis functions. In our case we will study solid-solid transformation. The numerical solutions will be compared with analytical solutions. Actually, in our work we will examine usefulness of radial basis functions (especially multiquadric-MQ) for one-dimensional Stefan's problems. The position of the moving boundary will be simulated by moving grid method. The resultant system of RBF-PDE will be solved by affine space decomposition.

1 INTRODUCTION

Many physical processes involve heat conduction and materials undergoing a change of phase. Examples include the safety studies of nuclear reactors (the molten corium concrete interaction), casting of metals, geophysics and industrial applications involving metals, oil, and plastics. The molten core discharged to the containment cavity will interact with the concrete basemat if it is not, or cannot be, cooled below the solidus temperature of the concrete. The molten core concrete interaction results in decomposition and melting of very large quantities of carbon dioxide and steam.

Due to their wide range of applications the phase change problems have drawn considerable attention of mathematicians, engineers and scientists. These problems are often called Stefan's or moving boundary value problems. One common feature of phase change problems is that the location of the solid-liquid or solid-solid interface is not known a priori and must be determined during the course of analysis.

Analytical solutions are only available for a limited number of model examples (e.g. the heat transfer regions are infinite or semi-infinite one dimensional-space) and hence solution of most practical cases requires the use of numerical techniques.

Several numerical methods have been developed to solve various Stefan's problems. Crank [1] provides a good introduction to the Stefan's problems and presents an elaborate collection of numerical methods for these problems. According to Crank the numerical methods for moving boundary problems can be classified in three categories: front-tracking methods, front-capturing methods and hybrid methods. We follow front-tracking methods (moving grid method) which use an explicit representation of the interface, given by a set of points lying on the interface location, which must be updated at each time step.

The meshless method has been widely investigated in the past and emerged as a new category of computational methods. One of the common characteristics of all mesh-free methods is their ability to construct functional approximation or interpolation entirely based on the information given at a set of scattered nodes. Three different approaches to develop meshless methods have been successfully proposed. The first one is based on the spirit of the finite element method and employs Petrov-Galerkin weak formulation [2]. The second approach is of boundary element type [3]. The third approach employs radial basis functions (RBFs) [4]. In our case we focused on using multiquadric basis functions (MQ) with collocation methods.

Heat treatment of metals is often used to optimize mechanical properties. During heat treatment, the metallurgical state of the alloy changes. This change can involve the phase present at a given location or the morphology of the various phases. One of these processes, which is both of large industrial and scientific interest and amenable to modelling, is the dissolution of the second-phase particles in a matrix with a uniform initial composition.

We will study usefulness of radial basis functions (especially multiquadric-MQ) for one-dimensional Stefan's problems. The position of the moving boundary will be simulated by moving grid method. The resultant system of RBF-PDE will be solved by an affine space decomposition that decouples the influence between the interior and boundary collocations.

2 RADIAL BASIS FUNCTION METHODS

The base of this approach is its employment of high-order interpolating functions to approximate solutions of differential equations. All RBFs possess the property that their values are determined only by distance and have nothing to do with directions. Kansa [4] introduced multiquadric functions to solve hyperbolic, parabolic and elliptic differential equations with collocation methods. This method is an asymmetric collocation set-up in which boundary conditions are treated separately from the interior problem. He found that

they had quite good convergence properties and achieved outstanding computational efficiency. One of the most powerful RBF methods is based on multiquadric basis functions (MQ), first used by R. L. Hardy [5]. It is important to mention that the MQ was till now efficiently used in transport modelling [6].

A radial basis function is a function $\varphi(\mathbf{x}) = \varphi(\| \mathbf{x} - \mathbf{x}_j \|)$, which depends only on the distance between $\mathbf{x} \in \mathbf{R}^d$ and a fixed point $\mathbf{x}_j \in \mathbf{R}^d$. Here, φ is continuous and bounded on any bounded sub-domain $\Omega \subseteq \mathbf{R}^d$. Let r denote the Euclidean distance between any pair of points in the domain Ω. The commonly used radial basis functions are: linear $(\varphi(r) = r)$, cubic $(\varphi(r) = r^3)$, thin-plate spline $(\varphi(r) = r^2 \log r)$, Gaussian $(\varphi(r) = e^{-\alpha^2 r})$ and multiquadric (MQ) $(\varphi(r) = (r^2 + c^2))^{\beta})$. Commonly used values for β are -1/2 and 1/2. The parameter $c > 0$ is a shape parameter controlling the fitting of a smoothing surface to the data. To introduce RBF collocation methods, we consider a PDE in the form of

$$\mathrm{L}u(\mathbf{x}) = f(\mathbf{x}), \quad \text{in} \quad \Omega \subset \mathbf{R}^d, \tag{1}$$

$$\mathrm{B}u(\mathbf{x}) = g(\mathbf{x}), \quad \text{on} \quad \partial\Omega, \tag{2}$$

where u is concentration, d denotes the dimension, $\partial\Omega$ is the boundary of the domain Ω, L is the differential operator on the interior, and B is the operator that specifies the boundary conditions of the Dirichlet, Neumann or mixed type. Both, f and g, are given functions mapping $\Re^d \to \Re$.

Using Kansa's asymmetric multiquadric collocation method, the unknown PDE solution u is approximated by RBFs in the form:

$$u \approx U(\mathbf{x}) = \sum_{j=1}^{N} \alpha_j \varphi_j(\mathbf{x}) + \sum_{l=1}^{M} \gamma_l v_l(\mathbf{x}), \tag{3}$$

where φ can be any of above mentioned radial basis function, $v_l, \ldots, v_M \in \prod_m^d$, is a polynomial of degree m or less. Let $(\mathbf{x}_j)_{j=1}^N$ be the N collocation points in $\Omega \cup \partial\Omega$. We assume the collocation points are arranged in such a way that the first N_I points are in Ω, whereas the last N_B points are on $\partial\Omega$. To evaluate $N+M$ unknown coefficients, $N+M$ linearly independent equations are needed. Ensuring that $U(\mathbf{x})$ satisfies (1) and (2) at the collocation points results in a good approximation of the solution u. The first N equations are given by

$$\sum_{j=1}^{N} \alpha_j \mathrm{L}\varphi_j(\mathbf{x}_i) + \sum_{l=1}^{M} \gamma_l \mathrm{L}v_l(\mathbf{x}) = f(\mathbf{x}_i), \quad \text{for } i = 1, \ldots, N_I, \tag{4}$$

$$\sum_{j=1}^{N} \alpha_j \mathrm{B}\varphi_j(\mathbf{x}_i) + \sum_{l=1}^{M} \gamma_l \mathrm{B}v_l(\mathbf{x}) = g(\mathbf{x}_i), \quad \text{for } i = N_I + 1, \ldots, N_I + N_B. \tag{5}$$

The last M equations could be obtained by imposing some extra condition on $v(\cdot)$:

$$\sum_{j=1}^{N} \alpha_j v_k(\mathbf{x}_j) = 0, \quad k = 1, \ldots, M. \tag{6}$$

The choice of basis function is another flexible feature of RBF methods. RBFs can be globally supported, infinitely differentiable, and contain a free parameter, c. This leads to a full coefficient matrix or a dense interpolation matrix. The shape parameter c affects both the accuracy of the approximation and the conditioning of the interpolation matrix. The optimal shape parameter c is still an open question. In our case we used an iterative mode by monitoring the spatial distribution of the residual errors in Ω and $\partial\Omega$ as a function of c. The iterations are terminated when errors are smaller then a specified bound. This map is then used to guide the search of the optimal shape parameter c that gives the best approximation the solution.

3 THE PROBLEM

3.1 The physical model

We consider the solid state phase transformation problem in binary metallic alloys which is described in [7]. In that problem a volume of constant composition is surrounded by a diffusive phase. In the interface between the particle and the diffusive phase a constant concentration is assumed, and the gradient of the concentration causes the movement of the interface.

3.2 The mathematical model

We studied the domain Ω containing a diffusive phase Ω_{dp} and the part where the material characteristic Ω_{part} remain of constant composition c^{part}. The particle dissolves due to Fickian diffusion in the diffusive phase. The concentration at the interface Γ, separating Ω_{part} and Ω_{dp}, is assumed to be given by the constant value c^{sol}. The concentration gradient on the side of Ω_{dp} at Γ causes its displacement. The governing equations and boundary conditions of this problem are:

$$\frac{\partial u}{\partial t}(\mathbf{x},t) = D\Delta u(\mathbf{x},t), \quad x \in \Omega_{dp}(\mathrm{t}), \mathrm{t} > 0, \tag{7}$$

$$u(\mathbf{x},t) = u^{part}, \quad x \in \Omega_{part}(\mathrm{t}), \mathrm{t} \geq 0, \tag{8}$$

$$u(\mathbf{x},t) = u^{sol}, \quad x \in \Gamma(\mathrm{t}), \mathrm{t} \geq 0, \tag{9}$$

$$(u^{part} - u^{sol})v_n(\mathbf{x},t) = D\frac{\partial u}{\partial \mathbf{n}}(\mathbf{x},t), \quad x \in \Gamma(\mathrm{t}), \mathrm{t} > 0, \tag{10}$$

$$\frac{\partial u}{\partial \mathbf{n}}(\mathbf{x},t) = 0, \quad x \in \partial\Omega_{dp}(t) \setminus \Gamma(\mathrm{t}), \mathrm{t} > 0, \tag{11}$$

where $\mathbf{x}$ is coordinate vector of a point in Ω, D means the diffusivity constant, $\mathbf{n}$ is the unit normal vector on the interface pointing outward with respect to Ω_{part} (t) and v_n is the normal component of the velocity of the interface. The initial concentration $u(\mathbf{x}, 0)$ inside the diffusive phase is given.

4 THE NUMERICAL SOLUTION METHOD

Our interest is to give an accurate discretization of the moving boundary conditions. Here we present an interpolative moving grid method, in which the grid is computed for each time step and the solution is interpolated from the old grid to the new. The equations are solved with collocation method using RBFs. An outline of the algorithm is:

- Compute the concentrations profiles solving equations (7-9) and (11).
- Predict the position of boundary s_1 at the new time-step: $s_1(t+\Delta t)$ using equation (10).
- Once the boundary is moved, the concentration u can be computed in the new region using equation (7). The solution is interpolated from the old point location to the new.

5 ANALYTICAL SOLUTIONS

In numerical experiments we will compare our numerical solutions with the analytical solutions that exist for the problem presented in chapter 3. These solutions are expressed as functions of $(x-s_0)/\sqrt{t}$, and the domain $\Omega=[0,1]$ has to be infinite or semi-infinite. The interface position is given by $s(t)=s_0+2\alpha\sqrt{t}$, where the constant α is obtained by solving the following equation:

$$\alpha=\frac{u^0-u^{sol}}{u^{part}-u^{sol}}\sqrt{\frac{D}{\pi}}\frac{\exp\left(-\frac{\alpha^2}{D}\right)}{\operatorname{erfc}\left(\frac{\alpha}{\sqrt{D}}\right)}. \tag{12}$$

When α is known, the concentration is given by

$$u(x,t)=\begin{cases} u^{part} & if\ x<s(t) \\ u^0+\dfrac{(u^{sol}-u^0)\operatorname{erfc}\left(\dfrac{x-s_0}{2\sqrt{Dt}}\right)}{\operatorname{erfc}\left(\dfrac{\alpha}{\sqrt{D}}\right)}, & if\ x\geq s(t), \end{cases} \tag{13}$$

where u^{part} is the concentration inside the particle u^{sol} is the concentration on the interface and u^0 is the initial concentration of the diffusive phase. s_0 is the initial position of the interface.

6 NUMERICAL EXAMPLE

For the simulations we used data from [7]: the concentration inside the part where the material characteristics remain constant $u^{part}=0.53$, the concentration on the interface $u^{sol}=0$, the initial concentration of the diffusive phase $u^0=0.1$, the diffusivity constant $D=1$, the domain length $l=1$ and the initial position of the interface $s_0=0.2$. Let N be the total number of points, r of those lie inside constant composition and $N-r$ lie inside the

diffusive phase. The distances between each phase are uniform and the interface is always located in the r^{th} node. Due to the movement of the interface, the point locations are adapted at each time step.

In numerical experiments we also included MQ exponent, β as an additional parameter to be optimized. The MQ exponent β had the values 0.5 and 1.5. In Figure 1 the movement of the interface positions calculated with different MQ exponent, β is presented. On the left side of the Figure 1 we show the results obtained by shape parameter c based on residual error calculated at collocation points, and on the right side of the Figure 1 the results obtained by shape parameter c based on residual error calculated at other points (those laying between collocation points).

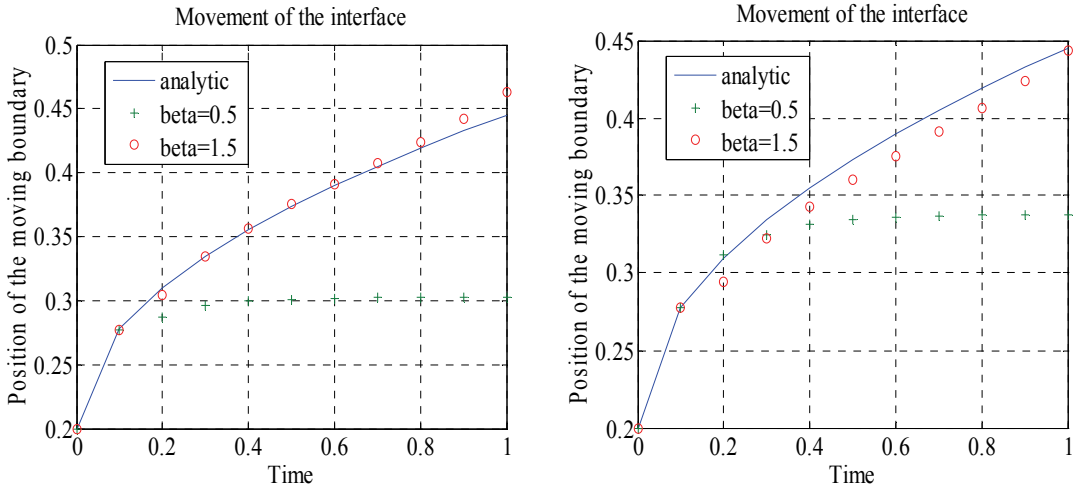

Figure 1: Interface position vs. time

7 DISCUSSION

Comparison of positions of the moving boundary calculated with MQ (β=0.5) and MQ (β=1.5) (Figure 1) shows that MQ (β=1.5) determines the position of the interfaces much more accurately than MQ (β=0.5). The simulations have also shown that the value of the shape parameter c which was computed by residual error procedure was in the range between 0.01 and 0.09. This confirms the fact that for a fixed number of centers N, smaller shape parameters produce more accurate approximations.

The results have shown that β should be greater than 0.5 if we want to get reasonable results. The shape parameter c determined at collocation points better fulfils equation than the shape parameter c determined at the other points. Probable reasons for bad results in Figure 1 (β=0.5) could be found in the facts that some centers were clustered (too close to each other). It has been also observed that in the case of (β=1.5) we had better fulfilment of the equation at collocations points (e.g. left picture of Figure 1) than at other points (e.g. right picture of Figure 1).

To achieve accuracy, the resultant system of RBF-PDE problem usually becomes badly conditioned. Several different strategies [9] have been somewhat successful in reducing the ill-conditioning problem when using RBF methods in PDE problems. The strategies include:

variable shape parameters, domain decomposition, preconditioning of the interpolation matrix, and optimizing the canter locations.

In our case we also used the affine space decomposition scheme of Ling and Hon [8]. The method decouples the influence between the interior and boundary collocations, and it is easy to implement. The resultant system (4-5) consists of two parts: the interior collocation matrix and the boundary collocation matrix, resulting from the interior operator L and boundary operators B, respectively (see details in [8]). The RBF unknown coefficient vector is decomposed by the orthonormal basis of the null space of the boundary collocation matrix.

In table 1 we present the results calculated with classical Gauss elimination with pivoting (GE) and affine space decomposition (ASD) compared with analytic solution.

Table 1: Solving numerical matrix system with affine space decomposition

Anal.	0.2000	0.2775	0.3097	0.3343	0.3551	0.3734	0.3899	0.4051	0.4193
GE	0.2000	0.2775	0.3048	0.3346	0.3568	0.3748	0.3917	0.4089	0.4264
ASD	0.2000	0.2775	0.3048	0.3346	0.3565	0.3752	0.3908	0.4071	0.4236

8 CONCLUSIONS

This study presents modelling of moving boundary value problems using a radial basis functions method (MQ). Simulations show that MQ (β=1.5) gives good results. In this case the method of evaluation was verified by comparing results with the analytical solutions. We explore the residual error from the equation as an indicator which provides a road map to the optimal selection of the shape parameter value.

The choice of basis function is flexible feature of RBF methods. Basis functions may have global or compact support and may have varying degrees of smoothness. The results show that the exponents β need not to be restricted to 0.5.

In that case of calculating the Stefan's problems we can conclude that the radial basis function methods could be an appropriate alternative to the analytic method due to its simpler implementation.

We used an affine space decomposition that decouples the influence between the interior and boundary collocations, and could be an appropriate alternative to the Gauss elimination with pivoting.

In our future work we will employ a Lagrangian approach to track the movement of the moving boundary and transform the problem to a time-independent domain.

In many nuclear accident sequences the reactor core attacks and fails the lower head of the pressure vessel and the core is released to containment cavity where the ex-vessel phase of the accident ensues. Therefore it will be possible to use the presented numerical method to model the attack on the basemat concrete by hot, often molten core materials where the effects of heat transfer, concrete ablation, cavity shape, gas generation, and debris/gas chemistry are included.

ACKNOWLEDGMENTS

The authors would like to thank the Slovenian Nuclear Safety Administration for their support.

REFERENCES

[1] J. Crank, Free and Moving Boundary Problems, Clarendon Press, Oxford, 1984.

[2] S. N. Atluri, S. Shen, the Meshless Local Petrov-Galerkin Method, Tech Science Press, Encino, CA, 2002.

[3] G. Li, S. N. Atluri, Boundary Cloud Method: A Combined Scattered Point/Boundary Integral Approach for Boundary-only Analysis, *Computer. Methods Appl. Engrg*., vol. 191, 2002, pp. 2337-2370.

[4] E. J. Kansa, Multiquadrics-A Scattered Data Approximation Scheme with Applications to Computational Fluid Dynamics-I. Surface Approximations and Partial Derivative Estimates, *Computer Math. Appl*, vol. 19, no. 8-9, 1990, pp. 127-145.

[5] R. L. Hardy, Multiquadric Equation of Topography and Other Irregular Surfaces, *J. Geophys. Res*., vol. 176, 1971, pp. 1905-1915.

[6] L. Vrankar, G. Turk, F. Runovc, Modelling of Radionuclide Migration through the Geosphere with Radial Basis Function Method and Geostatistics, *Journal of the Chinese Institute of Engineers*, vol. 27, No. 4, 2004, pp. 455-462.

[7] E. Javierre, C. Vuik, F.J. Vermolen, S. van der Zwaag, A Comparison of Numerical Models for One-Dimensional Stefan Problems, Reports of the Delft Institute of Applied Mathematics, Netherlands, 2005.

[8] L. Ling, Y.C. Hon, Improved Numerical Solver for Kansa's Method Based on Affine Space Decomposition, *Engineering with Boundary Elements*, vol. 29, 2005, pp. 1077-1085.

[9] E. J. Kansa, Y. C. Hon, Circumventing the Ill-Conditioning Problem with Multiquadric Radial Basis Functions: Applications to Elliptic Partial Differential Equations, *Computers Math. Applic,* vol. 39, No. 7-8, 2000, pp. 123-137.