Application of the dual reciprocity boundary element method on Stefan problems

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ABSTRACT

This paper describes the application of the dual reciprocity boundary element method for the solution of Stefan problem that appears when treating multidimensional Fourier conduction melting and solidification in rigid systems. The physical model is based on the mixture continuum formulation and includes temperature dependent thermal conductivities and specific heats of the solid and liquid phase. Phase-change could take place at distinct melting temperature or continuously on a solidus-liquidus temperature interval. The resulting governing equation is reformulated by the Kirchhoff transform and cast in the latent heat source term shape. Boundary element method solution procedure is structured by the Green's function of the Laplace equation and by the dual reciprocity boundary-only representation of domain integrals based on the $1 + r$ space splines. The highly non-linear source term updating is made following the recently deduced efficient Voller and Swaminathan scheme. The numerical solution is constructed by straight line boundary elements with constant space and linear time splines. The sensitivity of the solution with respect to space-time discretization was investigated on a two-phase Rathjen and Jiji's analytical solution for the solidification of an infinite rectangular corner.

INTRODUCTION

The research of the solid-liquid phase change involves interdisciplinary theoretical, experimental, and computational modelling of phase transformation kinetics, solid mechanics, and transport phenomena. It has an important impact on many basic-science, engineering, and medical developments. An overview of the discipline could be found in [1]. A data base of relevant references, including several key words is listed in [2].

Due to the demonstrated [3] suitability of the Boundary Element Method (BEM) for discrete approximative solution of nonlinear transport phenomena models, a great interest also exists to enable this method to cope with melting and solidification. A comprehensive survey of the related BEM applications is published in [4].

The principal incitement for present work was an advanced numerical solution of the boundary-domain integral equation describing the mixture continuum formulation [5] of the energy transport based on a simple conduction governed monoconstituent sub-model. This equation was deduced in [6] and forms a part of the Laplace equation fundamental solution structured boundary-domain integral equations of the general mixture continuum formulation for the extremely non-linear coupled transport of mass, energy, momentum, and species during melting and solidification.
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FORMULATION

Geometry and Material Properties
Consider a connected fixed domain \( \Omega \) with boundary \( \Gamma \) occupied by a rigid phase change material described with the density \( \rho_0 \) the temperature dependent specific heat \( c_\rho \) and the thermal conductivity \( k_\rho \) of the solid \( \rho = s \) and the liquid \( \rho = l \) phase, and the specific latent heat of solid-liquid phase change \( H_\rho^0 \).

Governing Equation
The mixture continuum formulation of the energy transport for the assumed system is

\[
\rho_0 \frac{\partial}{\partial t} \left( f_s H_s + f_l H_l \right) = -\nabla \cdot \left( f_s F_s + f_l F_l \right) + f_s q_s + f_l q_l, \quad f_s + f_l = 1. \tag{1}
\]

Function \( f_\rho \) presents the temperature dependent volume fraction, \( H_\rho \) the specific enthalpy, \( F_\rho \) heat flux, and \( q_\rho \) heat source of the phase \( \rho \). Heat sources could depend arbitrary on temperature and independent time and position variables. Due to the local thermal equilibrium between the phases, the mixture temperature \( T \) and the phase temperatures \( T_s \) and \( T_l \) are equal.

Constitutive equations for the two heat fluxes are based on the Fourier relation

\[
F_s = -k_s \nabla T, \quad F_l = -k_l \nabla T, \tag{2}
\]

and the enthalpy-temperature relationship is defined as

\[
H_s = c_s (T_H) T_H + \int_{T_H}^{T} c_s (\theta) \, d\theta, \quad H_l = c_l (T_H) T_H + \int_{T_H}^{T} c_l (\theta) \, d\theta + H_\rho^0, \tag{3}
\]

with \( T_H \) representing the enthalpy reference temperature. The governing equation could be rewritten in the following latent heat source term form

\[
\rho_0 c \frac{\partial T}{\partial t} = \nabla \cdot \left( k \nabla T \right) + q - \rho_0 \frac{dH_\rho}{dT} \frac{\partial T}{\partial t}, \tag{4}
\]

with

\[
q = f_s q_s + f_l q_l, \quad \frac{dH_\rho}{dT} = (H_l - H_s) \frac{df_l}{dT} = -(H_l - H_s) \frac{df_s}{dT}. \tag{5}
\]

The thermal conductivity \( k \) and the specific heat \( c \) of the mixture are defined as

\[
k = k_0 + k_T = f_s k_s + f_l k_l, \quad c = c_0 + c_T = f_s c_s + f_l c_l. \tag{6}
\]

Constants \( k_0, c_0 \) present mean values, and functions \( k_T, c_T \) temperature behaviour of the respective mixture quantities.

Initial and Boundary Conditions
We seek the solution of the governing equation for mixture temperature at final time \( t = t_0 + \Delta t \), where \( t_0 \) presents initial time and \( \Delta t \) positive time increment. The solution is constructed by the initial and boundary conditions that follow.

The initial temperature \( T(p, t_0) \) at point with position vector \( p \) and time \( t_0 \) is defined through known function \( T_0 \)

\[
T(p, t_0) = T_0; \quad p \in \Omega \oplus \Gamma. \tag{7}
\]

The boundary \( \Gamma \) is divided into not necessary connected parts \( \Gamma^P, \Gamma^N, \) and \( \Gamma^R \)

\[
\Gamma = \Gamma^P \oplus \Gamma^N \oplus \Gamma^R, \tag{8}
\]
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with Dirichlet, Neumann, and Robin type of boundary conditions respectively. These boundary conditions are at point \( p \) and time \( t_0 \leq t \leq t_0 + \Delta t \) defined through known functions \( T_r, F_r, \) and \( h \)

\[
T(p, t) = T_r; \quad p \in \Gamma_D, \quad (9)
\]

\[
-k \nabla T(p, t) \cdot n_r(p) = F_r; \quad p \in \Gamma_N, \quad (10)
\]

\[
-k \nabla T(p, t) \cdot n_r(p) = h \left[ T(p, t) - T_r \right]; \quad p \in \Gamma_R, \quad (11)
\]

where the heat transfer coefficient \( h \) and other known functions are allowed to depend arbitrary on thermal field. The outward pointing normal on \( \Gamma \) is denoted by \( n_r(p) \).

Constraint

\[
T_0 = T_r; \quad p \in \Gamma_D, \quad t = t_0, \quad (12)
\]

is required for the problem to be well-posed.

Governing Discretization Equation

The equation (4) is rewritten into boundary-domain integral shape by the introduction of the Kirchhoff variable

\[
T = T_T + \int_{T_T}^T k(\theta) d\theta = T + \int_{T_T}^T \frac{k_T(\theta)}{k_0} d\theta, \quad (13)
\]

with \( T_T \) denoting the Kirchhoff variable reference temperature, and by weighting it over space-time \( [\Omega] \times [t_0, t_0 + \Delta t] \) with the fundamental solution of the Laplace equation \( T^*(p; s) \). After lengthy procedure, detailed in [7], the following boundary-domain integral expression is obtained

\[
\int_\Omega \rho_0 c_0 T(p, t_0 + \Delta t) T^*(p; s) d\Omega - \int_\Omega \rho_0 c_0 T(p, t_0) T^*(p; s) d\Omega
\]

\[
= \int_{t_0}^{t_0+\Delta t} \int_\Gamma k_0 T^* \nabla T \cdot d\Gamma dt - \int_{t_0}^{t_0+\Delta t} \int_\Gamma k_0 T \nabla T^* \cdot d\Gamma dt + \int_{t_0}^{t_0+\Delta t} c^*(\Omega, s) k_0 T(s, t) dt
\]

\[
+ \int_{t_0}^{t_0+\Delta t} \int_\Omega \left[ q + Q \frac{\partial T}{\partial t} \right] T^* \, d\Omega dt; \quad Q = \rho_0 \left[ c_0 - \frac{k_0}{k} (c + \frac{dH_M}{dt}) \right],
\]

\[
c^*(\Omega, s) = \int_\Omega \nabla^2 T(p; s) d\Omega, \quad T^*_2(p; s) = \frac{1}{2\pi} \log \frac{r_0}{|p - s|}, \quad T^*_3(p; s) = \frac{1}{4\pi} \frac{p - s}{|p - s|^3}. \quad (14)
\]

Functions \( T^*_2 \) and \( T^*_3 \) represent the two and the three dimensional planar symmetry form of the fundamental solution \( T^* \). Equation (14) is solved by the related Kirchhoff transformed initial and boundary conditions

\[
T(p, t_0) = \int_{T_T}^{T_0} k \frac{d\theta}{k_0}; \quad p \in \Omega \oplus \Gamma, \quad (15)
\]

\[
T(p, t) = \int_{T_T}^{T_C} k \frac{d\theta}{k_0}; \quad p \in \Gamma_D, \quad (16)
\]

\[
-k_0 \nabla T(p, t) \cdot n_r(p) = F_r; \quad p \in \Gamma_N, \quad (17)
\]

\[
-k_0 \nabla T(p, t) \cdot n_r(p) = h \left[ T(p, t) - T_r - \int_{T_T}^{T[T(p, t)]} \frac{k_T}{k_0} d\theta \right]; \quad p \in \Gamma_R. \quad (18)
\]
SOLUTION PROCEDURE

Transformation of Domain Integrals into Boundary Integrals

The solution procedure is based on the Dual Reciprocity Method (DRM) [8] that handles the boundary-domain integral equation of the type (14) through the calculation of the boundary integrals only.

An arbitrary function $\mathcal{F}(p, t)$ is approximated over the domain $\Omega$ with $n = 1, 2, \ldots, N$ space $\Psi_n^p(p)$ and time splines $\Psi_n^t(t)$

$$\mathcal{F}(p, t) \approx \sum_{n} \Psi_n^p(p, t) \Psi_n^t(t), \quad \mathcal{F}(p_m, t) = \sum_{n} \Psi_n^p(p_m, t) \Psi_n^t(t), \quad \Psi_n^t(t) = [\Psi_{nm}^p]^t \mathcal{F}(p_m, t). \quad (19)$$

The Einstein summation is used in this text wherever possible.

Using the Green’s second identity and the definition for the functions $\Psi_n^p$ the domain integral of function $\mathcal{F}(p, t)$ weighted with the Green function $T^*$ over $\Omega$ approximately transforms into a series of $N$ integrals over its boundary

$$\int_{\Omega} \mathcal{F}(p, t) T^*(p; s) d\Omega \approx \sum_{n} \int_{\Gamma} \Psi_n^p(p) \Psi_n^t(t) T^*(p; s) d\Gamma$$

The efficiency of the transformation (20) strongly depends on the choice of the splines $\Psi_n^p$ which is not unique. We select the form

$$\Psi_n^p(p) = \sum_{i=0}^{I_p} |p - p_n|^i \ast, \quad \hat{\Psi}_n^p(p) = \sum_{i=0}^{I_p} \frac{|p - p_n|^i + 2}{(i + 2)(i + I_{dim})}, \quad (21)$$

with $I_p = 1$, as suggested by Partridge and Brebbia [9]. Parameter $I_{dim}$ = 2 stands for problems defined in two, and $I_{dim}$ = 3 for problems defined in three dimensions.

Nonlinear Source Term Updating, Time and Space Discretization

The numerical solution of the nonlinear integral equation (14) inherently requires timestep iterations. The recently developed robust and accurate Voller and Swaminathan scheme [10] has been used for the iterative updating of the nonlinear source term. Its DRM adapted essentials of the scheme could be perceived from the equation (28).

The governing discretization equation (14) is discretized by the introduction of the linear time splines over the time interval $[t_0, t_0 + \Delta t]$. The boundary is discretized by $N_\Gamma$ boundary elements $\Gamma_k$ with piecewise straight-line geometry and piecewise constant space splines. The first $N_\Gamma$ points $p_n$ in the splines (21) coincide with the nodes (geometric centers) of the boundary elements, and the last $N_\Omega$ points are arbitrary distributed in $\Omega$. All subsequently involved boundary integrals have been evaluated analytically.

Setup of Algebraic Equations System

The equation (14) is solved by constructing an algebraic equation system of $j = 1, 2, \ldots, N$ equations. These equations are obtained by writing the discretized form of equation (14) for source point $s$ to coincide with the nodal points $p_n$. The deduced system of algebraic equations could be cast in a symbolic form

$$F_{j_0 + \Delta t}^t T(p_m, t_0 + \Delta t) + T_{j_0 + \Delta t}^{j_m} \cdot \nabla T(p_m, t_0 + \Delta t)$$

$$= F_{j_0}^t T(p_m, t_0) + T_{j_0}^{j_m} \cdot \nabla T(p_m, t_0) + q_{j_0 + \Delta t}^{j_m} q(p_m, t_0 + \Delta t) + q_{j_0}^{j_m} q(p_m, t_0), \quad (22)$$
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which has to be rearranged according to the boundary condition types before the solution. Superscript \( i \) denotes the value of quantity at \( i \)-th iteration. The matrix elements are defined by

\[
F_{jm}^{i+\Delta t} = \Psi_{jn} \left[ \Psi_{nm} \right]^{-1} \left[ \rho_0 c_0 - Q_{t_0 + \Delta t}^i + \frac{1}{2} \left( \frac{dQ}{dT} \right)_{t_0 + \Delta t}^i \right]
\]

\[
+ \delta_{km} \frac{\Delta t k_0}{2} \int_{\Gamma_k} \nabla T^* (p, s_j) \cdot d\Gamma - \delta_{jm} \frac{\Delta t c^* (\Omega, s_j) k_0}{2},
\]

\[
F_{jm}^{t_0} = \Psi_{jn} \left[ \Psi_{nm} \right]^{-1} \left[ \rho_0 c_0 - Q \left[ T (p_m, t_0) \right] + \frac{1}{2} \frac{dQ}{dT} \left[ T (p_m, t_0) \right] T (p_m, t_0) \right]
\]

\[
- \delta_{km} \frac{\Delta t k_0}{2} \int_{\Gamma_k} \nabla T^* (p, s_j) \cdot d\Gamma + \delta_{jm} \frac{\Delta t c^* (\Omega, s_j) k_0}{2},
\]

\[
T_{jm}^{t_0 + \Delta t} = -T_{jm}^{t_0} = -\delta_{km} \frac{\Delta t k_0}{2} \int_{\Gamma_k} T^* (p; s_j) d\Gamma,
\]

\[
Q_{jm}^{t_0 + \Delta t} = Q_{jm}^{t_0} = \Psi_{jn} \left[ \Psi_{nm} \right]^{-1} \frac{\Delta t}{2},
\]

The value of \( Q_{t_0 + \Delta t} \) at \((i+1)\)-th iteration level is obtained through the values at \( i \)-th and \((i-1)\)-th iteration level

\[
Q_{t_0 + \Delta t}^{i+1} = Q_{t_0 + \Delta t}^i + \frac{dQ}{dT} \left[ T (p_m, t_0 + \Delta t) \right] \left[ T (p_m, t_0 + \Delta t) - T (p_m, t_0 + \Delta t) \right],
\]

\[
\left( \frac{dQ}{dT} \right)_{t_0 + \Delta t}^{i+1} = \frac{dQ}{dT} \left[ T (p_m, t_0 + \Delta t) \right] \left[ 2 T (p_m, t_0 + \Delta t) - T (p_m, t_0 + \Delta t) \right].
\]

The timestep iterations are stopped when the absolute Kirchhoff variable difference of the two successive iterations does not exceed some predetermined positive margin \( T_\delta \) in any of the meshpoints \( p_m \).

**NUMERICAL EXAMPLE**

**Solidification of an Infinite Rectangular Corner**

A comparison with the standard two-dimensional planar symmetry two-phase Rath- jen and Jihi’s [11] quasi-analytical solution is chosen to benchmark the deduced solution procedure. It represents a solidification of a planar semi-infinite rectangular corner with cartesian coordinates \( X \geq 0 \) [m], \( Y \geq 0 \) [m] approximated by a finite square region \( 0 \leq X \leq 1.5 \) [m] and \( 0 \leq Y \leq 1.5 \) [m]. It is initially filled with material at constant temperature \( T_0 = 1.3 \) [K]. Dirichlet boundary conditions with \( T = 0 \) [K] are imposed on boundaries \( X = 0 \) [m] and \( Y = 0 \) [m]. Boundary conditions at \( X = 1.5 \) [m] and \( Y = 1.5 \) [m] are approximated by Neumann type ones with \( F = 0 \) [W/(mK)]. The material properties are \( \rho_0 = 1 \) [kg/m³], \( c_s = c_v = 1 \) [J/(kgK)], \( k_s = k_n = 1 \) [W/(mK)], \( H_f = 0.25 \) [J/kg] with melting temperature \( T_m = 1 \) [K]. Distinct phase change is for computational purposes approximated by a narrow continuous range from \( T_m = T_m^0 - \Delta T_m^0 \) to \( T_m = T_m^0 + \Delta T_m^0 \) with \( \Delta T_m = 0.01 \) [K].

\[
f_c = \begin{cases} 
0; & \text{if } T < T_m^0 \\
(T - T_m^0)/(T - T_m^0); & T_m^0 \leq T \leq T_m^0 + \Delta T_m^0 \\
1; & T > T_m^0 + \Delta T_m^0
\end{cases}
\]
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<table>
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<tr>
<th>meshes</th>
<th>( N_r )</th>
<th>( N_H )</th>
<th>( N )</th>
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<td>25</td>
<td>45</td>
</tr>
<tr>
<td>2( M )</td>
<td>40</td>
<td>100</td>
<td>140</td>
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<tr>
<td>3( M )</td>
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<th>timesteps</th>
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<td>1( \Delta t )</td>
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<tr>
<td>2( \Delta t )</td>
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<tr>
<td>3( \Delta t )</td>
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</tr>
</tbody>
</table>

Table 1: Discretization parameters used in calculations.

Figure 1: Arrangement of the mesh 2\( M \). Boundary nodes are denoted with o and the domain nodes with . Meshes 1\( M \) and 3\( M \) have similar displaced configuration.

The numerically obtained temperatures \( T_{cal} = \Psi_n^p(p) \Psi_n^p(t) \) have been compared with the solution from [11] in \( N_{com} = 10201 \) uniform meshpoints \( p_{com} \) (these points coincide with the crossections of the lines \( Y = const. \) and \( X = const. \) in Figure 2). The maximum \( T_{max} \) absolute error and the average \( T_{ave} \) absolute error of the numerical solution are

\[
T_{max} = \max |T_{cal}(p_{com,n},t) - T_{ana}(p_{com,n},t)|; \quad n = 1, 2, \ldots, N_{com}, \quad (30)
\]

\[
T_{ave} = \frac{1}{N_{com}} \sum_{n=1}^{N_{com}} |T_{cal}(p_{com,n},t) - T_{ana}(p_{com,n},t)|. \quad (31)
\]

CONCLUSIONS

This paper presents the first attempts to computationally solve a multidimensional moving boundary problem through calculations that reduce to the integration of the fixed boundary quantities only. The results preliminary confirm the suitability of the described method for coping with such Stefan type of problems.

In addition, complementary benchmarking of the developed method is needed. It will concentrate on the one-phase classical Stefan problem recalculation and research of the solution sensitivity with respect to the Stefan number for both one- and two-phase problems and will include all aspects as treated in the excellent Dalhuijsen and Segal’s study [12].

The principal advantages of the method are the ease of the implementation of the different boundary condition types, straightforward mesh generation, sequel elimination of large data handling, and the potential ability to easily cope with geometrically moving boundaries as well.

The main disadvantage of the method is the resulting large algebraic system of equations, since the domain meshpoints have to be present. This unfavourable property could be set out efficiently by substructuring technique in combination with the adaptive strategy, that are both under development.

The convective term will be included in the future upgradings, thus enabling us to solve the complete energy transport equation in the discussed context.
Table 2: Absolute error in the numerically calculated temperatures for different space-time discretizations at time $t = 0.1$ [s]. The Table shows convergence of the method with the shorter timesteps and finer meshes. The timestep iteration margin $T_s$ used in calculations is 0.002 [K].

The computer time for solving one iteration on mesh $^1M$, $^2M$, and $^3M$ is approximately 45, 200, and 1000 CPU seconds respectively on 25 MHz PC i486 based compatible with NDP Fortran 77 compiler.

<table>
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<th>discretization</th>
<th>$^1M^2\Delta t$</th>
<th>$^2M^2\Delta t$</th>
<th>$^2M^3\Delta t$</th>
<th>$^3M^2\Delta t$</th>
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<td>$T_{\text{max}}$ [K]</td>
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<tr>
<td>$T_{\text{ave}}$ [K]</td>
<td>0.059</td>
<td>0.035</td>
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</table>

Figure 2: Axonometric view of the interpolated solution for the discretization $^2M^2\Delta t$. The bold isotherm represents the solid-liquid interphase boundary and the dimensionless scales are simply $T^* = T/(1$ [K]), $X^* = X/(1$ [m]), and $Y^* = (Y/1$ [m]). The positions of the maximum errors are in the corners of the square.
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REFERENCES