



A boundary element method for phase change problems

A. J. Davies, M. E. Honnor & S. J. Kane

Department of Mathematics, University of Hertfordshire, UK

Abstract

This paper presents the Generalized Newmark Dual Reciprocity Boundary Element Method, GNDRM, for solving nonlinear transient field problems with phase change. GNDRM is a combination of the Generalized Newmark family of single step time marching schemes and the Dual Reciprocity Boundary Element Method. Iterations are performed at each time step using the Newton-Raphson method with line searches. Latent heat effects due to phase change are incorporated using a fixed-grid apparent heat capacity method.

1 Introduction

The Generalized Newmark, or GNpj, method was originally called the Beta-m method [1]. The GNpj method is a generalization of the Newmark method and is a general family of single step time marching schemes, choice of integration parameters controls accuracy and stability. Other well-known methods (e.g. Newmark, Wilson, Houbolt, etc.) are contained within the GNpj family.

An initial restriction of the boundary element method was that the fundamental solution to the original partial differential equation was required in order to obtain an equivalent boundary integral equation. Another restriction was that domain integrals were needed to account for non-homogeneous terms arising from initial conditions and body loads. One widely used method to overcome both these problems is the dual reciprocity method. The method uses a fundamental solution to a much simpler partial differential equation and treats the remaining terms using global approximating functions [2].

Transient field problems with phase change can be solved numerically by either front-tracking methods or fixed-grid methods. In front-tracking methods the phase change front is tracked continuously and the latent heat effects are

treated as moving boundary conditions. Fixed-grid methods can be divided into source based methods and apparent heat capacity methods. In source based methods latent heat effects of phase change are incorporated by fictitious sources and sinks. This paper deals with two-dimensional transient field problems with phase change using a fixed-grid apparent heat capacity method.

2 Generalized Newmark dual reciprocity method - GNDRM

The GNpj method is a generalization of the Newmark method where p is the order of the approximation function and j is the order of differential equation. The p integration parameters provide a subfamily of methods, which control accuracy and stability as well as options for explicit and implicit algorithms.

The method can be defined by writing the k^{th} derivative of w with respect to time as [1]

$$w^{(k)} = q_k + b_k \Delta w^{(m)} \quad (1)$$

where

$$q_k = \sum_{j=k}^m \frac{w_n^{(j)} h^{(j-k)}}{(j-k)!} \quad (2)$$

and

$$b_k = \frac{\beta_k h^{(m-k)}}{(m-k)!} \quad (3)$$

Δ is the forward difference operator

$$\Delta w = w_{n+1}^{(m)} - w_n^{(m)} \quad (4)$$

where subscripts n and $n+1$ refer to time n and $n+1$ and h is the time step.

In the above, q_k is the Taylor series expansion of $w_{n+1}^{(k)}$ up to the term $w_n^{(m)}$. Thus each q_k is a known history vector. The last term in equation (1), which contains the unknown increment $\Delta w^{(m)}$, may be interpreted as an approximation to the next Taylor series term $w_n^{(m+1)}$. The accuracy of the approximation is controlled by the choice of the integration parameters, $\beta_0, \beta_1, \dots, \beta_{m-1}$. By choosing $\beta_k = 1/(m-k+1)$ the scalar terms b_k become the recognizable Taylor series coefficients for the term $w_n^{(m+1)}$. However this is not necessarily an optimal choice. It is applicable to any system of initial value problems providing we choose m greater than or equal to the highest order differential appearing in the system. Table 1 lists selected methods [1].

The heat conduction equation for two-dimensional problems for isotropic materials is

$$\frac{\partial}{\partial x} \left(K \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(K \frac{\partial u}{\partial y} \right) + V = \rho c \frac{\partial u}{\partial t} \quad (5)$$

where u is the temperature, K is the thermal conductivity, V is the heat generated, ρ is the density, c is the specific heat. Equation (5) can be written as

$$\nabla^2 u = \frac{\rho c}{K} \frac{\partial u}{\partial t} - \frac{V}{K} - \frac{1}{K} \left(\frac{\partial K}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial K}{\partial y} \frac{\partial u}{\partial y} \right) \quad (6)$$

Applying the dual reciprocity boundary element method [2] to equation (6) gives

$$H_{ik} u_k - G_{ik} q_k = S_{ik} \left[\frac{\rho c_k}{K_k} \frac{\partial u_k}{\partial t} - \frac{V_k}{K_k} - \frac{1}{K_k} \left(\frac{\partial K_k}{\partial x} \frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y} \frac{\partial u_k}{\partial y} \right) \right] \quad (7)$$

In general equation (7) is a nonlinear equation. Matrices \mathbf{H} , \mathbf{G} and \mathbf{S} are independent of temperature but vectors \mathbf{K} , and \mathbf{V} may be dependent upon temperature. Rearranging equation (7) for the residual, or out of balance, ψ gives

$$\psi_i = H_{ik} u_k - G_{ik} q_k - S_{ik} \left[\frac{\rho c_k}{K_k} \frac{\partial u_k}{\partial t} - \frac{V_k}{K_k} - \frac{1}{K_k} \left(\frac{\partial K_k}{\partial x} \frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y} \frac{\partial u_k}{\partial y} \right) \right] \quad (8)$$

Applying the Newton-Raphson method

$$(K_T)_{ij} dw_j = -\psi_i \quad (9)$$

where

$$(K_T)_{ij} = \frac{\partial \psi_i}{\partial w_j} \quad (10)$$

and \mathbf{w} represents the vector of unknowns either $u^{(m)}$ or $q^{(m)}$ depending upon the conditions at the node.

If $q_j^{(m)}$ is the unknown, then

$$(K_T)_{ij} = \frac{\partial \psi_i}{\partial w_j} = \frac{\partial \psi_i}{\partial q_j^{(m)}} = -G_{ik} \frac{\partial q_k}{\partial q_j^{(m)}} = -G_{ik} b_0 \delta_{kj} = -G_{ij} b_0 \quad (11)$$

for all i .

If $u_j^{(m)}$ is the unknown

$$\begin{aligned} (K_T)_{ij} = \frac{\partial \psi_i}{\partial w_j} = \frac{\partial \psi_i}{\partial u_j^{(m)}} = H_{ik} \frac{\partial u_k}{\partial u_j^{(m)}} - S_{ik} \left[\frac{\rho c_k}{K_k} \frac{\partial}{\partial u_j^{(m)}} \left(\frac{\partial u_k}{\partial t} \right) - \frac{\rho c_k}{K_k^2} \frac{\partial K_k}{\partial u_j^{(m)}} \frac{\partial u_k}{\partial t} \right. \\ \left. + \frac{1}{K_k} \frac{\partial (\rho c)_k}{\partial u_j^{(m)}} \frac{\partial u_k}{\partial t} - \frac{1}{K_k} \frac{\partial V_k}{\partial u_j^{(m)}} + \frac{V_k}{K_k^2} \frac{\partial K_k}{\partial u_j^{(m)}} \right] \end{aligned}$$

$$-\frac{1}{K_k} \frac{\partial}{\partial u_j^{(m)}} \left(\frac{\partial K_k}{\partial x} \frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y} \frac{\partial u_k}{\partial y} \right) + \frac{1}{K_k^2} \frac{\partial K_k}{\partial u_j^{(m)}} \left(\frac{\partial K_k}{\partial x} \frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y} \frac{\partial u_k}{\partial y} \right) \quad (12)$$

for all i .

Let α be the slope of the thermal conductivity curve, hence

$$\frac{\partial K_k}{\partial u_j^{(m)}} = \frac{\partial K_k}{\partial u_k} \frac{\partial u_k}{\partial u_j^{(m)}} = \alpha_k b_0 \delta_{kj} \quad (13)$$

and let β be the slope of the heat capacity curve

$$\frac{\partial (\rho c)_k}{\partial u_j^{(m)}} = \frac{\partial (\rho c)_k}{\partial u_k} \frac{\partial u_k}{\partial u_j^{(m)}} = \beta_k b_0 \delta_{kj} \quad (14)$$

Substituting into equation (12) gives

$$\begin{aligned} (K_T)_{ij} = & H_{ik} b_0 \delta_{kj} - S_{ik} \left\{ \frac{\rho c_k}{K_k} b_1 \delta_{kj} - \frac{\rho c_k}{K_k^2} \alpha_k b_0 \delta_{kj} \frac{\partial u_k}{\partial t} + \frac{1}{K_k} \beta_k b_0 \delta_{kj} \frac{\partial u_k}{\partial t} \right. \\ & \left. - \frac{1}{K_k} \frac{\partial V_k}{\partial u_k} b_0 \delta_{kj} + \frac{V_k}{K_k^2} \alpha_k b_0 \delta_{kj} \right. \\ & \left. - \frac{1}{K_k} \left[\frac{\partial}{\partial u_j^{(m)}} \left(\frac{\partial K_k}{\partial x} \right) \frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial x} \frac{\partial}{\partial u_j^{(m)}} \left(\frac{\partial u_k}{\partial x} \right) + \frac{\partial}{\partial u_j^{(m)}} \left(\frac{\partial K_k}{\partial y} \right) \frac{\partial u_k}{\partial y} + \frac{\partial K_k}{\partial y} \frac{\partial}{\partial u_j^{(m)}} \left(\frac{\partial u_k}{\partial y} \right) \right] \right. \\ & \left. + \frac{\alpha_k}{K_k^2} b_0 \delta_{kj} \left(\frac{\partial K_k}{\partial x} \frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y} \frac{\partial u_k}{\partial y} \right) \right\} \quad (15) \end{aligned}$$

Using the Dual Reciprocity Method approximations to a derivative of temperature or thermal conductivity with respect to a spatial coordinate, equation (15) becomes

$$\begin{aligned} (K_T)_{ij} = & H_{ik} b_0 \delta_{kj} - S_{ik} \left[\frac{\rho c_k}{K_k} b_1 \delta_{kj} - \frac{\rho c_k}{K_k^2} \alpha_k b_0 \delta_{kj} \frac{\partial u_k}{\partial t} + \frac{1}{K_k} \beta_k b_0 \delta_{kj} \frac{\partial u_k}{\partial t} \right. \\ & \left. - \frac{1}{K_k} \frac{\partial V_k}{\partial u_k} b_0 \delta_{kj} + \frac{V_k}{K_k^2} \alpha_k b_0 \delta_{kj} - \frac{1}{K_k} \left(\frac{\partial F_{km}}{\partial x} F_{mn}^{-1} \alpha_n b_0 \delta_{nj} \frac{\partial F_{kr}}{\partial x} F_{rs}^{-1} \right) \right. \\ & \left. + \frac{\partial F_{km}}{\partial x} F_{mn}^{-1} K_n \frac{\partial F_{kr}}{\partial x} F_{rs}^{-1} b_0 \delta_{sj} + \frac{\partial F_{km}}{\partial y} F_{mn}^{-1} \alpha_n b_0 \delta_{nj} \frac{\partial F_{kr}}{\partial y} F_{rs}^{-1} u_s \right. \\ & \left. + \frac{\partial F_{km}}{\partial y} F_{mn}^{-1} K_n \frac{\partial F_{kr}}{\partial y} F_{rs}^{-1} b_0 \delta_{sj} \right) \\ & \left. + \frac{\alpha_k}{K_k^2} b_0 \delta_{kj} \left(\frac{\partial F_{km}}{\partial x} F_{mn}^{-1} K_n \frac{\partial F_{kr}}{\partial x} F_{rs}^{-1} u_s + \frac{\partial F_{km}}{\partial y} F_{mn}^{-1} K_n \frac{\partial F_{kr}}{\partial y} F_{rs}^{-1} u_s \right) \right] \quad (16) \end{aligned}$$

Which can be rewritten as

$$\begin{aligned}
 (K_T)_{ij} = & H_{ij} b_0 - S_{ij} \left(\frac{\rho c_j}{K_j} b_1 - \frac{\rho c_j}{K_j^2} \alpha_j b_0 \frac{\partial u_j}{\partial t} + \frac{1}{K_j} \beta_j b_0 \frac{\partial u_j}{\partial t} - \frac{1}{K_j} \frac{\partial V_j}{\partial u_j} b_0 \right. \\
 & \left. + \frac{V_j}{K_j^2} \alpha_j b_0 \right) + \frac{S_{ik}}{K_k} \left(\frac{\partial F_{km}}{\partial x} F_{mj}^{-1} \alpha_j b_0 \frac{\partial F_{kr}}{\partial x} F_{rs}^{-1} u_s + \frac{\partial F_{km}}{\partial x} F_{mn}^{-1} K_n \frac{\partial F_{kr}}{\partial x} F_{rj}^{-1} b_0 \right. \\
 & \left. + \frac{\partial F_{km}}{\partial y} F_{mj}^{-1} \alpha_j b_0 \frac{\partial F_{kr}}{\partial y} F_{rs}^{-1} u_s + \frac{\partial F_{km}}{\partial y} F_{mn}^{-1} K_n \frac{\partial F_{kr}}{\partial y} F_{rj}^{-1} b_0 \right) \\
 & - S_{ij} \frac{\alpha_j}{K_j^2} b_0 \left(\frac{\partial F_{jm}}{\partial x} F_{mn}^{-1} K_n \frac{\partial F_{jr}}{\partial x} F_{rs}^{-1} u_s + \frac{\partial F_{jm}}{\partial y} F_{mn}^{-1} K_n \frac{\partial F_{jr}}{\partial y} F_{rs}^{-1} u_s \right) \quad (17)
 \end{aligned}$$

no sum on j .

For the Dirichlet boundary condition, prescribed temperature, $u = \bar{u}$

$$\bar{u} = q_0 + b_0 \Delta^{(m)} u \quad (18)$$

$$\Delta^{(m)} u = \frac{\bar{u} - q_0}{b_0} \quad (19)$$

For the Neumann boundary condition, prescribed flux, $q_f = \bar{q}_f = K \frac{\partial u}{\partial n}$

$$\bar{q}_f = K \frac{\partial u}{\partial n} = K \left(q_0 + b_0 \Delta^{(m)} q \right) \quad (20)$$

$$\Delta^{(m)} q = \frac{\bar{q}_f - q_0}{b_0} \quad (21)$$

For the Convection boundary condition, $q_c = K \frac{\partial u}{\partial n} = h_c (u_c - u)$, where h_c is the convection transfer coefficient and u_c is the ambient temperature for convection. Hence an extra term appears in K_T

$$(K_T)_{ij} = (K_T)_{ij} + \frac{1}{K_j} G_{ij} h_c b_0 \quad (22)$$

no sum on j .

For the Radiation boundary condition, $q_R = K \frac{\partial u}{\partial n} = \sigma \varepsilon (u_R^4 - u^4)$, where σ is the Stefan-Boltzmann constant = 5.667×10^{-8} , ε is the surface emissivity and u_R is the ambient temperature for radiation. Hence an extra term appears in K_T

$$(K_T)_{ij} = (K_T)_{ij} + \frac{4}{K_j} G_{ij} \sigma \varepsilon u_j^3 b_0 \quad (23)$$

no sum on j .

3 Phase change

In the apparent heat capacity method equation (5) is replaced by

$$\frac{\partial}{\partial x} \left(K \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(K \frac{\partial u}{\partial y} \right) + V = \frac{\partial h}{\partial t} \quad (24)$$

where h is the enthalpy defined as

$$h = \int_{u_{ref}}^u \rho c dT + \rho L \quad (25)$$

and u_{ref} is the reference temperature and L is the latent heat. The right hand side of equation (24) can be rewritten as

$$\frac{\partial h}{\partial t} = \frac{\partial h}{\partial u} \frac{\partial u}{\partial t} = (\rho c)_a \frac{\partial u}{\partial t} \quad (26)$$

where $(\rho c)_a$ is termed the apparent heat capacity. Using the apparent heat capacity directly leads to numerical problems due to the step like behaviour of $(\rho c)_a$. In order to overcome these problems both space-averaging and time-averaging methods have been used in the finite element literature. Del Giudice et al [3] used a space averaging method and evaluated the apparent heat capacity, for two dimensions, using

$$(\rho c)_a = \frac{\partial h}{\partial u} = \left[\frac{\frac{\partial h}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial h}{\partial y} \frac{\partial u}{\partial y}}{\frac{\partial u}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} \frac{\partial u}{\partial y}} \right] \quad (27)$$

It has been reported [5] that the space averaging technique of Del Giudice, equation (27), can lead to problems in certain circumstances. In this work we use the space-averaging technique of Lemmon [4] where, for two dimensions, the apparent heat capacity is evaluated using

$$(\rho c)_a = \frac{\partial h}{\partial u} = \left[\frac{\frac{\partial h}{\partial x} \frac{\partial h}{\partial x} + \frac{\partial h}{\partial y} \frac{\partial h}{\partial y}}{\frac{\partial u}{\partial x} \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} \frac{\partial u}{\partial y}} \right]^{\frac{1}{2}} \quad (28)$$

Using the Dual Reciprocity Method approximation to a derivative with respect to a spatial coordinate, say x , the terms of equation (28) are evaluated using

$$\frac{\partial h_i}{\partial x} = \frac{\partial F_{ij}}{\partial x} F_{jk}^{-1} h_k \quad (29)$$

and

$$\frac{\partial u_i}{\partial x} = \frac{\partial F_{ij}}{\partial x} F_{jk}^{-1} u_k \quad (30)$$

4 Line searches

The direction of the line search is given by the Newton-Raphson iteration equation (9)

$$d\mathbf{w} = -(\mathbf{K}_T)^{-1} \boldsymbol{\psi} \quad (31)$$

The vector of unknowns \mathbf{w} , either u or q depending upon the conditions at each node, is then updated according to

$$\mathbf{w}^{i+1} = \mathbf{w}^i + \eta d\mathbf{w} \quad (32)$$

where the superscript refers to iteration number and η is a scalar quantity chosen to minimise the residual, or out of balance, $\boldsymbol{\psi}$. Performing line searches at every iteration would be expensive since most iterations would not benefit. Fortunately it is easy to check if the current iteration is a good or bad iteration in terms of reducing the residual at virtually no cost before deciding if line searches would benefit the current iteration. Equation (32) is used to update the vector of unknowns w , with η set to unity. Then if

$$\frac{\psi_j^{i+1} \psi_j^{i+1}}{\psi_k^i \psi_k^i} \leq 0.5 \quad (33)$$

is not satisfied then the current iteration is deemed not good and line searches are then performed. Defining the scalar $\phi = \psi_i \psi_i$ and subscripts on the scalars η and ϕ to denote the line search number, then for iteration $i+1$ we have starting conditions $\eta_0 = 0$, $\phi_0 = \psi_k^i \psi_k^i$ and $\eta_1 = 1$, ϕ_1 obtained from the standard iteration. The line search parameter is then continually updated from

$$\eta_{i+1} = \eta_i + d\eta = \eta_i - \phi_i \left(\frac{\eta_i - \eta_{i-1}}{\phi_i - \phi_{i-1}} \right) \quad (34)$$

until equation (33) is satisfied. Limits on the line searches have to be imposed in order to avoid numerical problems. The first is that $|d\eta|$ is limited to 25% of η . The second is that $0.25 < \eta < 25$. The third is if equation (33) is not satisfied within 25 line searches. When iteration stops due to condition two or three then η is set to the value that was nearest to satisfying equation (33) during the line search procedure.

5 Results

In this example taken for reference [6] a unit square of liquid with an initial temperature of $0.3^\circ C$ is subjected to a constant temperature of $-1^\circ C$ on the surfaces of the wedge AB and AD, surfaces BC and CD are perfectly insulated, as shown in figure 1.

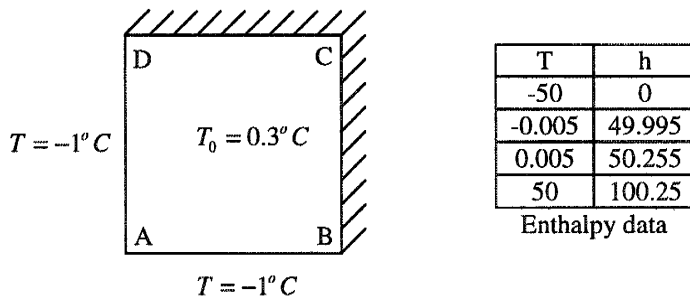


Figure 1: Problem definition.

The material properties are $K = 1 \text{ J/m}^3$, $c = 1 \text{ J/Kg}^\circ\text{C}$, $\rho = 1 \text{ Kg/m}^3$, Latent heat = 0.25 J/m^3 , Liquidus temperature = 0.005°C and Solidus temperature = -0.005°C . From these material properties the enthalpy data given in figure 1 is derived. The problems associated with corners and discontinuous boundary conditions have been handled via the gradient approach [7]. The boundary was divided into 40 elements with 81 equally spaced internal points. Linear radial basis functions $f = 1+r$ are used for the dual reciprocity method. Figure 2 shows the phase front, determined by the 0°C contour, at 0.02, 0.04, 0.06 and 0.08 seconds obtained using the $U1$, $\beta = 1$, scheme and very small timesteps, $dt = 0.1 \times 10^{-6}$ seconds.

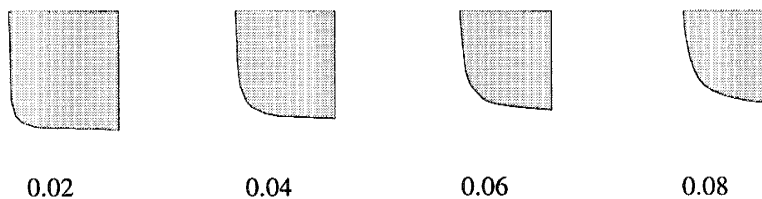


Figure 2: Phase front location.

6 Conclusions

The generalized Newmark dual reciprocity boundary element method, GNDRM, is presented for nonlinear transient field problems with phase change. Since the method is a fixed-grid apparent heat capacity method it can easily be extended to three dimensions without difficulty, unlike the front tracking methods previously used for this type of problem using boundary element methods. Due to the complexity of the problem there are very few analytical results available in order

to verify the results so no comparison of the results presented is made. The authors have verified the results presented by comparing the results obtained from GNDRM to the results produced from a commercially available finite element code and very good agreement was found. The line search technique is fundamental to obtaining convergence in some situations when using GNDRM for phase change problems

The authors were unable to obtain convergence at all using any of the timestepping schemes for any timestep lengths using the space averaging technique of Del Giudice et al [3], equation (27), or the time averaging technique of Morgan et al [5], using a simple backward difference approximation.

References

- [1] Katona, M.G., 'A general family of single-step methods for numerical time integration of structural dynamic equations', Proceedings of the NUMETA 85 Conference, pp 213-225, 1985.
- [2] Partridge, P.W., Brebbia, C.A. and Wrobel, L.C., 'The Dual Reciprocity Boundary Element Method', Computational Mechanics Publications, 1992.
- [3] Del Giudice, S., Comini, G. and Lewis, R.W., 'Finite element simulation of freezing process in solids', International Journal for Numerical and Analytical Methods in Geomechanics, 2, pp 223-235, 1978.
- [4] Lemmon, E.C., 'Phase-change techniques for finite element conduction codes', Proceedings of the Conference on Numerical Methods in Thermal Problems, pp 149-158, 1979.
- [5] Morgan, K., Lewis, R.W. and Zienkiewicz, O.C., 'An improved algorithm for heat conduction problems with phase change', International Journal for Numerical Methods in Engineering, 12, pp 1191-1195, 1978.
- [6] Budhia, H. and Kreith, F., 'Heat transfer with melting or freezing in a wedge', International Journal of Heat and Mass Transfer, 16, pp195-211, 1973.
- [7] Paris, F. and Canas, J., 'Boundary Element Method, Fundamentals and Applications', Oxford University Press, 1997.

