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Nonlinear transient field problems with phase change using the boundary element method

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Abstract

This paper presents the Generalized Newmark Dual Reciprocity Boundary Element Method and the Single Step Dual Reciprocity Boundary Element Method for solving nonlinear transient field problems with phase change. Both are a combination of a general 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.

Keywords: Generalized newmark; Single step; Dual reciprocity; Boundary element; Phase change; Time marching; Latent heat; Apparent heat capacity

1. Introduction

A number of physical processes are governed by the so-called quasi-harmonic equation including heat conduction, gas diffusion, seepage and compressible flow, magnetostatics, torsion and Reynolds film lubrication. These processes are generally termed field problems.

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 [1].

The Generalized Newmark, or GN*pj*, method was originally called the Beta-m method [2]. The GN*pj* 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 GN*pj* family. The SS*pj* method [3] is another general family of single step time marching schemes.

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. Heat conduction

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

$$\frac{\partial}{\partial x}\left(K\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(K\frac{\partial u}{\partial y}\right)+V=\rho c\frac{\partial u}{\partial t} \qquad (1)$$

subject to boundary conditions:

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- Dirichlet boundary condition, prescribed temperature

$$u = \bar{u} \tag{2}$$

- Neumann boundary condition, prescribed flux

$$q_{\mathrm{f}} = \bar{q}_f = K\frac{\partial u}{\partial n} \tag{3}$$

- Convection boundary condition

$$q_{\mathrm{C}} = h(u_{\mathrm{C}} - u) \tag{4}$$

- Radiation boundary condition

$$q_{\mathrm{R}} = \sigma\varepsilon(u_{\mathrm{R}}^4 - u^4) \tag{5}$$

Here u is the temperature, K is the thermal conductivity, V is the heat generated, ρ is the density, c is the specific heat, h is the convection transfer coefficient, u_{C} is the ambient temperature for convection, σ is the Stefan–Boltzmann constant $= 5.667 \times 10^{-8}$, ε is the surface emissivity and u_{R} is the ambient temperature for radiation.

3. The dual reciprocity method

The Laplace operator is isolated on the left hand side and all other terms are transferred to the right hand side to form an equation of the type

$$\nabla^2 u = b(x, y, u) \tag{6}$$

In order to take the right hand side $b(x, y, u)$ to the boundary, the approximation of b is written as

$$b_i = \sum_{j=1}^{N+L} f_{ij}\alpha_j \tag{7}$$

where b_i is the function b at node i, f_{ij} are approximating functions and α_i unknown coefficients. The approximation is performed at $(N + L)$ nodes called DRM collocation points, N boundary nodes and L internal nodes. The functions f are defined by

$$\nabla^2 \hat{u} = f \tag{8}$$

where $\hat{u}$ is a particular solution. Combining Eqs. (6)–(8) gives

$$\nabla^2 u = \sum_{j=1}^{N+L} (\nabla^2 \hat{u}_j)\alpha_j \tag{9}$$

Multiplying by the fundamental solution u^* and integrating by parts gives [4]

$$c_i u_i + \int_\Gamma q^* u \, \mathrm{d}\Gamma - \int_\Gamma u_i^* q \, \mathrm{d}\Gamma = \sum_{j=1}^{N+L} \left\{ \alpha_j \left(c_i \hat{u}_{ij} + \int_\Gamma q^* \hat{u}_j \, \mathrm{d}\Gamma - \int_\Gamma u^* \hat{q}_j \, \mathrm{d}\Gamma \right) \right\} \tag{10}$$

where $q = \partial u/\partial n$, after discretization this becomes

$$c_i u_i + \sum_{k=1}^{N} H_{ik}u_k - \sum_{k=1}^{N} G_{ik}q_k = \sum_{j=1}^{N+L} \alpha_j \left(c_i \hat{u}_{ij} + \sum_{k=1}^{N} H_{ik}\hat{u}_{kj} - \sum_{k=1}^{N} G_{ik}\hat{q}_{kj} \right) \tag{11}$$

which is written for each of the $(N + L)$ nodes i and incorporating the c_i terms into the diagonal of H gives

$$\mathbf{Hu} - \mathbf{Gq} = (\mathbf{H}\hat{\mathbf{U}} - \mathbf{G}\hat{\mathbf{Q}})\boldsymbol{\alpha} \tag{12}$$

From Eq. (7), $\mathbf{b} = \mathbf{F}\boldsymbol{\alpha}$, hence

$$\boldsymbol{\alpha} = \mathbf{F}^{-1}\mathbf{b} \tag{13}$$

which is substituted into Eq. (12) to give

$$\mathbf{Hu} - \mathbf{Gq} = \mathbf{Sb} \tag{14}$$

where

$$\mathbf{S} = (\mathbf{H}\hat{\mathbf{U}} - \mathbf{G}\hat{\mathbf{Q}})\mathbf{F}^{-1} \tag{15}$$

The matrices $\hat{\mathbf{U}}$, $\hat{\mathbf{Q}}$ and $\mathbf{F}$ are all known if f is defined.

4. Generalized Newmark dual reciprocity method

The GNpj method was originally called the Beta-m method [2]. 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 kth derivative of w with respect to time as

$$\overset{(k)}{w} = q_k + b_k \Delta \overset{(m)}{w} \tag{16}$$

where

$$q_k = \sum_{j=k}^{m} \frac{\overset{(j)}{w}_n h^{(j-k)}}{(j-k)!} \tag{17}$$

and

$$b_k = \frac{\beta_k h^{(m-k)}}{(m-k)!} \tag{18}$$

Δ is the forward difference operator

$$\Delta \overset{(m)}{w} = \overset{(m)}{w}_{n+1} - \overset{(m)}{w}_n \tag{19}$$

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 $\overset{(k)}{w}_{n+1}$ up to the term $\overset{(m)}{w}_n$. Thus each q_k is a known history vector. The last term in Eq. (16), which contains the unknown increment $\Delta \overset{(m)}{w}$, may be interpreted as an approximation to the next Taylor series term $\overset{(m+1)}{w}_n$. The accuracy of the approximation is controlled by the choice of the integration parameters, $\beta_0, \beta_1, \ldots, \beta_{m-1}$. By choosing $\beta_k = 1/(m-k+1)$, the scalar terms b_k become the recognizable Taylor series coefficients for the term $\overset{(m+1)}{w}_n$. 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.

Eq. (1) can be written as

$$\nabla^2 u = \frac{\rho c}{K}\frac{\partial u}{\partial t} - \frac{V}{K} - \frac{1}{K}\left(\frac{\partial K}{\partial x}\frac{\partial u}{\partial x} + \frac{\partial K}{\partial y}\frac{\partial u}{\partial y}\right) \tag{20}$$

Applying the dual reciprocity boundary element method to Eq. (20) gives

$$H_{ik}u_k - G_{ik}q_k = S_{ik}\left[\frac{\rho c_k}{K_k}\frac{\partial u_k}{\partial t} - \frac{V_k}{K_k} - \frac{1}{K_k}\left(\frac{\partial K_k}{\partial x}\frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y}\frac{\partial u_k}{\partial y}\right)\right] \tag{21}$$

In general, Eq. (21) is a nonlinear equation. Matrices **H**, **G** and **S** are independent of temperature but vectors **K**, **ρc** and **V** may be dependent upon temperature. Rearranging Eq. (21) for the residual, or out of balance, $\boldsymbol{\psi}$ gives

$$\psi_i = H_{ik}u_k - G_{ik}q_k - S_{ik}\left[\frac{\rho c_k}{K_k}\frac{\partial u_k}{\partial t} - \frac{V_k}{K_k} - \frac{1}{K_k}\left(\frac{\partial K_k}{\partial x}\frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y}\frac{\partial u_k}{\partial y}\right)\right] \tag{22}$$

Applying the Newton–Raphson method

$$(K_T)_{ij}\, \mathrm{d}w_j = -\psi_i \tag{23}$$

where

$$(K_T)_{ij} = \frac{\partial \psi_i}{\partial w_j} \tag{24}$$

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

If $\overset{(m)}{q}_j$ is unknown, then

$$(K_T)_{ij} = \frac{\partial \psi_i}{\partial w_j} = \frac{\partial \psi_i}{\partial \overset{(m)}{q}_j} = -G_{ik}\frac{\partial q_k}{\partial \overset{(m)}{q}_j} = -G_{ik}b_0\delta_{kj} = -G_{ij}b_0 \tag{25}$$

for all i.

If $\overset{(m)}{u}_j$ is unknown

$$\begin{aligned}(K_T)_{ij} &= \frac{\partial \psi_i}{\partial w_j} = \frac{\partial \psi_i}{\partial \overset{(m)}{u}_j} \\ &= H_{ik}\frac{\partial u_k}{\partial \overset{(m)}{u}_j} - S_{ik}\Bigg[\frac{\rho c_k}{K_k}\frac{\partial}{\partial \overset{(m)}{u}_j}\left(\frac{\partial u_k}{\partial t}\right) \\ &\quad - \frac{\rho c_k}{K_k^2}\frac{\partial K_k}{\partial \overset{(m)}{u}_j}\frac{\partial u_k}{\partial t} + \frac{1}{K_k}\frac{\partial (\rho c)_k}{\partial \overset{(m)}{u}_j}\frac{\partial u_k}{\partial t} \\ &\quad - \frac{1}{K_k}\frac{\partial V_k}{\partial \overset{(m)}{u}_j} + \frac{V_k}{K_k^2}\frac{\partial K_k}{\partial \overset{(m)}{u}_j} - \frac{1}{K_k}\frac{\partial}{\partial \overset{(m)}{u}_j} \\ &\quad \times \left(\frac{\partial K_k}{\partial x}\frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y}\frac{\partial u_k}{\partial y}\right) \\ &\quad + \frac{1}{K_k^2}\frac{\partial K_k}{\partial \overset{(m)}{u}_j}\left(\frac{\partial K_k}{\partial x}\frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y}\frac{\partial u_k}{\partial y}\right)\Bigg]\end{aligned} \tag{26}$$

for all i.

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

$$\frac{\partial K_k}{\partial \overset{(m)}{u}_j} = \frac{\partial K_k}{\partial u_k}\frac{\partial u_k}{\partial \overset{(m)}{u}_j} = \alpha_k b_0 \delta_{kj} \tag{27}$$

and let β be the slope of the heat capacity curve

$$\frac{\partial (\rho c)_k}{\partial \overset{(m)}{u}_j} = \frac{\partial (\rho c)_k}{\partial u_k}\frac{\partial u_k}{\partial \overset{(m)}{u}_j} = \beta_k b_0 \delta_{kj} \tag{28}$$

Substituting into Eq. (26) gives

$$\begin{aligned}(K_T)_{ij} &= H_{ik}b_0\delta_{kj} - S_{ik}\Bigg\{\frac{\rho c_k}{K_k}b_1\delta_{kj} - \frac{\rho c_k}{K_k^2}\alpha_k b_0\delta_{kj}\frac{\partial u_k}{\partial t} \\ &\quad + \frac{1}{K_k}\beta_k b_0\delta_{kj}\frac{\partial u_k}{\partial t} - \frac{1}{K_k}\frac{\partial V_k}{\partial u_k}b_0\delta_{kj} + \frac{V_k}{K_k^2}\alpha_k b_0\delta_{kj} \\ &\quad - \frac{1}{K_k}\Bigg[\frac{\partial}{\partial \overset{(m)}{u}_j}\left(\frac{\partial K_k}{\partial x}\right)\frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial x}\frac{\partial}{\partial \overset{(m)}{u}_j}\left(\frac{\partial u_k}{\partial x}\right) \\ &\quad + \frac{\partial}{\partial \overset{(m)}{u}_j}\left(\frac{\partial K_k}{\partial y}\right)\frac{\partial u_k}{\partial y} + \frac{\partial K_k}{\partial y}\frac{\partial}{\partial \overset{(m)}{u}_j}\left(\frac{\partial u_k}{\partial y}\right)\Bigg] \\ &\quad + \frac{\alpha_k}{K_k^2}b_0\delta_{kj}\left(\frac{\partial K_k}{\partial x}\frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y}\frac{\partial u_k}{\partial y}\right)\Bigg\}\end{aligned} \tag{29}$$

The Dual Reciprocity Method approximation to a derivative of temperature with respect to a spatial coordinate, say x, can be written as [1]

$$\frac{\partial u}{\partial x} = \frac{\partial F}{\partial x}F^{-1}u \tag{30}$$

Similarly for thermal conductivity

$$\frac{\partial K}{\partial x} = \frac{\partial F}{\partial x}F^{-1}K \tag{31}$$

Substituting Eqs. (30) and (31) into Eq. (29) gives

$$(K_T)_{ij} = H_{ik}b_0\delta_{kj} - S_{ik}\Bigg[\frac{\rho c_k}{K_k}b_1\delta_{kj} - \frac{\rho c_k}{K_k^2}\alpha_k b_0\delta_{kj}\frac{\partial u_k}{\partial t} + \frac{1}{K_k}\beta_k b_0\delta_{kj}\frac{\partial u_k}{\partial t} - \frac{1}{K_k}\frac{\partial V_k}{\partial u_k}b_0\delta_{kj} + \frac{V_k}{K_k^2}\alpha_k b_0\delta_{kj} - \frac{1}{K_k}\bigg(\frac{\partial F_{km}}{\partial x}F_{mn}^{-1}\alpha_n b_0\delta_{nj}\frac{\partial F_{kr}}{\partial x}F_{rs}^{-1}u_s + \frac{\partial F_{km}}{\partial x}F_{mn}^{-1}K_n\frac{\partial F_{kr}}{\partial x}F_{rs}^{-1}b_0\delta_{sj} + \frac{\partial F_{km}}{\partial y}F_{mn}^{-1}\alpha_n b_0\delta_{nj} \times \frac{\partial F_{kr}}{\partial y}F_{rs}^{-1}u_s + \frac{\partial F_{km}}{\partial y}F_{mn}^{-1}K_n\frac{\partial F_{kr}}{\partial y}F_{rs}^{-1}b_0\delta_{sj}\bigg) + \frac{\alpha_k}{K_k^2}b_0\delta_{kj}\bigg(\frac{\partial F_{km}}{\partial x}F_{mn}^{-1}K_n\frac{\partial F_{kr}}{\partial x}F_{rs}^{-1}u_s + \frac{\partial F_{km}}{\partial y}F_{mn}^{-1}K_n\frac{\partial F_{kr}}{\partial y}F_{rs}^{-1}u_s\bigg)\Bigg] \quad (32)$$

which can be rewritten as

$$(K_T)_{ij} = H_{ij}b_0 - S_{ij}\bigg(\frac{\rho c_j}{K_j}b_1 - \frac{\rho c_j}{K_j^2}\alpha_j b_0\frac{\partial u_j}{\partial t} + \frac{1}{K_j}\beta_j b_0\frac{\partial u_j}{\partial t} - \frac{1}{K_j}\frac{\partial V_j}{\partial u_j}b_0 + \frac{V_j}{K_j^2}\alpha_j b_0\bigg) + \frac{S_{ik}}{K_k}\bigg(\frac{\partial F_{km}}{\partial x}F_{mj}^{-1}\alpha_j b_0 \times \frac{\partial F_{kr}}{\partial x}F_{rs}^{-1}u_s + \frac{\partial F_{km}}{\partial x}F_{mn}^{-1}K_n\frac{\partial F_{kr}}{\partial x}F_{rj}^{-1}b_0 + \frac{\partial F_{km}}{\partial y}F_{mj}^{-1}\alpha_j b_0\frac{\partial F_{kr}}{\partial y}F_{rs}^{-1}u_s + \frac{\partial F_{km}}{\partial y}F_{mn}^{-1}K_n \times \frac{\partial F_{kr}}{\partial y}F_{rj}^{-1}b_0\bigg) - S_{ij}\frac{\alpha_j}{K_j^2}b_0\bigg(\frac{\partial F_{jm}}{\partial x}F_{mn}^{-1}K_n\frac{\partial F_{jr}}{\partial x} \times F_{rs}^{-1}u_s + \frac{\partial F_{jm}}{\partial y}F_{mn}^{-1}K_n\frac{\partial F_{jr}}{\partial y}F_{rs}^{-1}u_s\bigg) \quad (33)$$

no sum on j.

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

$$\bar{u} = q_0 + b_0\Delta\overset{(m)}{u} \quad (34)$$

$$\Delta\overset{(m)}{u} = \frac{\bar{u} - q_0}{b_0} \quad (35)$$

For Neumann boundary condition, prescribed flux

$$q_f = \bar{q}_f = K\frac{\partial u}{\partial n}$$

$$\bar{q}_f = K\frac{\partial u}{\partial n} = K\Big(q_0 + b_0\Delta\overset{(m)}{q}\Big) \quad (36)$$

$$\Delta\overset{(m)}{q} = \frac{\frac{\bar{q}_f}{K} - q_0}{b_0} \quad (37)$$

For convection boundary condition, $q_C = K\dfrac{\partial u}{\partial n} = h(u_C - u)$

$$\psi_i = H_{ik}u_k - G_{ik}\frac{\partial u_k}{\partial n} - S_{ik}\bigg[\frac{\rho c_k}{K_k}\frac{\partial u_k}{\partial t} - \frac{V_k}{K_k} - \frac{1}{K_k}\bigg(\frac{\partial K_k}{\partial x}\frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y}\frac{\partial u_k}{\partial y}\bigg)\bigg] \quad (38)$$

Hence an extra term appears in K_T

$$(K_T)_{ij} = (K_T)_{ij} + \frac{1}{K_j}G_{ij}hb_0 \quad (39)$$

no sum on j.

For radiation boundary condition

$$q_R = K\frac{\partial u}{\partial n} = \sigma\varepsilon(u_R^4 - u^4)$$

$$\psi_i = H_{ik}u_k - G_{ik}\frac{\partial u_k}{\partial n} - S_{ik}\bigg[\frac{\rho c_k}{K_k}\frac{\partial u_k}{\partial t} - \frac{V_k}{K_k} - \frac{1}{K_k}\bigg(\frac{\partial K_k}{\partial x}\frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y}\frac{\partial u_k}{\partial y}\bigg)\bigg] \quad (40)$$

Hence an extra term appears in K_T

$$(K_T)_{ij} = (K_T)_{ij} + \frac{4}{K_j}G_{ij}\sigma\varepsilon u_j^3 b_0 \quad (41)$$

no sum on j.

5. Single Step dual reciprocity method—SSDRM

The SS*pj* family of algorithms was motivated by supposing that $\underset{\sim}{u}(t)$ is represented in the time step by a polynomial. Writing the kth derivative of $\underset{\sim}{u}$ with respect to time, $\overset{(k)}{\underset{\sim}{u}}$, at a time τ between time steps n and $n+1$, i.e. $0 \le \tau \le \Delta t$, as

$$\overset{(k)}{\underset{\sim}{u}}_\tau = \overset{(k)}{\tilde{\underset{\sim}{u}}}_\tau + \underset{\sim}{\alpha}_n^p\frac{\tau^{(p-k)}}{(p-k)!} \quad (42)$$

where

$$\overset{(k)}{\tilde{\underset{\sim}{u}}}_\tau = \sum_{q=k}^{p-1}\overset{(q)}{\underset{\sim}{u}}_n\frac{\tau^{(q-k)}}{(q-k)!} \quad (43)$$

The vector $\underset{\sim}{\alpha}_n^p$ is determined by substituting for $\underset{\sim}{u}(\tau)$ and its derivatives into the weighted residual equation

$$\int_0^{\Delta t} W(\tau)(C_{ij}\dot{u}_j + K_{ij}u_j - f_i)\,\mathrm{d}\tau = 0 \quad (44)$$

Labelling a set of $p+1$ parameters θ_q, $q = 0, 1, \ldots, p$ thus

$$\theta_0 = 1, \qquad \frac{\int_0^{\Delta t} W(\tau)\tau^q\,\mathrm{d}\tau}{\int_0^{\Delta t} W(\tau)\,\mathrm{d}\tau} = \theta_q\Delta t^q \quad (45)$$

gives

$$\frac{\int_0^{\Delta t} W(\tau)\underset{\sim}{u}\,\mathrm{d}\tau}{\int_0^{\Delta t} W(\tau)\,\mathrm{d}\tau} = \sum_{q=0}^{p-1} \overset{(q)}{\underset{\sim}{u}_n} \frac{\Delta t^q}{q!}\theta_q + \underset{\sim}{\alpha}_n^p \frac{\Delta t^p}{p!}\theta_p \tag{46}$$

$$\frac{\int_0^{\Delta t} W(\tau)\dot{\underset{\sim}{u}}\,\mathrm{d}\tau}{\int_0^{\Delta t} W(\tau)\,\mathrm{d}\tau}$$

$$= \sum_{q=1}^{p-1} \overset{(q)}{\underset{\sim}{u}_n} \frac{\Delta t^q}{(q-1)!}\theta_{(q-1)} + \underset{\sim}{\alpha}_n^p \frac{\Delta t^{(p-1)}}{(p-1)!}\theta_{(p-1)} \tag{47}$$

$$\frac{\int_0^{\Delta t} W(\tau)\underset{\sim}{f}\,\mathrm{d}\tau}{\int_0^{\Delta t} W(\tau)\,\mathrm{d}\tau} = \bar{\underset{\sim}{f}} = \theta_1 \underset{\sim}{f}_{n+1} + (1-\theta_1)\underset{\sim}{f}_n \tag{48}$$

Substituting into the weighted residual equation (44) gives

$$\underset{\approx}{C}\left[\sum_{q=1}^{p-1} \overset{(q)}{\underset{\sim}{u}_n} \frac{\Delta t^q}{(q-1)!}\theta_{(q-1)} + \underset{\sim}{\alpha}_n^p \frac{\Delta t^{(p-1)}}{(p-1)!}\theta_{(p-1)}\right] + \underset{\approx}{K}\left[\sum_{q=0}^{p-1} \overset{(q)}{\underset{\sim}{u}_n} \frac{\Delta t^q}{q!}\theta_q + \underset{\sim}{\alpha}_n^p \frac{\Delta t^p}{p!}\theta_p\right] - \bar{\underset{\sim}{f}} = \underset{\sim}{0} \tag{49}$$

Solving for $\underset{\sim}{\alpha}_n^p$ gives

$$\left[\underset{\approx}{C}\frac{\Delta t^{(p-1)}}{(p-1)!}\theta_{(p-1)} + \underset{\approx}{K}\frac{\Delta t^p}{p!}\theta_p\right]\underset{\sim}{\alpha}_n^p = \left[\bar{\underset{\sim}{f}} - \underset{\approx}{C}\sum_{q=1}^{p-1} \overset{(q)}{\underset{\sim}{u}_n} \frac{\Delta t^q}{(q-1)!}\theta_{(q-1)} - \underset{\approx}{K}\sum_{q=0}^{p-1} \overset{(q)}{\underset{\sim}{u}_n} \frac{\Delta t^q}{q!}\theta_q\right] \tag{50}$$

Once $\underset{\sim}{\alpha}_n^p$ is evaluated then Eq. (43) gives

$$\overset{(k)}{\tilde{\underset{\sim}{u}}_{n+1}} = \sum_{q=k}^{p-1} \overset{(q)}{\underset{\sim}{u}_n} \frac{\Delta t^{(q-k)}}{(q-k)!} \tag{51}$$

and finally Eq. (42) gives the values at the next time step

$$\overset{(k)}{\underset{\sim}{u}_{n+1}} = \overset{(k)}{\tilde{\underset{\sim}{u}}_{n+1}} + \underset{\sim}{\alpha}_n^p \frac{\Delta t^{(p-k)}}{(p-k)!} \tag{52}$$

Applying the dual reciprocity boundary element method to Eq. (20) gives

$$H_{ik}u_k - G_{ik}q_k = S_{ik}\left[\frac{\rho c_k}{K_k}\frac{\partial u_k}{\partial t} - \frac{V_k}{K_k} - \frac{1}{K_k}\left(\frac{\partial K_k}{\partial x}\frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y}\frac{\partial u_k}{\partial y}\right)\right] \tag{53}$$

Let $\underset{\sim}{w}$ be the vector of unknowns, either u_k or q_k, depending upon the conditions at the node. Writing the kth derivative of $\underset{\sim}{w}$ with respect to time, $\overset{(k)}{\underset{\sim}{w}}$, at a time τ between time steps n and $n+1$, i.e. $0 \le \tau \le \Delta t$, as

$$\overset{(k)}{\underset{\sim}{w}_\tau} = \overset{(k)}{\tilde{\underset{\sim}{w}}_\tau} + \underset{\sim}{\alpha}_n^p \frac{\tau^{(p-k)}}{(p-k)!} \tag{54}$$

where

$$\overset{(k)}{\tilde{\underset{\sim}{w}}_\tau} = \sum_{q=k}^{p-1} \overset{(q)}{\underset{\sim}{w}_n} \frac{\tau^{(q-k)}}{(q-k)!} \tag{55}$$

The vector $\underset{\sim}{\alpha}_n^p$ is determined by substituting for $\underset{\sim}{w}(\tau)$ and its derivatives into the weighted residual equation

$$\int_0^{\Delta t} W(\tau)\left\{H_{ik}u_k - G_{ik}q_k - S_{ik}\left[\frac{\rho c_k}{K_k}\frac{\partial u_k}{\partial t} - \frac{V_k}{K_k} - \frac{1}{K_k}\left(\frac{\partial K_k}{\partial x}\frac{\partial u_k}{\partial x} + \frac{\partial K_k}{\partial y}\frac{\partial u_k}{\partial y}\right)\right]\right\}\mathrm{d}\tau = \underset{\sim}{0} \tag{56}$$

Labelling a set of $p+1$ parameters θ_q, $q = 0, 1, \ldots, p$ thus

$$\theta_0 = 1, \qquad \frac{\int_0^{\Delta t} W(\tau)\tau^q\,\mathrm{d}\tau}{\int_0^{\Delta t} W(\tau)\,\mathrm{d}\tau} = \theta_q \Delta t^q \tag{57}$$

gives

$$\frac{\int_0^{\Delta t} W(\tau)\underset{\sim}{w}\,\mathrm{d}\tau}{\int_0^{\Delta t} W(\tau)\,\mathrm{d}\tau} = \sum_{q=0}^{p-1} \overset{(q)}{\underset{\sim}{w}_n} \frac{\Delta t^q}{q!}\theta_q + \underset{\sim}{\alpha}_n^p \frac{\Delta t^p}{p!}\theta_p \tag{58}$$

$$\frac{\int_0^{\Delta t} W(\tau)\dot{\underset{\sim}{w}}\,\mathrm{d}\tau}{\int_0^{\Delta t} W(\tau)\,\mathrm{d}\tau}$$

$$= \sum_{q=1}^{p-1} \overset{(q)}{\underset{\sim}{w}_n} \frac{\Delta t^{(q-1)}}{(q-1)!}\theta_{(q-1)} + \underset{\sim}{\alpha}_n^p \frac{\Delta t^{(p-1)}}{(p-1)!}\theta_{(p-1)} \tag{59}$$

$$\frac{\int_0^{\Delta t} W(\tau)\underset{\sim}{V}\,\mathrm{d}\tau}{\int_0^{\Delta t} W(\tau)\,\mathrm{d}\tau} = \bar{\underset{\sim}{V}} = \theta_1 \underset{\sim}{V}_{n+1} + (1-\theta_1)\underset{\sim}{V}_n \tag{60}$$

Let α be the slope of the thermal conductivity curve, as before, thus

$$\frac{\partial K_k}{\partial x} = \frac{\partial K_k}{\partial u_k}\frac{\partial u_k}{\partial x} = \alpha_k \frac{\partial u_k}{\partial x} \tag{61}$$

The Dual Reciprocity Method approximation to a derivative of temperature with respect to a spatial coordinate, say x, can be written as [1]

$$\frac{\partial u_k}{\partial x} = \frac{\partial F_{kl}}{\partial x}F_{lm}^{-1}u_m \tag{62}$$

Thus, the last term in Eq. (56) is

$$\frac{1}{K_k}\left(\frac{\partial K_k}{\partial x}\frac{\partial u_k}{\partial x}+\frac{\partial K_k}{\partial y}\frac{\partial u_k}{\partial y}\right) = \frac{\alpha_k}{K_k}\left(\frac{\partial F_{kl}}{\partial x}F_{lm}^{-1}u_m\frac{\partial F_{kr}}{\partial x}F_{rs}^{-1}u_s+\frac{\partial F_{kl}}{\partial y}F_{lm}^{-1}u_m\frac{\partial F_{kr}}{\partial y}F_{rs}^{-1}u_s\right) \tag{63}$$

In general Eq. (56) is a nonlinear equation. Rearranging Eq. (56) for the residual, or out of balance, ψ gives

If u_j is the unknown, then

$$\bar{u}_k = \sum_{q=0}^{p-1}\left(\overset{(q)}{u}_k\right)_n\frac{\Delta t^q}{q!}\theta_q+(\alpha_k^p)_n\frac{\Delta t^p}{p!}\theta_p \tag{69}$$

$$\frac{\partial \bar{u}_k}{\partial \alpha_j^p} = \frac{\partial}{\partial \alpha_j^p}(\alpha_k^p)_n\frac{\Delta t^p}{p!}\theta_p = \delta_{kj}\frac{\Delta t^p}{p!}\theta_p \tag{70}$$

$$\begin{aligned}\psi_i = {} & H_{ik}\Bigg\langle\underbrace{\sum_{q=0}^{p-1}\left(\overset{(q)}{u}_k\right)_n\frac{\Delta t^q}{q!}\theta_q+(\alpha_k^p)_n\frac{\Delta t^p}{p!}\theta_p}_{\bar{u}_k}\Bigg\rangle - G_{ik}\Bigg\langle\underbrace{\sum_{q=0}^{p-1}\left(\overset{(q)}{q}_k\right)_n\frac{\Delta t^q}{q!}\theta_q+(\alpha_k^p)_n\frac{\Delta t^p}{p!}\theta_p}_{\bar{q}_k}\Bigg\rangle \\ & - S_{ik}\Bigg[\frac{\rho c_k}{K_k}\Bigg\langle\underbrace{\sum_{q=1}^{p-1}\left(\overset{(q)}{u}_k\right)_n\frac{\Delta t^{(q-1)}}{(q-1)!}\theta_{(q-1)}+(\alpha_k^p)_n\frac{\Delta t^{(p-1)}}{(p-1)!}\theta_{(p-1)}}_{\frac{\partial \bar{u}_k}{\partial t}}\Bigg\rangle - \frac{\bar{V}_k}{K_k} \\ & - \frac{\alpha_k}{K_k}\Bigg(\frac{\partial F_{kl}}{\partial x}F_{lm}^{-1}\Bigg\langle\underbrace{\sum_{q=0}^{p-1}\left(\overset{(q)}{u}_m\right)_n\frac{\Delta t^q}{q!}\theta_q+(\alpha_m^p)_n\frac{\Delta t^p}{p!}\theta_p}_{\bar{u}_m}\Bigg\rangle\frac{\partial F_{kr}}{\partial x}F_{rs}^{-1}\Bigg\langle\underbrace{\sum_{q=0}^{p-1}\left(\overset{(q)}{u}_s\right)_n\frac{\Delta t^q}{q!}\theta_q+(\alpha_s^p)_n\frac{\Delta t^p}{p!}\theta_p}_{\bar{u}_s}\Bigg\rangle \\ & + \frac{\partial F_{kl}}{\partial y}F_{lm}^{-1}\Bigg\langle\underbrace{\sum_{q=0}^{p-1}\left(\overset{(q)}{u}_m\right)_n\frac{\Delta t^q}{q!}\theta_q+(\alpha_m^p)_n\frac{\Delta t^p}{p!}\theta_p}_{\bar{u}_m}\Bigg\rangle\frac{\partial F_{kr}}{\partial y}F_{rs}^{-1}\Bigg\langle\underbrace{\sum_{q=0}^{p-1}\left(\overset{(q)}{u}_s\right)_n\frac{\Delta t^q}{q!}\theta_q+(\alpha_s^p)_n\frac{\Delta t^p}{p!}\theta_p}_{\bar{u}_s}\Bigg\rangle\Bigg)\Bigg]\end{aligned} \tag{64}$$

Applying the Newton Raphson method

$$\frac{\partial \psi_i}{\partial \alpha_j^p}\mathrm{d}\alpha_j^p = -\psi_i \tag{65}$$

If q_j is the unknown, then

$$\bar{q}_k = \sum_{q=0}^{p-1}\left(\overset{(q)}{q}_k\right)_n\frac{\Delta t^q}{q!}\theta_q+(\alpha_k^p)_n\frac{\Delta t^p}{p!}\theta_p \tag{66}$$

$$\frac{\partial \bar{q}_k}{\partial \alpha_j^p} = \frac{\partial}{\partial \alpha_j^p}(\alpha_k^p)_n\frac{\Delta t^p}{p!}\theta_p = \delta_{kj}\frac{\Delta t^p}{p!}\theta_p \tag{67}$$

$$\frac{\partial \psi_i}{\partial \alpha_j^p} = -G_{ij}\frac{\Delta t^p}{p!}\theta_p \tag{68}$$

$$\frac{\partial \bar{u}_k}{\partial t} = \sum_{q=1}^{p-1}\left(\overset{(q)}{u}_k\right)_n\frac{\Delta t^{(q-1)}}{(q-1)!}\theta_{(q-1)}+(\alpha_k^p)_n\frac{\Delta t^{(p-1)}}{(p-1)!}\theta_{(p-1)} \tag{71}$$

$$\frac{\partial}{\partial \alpha_j^p}\left(\frac{\partial \bar{u}_k}{\partial t}\right) = \frac{\partial}{\partial \alpha_j^p}(\alpha_k^p)_n\frac{\Delta t^{(p-1)}}{(p-1)!}\theta_{(p-1)} = \delta_{kj}\frac{\Delta t^{(p-1)}}{(p-1)!}\theta_{(p-1)} \tag{72}$$

$$\begin{aligned}\frac{\partial \psi_i}{\partial \alpha_j^p} = {} & H_{ik}\frac{\partial \bar{u}_k}{\partial \alpha_j^p} - S_{ik}\Bigg[\frac{\rho c_k}{K_k}\frac{\partial}{\partial \alpha_j^p}\left(\frac{\partial \bar{u}_k}{\partial t}\right) - \frac{\rho c_k}{K_k^2}\frac{\partial K_k}{\partial \alpha_j^p}\frac{\partial \bar{u}_k}{\partial t} \\ & + \frac{1}{K_k}\frac{\partial(\rho c_k)}{\partial \alpha_j^p}\frac{\partial \bar{u}_k}{\partial t} - \frac{1}{K_k}\frac{\partial \bar{V}_k}{\partial \alpha_j^p} + \frac{\bar{V}_k}{K_k^2}\frac{\partial K_k}{\partial \alpha_j^p} \\ & - \frac{\alpha_k}{K_k}\frac{\partial}{\partial \alpha_j^p}\left(\frac{\partial \bar{u}_k}{\partial x}\frac{\partial \bar{u}_k}{\partial x}+\frac{\partial \bar{u}_k}{\partial y}\frac{\partial \bar{u}_k}{\partial y}\right) \\ & + \frac{\alpha_k}{K_k^2}\frac{\partial K_k}{\partial \alpha_j^p}\left(\frac{\partial \bar{u}_k}{\partial x}\frac{\partial \bar{u}_k}{\partial x}+\frac{\partial \bar{u}_k}{\partial y}\frac{\partial \bar{u}_k}{\partial y}\right)\Bigg]\end{aligned} \tag{73}$$

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

$$\frac{\partial K_k}{\partial \alpha_j^p} = \frac{\partial K_k}{\partial u_k}\frac{\partial u_k}{\partial \alpha_j^p} = \alpha_k \delta_{kj}\frac{\Delta t^p}{p!} = \alpha_j \frac{\Delta t^p}{p!} \tag{74}$$

and let β be the slope of the heat capacity curve

$$\frac{\partial(\rho c)_k}{\partial \alpha_j^p} = \frac{\partial(\rho c)_k}{\partial u_k}\frac{\partial u_k}{\partial \alpha_j^p} = \beta_k \delta_{kj}\frac{\Delta t^p}{p!} = \beta_j \frac{\Delta t^p}{p!} \tag{75}$$

Substituting into Eq. (73) gives

$$\begin{aligned}\frac{\partial \psi_i}{\partial \alpha_j^p} = {} & H_{ik}\delta_{kj}\frac{\Delta t^p}{p!}\theta_p - S_{ik}\Bigg\{\frac{\rho c_k}{K_k}\delta_{kj}\frac{\Delta t^{(p-1)}}{(p-1)!}\theta_{(p-1)} \\ & -\frac{\rho c_k}{K_k^2}\alpha_k\delta_{kj}\frac{\Delta t^p}{p!}\frac{\partial \bar{u}_k}{\partial t} + \frac{1}{K_k}\beta_k\delta_{kj}\frac{\Delta t^p}{p!}\frac{\partial \bar{u}_k}{\partial t} \\ & -\frac{1}{K_k}\frac{\partial \bar{V}_k}{\partial u_k}\delta_{kj}\frac{\Delta t^p}{p!}\theta_p + \frac{\bar{V}_k}{K_k^2}\alpha_k\delta_{kj}\frac{\Delta t^p}{p!}\theta_p \\ & -\frac{\alpha_k}{K_k}\Bigg[\frac{\partial}{\partial \alpha_j^p}\left(\frac{\partial \bar{u}_k}{\partial x}\right)\frac{\partial \bar{u}_k}{\partial x} + \frac{\partial \bar{u}_k}{\partial x}\frac{\partial}{\partial \alpha_j^p}\left(\frac{\partial \bar{u}_k}{\partial x}\right) \\ & + \frac{\partial}{\partial \alpha_j^p}\left(\frac{\partial \bar{u}_k}{\partial y}\right)\frac{\partial \bar{u}_k}{\partial y} + \frac{\partial \bar{u}_k}{\partial y}\frac{\partial}{\partial \alpha_j^p}\left(\frac{\partial \bar{u}_k}{\partial y}\right)\Bigg] \\ & + \frac{\alpha_k}{K_k^2}\alpha_k\delta_{kj}\frac{\Delta t^p}{p!}\left(\frac{\partial \bar{u}_k}{\partial x}\frac{\partial \bar{u}_k}{\partial x} + \frac{\partial \bar{u}_k}{\partial y}\frac{\partial \bar{u}_k}{\partial y}\right)\Bigg\}\end{aligned} \tag{76}$$

From Eq. (62) we have

$$\begin{aligned}\frac{\partial}{\partial \alpha_j^p}\left(\frac{\partial \bar{u}_k}{\partial x}\right) &= \frac{\partial}{\partial \alpha_j^p}\left(\frac{\partial F_{kl}}{\partial x}F_{lm}^{-1}\bar{u}_m\right) \\ &= \frac{\partial F_{kl}}{\partial x}F_{lm}^{-1}\delta_{mj}\frac{\Delta t^p}{p!}\theta_p\end{aligned} \tag{77}$$

substituting into Eq. (76) gives

$$\begin{aligned}\frac{\partial \psi_i}{\partial \alpha_j^p} = {} & H_{ik}\delta_{kj}\frac{\Delta t^p}{p!}\theta_p - S_{ik}\Bigg\{\frac{\rho c_k}{K_k}\delta_{kj}\frac{\Delta t^{(p-1)}}{(p-1)!}\theta_{(p-1)} \\ & -\frac{\rho c_k}{K_k^2}\alpha_k\delta_{kj}\frac{\Delta t^p}{p!}\frac{\partial \bar{u}_k}{\partial t} + \frac{1}{K_k}\beta_k\delta_{kj}\frac{\Delta t^p}{p!}\frac{\partial \bar{u}_k}{\partial t} \\ & -\frac{1}{K_k}\frac{\partial \bar{V}_k}{\partial u_k}\delta_{kj}\frac{\Delta t^p}{p!}\theta_p + \frac{\bar{V}_k}{K_k^2}\alpha_k\delta_{kj}\frac{\Delta t^p}{p!}\theta_p \\ & -\frac{\alpha_k}{K_k}\Bigg[\frac{\partial F_{kl}}{\partial x}F_{lm}^{-1}\delta_{mj}\frac{\Delta t^p}{p!}\theta_p\frac{\partial \bar{u}_k}{\partial x} + \frac{\partial \bar{u}_k}{\partial x}\frac{\partial F_{kl}}{\partial x}F_{lm}^{-1}\delta_{mj} \\ & \times\frac{\Delta t^p}{p!}\theta_p + \frac{\partial F_{kl}}{\partial y}F_{lm}^{-1}\delta_{mj}\frac{\Delta t^p}{p!}\theta_p\frac{\partial \bar{u}_k}{\partial y} + \frac{\partial \bar{u}_k}{\partial y}\frac{\partial F_{kl}}{\partial y} \\ & \times F_{lm}^{-1}\delta_{mj}\frac{\Delta t^p}{p!}\theta_p\Bigg] + \frac{\alpha_k}{K_k^2}\alpha_k\delta_{kj}\frac{\Delta t^p}{p!} \\ & \times\left(\frac{\partial \bar{u}_k}{\partial x}\frac{\partial \bar{u}_k}{\partial x} + \frac{\partial \bar{u}_k}{\partial y}\frac{\partial \bar{u}_k}{\partial y}\right)\Bigg\}\end{aligned} \tag{78}$$

which can be rewritten as

$$\begin{aligned}\frac{\partial \psi_i}{\partial \alpha_j^p} = {} & H_{ij}\frac{\Delta t^p}{p!}\theta_p - S_{ij}\Bigg\{\frac{\rho c_j}{K_j}\frac{\Delta t^{(p-1)}}{(p-1)!}\theta_{(p-1)} - \frac{\rho c_j}{K_j^2}\alpha_j\frac{\Delta t^p}{p!}\frac{\partial \bar{u}_j}{\partial t} \\ & + \frac{1}{K_j}\beta_j\frac{\Delta t^p}{p!}\frac{\partial \bar{u}_j}{\partial t} - \frac{1}{K_j}\frac{\partial \bar{V}_j}{\partial u_j}\frac{\Delta t^p}{p!}\theta_p + \frac{\bar{V}_j}{K_j^2}\alpha_j\frac{\Delta t^p}{p!}\theta_p\Bigg\} \\ & + S_{ik}\frac{\alpha_k}{K_k}\Bigg[\frac{\partial F_{kl}}{\partial x}F_{lj}^{-1}\frac{\Delta t^p}{p!}\theta_p\frac{\partial \bar{u}_k}{\partial x} + \frac{\partial \bar{u}_k}{\partial x}\frac{\partial F_{kl}}{\partial x}F_{lj}^{-1}\frac{\Delta t^p}{p!}\theta_p \\ & + \frac{\partial F_{kl}}{\partial y}F_{lj}^{-1}\frac{\Delta t^p}{p!}\theta_p\frac{\partial \bar{u}_k}{\partial y} + \frac{\partial \bar{u}_k}{\partial y}\frac{\partial F_{kl}}{\partial y}F_{lj}^{-1}\frac{\Delta t^p}{p!}\theta_p\Bigg] \\ & - S_{ij}\frac{\alpha_j}{K_j^2}\alpha_j\frac{\Delta t^p}{p!}\left(\frac{\partial \bar{u}_j}{\partial x}\frac{\partial \bar{u}_j}{\partial x} + \frac{\partial \bar{u}_j}{\partial y}\frac{\partial \bar{u}_j}{\partial y}\right)\end{aligned} \tag{79}$$

no sum on j

For convection boundary condition

$$q_C = K\frac{\partial \bar{u}}{\partial n} = h_C(u_C - u)$$

$$\begin{aligned}\psi_i = {} & H_{ik}\bar{u}_k - G_{ik}\frac{\partial \bar{u}_k}{\partial n} \\ & - S_{ik}\left[\frac{\rho c_k}{K_k}\frac{\partial \bar{u}_k}{\partial t} - \frac{\bar{V}_k}{K_k} - \frac{1}{K_k}\left(\frac{\partial \bar{K}_k}{\partial x}\frac{\partial \bar{u}_k}{\partial x} + \frac{\partial \bar{K}_k}{\partial y}\frac{\partial \bar{u}_k}{\partial y}\right)\right]\end{aligned} \tag{80}$$

Hence an extra term appears in K_T

$$(K_T)_{ij} = (K_T)_{ij} + \frac{1}{K_j}G_{ij}h_C\frac{\Delta t^p}{p!}\theta_p \tag{81}$$

no sum on j.

For radiation boundary condition

$$q_R = K\frac{\partial \bar{u}}{\partial n} = \sigma\varepsilon(u_R^4 - \bar{u}^4)$$

$$\begin{aligned}\psi_i = {} & H_{ik}\bar{u}_k - G_{ik}\frac{\partial \bar{u}_k}{\partial n} \\ & - S_{ik}\left[\frac{\rho c_k}{K_k}\frac{\partial \bar{u}_k}{\partial t} - \frac{\bar{V}_k}{K_k} - \frac{1}{K_k}\left(\frac{\partial \bar{K}_k}{\partial x}\frac{\partial \bar{u}_k}{\partial x} + \frac{\partial \bar{K}_k}{\partial y}\frac{\partial \bar{u}_k}{\partial y}\right)\right]\end{aligned} \tag{82}$$

Hence an extra term appears in K_T

$$(K_T)_{ij} = (K_T)_{ij} + \frac{4}{K_j}G_{ij}\sigma\varepsilon\bar{u}_j^3\frac{\Delta t^p}{p!}\theta_p \tag{83}$$

no sum on j.

There is a link between the GNpj and SSpj algorithms. They are very closely connected for linear problems but can give different effects when used on nonlinear problems [5]. For linear problems, the GNpj and SSpj algorithms can be matched exactly by taking $\theta_j = \beta_{p-j}$, $j = 1, 2, \ldots, p$, $\theta_0 = \beta_p = 1$. However, for nonlinear problems they can have quite different stability properties [5].

6. Phase change

In the apparent heat capacity method Eq. (1) is replaced by

$$\frac{\partial}{\partial x}\left(K\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(K\frac{\partial u}{\partial y}\right)+V=\frac{\partial h}{\partial t} \quad (84)$$

where h is the enthalpy defined as

$$h=\int_{u_{\mathrm{ref}}}^{u}\rho c\,\mathrm{d}T+\rho L \quad (85)$$

and u_{ref} is the reference temperature and L is the latent heat. The right hand side of Eq. (84) can be rewritten as

$$\frac{\partial h}{\partial t}=\frac{\partial h}{\partial u}\frac{\partial u}{\partial t}=(\rho c)_{\mathrm{a}}\frac{\partial u}{\partial t} \quad (86)$$

where $(\rho c)_{\mathrm{a}}$ is termed the apparent heat capacity. Using the apparent heat capacity directly leads to numerical problems due to the step like behaviour of $(\rho c)_{\mathrm{a}}$. In order to overcome these problems both space-averaging and time-averaging methods have been used in the finite element literature. Del Guidice et al. [6] used a space averaging method and evaluated the apparent heat capacity, for two dimensions, using

$$(\rho c)_{\mathrm{a}}=\frac{\partial h}{\partial u}=\left[\frac{\dfrac{\partial h}{\partial x}\dfrac{\partial u}{\partial x}+\dfrac{\partial h}{\partial y}\dfrac{\partial u}{\partial y}}{\dfrac{\partial u}{\partial x}\dfrac{\partial u}{\partial x}+\dfrac{\partial u}{\partial y}\dfrac{\partial u}{\partial y}}\right] \quad (87)$$

It has been reported by Hibbitt [7] that the space averaging technique of Del Guidice, Eq. (87), can lead to problems in certain circumstances. In this work, we use the space-averaging technique of Lemmon [8] where for two-dimensions, the apparent heat capacity is evaluated using

$$(\rho c)_{\mathrm{a}}=\frac{\partial h}{\partial u}=\left[\frac{\dfrac{\partial h}{\partial x}\dfrac{\partial h}{\partial x}+\dfrac{\partial h}{\partial y}\dfrac{\partial h}{\partial y}}{\dfrac{\partial u}{\partial x}\dfrac{\partial u}{\partial x}+\dfrac{\partial u}{\partial y}\dfrac{\partial u}{\partial y}}\right]^{1/2} \quad (88)$$

Using the Dual Reciprocity Method approximation to a derivative with respect to a spatial coordinate, say x, the terms of Eq. (88) are evaluated using

$$\frac{\partial h_i}{\partial x}=\frac{\partial F_{ij}}{\partial x}F_{jk}^{-1}h_k \quad (89)$$

and

$$\frac{\partial u_i}{\partial x}=\frac{\partial F_{ij}}{\partial x}F_{jk}^{-1}u_k \quad (90)$$

7. Line searches

The direction of the line search is given by the Newton–Raphson iteration equation

$$\mathrm{d}\mathbf{w}=-(\mathbf{K}_{\mathrm{T}})^{-1}\boldsymbol{\psi} \quad (91)$$

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

$$\mathbf{w}^{i+1}=\mathbf{w}^{i}+\eta\,\mathrm{d}\mathbf{w} \quad (92)$$

where the superscript refers to iteration number and η is a scalar quantity chosen to minimise the residual, or out of balance, ψ. 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. Eq. (92) is used to update the vector of unknowns w, with η set to unity. Then if

$$\frac{\psi_j^{i+1}\psi_j^{i+1}}{\psi_k^{i}\psi_k^{i}}\le 0.5 \quad (93)$$

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

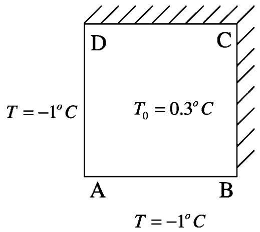
$$\eta_{i+1}=\eta_i+\mathrm{d}\eta=\eta_i-\phi_i\left(\frac{\eta_i-\eta_{i-1}}{\phi_i-\phi_{i-1}}\right) \quad (94)$$

until Eq. (93) is satisfied. Limits on the line searches have to be imposed in order to avoid numerical problems. The first is that $|\mathrm{d}\eta|$ is limited to 25% of η. The second is that $0.25<\eta<25$. The third is if Eq. (93) 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 Eq. (93) during the line search procedure.

8. Results

In this example taken from Ref. [9], a unit square of liquid with an initial temperature of 0.3 °C is subjected to a constant temperature of −1 °C on the surfaces of the wedge AB and AD, surfaces BC and CD are perfectly insulated, as shown in Fig. 1.

The material properties are $K=1$ J/m^3, $c=1$ J/Kg/°C, $\rho=1$ 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



T	h
-50	0
-0.005	49.995
0.005	50.255
50	100.25

Enthalpy Data

Fig. 1. Problem definition.

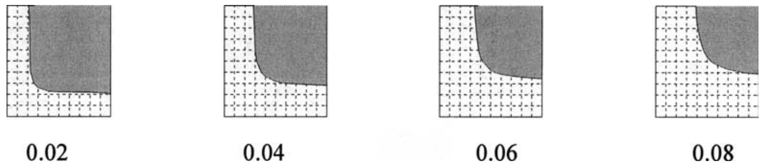


Fig. 2. Phase front location.

Fig. 1 is derived. The problems associated with corners and discontinuous boundary conditions have been handled via the gradient approach [10]. 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. Fig. 2 shows the phase front, determined by the 0 °C contour, at 0.02, 0.04, 0.06 and 0.08 s obtained using the GN11, $\beta_0 = 1$ scheme and very small timesteps, $\mathrm{d}t = 0.1 \times 10^{-6}$ s.

In order to compare the time-stepping schemes, we shall concentrate on where the 0 °C contour crosses the diagonal AC in Fig. 1 at 0.01 s intervals. Table 1 shows the average and maximum percentage difference in the phase front location when compared to the reference results for three timestep lengths for various time-stepping algorithms. The reference results were obtained using the GN11, $\beta_0 = 1$ backward difference algorithm with extremely small timesteps, $\mathrm{d}t = 0.1 \times 10^{-6}$ s, with timesteps this small all algorithms give the same results or do not converge at all. NC signifies that no convergence could be obtained even with the use of line searches. The * symbol in the table signifies that no convergence was obtained without the use of line searches.

In Table 1, algorithm code A is the backward difference algorithm for the first order scheme using parameters, GN11, $\beta_0 = 1$, and SS11, $\theta_1 = 1$. There is very little difference between GN11 and SS11 when using the backward difference algorithm. Algorithm code B is the Crank–Nicolson or trapezium algorithm for the first order scheme using parameters, GN11, $\beta_0 = 0.5$ and SS11, $\theta_1 = 0.5$. Both GN11 and SS11 have problems obtaining convergence when using the Crank–Nicolson algorithm. The persistent noise effects, i.e. troublesome oscillations, associated with the Crank–Nicolson method can off-set the advantage of the higher order error obtained over the backward difference algorithm [5]. Algorithm code C is Lees' [11] algorithm for the second order scheme using parameters, GN21, $\beta_0 = 2/3$, $\beta_1 = 1/2$ and SS21, $\theta_1 = 1/2$, $\theta_2 = 2/3$. Both GN21 and SS21 have problems obtaining convergence when using Lees' algorithm. Lees' algorithm is notoriously oscillatory [12]. Algorithm code D is the backward difference algorithm for the second order scheme using parameters, GN21, $\beta_0 = 2$, $\beta_1 = 3/2$ and SS21, $\theta_1 = 3/2$, $\theta_2 = 2$. GN21 has problems obtaining convergence and SS21 produces inaccurate results for large timesteps, $\mathrm{d}t = 0.01$ s, when using the backward difference algorithm. Algorithm code E is Liniger's [13] algorithm for the second order scheme using parameters, GN21, $\beta_0 = 1.292$, $\beta_1 = 1.218$ and SS21, $\theta_1 = 1.218$, $\theta_2 = 1.292$. GN21 provides slightly better results than SS21 when using Liniger's algorithm. Algorithm code F is Zlamal's [14] algorithm for the second order scheme using parameters, GN21, $\beta_0 = 8/9$, $\beta_1 = 5/6$ and SS21, $\theta_1 = 5/6$, $\theta_2 = 8/9$. Both GN21 and SS21 have problems obtaining convergence when using Zlamal's algorithm. Algorithm code G is the backward difference algorithm for the third order scheme using

Table 1
Phase front location, percentage differences to the reference solution

Method	Algorithm code	$\mathrm{d}t = 0.01$ s		$\mathrm{d}t = 0.001$ s		$\mathrm{d}t = 0.0001$ s	
		Average	Max	Average	Max	Average	Max
GN11	A	3.16	5.43	0.27*	0.36*	0.04	0.07
SS11	A	3.16	5.43	0.26*	0.36*	0.05	0.07
GN11	B	NC		0.48	1.11	0.02	0.04
SS11	B	1.04*	4.63*	0.20*	0.65*	NC	
GN21	C	NC		1.00	1.86	NC	
SS21	C	1.12	4.22	0.29*	0.90*	NC	
GN21	D	NC		0.55	1.21	NC	
SS21	D	12.78	44.04	1.27	2.71	0.12	0.25
GN21	E	8.57	16.99	0.49	1.11	0.03*	0.05*
SS21	E	10.51	24.43	0.84	1.76	0.07	0.11
GN21	F	NC		0.49*	1.11*	0.03*	0.05*
SS21	F	NC		0.34	0.65	NC	
GN31	G	9.01	16.64	0.48	1.06	0.02*	0.04*
SS31	G	23.05	53.95	1.52	3.67	0.13	0.25
GN31	H	8.68	18.90	0.47	1.06	0.02*	0.04*
SS31	H	17.52	52.09	1.16	2.31	0.11	0.20

parameters, GN31, $\beta_0 = 6$, $\beta_1 = 11/3$, $\beta_2 = 2$ and SS31, $\theta_1 = 2$, $\theta_2 = 11/3$, $\theta_3 = 6$. SS31 produces inaccurate results for large timesteps, $dt = 0.01$ s, when using the backward difference algorithm. Algorithm code H is the Shayya et al. [15] algorithm for the third order scheme using parameters, GN31, $\beta_0 = 2.86$, $\beta_1 = 2.0067$, $\beta_2 = 1.46$ and SS31, $\theta_1 = 1.46$, $\theta_2 = 2.0067$, $\theta_3 = 2.86$. SS31 produces inaccurate results for large timesteps, $dt = 0.01$ s, when using the Shayya et al. algorithm.

9. Conclusions

GN*pj* and SS*pj* time-stepping schemes have been presented for nonlinear transient field problems with phase change using the dual reciprocity boundary element method. 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 to the results produced from a commercially available finite element code and very good agreement was found. 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. The line search technique is fundamental to obtaining convergence in some situations, particularly when using time-stepping schemes that are known to be oscillatory. The authors were unable to obtain convergence at all using any of the time-stepping schemes for any time step length using the space averaging technique of Del Guidice et al. [6], Eq. (87), or the time averaging technique of Morgan et al. [7], using a simple backward difference approximation. The results show that the higher order schemes, GN21, SS21, GN31 and SS31, give less accurate results than the first order schemes, GN11 and SS11, when using large time steps. This could be because the higher order schemes are less able to model the discontinuity due to phase change than the first order schemes when using large time steps. There is very little difference between the results between the first order schemes, GN11 and SS11, whereas for higher order schemes, GN31 gives more accurate results than SS31 when using large time steps. Both GN11 and SS11 schemes using the backward difference algorithm are recommended for field problems with phase change using the dual reciprocity boundary element method.

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