High accuracy time-integration schemes for the dual reciprocity boundary element method

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Abstract

This work presents the development and testing of time integration schemes for the system of ordinary differential equations resulting from the Dual Reciprocity Boundary Element Method (DRM/BEM) for the transient diffusion and convection-diffusion equations. The article describes applications of two-level and three-level schemes and the numerical solutions are compared with available analytical solutions for different combinations of the time step numerical weighting factors. Also, a method is proposed based on the three-level scheme together with active polynomial Richardson extrapolation of the solution. This method is particularly recommended for problems that require very high accuracy such as long term simulations. Results demonstrate that the proposed method is more economic in computer time and gives more accurate results than the two and three-level schemes.

1 Introduction

The Boundary Element Method (BEM) has become a powerful tool in engineering analysis. Many problems, particularly steady state ones, can usually be solved more efficiently and accurately using boundary elements that with other numerical techniques. The application BEM to general time dependent problems like those governed by the diffusion and the convection-diffusion equations, was hampered for some time by the need to define internal cells in order to compute domain integrals that, although do not introduce any new unknown, made the method cumbersome to use.
The Dual Reciprocity Boundary Element Method (DRM/BEM) is a powerful and versatile technique to handle domain integrals without the use of internal cells. This method was introduced by Nardini and Brebbia [9] and has been later generalised to a wide range of engineering problems [10]. The method is straightforward to apply and use simple fundamental solutions, being capable of transforming domain terms to the boundary.

Many pollution and fluid dynamics problems require long term simulations. The production, flux and transport of many pollutants may be slow phenomena where the simulation time scale is usually large. Therefore, the numerical computation of these problems must assure high accuracy with minimum error increase in time.

The most frequently used time integration scheme for the time dependent application of the DRM/BEM was introduced by Wrobel et al. [15]. This scheme involves the discretization of the time derivative term using forward finite differences together with a weighted linear time interpolation for concentrations and fluxes resulting in a first order accurate scheme.

Singh and Kalra [13], proposed a least square method that involves the minimisation of a functional that represents the integral of the square of the error over a time step. This scheme was applied to solve a number of heat conduction problems, and its performance compared to other two-level schemes such as Crank-Nicholson, Galerkin and fully implicit, obtaining a quadratic rate of convergence.

Lahrmann and Haberland [8] derived a weighted time-step relation procedure that optimises the weighting factors of the first order Wrobel et al scheme [15], obtaining unconditional stability and accurate results compared to finite element method and DRM/BEM schemes.

This article first presents the formulation of three-level time integration schemes in the context of DRM/BEM which have the theoretical capabilities of obtaining second and higher order rates of convergence. The three-level algorithm is then compared with exact solutions of the convection-diffusion equation. Although the three-level schemes require more computer effort and the definition of several weighting parameters, the test performed in this work show that these schemes give slightly better results than the two-level schemes for a few sets of the weighting parameters. However, the method becomes unstable or give worst results than the two-level schemes for many of the standard parameters recommended in the literature. It is believed that this behaviour is due to the mixed characteristic of the matrices resulting from the DRM/BEM formulation where both concentrations and fluxes are simultaneously calculated.

Finally, this article presents a method that solves the system of ordinary differential equations that result from the DRM/BEM formulation, with a Three-level scheme enhanced with Active polynomial Richardson Extrapolation. This scheme will be referred hereafter as TARE and to the knowledge of the authors, has not been previously used in transient DRM/BEM formulations.
The TARE scheme is particularly useful for time dependent problems where very high accuracy is a requirement, it is more economic in computer time, and gives more accurate results than the standard two-level and three-level methods.

2 Time Dependent DRM/BEM Formulation

The 2-D convection-diffusion equation considered in this work may be written as

$$\frac{D_x \partial^2 u}{\partial x^2} + D_y \frac{\partial^2 u}{\partial y^2} - v_x \frac{\partial u}{\partial x} - v_y \frac{\partial u}{\partial y} - ku + \phi - \frac{\partial u}{\partial t} = 0$$  \hspace{1cm} (1)

where \(x\), and \(y\) are the co-ordinates, \(t\) is the time, \(u\) is the concentration of a substance, \(D_x\) and \(D_y\) are diffusion coefficients, \(v_x\) and \(v_y\) are velocities in \(x\) and \(y\) directions respectively, \(k\) is a decay parameter and \(\phi\) is a source term.

The time-dependent formulation of the DRM/BEM for the convection-diffusion equation may be written as the following system of ordinary differential equations

$$\frac{1}{D_x} S \frac{du}{dt} = (H - T) u - G q + S \phi$$ \hspace{1cm} (2)

where

$$T = S \left\{ V_x \frac{\partial F}{\partial x} F^{-1} + V_y \frac{\partial F}{\partial y} F^{-1} - \frac{(D_x - D_y)}{D_x} \frac{\partial^2 F}{\partial y^2} F^{-1} + K \right\}$$ \hspace{1cm} (3)

$$S = (H U - G Q) F^{-1}$$ \hspace{1cm} (4)

and \(H\) and \(G\) are the usual matrices resulting from the integration of the surface potentials (see [2]), and the matrices \(U\), \(Q\), \(K\), \(F\) and \(F^{-1}\) are explained in [11].

Note that equation (2) is a mixed system of ordinary differential equations where \(u\) and \(q\) are unknown.

3 Three-level Time Integration Schemes

In order to describe the three-level scheme, we first treat its formulation in the context of a general system of ordinary differential equations of the type

$$\frac{du}{dt} = L(u, t)$$ \hspace{1cm} (5)
Table 1: List of multi-level time integration schemes

where \( \mathbf{u} \) is a vector, \( t \) is the time, and \( \mathbf{L} \) is a non linear operator that may represent a numerical discretization of a partial differential equation as will be seen in the next section.

The most general three-level scheme applied to Eq. (5) may be written as (see details in [1])

\[
\frac{1}{\Delta t} \left[ (1 + \xi)\mathbf{u}^{n+1} - (1 + 2\xi)\mathbf{u}^{n} + \xi\mathbf{u}^{n-1} \right] = \left[ \theta\mathbf{L}^{n+1} + (1 - \theta + \phi)\mathbf{L}^{n} - \phi\mathbf{L}^{n-1} \right]
\]  

(6)

4 Three-level Time Integration Schemes for the DRM/BEM Formulation

The most general consistent three-level discretization scheme for the DRM/-BEM represented by system (2) may be formulated by approximating the time derivative term as shown in (6)

\[
\frac{d\mathbf{u}}{dt} = \frac{1}{\Delta t} \left[ (1 + \xi)\mathbf{u}^{n+1} - (1 + 2\xi)\mathbf{u}^{n} + \xi\mathbf{u}^{n-1} \right]
\]  

(7)
and approximating the $u$ and $q$ in the right hand terms of Eq. (2) as

$$u = \theta_u u^{n+1} + (1 - \theta_u + \phi_u)u^n - \phi_u u^{n-1}$$  \tag{8}$$

and

$$q = \theta_q q^{n+1} + (1 - \theta_q + \phi_q)q^n - \phi_q q^{n-1}$$  \tag{9}$$

Substituting Eqs. (7), (8) and (9) into (2) we obtain the following general DRM/BEM three-level scheme

$$
\left[ \theta_u (H - T) - \frac{(1 + \xi)}{D_x \Delta t} S \right] u^{n+1} - \theta_q Gq^{n+1} = \left[ (1 - \theta_u + \phi_u)(T - H) - \frac{(1 + 2\xi)}{D_x \Delta t} S \right] u^n + (1 - \theta_q + \phi_q)Gq^n + \left[ \phi_u (H - T) + \frac{\xi}{D_x \Delta t} S \right] u^{n-1} - \phi_q Gq^{n-1} - \frac{1}{D_x} S \phi
$$  \tag{10}$$

It may be readily seen that if $\xi = \phi_u = \phi_q = 0$, then Eq (10) reduces to the two-level scheme presented in [11].

Equation (10) may be rearranged according to which values of $u$ and $q$ are known at the boundaries in the following matrix form

$$Ax = p_1 + p_2$$  \tag{11}$$

Vector $x$ contains $N$ unknowns at boundary nodes (either $u$ or $q$ values), and $L$ unknowns at internal points.

Initially, $p_1$ is equal to $-1/D_x S \phi$. If $u^{n+1}$ is known at a certain node, then $\theta_u (H - T) - ((1 + \xi)/D_x \Delta t)S$ is retained on the left hand side in the same column of matrix $A$, otherwise it is multiplied by the known value and is added to $p_1$ in the right hand side. If $q^{n+1}$ is unknown, the column $-\theta_q G$ is retained in $A$, but if $q^{n+1}$ is known, it is multiplied by $\theta_q G$ and added to $p_1$.

For internal nodes we have

$$p_2 = \left[ (1 - \theta_u + \phi_u)(T - H) - \frac{(1 + 2\xi)}{D_x \Delta t} S \right] u^n + \left[ \phi_u (H - T) + \frac{\xi}{D_x \Delta t} S \right] u^{n-1}$$  \tag{12}$$

while for boundary nodes, $p_2$ is evaluated as

$$p_2 = \left[ (1 - \theta_u + \phi_u)(T - H) - \frac{(1 + 2\xi)}{D_x \Delta t} S \right] u^n$$
It is important to remark that Eq. (11) is a mixed algebraic system including \( u \) and \( q \) unknowns. Since Eq. (7) contains first derivatives only in \( u \), then \( q \) variables in (11) appear as unknowns only through the use of the weighting approximations used (Eqs. 8 and 9). This particular characteristic of the DRM/BEM formulation precludes the use of other ODE methods like the ones of the Runge-Kutta family.

The numerical implementation of the general three-level time integration scheme requires the values of the unknowns for \( n = 0 \) (initial conditions) as well as the values for the first time step, \( n = 1 \). To accomplish this, the two-level formulation described in [11] is used as a starting procedure. Thereafter, the three-level formulation is used for each time step.

It is important to remark that this formulation requires three arrays for \( u \) and three for the \( q \) unknowns representing an increase in memory requirements with respect to the two-level scheme that uses instead two arrays for each unknown. However, computer time is only increased slightly, since the matrix \( A \) is assembled and triangularized only once and the extra work is the multiplication of a matrix for a vector in the \( p_2 \) term for each time step. The tests performed in this work show that this general three-level scheme only gives slightly better results than those obtained with the two-level scheme, for a few sets of the weighting parameters.

5 Extrapolation Methods for the DRM/BEM Formulation

The proposed TARE method uses the concept of Richardson’s deferred approach to the limit. The purpose of this concept is to obtain the final answer of the numerical calculation as if it were an analytic function depending on \( \Delta t \) as an adjustable parameter. This analytic function may be evaluated for various \( \Delta t \) sizes none of them being small enough to obtain the desired accuracy. Once various values of the function have been calculated, we may fit these values with a known function and then evaluate it at \( \Delta t = 0 \).

Richardson method commonly uses either rational function extrapolation or straightforward polynomial extrapolation. The rational functions avoid certain limited radius of convergence encountered in power series. However, recent experience [12] suggest that for smooth problems polynomial extrapolation is slightly more efficient than rational function extrapolation.

There are many ways to apply Richardson extrapolation to initial-value problems. One way is called active extrapolation, which means that the
result of the extrapolation is used as input data for the remaining calculations. Another way is called passive extrapolation where the results of extrapolation are accepted as output data, but they are not used in the remaining calculations. Thus a passive extrapolation can be performed after the problem has been solved from start to finish with a number of step sizes. Although that active extrapolation may always be preferable, for certain types of systems, passive extrapolation is better because it is numerically more stable [4]. In this work active extrapolation is used together with the three-level scheme.

The TARE method advances the solution of (2) from \( t \) to \( t + T \) where \( T \) is a large time step consisting of many sub-steps of the three-level method.

The sequence of attempts to go from time \( t \) to time \( t + T \) is made with increased number of sub-steps \( n \). Some researchers [14] have proposed the sequence:

\[
\text{n} = 2, 4, 6, 8, 12, 16, 24, 32, \ldots, [n_i = 2^{2i}], \ldots, N
\]  
(14)

Recently, it was found that the following sequence is usually more efficient [5, 6]:

\[
\text{n} = 2, 4, 6, 8, 10, 12, 14, 16, \ldots, [n_i = 2i], \ldots, N
\]  
(15)

After each successive calculation for a particular \( n \), the Richardson polynomial extrapolation to zero \( \Delta t \) is performed resulting in an improved solution and a corresponding error estimate. If this error is not satisfactory, \( n \) is increased until a successful solution is obtained. If the solution is satisfactory, the next time step is started with \( n = 2 \).

6 Numerical Tests

6.1 Numerical Test Results for the Three-level Time Integration Scheme

The first test case, is the solution of a transient convection-diffusion problem in a rectangular region where the concentration is fixed at \( u = 300 \) upstream, \( q = 0 \) downstream and \( \nu_x = 20 \) and \( \nu_y = 0 \). The analytical solution for this problem is given in [7].

For this test the region is discretized with 38 linear boundary elements and 16 internal points. The initial concentration distribution is equal to zero. Also, \( D_x = D_y = 1m^2/s \), and \( \Delta t = 0.02 \) seconds.

In this case we test the sensitivity of the results to different values of \( \theta_u \), \( \theta_q \), \( \xi \), \( \phi_u \) and \( \phi_q \) between 0 and 1 and trying to follow the theoretical values reported in table 1.

Results presented in table 2 show that theoretical values of parameters that give high accuracy lead to instabilities when applied to the DRM/BEM formulation.
<table>
<thead>
<tr>
<th>Run</th>
<th>$\theta_u$</th>
<th>$\theta_q$</th>
<th>$\xi$</th>
<th>$\phi_u$</th>
<th>$\phi_q$</th>
<th>Solution</th>
</tr>
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<td>T₁</td>
<td>1/6</td>
<td>1/6</td>
<td>-1/2</td>
<td>-1/6</td>
<td>-1/6</td>
<td>large oscillations</td>
</tr>
<tr>
<td>T₂</td>
<td>1/3</td>
<td>1/3</td>
<td>-1/2</td>
<td>-1/6</td>
<td>-1/6</td>
<td>large oscillations</td>
</tr>
<tr>
<td>T₃</td>
<td>1/2</td>
<td>1</td>
<td>-1/2</td>
<td>-1/6</td>
<td>-1/6</td>
<td>stable</td>
</tr>
<tr>
<td>T₄</td>
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<td>1</td>
<td>1/2</td>
<td>0</td>
<td>0</td>
<td>stable</td>
</tr>
<tr>
<td>T₅</td>
<td>1/2</td>
<td>1</td>
<td>-0.6</td>
<td>0</td>
<td>0</td>
<td>large oscillations</td>
</tr>
<tr>
<td>T₆</td>
<td>1/2</td>
<td>1</td>
<td>0</td>
<td>1/2</td>
<td>1/2</td>
<td>unstable</td>
</tr>
<tr>
<td>T₇</td>
<td>5/2</td>
<td>0.7</td>
<td>0</td>
<td>1/2</td>
<td>1/2</td>
<td>stable</td>
</tr>
<tr>
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<td>-1/6</td>
<td>-2/9</td>
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<td>stable</td>
</tr>
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<td>0.2</td>
<td>1/12</td>
<td>1/12</td>
<td>stable</td>
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<tr>
<td>T₁₀</td>
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<td>0.9</td>
<td>-0.05</td>
<td>0.01</td>
<td>0.001</td>
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</tr>
<tr>
<td>W₃</td>
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<td>0</td>
<td>-1/2</td>
<td>-1/2</td>
<td>stable</td>
</tr>
<tr>
<td>W₄</td>
<td>1/2</td>
<td>1/2</td>
<td>-1/2</td>
<td>-1/2</td>
<td>-1/2</td>
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<tr>
<td>W₅</td>
<td>1/3</td>
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<td>1/6</td>
<td>-1/2</td>
<td>-1/6</td>
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<td>unstable</td>
</tr>
<tr>
<td>W₈</td>
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<td>1</td>
<td>0.087</td>
<td>0</td>
<td>0</td>
<td>stable</td>
</tr>
</tbody>
</table>

Table 2: Three-level test case: Fixed upstream concentration with positive velocity. Solution obtained for different values of $\theta_u$, $\theta_q$, $\xi$, $\phi_u$ and $\phi_q$. 
Amongst these theoretical high order schemes, runs W₄, W₅, W₆, W₇, and W₈, are worthy of special attention.

For run W₄ (Lees type scheme) the numerical results deviate from the analytical solution and a large oscillation appears close to the left hand boundary, although the numerical solution remains stable.

For run W₅ (third order implicit scheme) the numerical results compare well with the analytical solution for the first time intervals, but later the solution becomes unstable. Similar results were obtained for run W₆ (Adams-Moulton scheme) where good comparison is obtained initially, but later the numerical solution becomes unstable even for very small Δt.

Run W₇ corresponding to the theoretically very accurate Milne scheme (O(Δt⁴)) resulted in unstable results for all tested Δt.

The combination of parameters that leads to better results is run W₈ corresponding to ξ = 0.087, φₜ = φₚ = 0, θₜ = 0.5 and θₚ = 1.

Although there are some particular sets of weighting parameters that lead to accurate solutions it is seen that most sets produce unstable solutions.

6.2 Numerical Test Results for the Three-level Active Richardson Extrapolation Time Integration Scheme (TARE)

The test problem of heat diffusion in a square plate initially at 30° and cooled by the application of a thermal shock (u = 0°) all over the boundary was studied in [11] using the two-level DRM/BEM formulation and will be used here for comparison purposes. The exact solution of this problem is given in reference [3].

For the present test, the numerical values adopted are Lₓ = Lᵧ = 3, Kₓ = Kᵧ = 1.25 and u₀ = 30, where Lₓ and Lᵧ are the x and y side lengths of the plate respectively, Kₓ and Kᵧ are the thermal conductivities, u₀ is the initial temperature taken uniform over the plate.

The first test performed involved the study of convergence with increasing number of internal points L. The purpose of this test was to reproduce the results of ref. [11] where it was found that for a fixed time step Δt = 0.05, the results seem to converge to values that are slightly higher than the exact ones.

As shown in table 3, the numerical solutions using both the two-level and the three-level scheme converge to a value higher than the analytic solution for a fixed time step Δt = 0.05.

The explanation of this apparent erroneous numerical behaviour is that the convergence of the method should be tested increasing the number of internal points L and simultaneously reducing the time step Δt. To verify this, a series of runs was performed reducing the time step with the two-level scheme as well as with the three-level scheme. Table 3 shows that reduc-
<table>
<thead>
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<th>( L )</th>
<th>25</th>
<th>33</th>
<th>49</th>
<th>53</th>
<th>69</th>
<th>53</th>
<th>69</th>
<th>Ex</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta t )</td>
<td>0.05</td>
<td>0.05</td>
<td>0.05</td>
<td>0.05</td>
<td>0.05</td>
<td>0.005</td>
<td>0.005</td>
<td></td>
</tr>
<tr>
<td>two-level</td>
<td>1.787</td>
<td>1.877</td>
<td>1.891</td>
<td>1.887</td>
<td>1.926</td>
<td>1.784</td>
<td>1.813</td>
<td></td>
</tr>
<tr>
<td>three-level</td>
<td>N/A</td>
<td>1.813</td>
<td>N/A</td>
<td>1.824</td>
<td>1.860</td>
<td>1.788</td>
<td>1.807</td>
<td></td>
</tr>
</tbody>
</table>

Table 3: Two-level and trl schemes results for \( u \) at centre point, for \( t = 1.2 \) s.

Figure 1: Convergence rates of the two-level, three-level and TARE schemes.

Increasing the time step to \( \Delta t = 0.005 \), the numerical solution of both methods converges to the analytic solution as the number of internal points increases.

To compare the two-level, three-level and TARE method, the LI measure of the error will be used, defined as follows

\[
error_{L2} = \left[ \sum_{n=1}^{N} \frac{(u_{\text{num}}^n - u_a^n)^2}{u_a^n} \right]^{1/2}
\]

where \( n \) corresponds to \( t = n\Delta t \), \( N \) is the total number of sub-time steps \( n \), \( u_{\text{num}}^n \) is the numerical solution and \( u_a^n \) is the analytic solution for the time step \( n \).

This norm has the advantage of giving a more accurate measure of the error than simple comparison of numerical values.

Figure 1 shows the convergence rates for the two-level \( (\theta_u = 1/2, \theta_q = 1) \),
Figure 2: Error evolution with time for the two-level, three-level and TARE schemes at centre point.

It may be observed that both the two and three-level schemes show similar order of convergence although the later scheme gives lower overall errors. The new TARE method gives the lowest errors even when using relatively large time steps.

Figure 2 shows the time evolution of error $L_2$ for the two-level, three-level and TARE schemes at the centre point of the plate. Note that, for both the two-level and three-level schemes, errors start with relatively large values to later diminish. The three-level scheme shows more rapid error decrease. The proposed TARE scheme has much lower errors that the other methods.

Figure 3 presents the time evolution of error for the TARE scheme at the centre point of the plate as a function of the number of sub-steps $n$. Note that for $n \geq 8$ the errors are very similar showing very low values, making unnecessary to use large values of $n$ to obtain good results.

Table 4 compares the performance ratios of the methods measured in relative computer times $T^* = T_{TARE}/T_{TS}$, where $T_{TARE}$ is the computer time for the TARE scheme and $T_{TS}$ is the time for the three-level scheme. This table was constructed measuring the computer times required to obtain the solution with a relative error $L_2 = 0.03$ for both methods and for $n = 4, 8, 16$.

Note that the TARE scheme is much more efficient than the three-level scheme for $n < 16$, requiring only 1/3 of the time for $n = 4$. However, for
Figure 3: Error evolution with time for the TARE schemes at centre point as a function of the number of sub-steps $n$.

Table 4: Relative performance of the three-level and the TARE schemes

<table>
<thead>
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<th>$n$</th>
<th>4</th>
<th>8</th>
<th>16</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T^*$</td>
<td>0.3</td>
<td>0.7</td>
<td>1.5</td>
</tr>
</tbody>
</table>

large $n$ the TARE scheme becomes more expensive in computer time than the three-level scheme, with little increase in accuracy.

7 Conclusions

This article presents high accurate time integration schemes for the transient DRM/BEM formulation.

The three-level method is more accurate but requires more computer time than the two-level method and is also subject to instabilities for most values of the time integration parameters. It is believed that this behaviour is due to the mixed characteristic of the matrices resulting from the DRM/BEM formulation where both concentrations (or temperature) and fluxes are simultaneously calculated.

The TARE time integration method uses a three-level scheme together with active Richardson's extrapolation. Results from the tests presented show that the TARE method achieves high accuracy with less computer effort than existing methods. This formulation is particularly well suited to
solve problems requiring high accuracy as in long term simulations of many pollution and fluid dynamics problems.

Although the time integration schemes presented in this article have been limited to the diffusion and convection-diffusion equations, these algorithms may also be applied to the DRM/BEM formulations of other time dependent equations.

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