The two-dimensional reaction-diffusion Brusselator system: a dual-reciprocity boundary element solution

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Abstract

The dual-reciprocity boundary element method is applied for the numerical solution of a class of two-dimensional initial-boundary value problems governed by a non-linear system of partial differential equations. The system, known as the reaction-diffusion Brusselator, arises in the modeling of certain chemical reaction-diffusion processes. Numerical results are presented for some specific problems.

Keywords: Brusselator system, dual-reciprocity boundary element method.

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1 Introduction

Of particular interest here is the task of solving numerically the non-linear system of partial differential equations

$$\frac{\partial u}{\partial t} = B + u^2 v - (A+1)u + \alpha\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$
$$\frac{\partial v}{\partial t} = Au - u^2 v + \alpha\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) \quad (1)$$

for $u(x, y, t)$ and $v(x, y, t)$ in a two-dimensional region R bounded by a simple closed curve C subject to the initial-boundary conditions

$$(u(x, y, 0), v(x, y, 0)) = (f(x, y), g(x, y)) \text{ for } (x, y) \in R, \quad (2)$$

and

$$(u(x, y, t), v(x, y, t)) = (w(x, y, t), z(x, y, t)) \text{ for } (x, y) \in C_1 \text{ and } t > 0, \quad (3)$$
$$\left(\frac{\partial u}{\partial n}, \frac{\partial v}{\partial n}\right) = (p(x, y, t), q(x, y, t)) \text{ for } (x, y) \in C_2 \text{ and } t > 0, \quad (4)$$

where A, B and α are suitably given constants, f , g, w, z, p and q are suitably prescribed functions, C_1 and C_2 are non-intersecting curves such that $C_1 \cup C_2 = C$, $\partial u/\partial n = \underline{\mathbf{n}} \cdot \nabla u$, $\partial v/\partial n = \underline{\mathbf{n}} \cdot \nabla v$ and $\underline{\mathbf{n}}$ is the unit normal outward vector to R at the point (x, y) on C. Refer to Figure 1.

The non-linear system (1) arises in the modeling of certain chemical reaction-diffusion processes which involve a pair of variable intermediates with input and output chemicals whose concentrations are controlled, see e.g. Nicolis and Prigogine [8] and Prigogine and Lefever [10].

Adomian [2] and Wazwaz [13] showed how the Adomian decomposition method can be applied to solve (1) for a solution which satisfies only the initial condition (2). Twizell *et al.* [12] gave a finite-difference method for solving (1)-(4) numerically in a rectangular domain subject to a particular Neumann boundary condition ($\partial u/\partial n = 0$ and $\partial v/\partial n = 0$ on C).

In the present paper, the boundary element method (DRBEM) is applied for the numerical solution of (1)-(4). The partial derivatives of u and v with respect to time t are approximated using a finite-difference formula. The

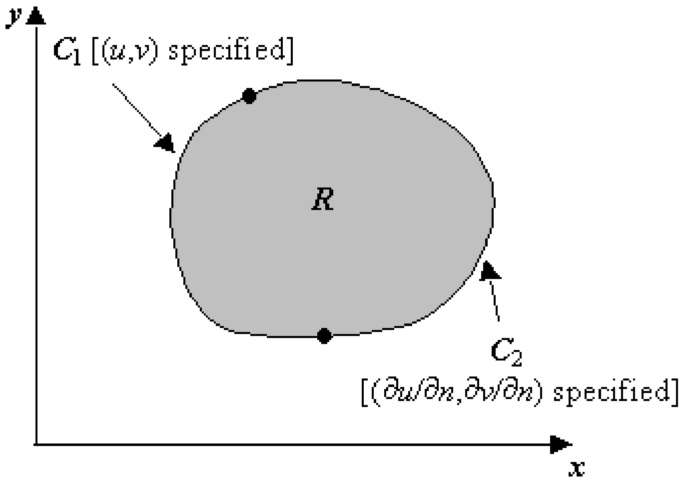

Figure 1: A geometrical sketch of the problem.

DRBEM is then used in an iterative scheme in which the non-linear term u^2v is "linearised" by superceding it with $\overline{u}^2v$, where $\overline{u}$ is the approximation of u from the "previous" iteration, to solve for u and v at each consecutive time level. The proposed method is applicable for solution domains of arbitrary shapes and mixed boundary conditions. It is applied to solve some specific problems.

The DRBEM was originally proposed by Brebbia and Nardini [3] for the numerical solution of dynamic problems in solid mechanics. The method has now been successfully extended to a wide range of problems in engineering, such as those involving diffusion processes, inhomogeneous media and non-linearity. For some examples of these problems, refer to Zhu *et al.* [15], Profit *et al.* [11], Harrouni *et al.* [7], Ang [1], and other references therein.

2 Integral equations

From the differential equations in (1), we derive the integral equations

$$\begin{aligned}\lambda(\xi,\eta)u(\xi,\eta,t) = & \iint\limits_R \alpha^{-1}[\frac{\partial}{\partial t}u(x,y,t) - B - u^2 v + (A+1)u] \\ & \times \Phi(x,y,\xi,\eta)dxdy \\ & + \oint_C [u(x,y,t)\Gamma(x,y,\xi,\eta) \\ & - \Phi(x,y,\xi,\eta)\frac{\partial}{\partial n}u(x,y,t)]ds(x,y), \end{aligned} \tag{5}$$

and

$$\begin{aligned}\lambda(\xi,\eta)v(\xi,\eta,t) = & \iint\limits_R \alpha^{-1}[\frac{\partial}{\partial t}v(x,y,t) - Au + u^2 v]\,\Phi(x,y,\xi,\eta)dxdy \\ & + \oint_C [v(x,y,t)\Gamma(x,y,\xi,\eta) \\ & - \Phi(x,y,\xi,\eta)\frac{\partial}{\partial n}v(x,y,t)]ds(x,y), \end{aligned} \tag{6}$$

where $\lambda(\xi,\eta) = 0$ if $(\xi,\eta) \notin R \cup C$, $\lambda(\xi,\eta) = 1$ if $(\xi,\eta) \in R$, $0 < \lambda(\xi,\eta) < 1$ if $(\xi,\eta) \in C$ and

$$\begin{aligned}\Phi(x,y,\xi,\eta) &= \frac{1}{4\pi}\ln\left[(x-\xi)^2 + (y-\eta)^2\right], \\ \Gamma(x,y,\xi,\eta) &= \frac{n_1(x,y)(x-\xi) + n_2(x,y)(y-\eta)}{2\pi\left[(x-\xi)^2 + (y-\eta)^2\right]}, \end{aligned} \tag{7}$$

where $[n_1(x,y), n_2(x,y)]$ is the unit normal vector to the curve C at the point (x,y) pointing away from R.

Notice that Φ as given in (7) is the well known fundamental solution of the two-dimensional Laplace equation. For an idea on how (5) and (6) can possibly be derived, one may refer to the monograph by Clements [4].

3 DRBEM

For the DRBEM, we discretize the boundary C into N straight line (boundary) elements $C^{(1)}$, $C^{(2)}$, $\cdots$, $C^{(N-1)}$ and $C^{(N)}$, where the i-th element $C^{(i)}$

has endpoints $(x^{(i)}, y^{(i)})$ and $(x^{(i+1)}, y^{(i+1)})$. [We take $(x^{(1)}, y^{(1)})$, $(x^{(2)}, y^{(2)})$, $\cdots$, $(x^{(N-1)}, y^{(N-1)})$ and $(x^{(N)}, y^{(N)})$ as N well-spaced out distinct points arranged consecutively in a counter-clockwise direction on C and we define $(x^{(N+1)}, y^{(N+1)}) = (x^{(1)}, y^{(1)})$.]

For a simple approximation, let

$$\left.\begin{array}{r} u(x,y,t) \simeq U^{(i)}(t) \\ v(x,y,t) \simeq V^{(i)}(t) \\ \partial[u(x,y,t)]/\partial n \simeq P^{(i)}(t) \\ \partial[v(x,y,t)/\partial n \simeq Q^{(i)}(t) \end{array}\right\} \text{ for } (x,y) \in C^{(i)}, \tag{8}$$

where $U^{(i)}(t)$, $V^{(i)}(t)$, $P^{(i)}(t)$ and $Q^{(i)}(t)$ are unknown parameters to be determined, i.e. the functions u and v and their normal derivatives are assumed to be spatially invariant over a boundary element.

Using (8) together with $C \simeq C^{(1)} \cup C^{(2)} \cup \cdots \cup C^{(N-1)} \cup C^{(N)}$, we replace (5) and (6) approximately by

$$\begin{aligned} \lambda(\xi,\eta)u(\xi,\eta,t) = & \iint\limits_R \alpha^{-1}[\frac{\partial}{\partial t}u(x,y,t) - B - u^2 v + (A+1)u] \\ & \times \Phi(x,y,\xi,\eta)dxdy \\ & + \sum_{j=1}^{N} U^{(j)}(t) \int_{C^{(j)}} \Gamma(x,y,\xi,\eta)ds(x,y) \\ & - \sum_{j=1}^{N} P^{(j)}(t) \int_{C^{(j)}} \Phi(x,y,\xi,\eta)ds(x,y), \end{aligned} \tag{9}$$

and

$$\begin{aligned} \lambda(\xi,\eta)v(\xi,\eta,t) = & \iint\limits_R \alpha^{-1}[\frac{\partial}{\partial t}v(x,y,t) - Au + u^2 v]\,\Phi(x,y,\xi,\eta)dxdy \\ & + \sum_{j=1}^{N} V^{(j)}(t) \int_{C^{(j)}} \Gamma(x,y,\xi,\eta)ds(x,y) \\ & - \sum_{j=1}^{N} Q^{(j)}(t) \int_{C^{(j)}} \Phi(x,y,\xi,\eta)ds(x,y). \end{aligned} \tag{10}$$

To deal with the domain integrals in (9) and (10), we apply the dual-reciprocity method (DRM) introduced by Brebbia and Nardini [3] and Partridge and Brebbia [9].

For the DRM, we choose $N + L$ collocation points in the region $R \cup C$ (L is a positive integer and recall that N is the number of boundary elements). The collocation points are denoted by $(\xi^{(1)}, \eta^{(1)})$, $(\xi^{(2)}, \eta^{(2)})$, $\cdots$, $(\xi^{(N+L-1)}, \eta^{(N+L-1)})$ and $(\xi^{(N+L)}, \eta^{(N+L)})$. For convenience, we take the first N collocation points to be the midpoints of the boundary elements, i.e. $(\xi^{(n)}, \eta^{(n)})$ is the midpoint of $C^{(n)}$ for $n = 1, 2, \cdots, N$.

We then make the approximations:

$$\alpha^{-1}[\frac{\partial}{\partial t}u(x,y,t) - u^2 v + (A+1)u] \simeq \sum_{j=1}^{N+L} \mu^{(j)}(t)\sigma^{(j)}(x,y),$$
$$\alpha^{-1}[\frac{\partial}{\partial t}v(x,y,t) - Au + u^2 v] \simeq \sum_{j=1}^{N+L} \phi^{(j)}(t)\sigma^{(j)}(x,y), \quad (11)$$

where $\mu^{(j)}$ and $\phi^{(j)}$ are yet unknown parameters and

$$\sigma^{(j)}(x,y) = 1 + \left([x-\xi^{(j)}]^2 + [y-\eta^{(j)}]^2\right) + \left([x-\xi^{(j)}]^2 + [y-\eta^{(j)}]^2\right)^{3/2}$$
$$\text{for } j = 1, 2, \cdots, N+L. \quad (12)$$

The local interpolating functions $\sigma^{(j)}(x,y)$ are those proposed in Zhang and Zhu [14].

With (11), we can express the domain integrals in (9) and (10) as

$$\iint\limits_R \alpha^{-1}[\frac{\partial}{\partial t}u(x,y,t) - B - u^2 v + (A+1)u]\,\Phi(x,y,\xi,\eta)dxdy$$
$$\simeq \sum_{j=1}^{N+L} \mu^{(j)}(t)\Psi^{(j)}(\xi,\eta) - \frac{1}{2}\alpha^{-1}B\lambda(\xi,\eta)\xi^2$$
$$- \alpha^{-1}B \oint_C [xn_1(x,y)\Phi(x,y,\xi,\eta)$$
$$- \frac{1}{2}x^2\Gamma(x,y,\xi,\eta)]ds(x,y), \quad (13)$$

and

$$\iint_R \alpha^{-1}[\frac{\partial}{\partial t}v(x,y,t) - Au + u^2v]\Phi(x,y,\xi,\eta)dxdy$$
$$\simeq \sum_{j=1}^{N+L} \phi^{(j)}(t)\Psi^{(j)}(\xi,\eta), \quad (14)$$

where

$$\Psi^{(j)}(\xi,\eta) = \lambda(\xi,\eta)\theta^{(j)}(\xi,\eta) + \oint_C \Phi(x,y,\xi,\eta)\beta^{(j)}(x,y)ds(x,y)$$
$$- \oint_C \Gamma(x,y,\xi,\eta)\theta^{(j)}(x,y)ds(x,y),$$

$$\theta^{(j)}(x,y) = \frac{1}{4}\left([x-\xi^{(j)}]^2 + [y-\eta^{(j)}]^2\right) + \frac{1}{16}\left([x-\xi^{(j)}]^2 + [y-\eta^{(j)}]^2\right)^2$$
$$+ \frac{1}{25}\left([x-\xi^{(j)}]^2 + [y-\eta^{(j)}]^2\right)^{5/2},$$
$$\beta^{(j)}(x,y) = n_1(x,y)\frac{\partial}{\partial x}[\theta^{(j)}(x,y)] + n_2(x,y)\frac{\partial}{\partial y}[\theta^{(j)}(x,y)]. \quad (15)$$

Equations (9), (10), (11), (13) and (14) may be used to obtain

$$\lambda(\xi^{(i)},\eta^{(i)})U^{(i)}(t) = -\frac{1}{2}\alpha^{-1}B\lambda(\xi^{(i)},\eta^{(i)})[\xi^{(i)}]^2$$
$$+ \alpha^{-1}\sum_{n=1}^{N+L}\{\frac{d}{dt}[U^{(n)}(t)] + (A+1)U^{(n)}(t)$$
$$- [U^{(n)}(t)]^2V^{(n)}(t)\}\sum_{j=1}^{N+L} b_{jn}\Psi^{(j)}(\xi^{(i)},\eta^{(i)})$$
$$+ \sum_{j=1}^{N}[U^{(j)}(t) + \frac{1}{2}\alpha^{-1}B(\xi^{(j)})^2]$$
$$\times \int_{C^{(j)}} \Gamma(x,y,\xi^{(i)},\eta^{(i)})ds(x,y)$$
$$- \sum_{j=1}^{N}[P^{(j)}(t) + \alpha^{-1}B\xi^{(j)}n_1^{(j)}]$$
$$\times \int_{C^{(j)}} \Phi(x,y,\xi^{(i)},\eta^{(i)})ds(x,y)$$
$$\text{for } i = 1,2,\cdots,N+L, \quad (16)$$

and

$$\lambda(\xi^{(i)},\eta^{(i)})V^{(i)}(t) = \alpha^{-1}\sum_{n=1}^{N+L}\{\frac{d}{dt}V^{(n)}(t) - AU^{(n)}(t)$$
$$+ [U^{(n)}(t)]^2V^{(n)}(t)\}\sum_{j=1}^{N+L} b_{jn}\Psi^{(j)}(\xi^{(i)},\eta^{(i)})$$
$$+\sum_{j=1}^{N}V^{(j)}(t)\int_{C^{(j)}}\Gamma(x,y,\xi^{(i)},\eta^{(i)})ds(x,y)$$
$$-\sum_{j=1}^{N}Q^{(j)}(t)\int_{C^{(j)}}\Phi(x,y,\xi^{(i)},\eta^{(i)})ds(x,y)$$
$$\text{for } i = 1,2,\cdots,N+L, \qquad (17)$$

where $[n_1^{(j)}, n_2^{(j)}]$ is the unit normal vector to the boundary element $C^{(j)}$ pointing away from R, $U^{(n)}(t) = u(\xi^{(n)},\eta^{(n)},t)$ and $V^{(n)}(t) = v(\xi^{(n)},\eta^{(n)},t)$ (for $n = 1, 2, \cdots, N+L$),and $[b_{ij}]$ is the inverse of $[a_{ij}]$ with $a_{ij} = \sigma^{(j)}(\xi^{(i)},\eta^{(i)})$.

Notice that in deriving (16) and (17) we collocate (11) by letting (x, y) be given by $(\xi^{(n)},\eta^{(n)})$ for $n = 1, 2, \cdots, N+L$ and invert the resulting linear equations to obtain $\mu^{(j)}(t)$ and $\phi^{(j)}(t)$ (for $j = 1, 2, \cdots, N+L$).

Now, (16) and (17) constitute a system of $2(N+L)$ non-linear differential equations in $2(N+L)$ unknown functions of t. The unknown functions are given by $(U^{(n)}(t), V^{(n)}(t))$ for $n = N+1, N+2, \cdots, N+L$, and either $(U^{(j)}(t), V^{(j)}(t))$ or $(P^{(j)}(t), Q^{(j)}(t))$ for $j = 1, 2, \cdots, N$.

The non-linear system is solved approximately using an iterative scheme as described below.

For $n = 1, 2, \cdots, N+L$, we make the approximation

$$\begin{aligned}
U^{(n)}(t) &\simeq \frac{1}{2}[U^{(n)}(t+\frac{1}{2}\Delta t) + U^{(n)}(t-\frac{1}{2}\Delta t)],\\
V^{(n)}(t) &\simeq \frac{1}{2}[V^{(n)}(t+\frac{1}{2}\Delta t) + V^{(n)}(t-\frac{1}{2}\Delta t)],\\
\frac{d}{dt}[U^{(n)}(t)] &\simeq \frac{U^{(n)}(t+\frac{1}{2}\Delta t) - U^{(n)}(t-\frac{1}{2}\Delta t)}{\Delta t},\\
\frac{d}{dt}[V^{(n)}(t)] &\simeq \frac{V^{(n)}(t+\frac{1}{2}\Delta t) - V^{(n)}(t-\frac{1}{2}\Delta t)}{\Delta t}.
\end{aligned} \qquad (18)$$

The non-linear term $[U^{(n)}(t)]^2V^{(n)}(t)$ in (16) and (17) is approximately "linearised" using

$$[U^{(n)}(t)]^2V^{(n)}(t) \simeq \frac{1}{2}[\overline{U}^{(n)}(t)]^2[V^{(n)}(t+\frac{1}{2}\Delta t)+V^{(n)}(t-\frac{1}{2}\Delta t)], \qquad (19)$$

where $\overline{U}^{(n)}(t)$ is given either by a *known* approximation of $U^{(n)}(t)$ or the boundary condition (3) (if it is applicable).

With (18) and (19), we find that (16) and (17) give rise to:

$$\begin{aligned}
&\frac{1}{2}\lambda(\xi^{(i)},\eta^{(i)})[U^{(i)}(t+\frac{1}{2}\Delta t)+U^{(i)}(t-\frac{1}{2}\Delta t)]\\
&=-\frac{1}{2}\alpha^{-1}B\lambda(\xi^{(i)},\eta^{(i)})[\xi^{(i)}]^2\\
&+\alpha^{-1}\sum_{n=1}^{N+L}\{\frac{U^{(n)}(t+\frac{1}{2}\Delta t)-U^{(n)}(t-\frac{1}{2}\Delta t)}{\Delta t}\\
&+\frac{1}{2}(A+1)[U^{(n)}(t+\frac{1}{2}\Delta t)+U^{(n)}(t-\frac{1}{2}\Delta t)]\\
&-\frac{1}{2}[\overline{U}^{(n)}(t)]^2[V^{(n)}(t+\frac{1}{2}\Delta t)+V^{(n)}(t-\frac{1}{2}\Delta t)]\}\\
&\times\sum_{j=1}^{N+L}b_{jn}\Psi^{(j)}(\xi^{(i)},\eta^{(i)})\\
&+\sum_{j=1}^{N}\frac{1}{2}[U^{(j)}(t+\frac{1}{2}\Delta t)+U^{(j)}(t-\frac{1}{2}\Delta t)+\alpha^{-1}B(\xi^{(j)})^2]\\
&\times\int_{C^{(j)}}\Gamma(x,y,\xi^{(i)},\eta^{(i)})ds(x,y)\\
&-\sum_{j=1}^{N}[P^{(j)}(t)+\alpha^{-1}B\xi^{(j)}n_1^{(j)}]\int_{C^{(j)}}\Phi(x,y,\xi^{(i)},\eta^{(i)})ds(x,y)\\
&\qquad\qquad\text{for } i=1,2,\cdots,N+L, \qquad (20)
\end{aligned}$$

and

$$\frac{1}{2}\lambda(\xi^{(i)},\eta^{(i)})\frac{1}{2}[V^{(i)}(t+\frac{1}{2}\Delta t)+V^{(i)}(t-\frac{1}{2}\Delta t)]$$

$$=\alpha^{-1}\sum_{n=1}^{N+L}\{\frac{V^{(n)}(t+\frac{1}{2}\Delta t)-V^{(n)}(t-\frac{1}{2}\Delta t)}{\Delta t}$$

$$-\frac{1}{2}A[U^{(n)}(t+\frac{1}{2}\Delta t)+U^{(n)}(t-\frac{1}{2}\Delta t)]$$

$$+\frac{1}{2}[\overline{U}^{(n)}(t)]^2[V^{(n)}(t+\frac{1}{2}\Delta t)+V^{(n)}(t-\frac{1}{2}\Delta t)]\}\sum_{j=1}^{N+L}b_{jn}\Psi^{(j)}(\xi^{(i)},\eta^{(i)})$$

$$+\sum_{j=1}^{N}\frac{1}{2}[V^{(j)}(t+\frac{1}{2}\Delta t)+V^{(j)}(t-\frac{1}{2}\Delta t)]\int_{C^{(j)}}\Gamma(x,y,\xi^{(i)},\eta^{(i)})ds(x,y)$$

$$-\sum_{j=1}^{N}Q^{(j)}(t)\int_{C^{(j)}}\Phi(x,y,\xi^{(i)},\eta^{(i)})ds(x,y)$$

$$\text{for } i=1,2,\cdots,N+L. \tag{21}$$

Now if we assume $(U^{(n)}(t-\frac{1}{2}\Delta t),V^{(n)}(t-\frac{1}{2}\Delta t))$ $(n=1,2,\cdots,N+L)$ are known, then (20) and (21) constitute a system of $2(N+L)$ linear algebraic equations containing $2(N+L)$ unknowns given by $(U^{(m)}(t+\frac{1}{2}\Delta t),V^{(m)}(t+\frac{1}{2}\Delta t))$ for $m=N+1$, $N+2$, $\cdots$, $N+L$, and either $(U^{(i)}(t+\frac{1}{2}\Delta t),V^{(i)}(t+\frac{1}{2}\Delta t))$ or $(P^{(i)}(t),Q^{(i)}(t))$ [not both] for $i=1$, 2, $\cdots$, N. Note the presence of $\overline{U}^{(n)}(t)$ which is given by either a known approximation of $U^{(n)}(t)$ or by the boundary condition (3).We can apply (20) and (21) to find the unknowns at time $t=(2k-1)\Delta t/2$ for $k=1$, 2, $\cdots$, as follows.

Begin a given time level $t=(2k-1)\Delta t/2$ by calculating $\overline{U}^{(n)}(t)=U^{(n)}(t-\frac{1}{2}\Delta t)$. With this, we can solve (20) and (21) as a system of linear algebraic equations for $(U^{(m)}(t+\frac{1}{2}\Delta t),V^{(m)}(t+\frac{1}{2}\Delta t))$ for $m=N+1$, $N+2$, $\cdots$, $N+L$, and for either $(U^{(i)}(t+\frac{1}{2}\Delta t),V^{(i)}(t+\frac{1}{2}\Delta t))$ or $(P^{(i)}(t),Q^{(i)}(t))$ [whichever is not known] for $i=1$, 2, $\cdots$, N, assuming that $(U^{(n)}(t-\frac{1}{2}\Delta t),V^{(n)}(t-\frac{1}{2}\Delta t))$ are known. Re-compute $\overline{U}^{(n)}(t)$ using

$$\overline{U}^{(n)}(t)=\frac{1}{2}[U^{(n)}(t+\frac{1}{2}\Delta t)+U^{(n)}(t-\frac{1}{2}\Delta t)], \tag{22}$$

where $U^{(n)}(t+\frac{1}{2}\Delta t)$ is either just obtained recently from solving (20) and (21) or from the boundary condition (3). Solve (20) and (21) with the re-computed value of $\overline{U}^{(n)}(t)$. We can iterate to and fro calculating $\overline{U}^{(n)}(t)$ using (22) and solving (20)-(21), until all the unknown quantities converge to within a prescribed number of significant figures, i.e. a predictor-corrector approach is adopted here. Once the prescribed convergence is achieved, we can move on to the following time level.

For the setting up of the system of linear algebraic equations, the line integrals over $C^{(j)}$ in (20)-(21) have to be evaluated. Details on the computation of these integrals may be found in Clements and Crowe [5] and Clements and Haselgrove [6].

4 Specific problems

Problem 1. For a specific test problem, consider solving the system

$$\begin{aligned}
\frac{\partial u}{\partial t} &= u^2 v - 2u + \frac{1}{4}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \\
\frac{\partial v}{\partial t} &= u - u^2 v + \frac{1}{4}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right)
\end{aligned} \tag{23}$$

in the region $R = \{(x, y) : x^2 + y^2 < 1,\ x > 0,\ y > 0\}$ subject to the initial-boundary conditions

$$\begin{aligned}
(u(x,y,0), v(x,y,0)) &= (\exp[-x-y], \exp[x+y]) \text{ for } (x,y) \in R, \\
(u(0,y,t), v(0,y,t)) &= (\exp[-\frac{t}{2} - y], \exp[\frac{t}{2} + y]) \text{ for } 0 < y < 1,\ t > 0, \\
(u(x,0,t), v(x,0,t)) &= (\exp[-\frac{t}{2} - x], \exp[\frac{t}{2} + x]) \text{ for } 0 < x < 1,\ t > 0, \\
(\frac{\partial u}{\partial n}, \frac{\partial v}{\partial n}) &= [x+y](-\exp[-\frac{t}{2} - x - y], \exp[\frac{t}{2} + x + y]) \\
&\qquad \text{for } x^2 + y^2 = 1,\ t > 0,
\end{aligned} \tag{24}$$

It is an easy matter to verify by direct substitution that (23) and (24) are satisfied by

$$(u, v) = (\exp[-\frac{t}{2} - x - y], \exp[\frac{t}{2} + x + y]). \tag{25}$$

For the purpose of obtaining some numerical results for this particular problem, the interior collocation points, the endpoints of the boundary elements and the time-step for the DRBEM are chosen as follows. For m, $n = 1, 2, \cdots, M-1$ (where M is a positive integer greater than 1), form the points $(m\ell_1, n\ell_1)$ with $\ell_1 = 1/M$, and take all those points that lie inside the domain solution (inside the quarter circle) as interior collocation points. The endpoints of the boundary elements are selected to be given by $(x^{(k+1)}, y^{(k+1)}) = (0, 1-k\ell_2,)$, $(x^{(k+1+2M)}, y^{(k+1+2M)}) = (k\ell_2, 0)$ and $(x^{(k+1+4M)}, y^{(k+1+4M)}) = (\cos[\pi k\ell_2/2], \sin[\pi k\ell_2/2])$ for $k = 0, 1, \cdots, 2M-1$, where $\ell_2 = 1/(2M)$. (Thus, $N = 6M$, i.e. there are $6M$ boundary elements.) The time-step Δt is chosen to be given by $\Delta t = 3\ell_1$.

The numerical values of (u, v) at the point $(0.40, 0.60)$ and at various time levels, as obtained using $M = 10$ and $M = 20$, are compared with the exact values from (25) in Table 1. [The given numerical values are those obtained after 6 iterations between calculating $\overline{U}^{(n)}(t)$ using (22) and solving (20)-(21).] The numerical values of (u, v) show an overall improvement in accuracy when M is doubled (i.e. when the number of boundary elements and collocation points is increased and the time-step is halved).

Table 1. A comparison of the numerical and the exact values of (u, v) at various time t at the point $(0.40, 0.60)$.

t	$M = 10$	$M = 20$	Exact
0.30	$(0.3168, 3.153)$	$(0.3166, 3.157)$	$(0.3166, 3.158)$
0.60	$(0.2724, 3.660)$	$(0.2725, 3.667)$	$(0.2725, 3.669)$
0.90	$(0.2345, 4.250)$	$(0.2345, 4.260)$	$(0.2346, 4.263)$
1.20	$(0.2016, 4.939)$	$(0.2018, 4.950)$	$(0.2019, 4.953)$
1.50	$(0.1739, 5.735)$	$(0.1737, 5.751)$	$(0.1738, 5.755)$
1.80	$(0.1489, 6.670)$	$(0.1495, 6.681)$	$(0.1496, 6.686)$

Problem 2. Solve

$$\begin{aligned} \frac{\partial u}{\partial t} &= 1 + u^2 v - \frac{3}{2}u + \frac{1}{500}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \\ \frac{\partial v}{\partial t} &= \frac{1}{2}u - u^2 v + \frac{1}{500}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) \end{aligned} \qquad (26)$$

in the region $R = \{(x, y) : 0 < x < 1,\ 0 < y < 1\}$ subject to

$$(u(x,y,0), v(x,y,0)) = (\frac{1}{2}x^2 - \frac{1}{3}x^3, \frac{1}{2}y^2 - \frac{1}{3}y^3) \text{ for } (x,y) \in R, \tag{27}$$

$$(\frac{\partial u}{\partial x}, \frac{\partial v}{\partial x}) = (0,0) \text{ at the points } (0,y) \text{ and } (1,y) \text{ for } 0 < y < 1 \text{ and } t > 0, \tag{28}$$

$$(\frac{\partial u}{\partial y}, \frac{\partial v}{\partial y}) = (0,0) \text{ at the points } (x,0) \text{ and } (x,1) \text{ for } 0 < x < 1 \text{ and } t > 0. \tag{29}$$

For m, $n = 1, 2, \cdots, M-1$ (where M is a positive integer greater than 1), form the points $(m\ell_1, n\ell_1)$ with $\ell_1 = 1/M$, and take them as collocation points for the DRBEM. The endpoints of the boundary elements are selected to be given by $(x^{(k+1)}, y^{(k+1)}) = (0, 1-k\ell_2,)$, $(x^{(k+1+2M)}, y^{(k+1+2M)}) = (k\ell_2, 0)$, $(x^{(k+1+4M)}, y^{(k+1+4M)}) = (1, k\ell_2)$ and $(x^{(k+1)}, y^{(k+1)}) = (1 - k\ell_2, 1)$ for $k = 0, 1, \cdots, 2M-1$, where $\ell_2 = 1/(2M)$. (Thus, $N = 8M$, i.e. there are $8M$ boundary elements and $8M + (M-1)^2$ collocation points.) As in the test problem above, the time-step Δt is chosen to be given by $\Delta t = 3\ell_1$.

We observe that the numerical values of u and v at all the collocation points seem to approach 1 and 1/2 respectively as time t increases. This is consistent with the observation of Twizell *et al.* [12], i.e. if $(\partial u/\partial n, \partial v/\partial n) = (0,0)$ on the boundary of the solution domain and if the diffusion coefficient α in (1) is small, we may expect the solution (u, v) to approach $(B, A/B)$ as t increases. [In (26), $A = 1/2$, $B = 1$ and $\alpha = 1/500$.]

For some typical numerical results, in Figures 2 and 3, we plot the numerical values of $u(0.50, 0.50, t)$ and $v(0.50, 0.50, t)$ obtained using $M = 8$ and $M = 16$ against time t ($t \in [0, 5.250]$). The iteration between calculating $\overline{U}^{(n)}(t)$ using (22) and solving (20)-(21) is stopped when all the numerical values of u and v at various selected points converge to at least 4 significant figures. At each time level, the number of iterations used is less than 6.

The numerical results obtained using $M = 8$ agree to at least 2 significant figures with those calculated using $M = 16$, i.e. convergence is observed when the number of collocation points and boundary elements is

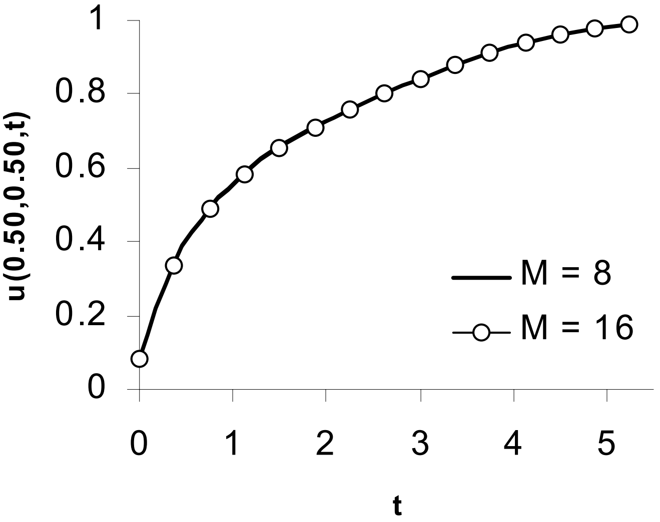

Figure 2: Graphs of $u(0.50, 0.50, t)$ against time t for Problem 2.

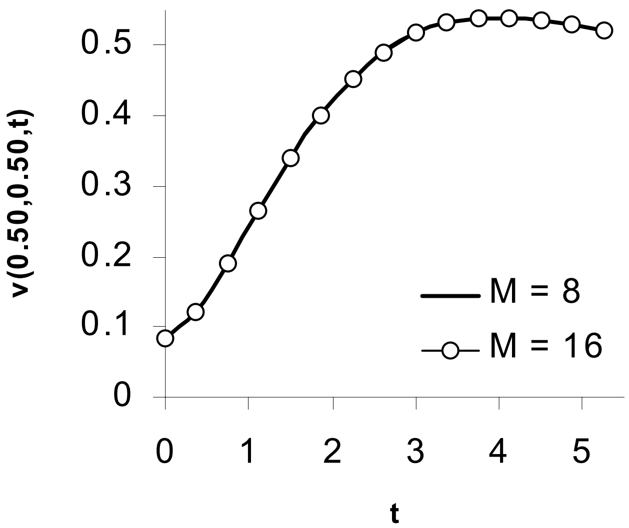

Figure 3: Graphs of $v(0.50, 0.50, t)$ against time t for Problem 2.

increased. In Figures 2 and 3, the difference between the two sets of numerical values (obtained using $M = 8$ and $M = 16$) is graphically almost indistinguishable. From the graphs, it is apparent that $(u, v) \to (1, 1/2)$ as $t \to \infty$.

5 Conclusion

A time-stepping DRBEM is described and successfully implemented on the computer for the numerical solution of two-dimensional initial-boundary value problems governed by the non-linear Brusselator system which arises in the modeling of chemical reaction-diffusion processes. At each time level, a rather efficient iterative scheme is introduced to deal with the non-linear terms in the Brusselator system.

Two specific problems are solved using the method. In the first problem, the numerical results obtained show good agreement with the exact solution. There is no known analytical solution for the second problem. However, the numerical solution exhibits the expected behaviour at large time t. In both problems, convergence is observed in the numerical results as the number of collocation points and boundary elements is increased and as the time-step is reduced correspondingly.

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References

[1] Ang WT. A Laplace transformation dual-reciprocity boundary element method for a class of two-dimensional microscale thermal problems. Engineering Computations 2002; 19: 467-478.

[2] Adomian G. The diffusion-Brusselator equation. Computers and Mathematics with Applications 1995; 29: 1-3.

[3] Brebbia CA, Nardini D, Dynamic analysis in solid mechanics by an alternative boundary element procedure. International Journal of Soil Dynamics and Earthquake Engineering 1983; 2: 228-233.

[4] Clements DL. Boundary value problems governed by second order elliptic systems. London: Pitman, 1981.

[5] Clements DL, Crowe J. A method of solution for the numerical solution of some elliptic boundary value problems for a strip. International Journal of Computer Mathematics 1980; 8: 345-355.

[6] Clements DL, Haselgrove MK. A method of solution of a class of boundary value problems governed by second order elliptic systems. Letters in Applied and Engineering Science 1981; 19: 1017-1029.

[7] Harrouni KE, Quazar D, Wrobel LC, Cheng AHD. Global interpolation function based DRBEM applied to Darcy's flow in heterogeneous media. Engineering Analysis with Boundary Elements 1995; 16: 281-285.

[8] Nicolis G, Prigogine I. Self-organization in non-equilibrium systems. New York: Wiley-Interscience, 1977.

[9] Partridge PW, Brebbia CA. The dual reciprocity boundary element method for the Helmholtz equation. In Proceedings of the International Boundary Elements Symposium, Brebbia, C. A. and A. Choudouet-Miranda (Editors), Computational Mechanics Publications/Springer, Berlin, pp. 543-555, 1990.

[10] Prigogine I, Lefever R. Symmetries breaking instabilities in dissipative systems II. Journal of Physical Chemistry 1968; 48: 1695-1700.

[11] Profit A, Chen K, Amini S. On a DRBEM model for time-dependent PDEs in semi-conductor simulation. Technical Report CMS-99-1, De-

partment of Computer and Mathematical Sciences, The University of Salford, 1999.

[12] Twizell EH, Gumel AB, Cao Q. A second-order scheme for the "Brusselator" reaction-diffusion system. Journal of Mathematical Chemistry 1999; 26: 297-316.

[13] Wazwaz AM. The decomposition method applied to systems of partial differential equations and to the reaction-diffusion Brusselator model. Applied Mathematics and Computation 2000; 110: 251-264.

[14] Zhang Y, Zhu S. On the choice of interpolation functions used in the dual-reciprocity boundary-element method. Engineering Analysis with Boundary Elements 1994; 13: 387-396.

[15] Zhu SP, Satravaha P, Lu XP. Solving linear diffusion equations with the dual reciprocity method in Laplace space. Engineering Analysis with Boundary Elements 1994; 13: 1-10.