A dual-reciprocity boundary element solution of a generalized non-linear Schrödinger equation

Whye-Teong Ang
Division of Engineering Mechanics
School of Mechanical and Production Engineering
Nanyang Technological University
50, Nanyang Avenue, Singapore 639798, Singapore

Keng-Cheng Ang
Mathematics and Mathematics Education
National Institute of Education
Nanyang Technological University
1, Nanyang Walk, Singapore 637616, Singapore

This is a preprint of the article in Numerical Methods for Partial Differential Equations 20 (2004) 843-854.
The publisher is located at: http://www.interscience.Wiley.com

A time-stepping dual-reciprocity boundary element method is presented for the numerical solution of an initial-boundary value problem governed by a generalized non-linear Schrödinger equation. To test the method, two specific problems with known exact solutions are solved. © (2004) John Wiley & Sons, Inc.

Keywords: Schrödinger equation; dual-reciprocity boundary element method; time-stepping scheme

I. INTRODUCTION

Of interest here is the non-linear Schrödinger equation of the form

$$i\frac{\partial \psi}{\partial t} + \sum_{k=1}^{2} \frac{\partial}{\partial x_k}\left(A(x_1, x_2)\frac{\partial \psi}{\partial x_k}\right) = \left(B(x_1, x_2, t) + C(x_1, x_2)|\psi|^p\right)\psi \qquad (1.1)$$

where $i = \sqrt{-1}$, x_k are the spatial Cartesian co-ordinates, t denotes time, ψ is an unknown complex-valued function of x_1, x_2 and t, $A(x_1, x_2)$ is a given real function such that $A(x_1, x_2)$ is strictly positive and and twice partially differentiable with respect to both x_1 and x_2 in the region of interest, $B(x_1, x_2, t)$ and $C(x_1, x_2)$ are given functions which may possibly be complex-valued, and p is a positive real constant.

Numerical Methods for Partial Differential Equations (20), 1–12 ((2004))
 CCC

We are interested in solving (1.1) in a two-dimensional region R subject to the initial-boundary conditions

$$\psi(x_1, x_2, 0) = f(x_1, x_2), \qquad (x_1, x_2) \in R \tag{1.2}$$

$$\psi(x_1, x_2, t) = g(x_1, x_2, t), \qquad (x_1, x_2) \in C_1 \tag{1.3}$$

$$\frac{\partial}{\partial n}\psi(x_1, x_2, t) = h(x_1, x_2, t), \qquad (x_1, x_2) \in C_2 \tag{1.4}$$

where f, g and h are suitably given complex-valued functions, C_1 and C_2 are non-intersecting curves such that $C_1 \cup C_2 = C$, C is the simple closed curve bounding the region R, $\partial\psi/\partial n = n_1\partial\psi/\partial x_1 + n_2\partial\psi/\partial x_2$ and $[n_1, n_2]$ is the unit normal vector to C pointing away from R.

The Schrödinger equation is an important partial differential equation in modern physics. It governs the quantum mechanical behaviours of dynamic systems. It can be solved analytically only for very simple systems. Thus, many researchers, such as Dai and Nassar [1], Ramos [2], Subaşi [3] and Ismail and Taha [4], have proposed finite-difference schemes for the numerical solution of various complicated forms of the Schrödinger equation. Although these schemes may be regarded as successful to a certain extent, it is still useful to develop alternative numerical approaches for solving the Schrödinger equation. An approach worthwhile considering is the boundary element method as it is well known for its flexibility and accuracy in dealing with the boundary conditions of many problems of practical interest in engineering.

In this paper, a dual-reciprocity boundary element method (DRBEM) is proposed for the numerical solution of the initial-boundary value problem defined by (1.1)–(1.4). The DRBEM was initially proposed by Brebbia and Nardini [5] for the numerical solution of dynamic problems in solid mechanics. It 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, one may refer to Partridge and Brebbia [6] (Helmholtz equation), Zhu *et al* [7] (diffusion problems), Profit *et al* [8] (semi-conductor simulation), Harrouni *et al* [9] (flow in porous media), Ang [10] (microscale heat conduction), Ang *et al* [11] (inverse problems) and other references therein.

For the purpose of deriving a DRBEM that does not require the partial derivatives of ψ with respect to x_i to be approximated, the Schrödinger equation (1.1) is re-written as:

$$\sum_{k=1}^{2} \frac{\partial^2}{\partial x_k^2}\left(\sqrt{A}\psi\right) = -\frac{i}{\sqrt{A}}\frac{\partial\psi}{\partial t} + \psi\left(F(x_1, x_2, \psi) + G(x_1, x_2, t)\right), \tag{1.5}$$

where

$$F(x_1, x_2, \psi) = \frac{C(x_1, x_2)}{\sqrt{A}}|\psi|^p \tag{1.6}$$

$$G(x_1, x_2, t) = \sum_{k=1}^{2} \frac{\partial^2}{\partial x_k^2}\left(\sqrt{A}\right) + \frac{1}{\sqrt{A}}B(x_1, x_2, t). \tag{1.7}$$

The DRBEM can be easily implemented on the computer for arbitrarily shaped solution domains with mixed boundary conditions. To test the method, specific problems are solved.

II. INTEGRO-DIFFERENTIAL EQUATION

If we treat (1.5) as a Poisson-like equation and use the fundamental solution of the two-dimensional Laplace's equation, we may apply the reciprocal theorem given in Clements [12] to derive an integro-differential equation for the Schrödinger equation under consideration. Specifically, we obtain

$$\begin{aligned}\gamma(\xi_1,\xi_2)\,\sqrt{A(\xi_1,\xi_2)}\,\psi(\xi_1,\xi_2,t) = \iint\limits_R \Big\{ &- \frac{i}{\sqrt{A(x_1,x_2)}}\frac{\partial}{\partial t}(\psi(x_1,x_2,t)) \\ &+(F(x_1,x_2,\psi(x_1,x_2,t)) + G(x_1,x_2,t))\Big\}\,\Phi(x_1,x_2,\xi_1,\xi_2)\,dx_1\,dx_2 \\ &+ \oint\limits_C \left(\Gamma(x_1,x_2,\xi_1,\xi_2)\sqrt{A(x_1,x_2)} - \Phi(x_1,x_2,\xi_1,\xi_2)\frac{\partial}{\partial n}\sqrt{A(x_1,x_2)}\right)\psi(x_1,x_2,t)\,ds(x_1,x_2) \\ &- \oint\limits_C \Phi(x_1,x_2,\xi_1,\xi_2)\sqrt{A(x_1,x_2)}\frac{\partial}{\partial n}(\psi(x_1,x_2,t))\,ds(x_1,x_2) \qquad (2.1)\end{aligned}$$

where $\gamma(\xi_1,\xi_2) = 0$ if $(\xi_1,\xi_2) \notin R \cup C$, $\gamma(\xi_1,\xi_2) = 1$ if $(\xi_1,\xi_2) \in R$, $0 < \gamma(\xi_1,\xi_2) < 1$ if $(\xi_1,\xi_2) \in C$ [$\gamma(\xi_1,\xi_2) = \frac{1}{2}$ if (ξ_1,ξ_2) lies on a smooth part of C], the fundamental solution of the Laplace's equation is given by

$$\Phi(x_1,x_2,\xi_1,\xi_2) \;=\; \frac{1}{2\pi}\mathrm{Re}\{\ln(x_1-\xi_1+i(x_2-\xi_2))\}, \qquad (2.2)$$

and its normal derivative by

$$\Gamma(x_1,x_2,\xi_1,\xi_2) \;=\; \frac{1}{2\pi}\mathrm{Re}\left\{\frac{n_1(x_1,x_2)+in_2(x_1,x_2)}{x_1-\xi_1+i(x_1-\xi_2)}\right\}. \qquad (2.3)$$

III. NUMERICAL SOLUTION

A. Overview of approach

We shall use (2.1) together with (1.2)–(1.4) to determine ψ numerically. In general, (2.1) is non-linear in ψ as F depends on ψ. To deal with the non-linearity, we adopt an iterative approach. We estimate $F(x_1,x_2,\psi(x_1,x_2,t))$ as $F(x_1,x_2,\tilde{\psi}(x_1,x_2,t))$, where $\tilde{\psi}(x_1,x_2,t)$ is the latest available approximation of $\psi(x_1,x_2,t)$. With this estimation, we solve (2.1) as a linear integro-differential equation in ψ. The newly obtained approximate ψ is used to re-calculate $F(x_1,x_2,\tilde{\psi}(x_1,x_2,t))$, and replacing $F(x_1,x_2,\psi(x_1,x_2,t))$ with the re-computed $F(x_1,x_2,\tilde{\psi}(x_1,x_2,t))$, we solve (2.1) again for ψ. We can iterate between estimating $F(x_1,x_2,\psi(x_1,x_2,t))$ and solving (2.1) approximately for ψ until a satisfactory convergence is achieved in the numerical solution.

A description of a time-stepping DRBEM for solving (2.1) with $F(x_1,x_2,\psi(x_1,x_2,t))$ superseded by $F(x_1,x_2,\tilde{\psi}(x_1,x_2,t))$ is given below.

B. DRBEM

The boundary C is discretized into N straight line elements denoted by $C^{(1)}$, $C^{(2)}$, …, $C^{(N-1)}$ and $C^{(N)}$. Over an element, ψ and $\partial\psi/\partial n$ are approximated as spatially invariant

functions, which, in general, may be complex-valued. That is,

$$\psi \approx \psi^{(k)}(t) \qquad \text{and} \qquad \frac{\partial \psi}{\partial n} \approx \mu^{(k)}(t) \qquad \text{for} \qquad (x_1, x_2) \in C^{(k)}. \tag{3.1}$$

For a given k, either $\psi^{(k)}(t)$ or $\mu^{(k)}(t)$, but not both, is known from the boundary conditions (1.3) and (1.4). Thus there are N unknown functions in (3.1).

To obtain an approximation for the domain integral over R in (2.1), we need to choose $N + M$ collocation points. The first N collocation points are taken to be the midpoints of the N elements. The remaining M collocation points are well-spaced points in the interior of the solution domain.

We denote all the $N+M$ collocation points by $(\xi_1^{(1)}, \xi_2^{(1)})$, $(\xi_1^{(2)}, \xi_2^{(2)})$, …, $(\xi_1^{(N)}, \xi_2^{(N)})$, $(\xi_1^{(N+1)}, \xi_2^{(N+1)})$, …, $(\xi_1^{(N+M-1)}, \xi_2^{(N+M-1)})$ and $(\xi_1^{(N+M)}, \xi_2^{(N+M)})$, where $(\xi_1^{(k)}, \xi_2^{(k)})$ is the midpoint of $C^{(k)}$ for $k = 1, 2, \ldots, N$.

Following Brebbia and Nardini [5], we make the approximation

$$\begin{aligned} -\frac{i}{\sqrt{A(x_1,x_2)}}\frac{\partial}{\partial t}\psi(x_1,x_2,t) + \psi(x_1,x_2,t)\left(G(x_1,x_2,t) + F(x_1,x_2,\tilde{\psi}(x_1,x_2,t))\right) \\ \approx \sum_{j=1}^{N+M} \omega^j(t)\sigma_j(x_1,x_2) \end{aligned} \tag{3.2}$$

where $\omega^j(t)$ are complex-valued functions of t and the interpolating functions $\sigma^{(j)}(x_1, x_2)$ are chosen to be given by

$$\begin{aligned} \sigma_j(x_1,x_2) = 1 + \left((x_1 - \xi_1^{(j)})^2 + (x_2 - \xi_2^{(j)})^2\right) \\ + \left((x_1 - \xi_1^{(j)})^2 + (x_2 - \xi_2^{(j)})^2\right)^{3/2} \quad \text{for} \quad j = 1, 2, \ldots, N+M. \end{aligned} \tag{3.3}$$

The choice of the interpolating functions is not unique. The ones used in (3.3) are those proposed by Zhang and Zhu [13].

With the approximation (3.2), it can be shown that

$$\begin{aligned} \iint_R \Big\{ &- \frac{i}{\sqrt{A(x_1,x_2)}}\frac{\partial}{\partial t}(\psi(x_1,x_2,t)) \\ &+ (F(x_1,x_2,\psi(x_1,x_2,t)) + G(x_1,x_2,t)) \Big\} \Psi(x_1,x_2,\xi_1,\xi_2)\, dx_1\, dx_2 \\ \approx &\sum_{j=1}^{N+M} \omega^j(t)\Psi^{(j)}(\xi_1,\xi_2), \end{aligned} \tag{3.4}$$

where

$$\begin{aligned} \Psi^{(j)}(\xi_1,\xi_2) \;=\; &\gamma(\xi_1,\xi_2)\theta^{(j)}(\xi_1,\xi_2) + \oint_C \Phi(x_1,x_2,\xi_1,\xi_2)\beta^{(j)}(x_1,x_2)\, dx_1\, dx_2 \\ &- \oint_C \Gamma(x_1,x_2,\xi_1,\xi_2)\theta^{(j)}(x_1,x_2)\, ds(x_1,x_2) \\ &\text{for } j = 1, 2, \ldots, N+M, \end{aligned} \tag{3.5}$$

with

$$\theta^{(j)}(x_1,x_2) = \frac{1}{4}\left((x_1-\xi_1^{(j)})^2+(x_2-\xi_2^{(j)})^2\right) + \frac{1}{16}\left((x_1-\xi_1^{(j)})^2+(x_2-\xi_2^{(j)})^2\right)^2 + \frac{1}{25}\left((x_1-\xi_1^{(j)})^2+(x_2-\xi_2^{(j)})^2\right)^{5/2} \quad (3.6)$$

and

$$\beta^{(j)}(x_1,x_2) = n_1(x_1,x_2)\frac{\partial}{\partial x_1}\left(\theta^{(j)}(x_1,x_2)\right) + n_2(x_1,x_2)\frac{\partial}{\partial x_2}\left(\theta^{(j)}(x_1,x_2)\right). \quad (3.7)$$

The functions $\Psi^{(j)}(\xi_1,\xi_2)$ in (3.5) can be computed approximately using

$$\Psi^{(j)}(\xi_1,\xi_2) \approx \gamma(\xi_1,\xi_2)\theta^{(j)}(\xi_1,\xi_2) + \sum_{k=1}^{N}\beta^{(j)}(\xi_1^{(k)},\xi_2^{(k)}) \int\limits_{C^{(k)}} \Phi(x_1,x_2,\xi_1,\xi_2)\, ds(x_1,x_2) + \sum_{k=1}^{N}\theta^{(j)}(\xi_1^{(k)},\xi_2^{(k)}) \int\limits_{C^{(k)}} \Gamma(x_1,x_2,\xi_1,\xi_2)\, ds(x_1,x_2). \quad (3.8)$$

To eliminate $\omega^{(j)}(t)$ from (3.4), we let (x_1,x_2) in (3.2) be given by $(\xi_1^{(n)},\xi_2^{(n)})$ for $n=1,2,\ldots,N+M$ to form a system of $N+M$ linear algebraic equations in $\omega^{(j)}(t)$. The system is then inverted to give

$$\omega^{(j)}(t) = \sum_{n=1}^{N+M} a^{(jn)}\Big\{ -\frac{i}{\sqrt{A(\xi_1^{(n)},\xi_2^{(n)})}}\frac{d}{dt}(\psi^{(n)}(t)) + \left(G(\xi_1^{(n)},\xi_2^{(n)},t)+F(\xi_1^{(n)},\xi_2^{(n)},\tilde{\psi}(\xi_1^{(n)},\xi_2^{(n)},t))\right)\psi^{(n)}(t)\Big\} \quad (3.9)$$

where $a^{(jn)}$ are implicitly defined by

$$\sum_{m=1}^{N+M} a^{(jm)}\sigma^{(k)}(\xi_1^{(m)},\xi_2^{(m)}) = \begin{cases} 1 & \text{if} \quad j=k \\ 0 & \text{if} \quad j\neq k \end{cases} \quad \text{for } j,k=1,2,\ldots,N+M. \quad (3.10)$$

Note that in (3.9), $\psi^{(n)}(t)=\psi(\xi_1^{(n)},\xi_2^{(n)},t)$ for $n=1,2,\ldots,N+M$. Also, see (3.1) where $\psi^{(n)}(t)$ are defined for $n=1,2,\ldots,N$.

Using all the approximations made above and letting (ξ_1,ξ_2) in (2.1) be $(\xi_1^{(m)},\xi_2^{(m)})$ for $m=1,2,\ldots,N+M$, we obtain

$$\gamma(\xi_1^{(m)},\xi_2^{(m)})\sqrt{A(\xi_1^{(m)},\xi_2^{(m)})}\,\psi^{(m)}(t) = \sum_{k=1}^{N+M}\Big\{ -\frac{i}{\sqrt{A(\xi_1^{(k)},\xi_2^{(k)})}}\frac{d}{dt}(\psi^{(k)}(t)) + \left(G(\xi_1^{(k)},\xi_2^{(k)},t)+F(\xi_1^{(k)},\xi_2^{(k)},\tilde{\psi}(\xi_1^{(k)},\xi_2^{(k)},t))\right)\psi^{(k)}(t)\Big\}\sum_{k=1}^{N+M} a^{(jk)}\Psi^{(j)}(\xi_1^{(m)},\xi_2^{(m)}) + \sum_{k=1}^{N}\left\{D^{(mk)}\psi^{(k)}(t)-E^{(mk)}\mu^{(k)}(t)\right\} \quad \text{for} \quad m=1,2,\ldots,N+M, \quad (3.11)$$

where

$$D^{(mk)} = \sqrt{A(\xi_1^{(k)},\xi_2^{(k)})} \int\limits_{C^{(k)}} \Gamma(x_1,x_2,\xi_1^{(m)},\xi_2^{(m)})\, ds(x_1,x_2) - \left.\frac{\partial\sqrt{A(x_1,x_2)}}{\partial n}\right|_{(x_1,x_2)=(\xi_1^{(k)},\xi_2^{(k)})} \int\limits_{C^{(k)}} \Phi(x_1,x_2,\xi_1^{(m)},\xi_2^{(m)})\, ds(x_1,x_2) \tag{3.12}$$

and

$$E^{(mk)} = \sqrt{A(\xi_1^{(k)},\xi_2^{(k)})} \int\limits_{C^{(k)}} \Phi(x_1,x_2,\xi_1^{(m)},\xi_2^{(m)})\, ds(x_1,x_2). \tag{3.13}$$

Note that $\gamma(\xi_1^{(m)},\xi_2^{(m)}) = \frac{1}{2}$ for $m = 1,2,\ldots,N$ and $\gamma(\xi_1^{(m)},\xi_2^{(m)}) = 1$ for $m = N+1, N+2,\ldots,N+M$. Also, $F(\xi_1^{(k)},\xi_2^{(k)},\tilde{\psi}(\xi_1^{(k)},\xi_2^{(k)},t))$ is assumed to be known since $\tilde{\psi}(\xi_1^{(k)},\xi_2^{(k)},t)$ is a known estimate of $\psi^{(k)}(t)$ at that particular time t, as described earlier.

The line integrals over $C^{(k)}$ in (3.8), (3.12) and (3.13) can be evaluated either analytically or numerically as described in Clements *et al* [14], [15].

C. Time-stepping scheme

To step forward in time in the numerical scheme, we make the approximations

$$\begin{aligned} \frac{d}{dt}\left(\psi^{(k)}(t)\right) &\approx \frac{\psi^{(k)}(t+\frac{1}{2}\Delta t) - \psi^{(k)}(t-\frac{1}{2}\Delta t)}{\Delta t} \\ \psi^{(k)}(t) &\approx \frac{1}{2}\left(\psi^{(k)}(t+\frac{1}{2}\Delta t) + \psi^{(k)}(t-\frac{1}{2}\Delta t)\right), \end{aligned} \tag{3.14}$$

where Δt is a small positive real number. In the above approximations, the errors are of order $\mathbf{O}\{(\Delta t)^2\}$.

Using (3.14) in (3.11), we obtain

$$\begin{aligned} &\frac{1}{2}\gamma(\xi_1^{(m)},\xi_2^{(m)})\sqrt{A(\xi_1^{(m)},\xi_2^{(m)})}\left(\psi^{(m)}(t+\frac{1}{2}\Delta t)+\psi^{(m)}(t-\frac{1}{2}\Delta t)\right) = \\ &\sum_{k=1}^{N+M}\Big\{-\frac{i\left(\psi^{(k)}(t+\frac{1}{2}\Delta t)+\psi^{(k)}(t-\frac{1}{2}\Delta t)\right)}{\Delta t\sqrt{A(\xi_1^{(k)},\xi_2^{(k)})}} + \frac{1}{2}\left(\psi^{(k)}(t+\frac{1}{2}\Delta t)+\psi^{(k)}(t-\frac{1}{2}\Delta t)\right) \\ &\times\left(G(\xi_1^{(k)},\xi_2^{(k)},t)+F(\xi_1^{(k)},\xi_2^{(k)},\tilde{\psi}(\xi_1^{(k)},\xi_2^{(k)},t))\right)\Big\}\sum_{k=1}^{N+M} a^{(jk)}\Psi^{(j)}(\xi_1^{(m)},\xi_2^{(m)}) \\ &+\sum_{k=1}^{N}\left\{\frac{1}{2}D^{(mk)}\left(\psi^{(m)}(t+\frac{1}{2}\Delta t)+\psi^{(m)}(t-\frac{1}{2}\Delta t)\right) - E^{(mk)}\mu^{(k)}(t)\right\} \\ &\qquad\qquad \text{for} \quad m = 1,2,\ldots,N+M. \end{aligned} \tag{3.15}$$

The time-stepping scheme is carried out as described below.

The system (3.15) is to be solved at consecutive time levels $t = (2s-1)\frac{1}{2}\Delta t$ for $s = 1,2,\ldots$, with $\psi^{(m)}(t-\frac{1}{2}\Delta t)$ regarded as known for $m = 1,2,\ldots,N+M$.

For the first time level, let $t = \frac{1}{2}\Delta t$ and so $\psi^{(m)}(t - \frac{1}{2}\Delta t) = \psi^{(m)}(0)$ are given by the initial conditions. We compute $F(\xi_1^{(k)}, \xi_2^{(k)}, \tilde{\psi}(\xi_1^{(k)}, \xi_2^{(k)}, \frac{1}{2}\Delta t))$ using $\tilde{\psi}(\xi_1^{(k)}, \xi_2^{(k)}, t) \approx \psi^{(k)}(0)$. With this, (3.15) is solved for the $N + M$ unknowns given by $\psi^{(m)}(\Delta t)$ for $m = N + 1, N + 2, \ldots, N + M$, and either $\psi^{(k)}(\Delta t)$ or $\mu^{(k)}(\frac{1}{2}\Delta t)$ for $k = 1, 2, \ldots, N$. The expression $F(\xi_1^{(k)}, \xi_2^{(k)}, \tilde{\psi}(\xi_1^{(k)}, \xi_2^{(k)}, \frac{1}{2}\Delta t))$ is then re-computed using $\tilde{\psi}(\xi_1^{(k)}, \xi_2^{(k)}, t) \approx \frac{1}{2}(\psi^{(k)}(0) + \psi^{(k)}(\Delta t))$. A new set of approximate values of the $N+M$ unknowns is again obtained by solving (3.15). We iterate between calculating $F(\xi_1^{(k)}, \xi_2^{(k)}, \tilde{\psi}(\xi_1^{(k)}, \xi_2^{(k)}, \frac{1}{2}\Delta t))$ and solving for approximate values of the unknowns, until two consecutive approximations agree to a prescribed number of significant figures. The final iteration then gives the approximate values required. These are then used in the next time step.

We proceed in this manner for $t = \frac{3}{2}\Delta t$, $\frac{5}{2}\Delta t$, $\frac{7}{2}\Delta t$ and so on until we reach the time level required.

IV. SPECIFIC TEST PROBLEMS

In this section, we describe two specific problems that are used to test the method described above. These are problems whose exact solutions are known and comparisons between the exact and numerical solutions are made and discussed.

In each of the problems discussed below, the boundary of the solution domain is discretized into N staight line elements of equal lengths. The midpoints of each element are then taken as collocation points on the boundary. Inside the region R, we choose M interior points which are well spaced out and as evenly distributed as possible.

A. A linear test problem

Consider solving the equation

$$i\frac{\partial \psi}{\partial t} + \sum_{k=1}^{2} \frac{\partial}{\partial x_k}\left(\left(1 + \frac{2}{\pi}x_1 + x_2^2\right)\frac{\partial \psi}{\partial x_k}\right) = -\frac{\pi^2}{4}\left(1 + \frac{2}{\pi}x_1 + x_2^2\right)\psi \qquad (4.1)$$

subject to

$$\psi(x_1, x_2, 0) = \exp\left(\frac{i\pi x_1}{2}\right), \quad \text{for} \quad (x_1, x_2) \in R, \qquad (4.2)$$

$$\psi(0, x_2, t) = \exp(-t), \quad \text{for} \quad 0 < x_2 < 1 \text{ and } t > 0, \qquad (4.3)$$

$$\psi(1, x_2, t) = i\exp(-t), \quad \text{for} \quad 0 < x_2 < 1 \text{ and } t > 0, \quad \text{and} \qquad (4.4)$$

$$\left.\frac{\partial \psi}{\partial n}\right|_{x_2=0} = \left.\frac{\partial \psi}{\partial n}\right|_{x_2=1} = 0, \quad \text{for} \quad 0 < x_1 < 1 \text{ and } t > 0, \qquad (4.5)$$

in the region R defined by $0 < x_1 < 1$ and $0 < x_2 < 1$.

The exact solution for this problem is

$$\psi(x_1, x_2, t) = \exp\left(-t + i\frac{\pi x_1}{2}\right). \qquad (4.6)$$

The N boundary elements are chosen to be evenly distributed on the boundary. Since R is a square, this means that each side has $\frac{N}{4}$ elements. Thus, N has to be divisible by 4. The test point chosen to make comparison with the exact solution is (0.5,0.5).

Therefore, to choose the interior points, we start by selecting this test point as one of the collocation points. The other interior collocation points are then generated by taking a fixed distance vertically and horizontally from already generated points, until the whole interior is covered with M points.

The DRBEM is applied to solve the problem using three different sets of boundary elements and interior collocation points. The three sets are (A) $N = 40$, $M = 25$ with $\Delta t = 0.3$, (B) $N = 80$, $M = 81$ with $\Delta t = 0.15$ and (C) $N = 120$, $M = 225$ with $\Delta t = 0.1$. Results obtained are summarized in Table 1. For the purpose of comparison, we define the error in each approximated value as the distance between the the approximation and the exact value in the complex plane. To show more clearly the improvement in the approximations as the number of boundary elements and interior collocation points is increased, Table 2 is presented.

TABLE I. Approximate and exact values of $\psi(0.5, 0.5, t)$ at selected values of t for the linear test problem

Time	Exact		(A)		(B)		(C)	
	Real	Imaginary	Real	Imaginary	Real	Imaginary	Real	Imaginary
0.30	0.52384	0.52384	0.52172	0.52227	0.52299	0.52354	0.52336	0.52380
0.60	0.38807	0.38807	0.38622	0.38946	0.38826	0.38830	0.38820	0.38810
0.90	0.28749	0.28749	0.28852	0.28754	0.28697	0.28705	0.28714	0.28749
1.20	0.21298	0.21298	0.21154	0.21133	0.21304	0.21348	0.21321	0.21293
1.50	0.15778	0.15778	0.15658	0.15949	0.15748	0.15727	0.15738	0.15778
1.80	0.11688	0.11688	0.11836	0.11653	0.11676	0.11739	0.11712	0.11696
2.10	0.08659	0.08659	0.08532	0.08540	0.08669	0.08602	0.08642	0.08655
2.40	0.06415	0.06415	0.06335	0.06550	0.06390	0.06455	0.06425	0.06394
2.70	0.04752	0.04752	0.04908	0.04750	0.04792	0.04704	0.04717	0.04777
3.00	0.03520	0.03520	0.03407	0.03364	0.03485	0.03545	0.03560	0.03515

TABLE II. Errors in the approximation for the linear test problem

Time	(A)	(B)	(C)
0.30	2.64×10^{-3}	9.01×10^{-4}	4.82×10^{-4}
0.60	2.31×10^{-3}	2.98×10^{-4}	1.33×10^{-4}
0.90	1.03×10^{-3}	6.81×10^{-4}	3.50×10^{-4}
1.20	2.19×10^{-3}	5.04×10^{-4}	2.35×10^{-4}
1.50	2.09×10^{-3}	5.92×10^{-4}	4.00×10^{-4}
1.80	1.52×10^{-3}	5.24×10^{-4}	2.53×10^{-4}
2.10	1.74×10^{-3}	5.79×10^{-4}	1.75×10^{-4}
2.40	1.57×10^{-3}	4.72×10^{-4}	2.33×10^{-4}
2.70	1.56×10^{-3}	6.25×10^{-4}	4.30×10^{-4}
3.00	1.93×10^{-3}	4.30×10^{-4}	4.03×10^{-4}

It is clear from the results presented that the numerical values obtained by the proposed DRBEM are in excellent agreement with the exact solution.

B. A non-linear test problem

As a second test problem, consider solving (1.1) to (1.4) with

$$A(x_1,x_2) = C(x_1,x_2) = 1 \tag{4.7}$$

$$B(x_1,x_2,t) = -(x_1^2-x_2^2)^2\exp(-2t) - (1+x_1x_2)^2 - \frac{i(x_1^2-x_2^2)\exp(-t)[(x_1^2-x_2^2)\exp(-t) - i(1+x_1x_2)]}{(x_1^2-x_2^2)^2\exp(-2t)+(1+x_1x_2)^2}, \tag{4.8}$$

$$p = 2, \tag{4.9}$$

and initial-boundary conditions given by

$$\psi(x_1,x_2,0) = (x_1^2-x_2^2) + i(1+x_1x_2) \quad \text{for} \quad (x_1,x_2)\in R, \tag{4.10}$$

$$\psi = i(1+x_1^2) \quad \text{on} \quad x_2 = x_1 \quad \text{for} \quad 0<x_1<1, \tag{4.11}$$

$$\frac{\partial\psi}{\partial n} = -ix_1 \quad \text{on} \quad x_2 = 0 \quad \text{for} \quad 0<x_1<1, \quad \text{and} \tag{4.12}$$

$$\frac{\partial\psi}{\partial n} = 2\exp(-t) + ix_2 \quad \text{on} \quad x_1 = 1 \quad \text{for} \quad 0<x_2<1, \tag{4.13}$$

where the region R is bounded by $x_2 = x_1$, $x_2 = 0$ and $x_1 = 1$.

The exact solution for this problem is

$$\psi(x_1,x_2,t) = (x_1^2-x_2^2)\exp(-t) + i(1+x_1x_2). \tag{4.14}$$

Using a similar approach as before, N boundary elements are chosen to discretize the boundary of the domain. For the problem considered here, the region R is triangular, and so each side has $\frac{N}{3}$ boundary elements. Thus, N has to be divisible by 3.

The interior collocation points are chosen to include the test point, which, in this case is (0.7,0.3). A procedure similar to that described earlier for the linear test problem is adopted to generate the other points to make a total of M well spaced out and evenly distributed interior collocation points.

Like before, the DRBEM is applied to solve the problem using three different sets of boundary elements and interior collocation points. Here, the three sets chosen are (A) $N = 60$, $M = 36$ with $\Delta t = 0.3$, (B) $N = 120$, $M = 171$ with $\Delta t = 0.1$ and (C) $N = 180$, $M = 630$ with $\Delta t = 0.05$.

For this problem, as described in Section 3.1, we need to iterate between finding an estimate for $\tilde{\psi}$ to re-compute $F(x_1,x_2,\tilde{\psi})$ and solving the system (3.15) for a new ψ. In all the cases considered, the iteration was stopped when the absolute values of all the unknowns in (3.15) from two consecutive iterations differ by less than 10^{-9}. Convergence was achieved after less than 10 iterations in all cases tested.

Results obtained are summarized in Table 3, and Table 4 shows the errors in these approximations. As can be seen from the tables, the approximations obtained using the proposed DRBEM agree very well with the exact solutions, even at large values of t. It is also clear from the results that as the number of boundary elements and interior collocation points is increased, better accuracy is attained.

TABLE III. Approximate and exact values of $\psi(0.7, 0.3, t)$ at selected values of t for the non-linear test problem

Time	Exact		(A)		(B)		(C)	
	Real	Imaginary	Real	Imaginary	Real	Imaginary	Real	Imaginary
0.30	0.29633	1.21000	0.29079	1.20655	0.29507	1.21036	0.29593	1.21018
0.60	0.21952	1.21000	0.21281	1.21473	0.22008	1.21013	0.21968	1.20997
0.90	0.16263	1.21000	0.16732	1.21098	0.16159	1.20989	0.16242	1.21013
1.20	0.12048	1.21000	0.11575	1.20540	0.12091	1.21043	0.12050	1.20999
1.50	0.08925	1.21000	0.08544	1.21516	0.08863	1.20985	0.08893	1.21008
1.80	0.06612	1.21000	0.07041	1.21032	0.06655	1.21022	0.06638	1.20993
2.10	0.04898	1.21000	0.04686	1.20651	0.04817	1.20986	0.04897	1.21033
2.40	0.03629	1.21000	0.03179	1.21320	0.03689	1.21062	0.03632	1.20984
2.70	0.02688	1.21000	0.03218	1.21255	0.02644	1.20956	0.02678	1.21002
3.00	0.01991	1.21000	0.01830	1.20443	0.02016	1.21049	0.02002	1.20985

TABLE IV. Errors in the approximation for the non-linear test problem

Time	(A)	(B)	(C)
0.30	6.53×10^{-3}	1.31×10^{-3}	4.39×10^{-4}
0.60	8.21×10^{-3}	5.75×10^{-4}	1.63×10^{-4}
0.90	4.79×10^{-3}	1.05×10^{-3}	2.47×10^{-4}
1.20	6.60×10^{-3}	6.08×10^{-4}	2.24×10^{-5}
1.50	6.41×10^{-3}	6.38×10^{-4}	3.30×10^{-4}
1.80	4.30×10^{-3}	4.83×10^{-4}	2.69×10^{-4}
2.10	4.08×10^{-3}	8.22×10^{-4}	3.30×10^{-4}
2.40	5.52×10^{-3}	8.63×10^{-4}	1.63×10^{-4}
2.70	5.88×10^{-3}	6.22×10^{-4}	1.02×10^{-4}
3.00	5.80×10^{-3}	5.50×10^{-4}	1.86×10^{-4}

V. FINAL REMARKS

A time-stepping DRBEM has been formulated and successfully implemented for solving a generalized non-linear Schrödinger equation. The method is applied to solve two specific test problems. The numerical results obtained are in excellent agreement with the exact solutions of the respective problems.

Only constant elements are used in the present work. That is, ψ and $\partial\psi/\partial n$ are assumed to be constant across a boundary element. The computation can possibly be refined by using higher order elements, although for the same number of boundary elements and interior collocation points this may result in a system of linear algebraic equations that would require more CPU time to set up. Furthermore, for the same number of boundary elements and interior collocation points, the system may be larger, such as in the case when discontinuous linear elements are used. However, with higher order elements, a better accuracy in the numerical results may be obtained using fewer elements.

In the current formulation, the bulk of the computational time is taken up when the time-independent coefficients of the linear algebraic equations are computed. However, this is done only once and it is not necessary to re-compute those coefficients from one time level to the next. Once they are computed and the necessary portions of the system

are set up, the computations of the approximate solutions take up only a relatively small amount of computational time.

REFERENCES

1. W. Dai and R. Nassar, A finite difference scheme for the generalized non-linear Schrödinger equation with variable coefficients, Journal of Computational Mathematics 18 (2000), 123–132.
2. J.I. Ramos, Linearly implicit methods for the nonlinear Schrödinger equation in nonhomogeneous media, Applied Mathematics and Computation 133 (2002) 1–28.
3. M. Subaşi, On the finite-difference schemes for the numerical solution of two-dimensional Schrödinger equation, Numerical Methods for Partial Differential Equations 18 (2002) 752–758.
4. M.S. Ismail and T.R. Taha, Numerical simulation of coupled nonlinear Schrödinger equation, Mathematics and Computers in Simulation 56 (2001) 547–562.
5. C.A. Brebbia and D. Nardini, Dynamic analysis in solid mechanics by an alternative boundary element procedure, International Journal of Soil Dynamics and Earthquake Engineering 2 (1983) 228–233.
6. P.W. Partridge and C.A. Brebbia, "The dual reciprocity boundary element method for the Helmholtz equation" in Proceedings of the International Boundary Elements Symposium, C.A. Brebbia and A. Choudouet-Miranda (Editors), Computational Mechanics Publications/Springer Berlin, 1990, pp. 543–555.
7. S.P. Zhu, P. Satravaha and X.P. Lu, Solving linear diffusion equations with the dual reciprocity method in Laplace space, Engineering Analysis with Boundary Elements 13 (1994) 1–10.
8. A. Profit, K. Chen and S. Amini, On a DRBEM model for time-dependent PDEs in semiconductor simulation, Technical Report CMS-99-1, Department of Computer and Mathematical Sciences, The University of Salford, 1999.
9. K.E. Harrouni, D. Quazar, L.C. Wrobel and A.H.D. Cheng, Global interpolation function based DRBEM applied to Darcy's flow in heterogeneous media, Engineering Analysis with Boundary Elements 16 (1995) 281–285.
10. W.T. Ang, A Laplace transformation dual-reciprocity boundary element method for a class of two-dimensional microscale thermal problems, Engineering Computations 19 (2002) 467–478.
11. W.T. Ang, K.C. Ang and M. Dehghan, The determination of a control parameter in a two-dimensional diffusion equation using a dual-reciprocity boundary element method, International Journal of Computer Mathematics 80 (2003) 65–74.
12. D.L. Clements, Boundary Value Problems governed by Second Order Elliptic Systems, Pitman, London, 1981.
13. Y. Zhang and S. Zhu, On the choice of interpolation functions used in the dual-reciprocity boundary-element method, Engineering Analysis with Boundary Elements 13 (1994) 387–396.
14. D.L. Clements and J. Crowe, A method of solution for the numerical solution of some elliptic boundary value problems for a strip, International Journal of Computer Mathematics 8 (1980) 345–355.

15. D.L. Clements and G.W. King, A method for the numerical solution of problems governed by elliptic systems in the cut plane, Journal of the Institute of Mathematics and its Applications 24 (1979) 81–83.