NUMERICAL SOLUTION OF NONLINEAR REACTION-DIFFUSION AND
WAVE EQUATIONS

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NUMERICAL SOLUTION OF NONLINEAR REACTION-DIFFUSION AND
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ABSTRACT

NUMERICAL SOLUTION OF NONLINEAR REACTION-DIFFUSION AND
WAVE EQUATIONS

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In this thesis, the two-dimensional initial and boundary value problems (IBVPs) and the one-dimensional Cauchy problems defined by the nonlinear reaction-diffusion and wave equations are numerically solved. The dual reciprocity boundary element method (DRBEM) is used to discretize the IBVPs defined by single and system of nonlinear reaction-diffusion equations and nonlinear wave equation, spatially. The advantage of DRBEM for the exterior regions is made use of for the latter problem. The differential quadrature method (DQM) is used for the spatial discretization of IBVPs and Cauchy problems defined by the nonlinear reaction-diffusion and wave equations.

The DRBEM and DQM applications result in first and second order system of ordinary differential equations in time. These systems are solved with three different time integration methods, the finite difference method (FDM), the least squares method (LSM) and the finite element method (FEM) and comparisons among the methods are made. In the FDM a relaxation parameter is used to

smooth the solution between the consecutive time levels.

It is found that DRBEM+FEM procedure gives better accuracy for the IBVPs defined by nonlinear reaction-diffusion equation. The DRBEM+LSM procedure with exponential and rational radial basis functions is found suitable for exterior wave problem. The same result is also valid when DQM is used for space discretization instead of DRBEM for Cauchy and IBVPs defined by nonlinear reaction-diffusion and wave equations.

Keywords: DRBEM, DQM, FDM, LSM, FEM, nonlinear reaction-diffusion equation, nonlinear wave equation

ÖZ

DOĞRUSAL OLMAYAN REAKSİYON-YAYILIM VE DALGA DENKLEMLERİNİN SAYISAL ÇÖZÜMÜ

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Bu tezde, doğrusal olmayan reaksiyon-yayılım ve dalga denklemleri tarafından tanımlanan iki boyutlu başlangıç ve sınır değer problemleri ile bir boyutlu Cauchy problemleri sayısal olarak çözülmüştür.

Karşılıklı sınır elemanları yöntemi, doğrusal olmayan reaksiyon-yayılım denklem ve denklem sistemleri, ve doğrusal olmayan dalga denklemleri tarafından tanımlanan başlangıç ve sınır değer problemlerinin uzay koordinatlarının ayrıklaştırılmasında kullanılmıştır. Sonuncu problemde metodun sonsuz bölgelerde uygulanabilme özelliği kullanılmıştır. Diferensiyel kareleme yöntemi, doğrusal olmayan reaksiyon-yayılım ve dalga denklemleri tarafından tanımlanan başlangıç ve sınır değer problemleri ile Cauchy problemlerinin uzay koordinatlarının ayrıklaştırılmasında kullanılmıştır. Her iki uygulama da birinci ve ikinci dereceden zamana bağlı adi diferensiyel denklem sistemleri ile sonuçlanmaktadır. Bu sistemlerin çözümleri için üç farklı zaman integrasyonu (sonlu farklar metodu, en küçük kareler metodu ve sonlu elemanlar metodu) kullanılmış ve metotlar arası

karşılaştırmalar yapılmıştır. Sonlu farklar metodunda çözümü ardışık zaman aralıklarında düzeltmek amacıyla yumuşatma parametresi kullanılmıştır.

Karşılıklı sınır elemanları metodu ve sonlu elemanlar metotları birleşimi ile doğrusal olmayan reaksiyon-yayılım denklemleri için elde edilen çözümün doğruluk bakımından daha iyi olduğu görülmüştür. Metodun, üstel ve rasyonel radyal temelli fonksiyonlar ile kullanıldığında, en küçük kareler yöntemi ile olan birleşimi ise, doğrusal olmayan dalga denklemleri ile dış bölgede elde edilen çözüm için uygun bulunmuştur. Doğrusal olmayan reaksiyon-yayılım ve dalga denklemleri tarafından tanımlanan başlangıç ve sınır değer problemleri ve Cauchy problemlerinin uzay türevlerinin ayrıklaştırılmasında, karşılıklı sınır elemanları metodu yerine diferensiyel kareleme metodunun kullanılması durumunda da aynı zaman integrasyonu metotlarının üstünlüğü geçerlidir.

Anahtar Kelimeler: Karşılıklı sınır elemanları metodu, diferensiyel kareleme metodu, sonlu farklar metodu, en küçük kareler metodu, sonlu elemanlar metodu, doğrusal olmayan reaksiyon-yayılım denklemi, doğrusal olmayan dalga denklemi

To my family and to the memory of my grandfather

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LIST OF ABBREVIATIONS AND SYMBOLS

BEM	Boundary Element Method
DRM	Dual Reciprocity Method
DRBEM	Dual Reciprocity Boundary Element Method
DQM	Differential Quadrature Method
PDQ	Polynomial Based Differential Quadrature Method
FDQ	Fourier Based Differential Quadrature Method
CGL	Chebyshev Gauss Lobatto
FDM	Finite Difference Method
LSM	Least Squares Method
FEM	Finite Element Method
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
IBVP	Initial and Boundary Value Problem
Ω	Computational domain
Γ	Boundary of the computational domain Ω
∇^2	Laplace operator
μ	Relaxation parameter in FDM time integration
$p(u)$	The nonlinear function of u
t^m	m-th time level
τ_m	Maximum absolute error for the m-th time level

u_{exact} Exact solution

u_{num} Numerical solution

ν The diffusivity constant

c The wave speed

$w_{ij}^{(m)}$ Weighting coefficient for the $m-$th derivative (in DQM formulation)

$l_i(x)$ $i-$th degree Lagrange polynomial

$P_N(x)$ $N-$th degree polynomial

N Number of boundary elements in DRBEM

   Number of discretized points in one direction in DQM

N_x Number of boundary elements in $x-$direction in DQM

N_y Number of boundary elements in $y-$direction in DQM

L Number of points in the solution domain in DRBEM

CHAPTER 1

INTRODUCTION

Nonlinear reaction-diffusion equations model a huge number of problems in biology, chemistry, ecology and biomedicine. With such a wide range of application fields, the solutions of nonlinear reaction-diffusion equations are very attractive among the researchers.

The group of particles such as cells, bacteria, chemicals, animals and so on usually move around in a random way which can be thought as a diffusion process [1]. Without loss of generality one can consider the one-dimensional case and assume that a particle moves randomly backward and forward along a line in fixed steps Δx that are taken in a fixed time Δt. It is important to know the probability that a particle reaches a point m space steps to the right $(m\Delta x)$ after n time steps $(n\Delta t)$.

The classical approach to diffusion (Fickian diffusion) says that in the n-dimensional case the flux J of material which can be cells, amount of chemical, number of animals etc., is proportional to the gradient of concentration of material, i.e.

$$J = -D\nabla u \tag{1.1}$$

where $u(\mathbf{x}, t)$ is the concentration of the species with $\mathbf{x} = (x_1, x_2, x_3, ..., x_n), \ n \geq 1$ and D is the diffusivity of the particles that measures how efficiently the particles disperse from a high to a low density. The minus sign in (1.1) indicates that the dispersion is from a high to a low concentration.

Using the general conservation equation which says that the rate of change of the

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amount of material in a region is equal to the rate of flow across the boundary plus any that is created within the boundary, the reaction-diffusion equation is obtained as [1]

$$\dot{u} = p + \nabla(D\nabla u) \tag{1.2}$$

where the upper dot denotes the time derivative , p represents the source of particles which is called the reaction term and may be a function of u, $\mathbf{x}$ and t and the diffusivity D may be a function of space and u.

For the case D is space-dependent, nonlinear reaction-diffusion equations take the form of nonlinear parabolic partial differential equations and can be written as [1]

$$\dot{u} = D\nabla^2 u + p(u) \tag{1.3}$$

where ∇^2 denotes the Laplacian operator. If the reaction term p vanishes, equation (1.3) is simply the heat equation. Equation (1.3) arises in the modeling of biomedical importance from diffusion of genetically engineered organisms in heterogeneous environments to effect of white and grey matter in the growth and spread of brain tumors.

In an ecological context the reaction term p in (1.3) could represent the birth-death process and u the population density. With the logistic population growth $p = ru(1 - \dfrac{u}{K})$ where r is the linear reproduction rate and K the carrying capacity of the environment the resulting equation

$$\dot{u} = ru(1 - \frac{u}{K}) + D\nabla^2 u \tag{1.4}$$

is known as Fisher-Kolmogorov equation and it is a model for the spread of an advantageous gene in a population [1].

In the more general case the so-called Zeldovich equation with $p(u) = u(1 -$

$u)(u - a)$ $(0 < a < 1)$ arises in combustion theory and its particular degenerate case with $p(u) = u^2 - u^3$ is also referred as Zeldovich equation in [2].

If two or more species are interacting such as cells, reactants, populations, bacteria or chemicals, the system of nonlinear reaction-diffusion equations are obtained in the form

$$\dot{\mathbf{u}} = \mathbf{D}\nabla^2\mathbf{u} + \mathbf{p}(\mathbf{u}) \tag{1.5}$$

where $\mathbf{u} = (u_1, u_2, ..., u_m)^T$ $(i = 1, 2, ..., m)$ is the vector of densities or concentrations each diffusing with its own diffusion coefficient D_i and interacting according to the vector source term (reaction term) $\mathbf{p}$. $\mathbf{D}$ is the matrix of the diffusivities which if there is no diffusion among the species, is simply a diagonal matrix.

One of the most important feature of the nonlinear parabolic equations is their ability to support travelling wave solutions. A travelling wave is the wave which travels without change of shape. Thus, a travelling wave solution has the same shape for all time levels and the speed of propagation of this shape is constant and denoted by c. It is noted in [3] that unlike the wave equation which is hyperbolic and propagates any wave profile with a specific speed, reaction-diffusion equations may only allow certain wave profiles to propagate, each one with its own characteristic velocity. The travelling wave solutions for the Fisher and Fisher-Kolmogorov equations are found in [3] and [1], respectively.

On the other hand, the wave equation models the wave and oscillation phenomena [4], such as transmission of sound in air, the spreading of ripples on a pond of water, the transmission of radio waves or the waves produced by earthquakes etc. [5]. These topics include the applications in engineering such as acoustics, electromagnetics and fluid dynamics.

The n-dimensional wave equation (the simplest of all hyperbolic differential equations) is given by

$$\ddot{u} = c^2 \nabla^2 u \qquad (1.6)$$

where u is a function of space and time with the second order time derivative $\ddot{u}$, ∇^2 is the Laplacian operator and c is the given fixed constant which is equal to the propagation speed of the wave and called as the wave speed. In the one-dimensional case, u can represent physically the normal displacement of the particles of a vibrating string, for two-dimensions it represents the waves on the surface of water whereas it can represent waves in acoustics or optics in three-dimensional case [6].

The equation

$$\ddot{u} = c^2 \nabla^2 u + p(u) \qquad (1.7)$$

is the most natural generalization of the wave equation with the nonlinear function p of u. It appears in many fields of physics. In the one-dimensional case, for a cubic nonlinearity $p(u) = u - u^3$(Klein-Gordon equation) it has been used as a model field theory, with the nonlinearity $p(u) = -\sin u$ (the sine-Gordon equation) equation (1.7) has applications in elementary particle theory, dislocations in crystals, one-dimensional molecular systems [7].

In order to develop a predictive understanding on these real life problems genuinely, one should be able to solve the initial and boundary value or Cauchy problems defined by the modeling equations (1.3) and (1.7). However, these problems do not have exact solution or not easy to solve, due to their complexity. Thus, it is important to find accurate and efficient approximate (numerical) solutions. The best known oldest approximation techniques are the finite difference method (FDM) and the finite element method (FEM). Such methods discretize the domain into a number of elements or cells and they are called 'domain discretization methods'.

FDM is a numerical technique, which approximates the solutions to differential equations by replacing its derivatives using truncated Taylor series, and expresses

them in terms of the values at a number of discrete mesh points. This transforms the problem to a system of algebraic equations. Although the method applies relatively straightforward internal discretization scheme and is computationally economical, main difficulties arise in the consideration of curved boundaries and the insertion of boundary conditions.

FEM was originally evolved to represent the geometry of the problem and to simplify the introduction of the boundary conditions. The method divides the domain of the problem into small parts, which are called elements, and the approximation is made using the polynomial interpolation functions on each element. A weighted residual statement is constructed and this produces the influence matrices, which express the properties of each element in terms of a discrete number of nodal values. A global matrix is obtained by assembling all of the influence matrices and this enables a simpler way for the insertation of boundary conditions comparing to FDM. The disadvantages of FEM are that large quantities of data are needed to discretize the full domain and there are also difficulties when modeling infinite regions and moving boundary problems.

The boundary element method (BEM) is a well established numerical method, which is emerged as a powerful alternative to the finite difference and particularly to finite elements. The basic idea behind the method is to transform the partial differential equation (PDE) into an integral equation which can be obtained as a special case of the general weighted residual statement [8]. The fundamental solution of the differential equation is used as the weight function and this transforms the weighting residual statement involving domain integrals into a formula containing only boundary integrals. Then, the method uses the given boundary conditions to fit the boundary values into the integral equation. Once this is done, the integral equation can then be used again to calculate the solution numerically at any desired point in the interior of the solution domain. The most important future of the BEM is that it only requires discretization of the surface rather than the volume. Hence, the method results in a much smaller systems of equations comparing to domain discretization methods. The BEM coefficient matrices are not sparsed but contain lots of scattered zeros. As is marked in [9], the numerical accuracy of boundary elements is generally

greater than that of finite elements. BEM can also be used for analyzing problems with stress (or flux) concentration, which is not the case for FEM. The main advantage of the BEM is that contrary to the classical domain methods it is well-suited to solve the problems in infinite domains which arise for instance in solid mechanics, hydraulics, stress analysis, etc.

The BEM considered as an integral equation method has a long history that can be traced back to the beginning of 20-th century. The word BEM is first appeared in literature in 1977 in the work of Brebbia and Dominguez [10] which indicates the surface discretization character of the method. Since then the method has an increasing popularity and it has become a widely used technique with applications in many areas of science and engineering including fluid mechanics, acoustics, electromagnetics, fracture mechanics, elastodynamics and magneto-hydrodynamics. Furthermore, the time dependent problems such as transient heat conduction and wave propagation are also handled by BEM [5, 8, 9, 11].

Numerical simulations with FDM, FEM and BEM can be carried out using a large number of grid points. However, in some practical applications the numerical solutions of PDEs are required at only a few specified points in the physical domain. To achieve an acceptable degree of accuracy, these methods still require the use of a large number of grid points to obtain accurate solutions at these specified points. As a result, they require more storage and computational effort.

The differential quadrature method (DQM) is an efficient discretization technique to obtain accurate numerical solutions using considerably small number of grid points. The method is introduced by R. E. Bellman and his associates [12, 13] in the early 1970's and since then it has been successfully employed to many problems in engineering and science. The DQM depends on the idea of integral quadrature. It approximates a partial derivative of the solution with respect to a coordinate direction as a linear weighted sum of all functional values of the solution at all mesh points along that direction. The key to DQM is to determine the weighting coefficients for the discretization of a derivative of any order. In the early work [12] two different methods to determine the weighting coefficients are suggested. The first method solves an algebraic equation system

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whereas the second one uses a simple algebraic formulation with the coordinates of grid points chosen as the roots of the shifted Legendre polynomial. The current methods for determination of the weighting coefficients are generalized under the analysis of a high order polynomial approximation and the analysis of a linear vector space in [14]. In this approach the weighting coefficients for the first order derivative are determined by a simple algebraic formulation without any restriction on the choice of grid points and the second and higher order derivatives are determined by a recurrence relation, and this method is called as the polynomial based differential quadrature method (PDQ). Another approach to compute the weighting coefficients of the first and second order derivatives is used in [15] when the solution of a PDE is approximated by a Fourier series expansion. This approach is called the Fourier expansion based differential quadrature method (FDQ). For both PDQ and FDQ methods a linear vector space analysis is employed.

In this thesis, both the DRBEM and DQM are applied spatially to solve initial and boundary value and Cauchy problems defined by nonlinear reaction-diffusion and nonlinear wave equations. The advantage of DRBEM is made use of in solving the exterior nonlinear wave problem by using only the interior boundary. Three types of time integration methods (FDM, FEM, LSM) are combined with DRBEM and DQM successfully for obtaining accurate results. These constitute the main original contribution of this thesis.

1.1   Mathematical Problems

In the thesis, we consider the initial and boundary value problems, and the Cauchy problems defined by nonlinear reaction-diffusion (1.3) and nonlinear wave equations (1.7).

1.1.1   Initial and Boundary Value Problems

The initial and boundary value problems

$$
\begin{cases}
\dfrac{\partial^i u(x,y,t)}{\partial t^i} = \nabla^2 u(x,y,t) + p(u(x,y,t)) & (x,y) \in \Omega, \quad t > 0 \\[3mm]
\beta(x,y,t)u + \gamma(x,y,t)q = 0 & (x,y) \in \Gamma, \qquad t > 0 \\[3mm]
\dfrac{\partial^{k-1} u(x,y,0)}{\partial t^{k-1}} = u_{k-1}(x,y) & k = 1, i
\end{cases}
\tag{1.8}
$$

defined by the nonlinear reaction-diffusion (i=1) and wave ($i = 2$) equations are considered. In equation (1.8) Ω denotes a two-dimensional region in $\mathbb{R}^2$ with boundary Γ, $\beta(x,y,t)$, $\gamma(x,y,t)$ and $u_{k-1}(x,y)$ ($k = 1, i$) are given functions, $p(u(x,y,t))$ is the given nonlinear function, and q denotes the normal derivative $\dfrac{\partial u}{\partial n}$.

In such problems, it is not an easy task to find the corresponding fundamental solution necessary in obtaining boundary element formulation, since they involve time derivatives and the nonlinearity. In [16, 17, 18], the time-dependent fundamental solution is used and the resulting integral equations have been found with some domain integrals, which removes one of the main advantage (the boundary only character) of the BEM.

In the case that the problem includes time derivatives and nonlinear terms, an effective technique to treat the domain integrals is the dual reciprocity method (DRM). The technique approximates the integrands of the domain integrals using radial basis functions and converts the domain integrals into boundary integrals. This method is called the dual reciprocity BEM (DRBEM) and it gives the linear algebraic equations approximating the problem, being considered, at chosen points inside the solution domain and at the discretized boundary nodes.

The DRBEM is introduced in the early 1980's and the method is extended to more general problems including nonlinearity and infinite regions in [19, 20].

The basic idea behind the DRBEM is to employ a fundamental solution corresponding to a simpler equation and treat the remaining terms in the original equation as nonhomogenity. This may contain the time derivatives and nonlinear

terms, and is expressed through a procedure which involves a series expansion using global approximating functions, and the application of reciprocity rules [20].

In the first part of the thesis, the DRBEM is described for the Poisson equation [20]. Then, the method is extended to a more general case in which the right-hand side of the governing equation is taken as an unknown nonlinear function of the problem variable as well as a function of time derivatives and space. The right-hand side is approximated using several types of radial basis functions (linear, exponential and rational) [20, 21, 22, 23] suitable for the problems defined in both finite and infinite regions. Then, the DRBEM formulations are given for the initial and mixed type boundary value problems defined by the nonlinear reaction-diffusion and wave equations. The latter problem is defined in an exterior region and the advantage of using DRBEM in such domains is made use of. In the applications, the numerical solutions to initial and boundary value problems defined by the nonlinear reaction-diffusion and nonlinear wave equations are considered. First, the nonlinear reaction-diffusion problem in a rectangular region with mixed type boundary conditions is solved. Next, two problems are given in terms of system of nonlinear reaction-diffusion equations. The last application of this chapter is an initial and boundary value problem defined by the nonlinear wave equation given in a region which is outside of an obstacle.

DRBEM application to nonlinear reaction-diffusion and wave equations results with a nonlinear system of first and second order ordinary differential equations (ODEs) in time, respectively. The linerization is made, by taking the nonlinearity in the previous time level.

In the second part of the thesis, DQM is developed for the solution of equations containing Laplace operator on the left-hand side, and the right-hand side may be a function of first and second order time derivatives of the solution and nonlinearity. Then, corresponding DQM equations for the nonlinear reaction-diffusion and wave equations are derived. Since DQM is a domain discretization method, the resulting linear ordinary differential equations in time are obtained

in terms of matrix-matrix equations, instead of matrix-vector equations as in the case of DRBEM. Then, the equations are reorganized as the matrix-vector equations to be able to apply a time integration method.

Although DQM is a domain discretization method, it gives the advantage of using small number of freedom comparing to DRBEM. The computational domain is discretized using Chebyshev-Gauss-Lobatto (CGL) points, which leads to stable solutions [14]. In the applications, the initial and boundary value problems defined by the nonlinear reaction-diffusion and wave equations are solved. The applications are limited to finite rectangular domains for initial and boundary value problems.

The obtained linear system of differential equations in time after the space discretizations require a time integration scheme for obtaining the solution at the desired time level or at steady-state. There are several time integration methods to treat these ODEs such as FDM, least squares method (LSM), FEM, DQM etc.

Throughout the thesis, three different time integration schemes are used, FDM, LSM and FEM. A comparison among the methods is made and the superiority of the methods is discussed in terms of accuracy.

The explicit FDMs (forward and central differences for the nonlinear reaction-diffusion and wave equations, respectively) are used for the solution of ODEs. Since explicit methods may lead to instabilities and need small time increments, a relaxation procedure [20] is used for the solutions which is a linear approximation for the variation of the solution in time.

The application of LSM for the ODEs resulting from the one-dimensional transient problems was first formulated in 1974 in [24] and since then it is used in several studies (e.g. [25, 26, 27, 28]). The method approximates the unknown function, which now depends on time only after the space discretization, by using interpolation functions of time. Then, the residual vector is obtained using this approximate solution and the error functional is constructed in terms of the residual vector. The method is based on the idea of minimizing the error func-

tional with respect to the unknown (either the solution or its normal derivative on the boundary depending on the boundary conditions and the solution itself in the interior domain).

The same initial value problems are solved also by using the FEM. The time domain is divided into finite elements. This method is a direct method for the solution but since the nonlinearity is taken in the previous time level, we prefer to apply the method in the selected time intervals and use the found values from the previous time interval as the initial values.

The DQM may also be used for the time integration and it is used in [29, 30] as a time integration scheme for the system of ODEs in time resulting from the DRBEM application in space variables. As in the FEM it gives the solutions at once.

1.1.2   Cauchy Problems

The Cauchy problems

$$
\begin{cases}
\dfrac{\partial^i u(x,t)}{\partial t^i} = \kappa \dfrac{\partial^2 u(x,t)}{\partial x^2} + p(u(x,t)) & x \in \mathbb{R} \\[4mm]
\dfrac{\partial^{k-1} u(x,0)}{\partial t^{k-1}} = u_{k-1}(x) & x \in \mathbb{R} \qquad k = 1, i
\end{cases}
\tag{1.9}
$$

defined by the one-dimensional nonlinear reaction-diffusion(i=1) and wave equations ($i = 2$) are solved. In equation (1.9) $u_{k-1}(x)$ (k=1 or k=1,2 for the non-linear reaction-diffusion and nonlinear wave equations, respectively) are known functions of space, p is the given nonlinear function and κ denotes the diffusivity constant ν or the square of the wave speed c for the nonlinear reaction-diffusion and wave equations, respectively.

The Cauchy problems do not involve boundary conditions and are not easy to treat. DRBEM and the domain discretization methods other than DQM require the implementation of boundary conditions. The DRBEM also is not suitable

for such one-dimensional problems, since boundary of the computational domain consists of only two points.

In the second part of the thesis, the DQM is applied for the one-dimensional Cauchy problems in the form of problem (1.9). Quite small number of discretization points are seen to be enough to obtain the solution. In all the applications the CGL points are used. Then, the obtained time dependent system of ODEs, which is first or second order for the nonlinear reaction-diffusion or nonlinear wave equations, respectively are solved using three different time integration schemes, FDM, LSM and FEM. The comparison among the methods is made in terms of accuracy.

1.2   Review of the Existing Literature

Solving the nonlinear reaction-diffusion equation has attracted much interest for a long time and several numerical methods have been developed over the last four decades.

In the early work of Gazdag and Canosa in 1974 [31] Fisher equation was solved by finite Fourier series for the numerical evaluation of the space derivative which is called accurate space derivative method. It has been shown that the accuracy of this approach is orders of magnitude higher than that obtained by using FDM for space derivatives. In [32, 33, 34] and [35] FDM was made use of for solving one-dimensional Fisher equation and system of Fisher equations, respectively. They have used nonstandard FDM to eliminate instabilities. For the Fisher equation Carey and Shen have developed a least squares finite element formulation in space, combined with the Euler scheme in time, which produces stable results for the test cases investigated [36]. Viability of the moving mesh finite difference methods for the traveling wave solutions of Fisher's equation was investigated in [37], and it has been shown that equidistribution of arc-length or curvature is not suitable. The nonstandard finite difference schemes preserving the positivity property of the solution have been used for the system of one-dimensional reaction-diffusion equations, and the functional relation between

the space and time step sizes has been determined in the paper of Mickens' [35]. Then, the comparison between the nodal integral method and nonstandard finite difference schemes has been made using the Fisher equation as a model problem [38]. In [39], the Sinc collocation method has been used to solve the Fisher equation and the error in the approximation of the solution has been shown to converge at an exponential rate. Another comparison among the discrete singular convolution and three other time integration schemes (Accurate space derivative method, Fourier pseudospectral method and Crank-Nicolson scheme) has been made in [40]. In [41], the noniterative exponential time-linearization and the iterative exponential quasilinearization techniques for one-dimensional reaction-diffusion equations based on the discretization of the time derivative have been presented and applied to the Nagumo and Fisher equations. The Fisher-Kolmogorov equation has been solved numerically by Mittal and Kumar [42] using wavelet Galerkin method and their results have been seen to be available for the large values of linear growth rate (the linear reproduction rate given in equation (1.4)). Branco et al. [43] have proposed numerical methods for solving integro-differential equations which generalize the Fisher equation (one-dimensional nonlinear reaction-diffusion equation). The stability and convergence of the methods are studied. In the latest two studies [44, 45], the numerical solution of one-dimensional nonlinear reaction-diffusion equation is given by using, the finite volume method and proper orthogonal decomposition method, respectively.

The two-dimensional nonlinear reaction-diffusion equation has been discretized by Galerkin FEM spatially leading to a nonlinear ODE system with quite large size, and the solution of Fisher equation has been obtained using a standard ODE solver in [46]. The travelling wave solutions of two-dimensional nonlinear reaction-diffusion (quadratic Fisher equation in two spatial dimensions) equation have been studied by Brazhnik and Tyson [47], and the existence of several other traveling waves with nontrivial front geometry along with a plane wave has been shown. FDM (An extended trapezoidal formula) is used in both directions for the solutions of two-dimensional linear diffusion, convection-diffusion and nonlinear reaction-diffusion equations [48]. This locally one-dimensional time

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integration scheme is unconditionally stable.

A class of a system of second order nonlinear reaction-diffusion equations in two-space dimensions known as Brusselator system has been solved in [49] using a linear combination of first-order finite difference schemes leading to a second-order approximations for the components of the solution. In [50], the one-dimensional systems of linear and nonlinear PDEs and the reaction-diffusion Brusselator model have been handled by Adomain decomposition method. The decomposition method has the advantage of being more coincise for analytical and numerical purposes. An efficient higher-order FDM has been presented for the system of two-dimensional nonlinear reaction-diffusion equations, and the method has been found fourth-order accurate in both the temporal and spatial dimensions [51]. The DRBEM has been used for the spatial discretization of the two-dimensional Brusselator system by Ang [52]. In this study, a predictor-corrector approach has been adopted by using finite difference approximations for the time derivatives to linearize the nonlinear terms. Then, DRBEM idea has constituted a linear system of algebraic equations. The Galerkin finite element method has been used for the spatial discretization of the solution of one-dimensional reaction-diffusion equations combined with the first- and second-order semi-implicit, fully-implicit, operator splitting time integration techniques in [53]. The variational iteration method has also been used for three different kinds of nonlinear PDEs including the system of nonlinear reaction-diffusion equations [54].

One of the earliest work by Strauss and Vazquez [55] for the numerical solution of one-dimensional nonlinear wave equation used the implicit FDM and Newton's method to solve the resulting system. Later in [21] the two-dimensional linear wave equation has been solved in an infinite domain using DRBEM with rational type radial basis functions. A FEM has been used for the solution of the nonlinear exterior wave problems in [56]. In their solution procedure the infinite domain is divided into two parts (finite and infinite) with an artificial boundary between them. By analyzing the problem in infinite domain a Dirichlet to Neumann relation is derived on the artificial boundary, then a new well-posed problem is obtained in the finite domain. The multisympletic structure of the

nonlinear Klein-Gordon equation was derived directly from the variational principle by Wang and Quin [57], and the higher order and Fourier pseudospectral multi-sympletic schemes, which satisfy the multi-sympletic conservation law, were used in [58] and [59], respectively. The Adomain decomposition method was implemented to one-dimensional nonlinear Klein-Gordon equation, and the convergence of the method was proved in [60]. Existence and uniqueness of the solution of the special type of the nonlinear wave equation, the damped Klein-Gordon equation with damping term $(\frac{\partial y}{\partial t})$ have been established, and a numerical method has been developed based on FEM in [61]. The same equation has also been solved using a method based on variational method and FEM approach for the space discretization [62]. In this study, the Gauss-Legendre quadrature has been utilized for numerical integrations of nonlinear terms, and Runge-Kutta method is used for solving resulting ODEs in time. Yusufoğlu [64] has used He's variational iteration method for solving the linear and nonlinear Klein Gordon equation. Bratsos [65] proposed a three-time-level finite difference scheme based on a fourth-order rational approximant to the matrix-exponential term for the solution of sine-Gordon equation. Then, the obtained second order system of ODEs was solved using a predictor-corrector scheme. Differential transform method for solving linear and nonlinear Klein-Gordon equations has been implemented in [66]. The Adomain decomposition method has been used to solve nonlinear Klein-Gordon equation in [67].

1.3 Plan of the Thesis

In Chapter 2, the combinations of the dual reciprocity boundary element method with three different time integration methods (FDM, LSM and FEM) are introduced for solving the initial and boundary value problems defined by the nonlinear reaction-diffusion and wave equations. The DRBEM is used for the discretization of the spatial domain by taking the solution and its normal derivative values as unknowns on the boundary nodes. Solution can also be obtained at any required interior point. The DRBEM is applied using the fundamental solution of Laplace equation keeping the time derivative and the nonlinear func-

tion as the nonhomogenity. The corresponding formulations are derived for the initial and mixed-type boundary value problems in finite domains in the case of the nonlinear reaction-diffusion equation (Section 2.2) and for the initial and boundary value problems defined by the nonlinear wave equation in infinite regions (Section 2.3). The formulations are extended to the system of nonlinear reaction-diffusion equations in Section 2.5. The advantage of using DRBEM in infinite domains is made use of in solving nonlinear wave equation in an exterior domain. The nonlinear wave equation is solved using three different radial basis functions, linear, exponential and rational radial basis functions. The former is known to be not suitable to the nature of the problem, since it tends to infinity for the points far enough from the obstacle boundary. It was possible to obtain results even with linear radial basis functions with the help of relaxation parameter in time discretization. The other radial basis functions are suitable for infinite regions. The DRBEM solution of all of these problems result with the time dependent system of ODEs. The corresponding first-order system of ODEs for the nonlinear reaction-diffusion equation is solved using three different time integration methods, FDM, LSM and FEM. For the solution of ODEs obtained after DRBEM discretization of the nonlinear wave equation, FDM and LSM are made use of. In all these solution procedures, the linearization for the system of ODEs obtained from the DRBEM application, is made via taking the nonlinear function at the previous time level. The applications of the proposed methods are given in Section 2.6. These methods are applied initially to nonlinear reaction-diffusion equation in a unit square . Then, the method is applied to two systems of nonlinear reaction-diffusion equations. The first system contains an exact solution and thus the comparison among the solutions is made in terms of accuracy. Second system (Brusselator system) does not have an exact solution, but the solutions are seen to satisfy the expected behaviour of the solution. The last application in this chapter is the solution of nonlinear exterior wave equation in an infinite region, which is defined for the outside of an obstacle. In the application procedure, the above mentioned three different radial basis functions are used. The solution by using linear radial basis functions are only obtained using FDM with the help of relaxation parameter. The problem does not have an exact solution, either. The expected behaviour of the solution is seen to be

satisfied by all the methods with the proper radial basis functions used.

In Chapter 3, the one-dimensional Cauchy problems and the two-dimensional initial and boundary value problems for the nonlinear reaction-diffusion equations are solved using the combined application of DQM and the time integration methods FDM, LSM and FEM. The DQM is a suitable method for the one-dimensional Cauchy problems, since it may be used without boundary conditions. The corresponding formulations are derived through Sections 3.2-3.5. Numerical results are given in Section 3.6. Several test problems are solved (Problems 3.6.1-3.6.8). The comparison among the time integration methods is made.

Finally, in Chapter 4 the conclusions obtained in Chapters 2 and 3 are combined, and comparisons among the methods in space direction (DRBEM and DQM), and among the time integration methods (FDM, LSM and FEM) are given.

CHAPTER 2

THE DUAL RECIPROCITY BOUNDARY ELEMENT METHOD SOLUTION OF NONLINEAR REACTION-DIFFUSION AND WAVE EQUATIONS

The numerical solution of nonlinear reaction-diffusion equation and the nonlinear wave equation are demanding tasks, since they appear in many branches of science and engineering.

The governing equation for reaction-diffusion mechanisms are given by

$$\frac{\partial u}{\partial t} = p + \nabla(D\nabla u) \tag{2.1}$$

where D may be a function of x and u, and p a function of u, x and t [1, 68]. Diffusion of genetically engineered organisms in heterogeneous environments, effect of white and grey matter in the growth and spread of brain tumours are some of the areas where equation (2.1) models.

In an ecological context, the nonlinear term p could represent the birth-death process with the population density u. With logistic population growth $p = ru\left(1 - u/K\right)$ where r is the linear reproduction rate and K the carrying capacity of the environment, the resulting equation is the well known Fisher-Kolmogorov equation [1].

Nonlinear wave equation in an unbounded domain is also encountered in a variety of applications. The nonlinearity may originate from the material constitutive relations, from the large amplitude of the motion or from the presence of a variable boundary [56].

With such important applications, it is desirable to find efficient numerical solutions for these time dependent nonlinear partial differential equations. A number of combined methods for the time dependent partial differential equations is applied in the literature. For solving these problems classical methods discretize the spatial domain of the problem with one of the known methods such as boundary element method (BEM), finite element method (FEM), differential quadrature method (DQM) and finite difference method (FDM); then the resulting system of time dependent equations is solved by using the time integration schemes such as FDM, RKM (Runge-Kutta Method), LSM (Least Squares Method) etc.

In this chapter, the numerical solution of the system of nonlinear reaction-diffusion equations as well as the single nonlinear reaction-diffusion equation and the nonlinear exterior wave equation (defined in an exterior domain) are considered. The dual reciprocity boundary element method is explained in Section 2.1. The boundary integral equations and the DRBEM for the Poisson equation are derived in Sections 2.1.1 and 2.1.2, respectively. Then, in Section 2.1.4, the method is extended to a more general form where the right-hand side includes a function of position, time, the time derivative of the unknown function and a function containing unknown function. Thus, the right-hand side function may include a nonlinear term. In the solution procedure, the DRBEM is employed for the discretization of spatial partial derivatives. For the DRBEM discretization, the fundamental solution of the Laplace equation is used; the nonlinearity, and the time derivatives which are first and second order for the nonlinear reaction-diffusion and wave equations respectively, are treated as the nonhomogenity. The usage of the fundamental solution of the Laplace equation gives the resulting DRBEM matrices in terms of integrals of logarithmic function and its normal derivative, which can be computed easily and accurately. The right-hand side function is approximated by using linear radial basis functions for the nonlinear reaction-diffusion and for the nonlinear exterior wave equations. Several kinds of radial basis functions are used for exterior wave equation in order to fulfill the regularity condition at infinity and the usage as well as the suitable choice among them are explained in Sections 2.1.3 and 2.3. The DRBEM application to the spatial derivatives results in a time dependent sys-

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tem of ordinary differential equations (ODE) of first and second order for the nonlinear reaction-diffusion and nonlinear wave equations, respectively. These systems of ODEs are then solved with three different time integration schemes: FDM, LSM and FEM, which are explained in Section 2.4. These schemes are used for the time integration in order to see the advantages and disadvantages of the methods, and make a comparison among the methods. In all time integration methods, the nonlinearity is evaluated at the previous time level and the combined application of the DRBEM with the mentioned time integration methods ends up with a linear system of equations. The resulting system of linear equations are solved by using any direct method (Gaussian type) to have the solution at any required time level at the discretized nodal space points, iteratively. The FEM as applied to the system of initial value problems is described in Section 2.4.5, and it needs less iteration comparing to the other two time integration methods, since it divides the time interval into blocks and the iteration is run between these blocks. Section 2.5 contains DRBEM application to the system of nonlinear reaction-diffusion equations with above mentioned time integration schemes. The applications of the proposed methods including the comparison among them are made in Section 2.6 by solving several test problems for the nonlinear reaction-diffusion equation, and the DRBEM with the combination of FDM and LSM is applied to a test problem in an exterior region using different radial basis functions.

2.1 The Dual Reciprocity Boundary Element Method

The boundary element method is a well established numerical technique, that leads numerical solutions to a wide range of problems in science and engineering [20]. The main advantage of the method is that it provides the solution in terms of boundary values only which needs less computational time and data preparation effort.

However, the BEM applications always require the fundamental solution of the original differential equation in order to have boundary integrals only in the formulation, which is one of the disadvantage of the method. In many cases,

especially for the nonlinear equations, it is hard to find a fundamental solution and the BEM discretization of the problem ceases with not only the boundary integrals but also with the domain integrals. This implies an internal discretization which increases the amount of needed data to run the program substantially and the method loses its attraction in this case.

One of the techniques, which enables a "boundary only solution" and does not depend on obtaining a fundamental solution is the dual reciprocity boundary element method. This is a very useful technique to treat the domain integral without discretizing the domain. It depends on the approximation of the integrand using radial basis functions and converts the domain integral into the boundary integral at the selected points in the domain as well as on the boundary.

In this section, the dual reciprocity boundary element method will be explained for the Poisson equation, in which the nonhomogenity is a known function of space. Moreover, the method will be extended to the time dependent nonlinear problems, where nonhomogeneous term may also be a function of the unknown function of the problem as well as a function of space and time.

2.1.1 Boundary Integral Equation for the Poisson Equation

In this section, the boundary integral equations are going to be derived for the Poisson equation as in [69]. The Poisson equation is given by

$$\nabla^2 u = b(x, y) \qquad \text{in} \quad \Omega \tag{2.2}$$

with the following boundary conditions:

$$
\begin{aligned}
&\text{i. } \textit{Essential} \text{ conditions of the type} \qquad u = \bar{u} \text{ on } \Gamma_1 \\
&\text{ii. } \textit{Natural} \text{ conditions such as,} \qquad q = \frac{\partial u}{\partial n} = \bar{q} \text{ on } \Gamma_2
\end{aligned}
\tag{2.3}
$$

where $\nabla^2 = \dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2}$ is the Laplace operator, n is the outward normal to the

boundary $\Gamma = \Gamma_1 + \Gamma_2$ of Ω, and the bars indicate known values. In equation (2.2), $b(x, y)$ denotes a known function of position.

In order to find the boundary integral equation corresponding to Poisson equation, one should multiply the equation by the fundamental solution of Laplace equation which is denoted by u^*. The fundamental solution u^* satisfies Laplace's equation and represents the field generated by a concentrated unit charge acting at a point i. The effect of this charge is propagated from i to infinity without any consideration of boundary conditions. Thus, the solution can be written

$$\nabla^2 u^* + \Delta^i = 0 \tag{2.4}$$

where Δ^i represents the Dirac delta function which tends to infinity at the point $x = x_i$ and is equal to zero everywhere else. The integral of Δ^i over the domain is equal to one. Moreover, the integral of the Dirac delta function multiplied by any other function is equal to the value of the latter at the point i (x_i).

For a two-dimensional isotropic domain the fundamental solution of equation (2.4) is

$$u^* = \frac{1}{2\pi} \ln\left(\frac{1}{r}\right) \tag{2.5}$$

where r is the distance from the point i of application of the delta function to any point under consideration.

When equation (2.2) is multiplied by the fundamental solution of Laplace equation and integrated over the domain Ω, one obtains,

$$\int_\Omega (\nabla^2 u - b) u^* d\Omega = 0. \tag{2.6}$$

Integrating the equation (2.6) by parts in x and y twice gives,

$$\int_\Omega (\nabla^2 u^* u - b u^*) d\Omega + \int_\Gamma \frac{\partial u}{\partial n} u^* d\Gamma - \int_\Gamma u \frac{\partial u^*}{\partial n} d\Gamma = 0. \tag{2.7}$$

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If one makes use of the boundary conditions given in equation (2.3)

$$\int_\Omega (\nabla^2 u^*) u\, d\Omega - \int_\Omega b u^*\, d\Omega = \quad -\int_{\Gamma_2} \bar{q} u^*\, d\Gamma - \int_{\Gamma_1} q u^*\, d\Gamma$$

$$+ \int_{\Gamma_2} u q^*\, d\Gamma + \int_{\Gamma_1} \bar{u} q^*\, d\Gamma$$

(2.8)

where $q^* = \dfrac{\partial u^*}{\partial n}$. After using the properties of the fundamental solution of Laplace equation and grouping all the boundary terms together (i.e. in $\Gamma = \Gamma_1 + \Gamma_2$) equation (2.8) gives the boundary integral equation for the Poisson equation at the point i

$$c_i u_i + \int_\Gamma u q^*\, d\Gamma + \int_\Omega b u^*\, d\Omega = \int_\Gamma q u^*\, d\Gamma. \tag{2.9}$$

with the constant c_i

$$c_i = \begin{cases} \dfrac{\theta_i}{2\pi}, & \text{if } i \in \Gamma \\[2em] 1, & \text{if } i \in \Omega/\Gamma \end{cases} \tag{2.10}$$

where θ_i denotes the internal angle at the point i in radians.

The domain integral in (2.9) due to the right-hand side function $b(x, y)$ in (2.2) is also going to be transformed to boundary integrals with the help of the dual reciprocity boundary element method.

2.1.2 DRBEM for the Poisson Equation

The dual reciprocity boundary element method is explained for the boundary value problem defined by the Poisson equation (2.2) following the reference [20].

The solution to equation (2.2) can be expressed as the sum of the solution of the Laplace equation and a particular solution $\hat{u}$ to (2.2) such that

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$$\nabla^2 \hat{u} = b. \tag{2.11}$$

It is generally difficult to find a particular solution $\hat{u}$, especially in the case of nonlinear or time dependent problems. The DRBEM proposes the use of a series of particular solutions $\hat{u}_j$ instead of a single function $\hat{u}$. The number of $\hat{u}_j$ used is equal to the total number of points to be used in the region of the problem.

The following approximation for b is then proposed

$$b \approx \sum_{j=1}^{N+L} \alpha_j f_j \tag{2.12}$$

where the α_j are a set of initially unknown coefficients and the f_j are the approximating or interpolating functions. The values N and L are the numbers of boundary and internal points (nodes), respectively, which are going to be used in the boundary discretization and inside evaluations. The particular solutions $\hat{u}_j$, and the approximating functions f_j, are linked through the relation

$$\nabla^2 \hat{u}_j = f_j. \tag{2.13}$$

The functions f_j are only geometry-dependent and there is no restriction on these functions. In fact, many different types may be used, each of which results in a different function $\hat{u}_j$ as determined from equation (2.13).

Substituting equation (2.13) into equation (2.12) yields

$$b = \sum_{j=1}^{N+L} \alpha_j \nabla^2 \hat{u}_j \tag{2.14}$$

which can be substituted into the boundary integral equation (2.9) to give the following expression

$$c_i u_i + \int_\Gamma u q^* d\Gamma - \int_\Gamma u^* q d\Gamma = -\sum_{j=1}^{N+L} \alpha_j \int_\Omega (\nabla^2 \hat{u}_j) u^* d\Omega. \tag{2.15}$$

Integration by parts can be used twice for the right-hand side of equation (2.15) which produces the following integral equation for each source node i,

$$c_i u_i + \int_\Gamma u q^* d\Gamma - \int_\Gamma u^* q d\Gamma = \sum_{j=1}^{N+L} \alpha_j (c_i \hat{u}_{ij} + \int_\Gamma q^* \hat{u}_j d\Gamma - \int_\Gamma u^* \hat{q}_j d\Gamma). \quad (2.16)$$

The term $\hat{q}_j$ is defined as $\hat{q}_j = \dfrac{\partial \hat{u}_j}{\partial n}$, where n is the unit outward normal to Γ, and given by

$$\hat{q}_j = \frac{\partial \hat{u}_j}{\partial x}\frac{\partial x}{\partial n} + \frac{\partial \hat{u}_j}{\partial y}\frac{\partial y}{\partial n}. \quad (2.17)$$

The domain integral due to the source term b in equation (2.9) has been substituted by equivalent boundary integrals and consequently equation (2.16) involves no domain integrals. This is achieved by first approximating b using equation (2.14) and then expressing both right- and left-hand sides of the resulting expression as boundary integrals using integration by parts twice.

Equation (2.16) can be discretized to obtain a system of linear equations. Assume that the boundary of the two-dimensional domain Ω is divided into N segments or elements. The points where the unknown values are considered are called "nodes" and taken to be in the middle of the element for the so-called constant elements, which are used in the applications of the thesis. In the case of the constant elements the values of u and q are assumed to be constant over each element and equal to the value at the mid-element node. The points on the extreme of the elements are used only for defining the geometry of the problem.

The u and q values can be taken out of the integrals, since they are assumed to be constant over each element. This gives for a source node i the expression

$$c_i u_i + \sum_{k=1}^{N} u_k \int_{\Gamma_k} q^* d\Gamma - \sum_{k=1}^{N} q_k \int_{\Gamma_k} u^* d\Gamma =$$

$$\sum_{j=1}^{N+L} \alpha_j \left(c_i \hat{u}_{ij} + \sum_{k=1}^{N} \int_{\Gamma_k} q^* \hat{u}_j d\Gamma - \sum_{k=1}^{N} \int_{\Gamma_k} u^* \hat{q}_j d\Gamma \right) \tag{2.18}$$

for $i = 1, 2, ..., N$.

There is no need to approximate the variation of $\hat{u}$ and $\hat{q}$ within each boundary element by using interpolation functions and nodal values as done for u and q, since they are known functions once f is defined.

After integrating over each boundary element with the substitution of the fundamental solution u^* and its normal derivative q^*, equation (2.18) can be written in terms of nodal values as

$$c_i u_i + \sum_{k=1}^{N} H_{ik} u_k - \sum_{k=1}^{N} G_{ik} q_k = \sum_{j=1}^{N+L} \alpha_j \left(c_i \hat{u}_{ij} + \sum_{k=1}^{N} H_{ik} \hat{u}_{kj} - \sum_{k=1}^{N} G_{ik} \hat{q}_{kj} \right)$$
$$i = 1, ..., N. \tag{2.19}$$

The index k is used for the boundary nodes which are the field points. After application to all boundary nodes using a collocation technique, equation (2.19) can be expressed in matrix-vector form as

$$\mathbf{Hu} - \mathbf{Gq} = \sum_{j=1}^{N+L} \alpha_j (\mathbf{H\hat{u}_j} - \mathbf{G\hat{q}_j}) \tag{2.20}$$

where

$$H_{ik} = \int_{\Gamma_k} q^* d\Gamma_k + c_i \delta_{ik} = \frac{1}{2\pi} \int_{\Gamma_k} \frac{(r - r_i).n}{|r - r_i|^2} d\Gamma_k + c_i \delta_{ik} \qquad i \neq k,$$

$$G_{ik} = \int_{\Gamma_k} u^* d\Gamma_k = \frac{1}{2\pi} \int_{\Gamma_k} \ln \frac{1}{|r - r_i|} d\Gamma_k \qquad i \neq k,$$

$$(2.21)$$

$$H_{ii} = c_i,$$

$$G_{ii} = \frac{l}{2\pi} (\ln \frac{2}{l} + 1)$$

with δ being the Kronecker delta function defined as

$$\delta_{ik} = \begin{cases} 1, & \text{if } i = k \\ \\ 0, & \text{if } i \neq k \end{cases}$$

for $i, k = 1, 2, ..., N$, and l is the element length, c_i are given in equation (2.10).

If each of the vectors $\hat{u}_j$ and $\hat{q}_j$ is considered to be one column of the matrices $\hat{U}$ and $\hat{Q}$ respectively, then equation (2.20) may be written without summation to produce

$$\mathbf{Hu} - \mathbf{Gq} = (\mathbf{H}\hat{\mathbf{U}} - \mathbf{G}\hat{\mathbf{Q}})\boldsymbol{\alpha}. \tag{2.22}$$

The sizes of the matrices $\mathbf{H}$ and $\mathbf{G}$ are $N \times N$ and $\hat{\mathbf{U}}$, $\hat{\mathbf{Q}}$ are $N \times (N + L)$, the vector $\boldsymbol{\alpha}$ is of size $(N + L) \times 1$. The vectors $\mathbf{u}$ and $\mathbf{q}$ are defined on the boundary with size $N \times 1$.

Equation (2.22) is the basic equation for the application of the DRBEM and involves discretization of the boundary only. The definition of interior nodes is not normally a necessary condition to obtain a boundary solution; however, the solution will usually be more accurate if a number of such nodes is used. An obvious situation where interior nodes are necessary in order to obtain a solution

arises if a homogeneous boundary condition is applied at all boundary nodes. When interior nodes are defined, each one is independently placed, and they do not form part of any element or cell, thus only the coordinates are needed as input data. Hence, they can be defined in any order.

The α vector in (2.22) can be computed by using the approximation (2.12) [20]. Since b is a known function of space one can take the value of b at $(N + L)$ different points leading to a set of equations which can be expressed in matrix form as

$$\mathbf{b} = \mathbf{F}\boldsymbol{\alpha} \tag{2.23}$$

where each column of $\mathbf{F}$ consists of a vector $\mathbf{f_j}$ containing the values of the function f_j at the $(N + L)$ DRBEM collocation points. Thus equation (2.23) may be inverted to obtain $\boldsymbol{\alpha}$, i.e.,

$$\boldsymbol{\alpha} = \mathbf{F}^{-1}\mathbf{b}. \tag{2.24}$$

Writing equation (2.22) as

$$\mathbf{Hu} - \mathbf{Gq} = \mathbf{d} \tag{2.25}$$

where

$$\mathbf{d} = (\mathbf{H}\hat{\mathbf{U}} - \mathbf{G}\hat{\mathbf{Q}})\mathbf{F}^{-1}\mathbf{b} \tag{2.26}$$

it is seen that the calculation of the vector $\mathbf{d}$ is a matter of the multiplication and subtraction of the known matrices $\mathbf{H}, \hat{\mathbf{U}}, \mathbf{G}, \hat{\mathbf{Q}}, \mathbf{F}^{-1}$ and the known vector $\boldsymbol{b}$.

The values at any internal point i can be calculated from equation (2.19) with $c_i = 1$ as

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

$$i = 1, ..., L$$

$$(2.27)$$

and it can be written in the matrix-vector form

$$\mathbf{Iu}^i = \mathbf{Gq} - \mathbf{Hu} + (\mathbf{H\hat{U}} - \mathbf{G\hat{Q}})\boldsymbol{\alpha} + \mathbf{\hat{U}}^i\boldsymbol{\alpha}. \tag{2.28}$$

Here $\mathbf{I}$ is the $L \times L$ identity matrix, $\mathbf{G}$, $\mathbf{H}$ are now $L \times N$ and $\mathbf{\hat{U}}$, $\mathbf{\hat{Q}}$ are $N \times (N+L)$ matrices; $\mathbf{u}$, $\mathbf{q}$, and α are vectors of length N and $(N + L)$, respectively. $\boldsymbol{u}^i$ vector contains computed interior values and of size $L \times 1$ and the matrix $\boldsymbol{\hat{U}}^i$ is formed from $(N + L)$ columns computed at L interior points, thus has the size $L \times (N + L)$. The $\mathbf{H}$ and $\mathbf{G}$ matrices are produced by integrating over the boundary by taking the distance r from each internal node and are not, therefore, the same partitions of $\mathbf{H}$ and $\mathbf{G}$ given in (2.22).

Equation (2.22), the system for the boundary nodes can be schematized in Figure 2.1 and Figure 2.2 gives the schema for the system (2.28) which is obtained for interior points [20].

Figure 2.1:   Matrix-vector equations for boundary nodes

Figure 2.2:   Matrix-vector equations for interior nodes

The last term in the second schema, Figure 2.2, is extremely important. It is an extra term, since it does not come out on the right-hand side of the first schema. It is generated by the term $\alpha_j \hat{u}_{ij}$ of equation (2.27) and it can be incorporated onto the main diagonal of $\mathbf{H}$. At this point, one starts to see the superiority of the DRBEM to the BEM, since the matrix-vector equations in these two schemas, Figure 2.1 and Figure 2.2 can be combined in a third schema (Figure 2.3).

The abbreviations BS and IS for the matrix blocks in the third schema (Figure (2.3)) are used for the boundary and interior solutions, respectively. Thus, equations (2.22) and (2.28) can be represented together by the matrix-vector equation

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$$\mathbf{Hu} - \mathbf{Gq} = (\mathbf{H}\hat{\mathbf{U}} - \mathbf{G}\hat{\mathbf{Q}})\boldsymbol{\alpha} \qquad (2.29)$$

with the third schema (Figure 2.3). Now all the matrices are of size $(N + L) \times (N + L)$ and vectors are of size $(N + L) \times 1$.

It can be seen from Figure 2.3 and equation (2.29) that, it is enough to use $(N + L)$ DRBEM collocation points in order to obtain the solution at boundary and interior nodes at once using equation (2.29), which is one of the main advantages of the method comparing to the BEM.

Figure 2.3:   Final DRBEM matrix-vector equations

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2.1.3 Different f Expansions

The particular solution $\hat{u}$, its normal derivative $\hat{q}$ and the corresponding approximating functions f used in DRBEM formulation should be chosen in such a way that the resulting matrix $\mathbf{F}$ in (2.23) should be nonsingular. Many types of f may be proposed. f is given in terms of the distance functions r, used in the definition of the fundamental solution (2.5), which is found to be the simplest and most accurate alternative.

If the approximating functions f_j are distance or radial basis functions of the form

$$f = 1 + r + r^2 + ... + r^m \tag{2.30}$$

where r is the distance between the fixed and the field points, then it can be shown that the corresponding $\hat{u}$ and $\hat{q}$ functions are obtained using equation (2.13) in the form

$$\hat{u} = \frac{r^2}{4} + \frac{r^3}{9} + ... + \frac{r^{(m+2)}}{(m+2)^2} \tag{2.31}$$

and

$$\hat{q} = (\frac{r}{2} + \frac{r^2}{3} + ... + \frac{r^{m+1}}{(m+2)})\frac{\partial r}{\partial n}. \tag{2.32}$$

In principle, any combination of terms may be selected from equation (2.30). In all cases, however, results are found to differ little from those obtained using $f = 1 + r$ which is the simplest alternative [20].

As can be seen, for the bounded domains the choice of the radial basis functions is quite arbitrary and the simple ones should be preferred. However, for the unbounded domains, this is not the case and one can not be free to choose these functions. They should be chosen in such a way that the far field contribution vanishes,i.e., [21, 22, 23]

$$\lim_{\Gamma \to \infty} \int_{\Gamma_\infty} (\hat{u}q^* - \hat{q}u^*)d\Gamma_\infty = 0 \tag{2.33}$$

and thus the only contribution is coming from the inner boundary.

For the solution of the nonlinear wave equation in an infinite region, two different kinds of radial basis functions are used [21, 22, 23] and they are given with the corresponding $\hat{u}$ and $\hat{q}$ functions as,

$$f = \frac{2c - r}{(r + c)^4}, \quad \hat{u} = -\frac{c + 2r}{2(r + c)^2}, \quad \hat{q} = \frac{r}{(r + c)^3}\frac{\partial r}{\partial n} \tag{2.34}$$

and

$$f = \exp(-r^2), \quad \hat{u} = \frac{1}{4}(\ln r^2 + E_1(r^2)), \quad \hat{q} = \frac{1}{2r}(1 - \exp(-r^2))\frac{\partial r}{\partial n} \tag{2.35}$$

where c is an arbitrary constant and E_1 is the exponential integral given by [23]

$$E_1(X) = \int_X^\infty \frac{\exp(-t)}{t}dt. \tag{2.36}$$

The choice of the radial basis functions as in (2.34) and (2.35) gives the opportunity to eliminate the boundary integral coming from far field boundary by the decay of functions $\hat{u}$ and $\hat{q}$ in the far boundary.

2.1.4   DRBEM for the Equation $\nabla^2 u = b(x, y, t, p(u), \dot{u}, \ddot{u})$

In this section the application of the DRBEM to the Poisson equation, which is described in the previous section, is extended to the problems governed by the equations [20]

$$\nabla^2 u = b(x, y, t, p(u), \dot{u}, \ddot{u}). \tag{2.37}$$

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Comparing to equation (2.2), in equation (2.37) the nonhomogenous term b now contains the time, a function of the unknown u itself, which means that the original partial differential equation may have a nonlinear term, and the first and second order time derivatives $\dot{u}$ and $\ddot{u}$, respectively.

Assume that b is given as a linear function of $p(u)$, $\dot{u}$, $\ddot{u}$ and thus can be written as

$$b = b_0(x, y) + b_1(x, y)p(u) + k_1\dot{u} + k_2\ddot{u} \qquad (2.38)$$

where b_0 and b_1 are functions of position, k_1 and k_2 are constants and $p(u)$ is the nonlinear function which is given in terms of the unknown u.

The function b can be approximated by means of a set of coordinate functions f_j as

$$b = b_0 + b_1 p(u) + k_1\dot{u} + k_2\ddot{u} \approx \sum_{j=1}^{N+L} \alpha_j(t)f_j(x, y) \qquad (2.39)$$

where α_j are unknown functions of time. The approximating functions are known functions of geometry and are linked with particular solutions $\hat{u}_j$ through $\nabla^2\hat{u}_j = f_j$. This relation between $\hat{u}_j$ and f_j gives the approximation in terms of a Laplacian operator for b in the form

$$b \approx \sum_{j=1}^{N+L} \alpha_j(t)\nabla^2\hat{u}_j. \qquad (2.40)$$

If we multiply both sides of equation (2.37) by the fundamental solution of the Laplace equation, integrate over the domain Ω and apply integration by parts twice, then follow the same steps as in Section 2.1.2, we obtain the matrix equation

$$\mathbf{Hu} - \mathbf{Gq} = (\mathbf{H\hat{U}} - \mathbf{G\hat{Q}})\boldsymbol{\alpha} \qquad (2.41)$$

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where the time dependent vector $\boldsymbol{\alpha}$ now is

$$\boldsymbol{\alpha} = \mathbf{F}^{-1}(k_1\dot{\mathbf{u}} + k_2\ddot{\mathbf{u}} + \mathbf{b_0} + \mathbf{B_1}\mathbf{p}(\mathbf{u})). \tag{2.42}$$

The matrices $\mathbf{H}$ and $\mathbf{G}$ whose entries are given in terms of the normal derivative of the fundamental solution and the fundamental solution itself, respectively, are given in equation (2.21).

In equations (2.41) and (2.42) , $\hat{\mathbf{U}}$, $\hat{\mathbf{Q}}$ and $\mathbf{F}$ compromise the columns $\hat{u}_j$, $\hat{q}_j$ and f_j at the $(N + L)$ nodal points , respectively, $\mathbf{b_0}$ is the vector with components $b_0\,(x_i, y_i)$ at the nodes $i = 1, ..., N + L$. The matrix $\mathbf{B_1}$ refers to the diagonal matrix with $b_1\,(x_i, y_i)$ on the diagonals $(i = 1, ..., (N + L))$ and is of the size $(N + L) \times (N + L)$. The $\mathbf{H}$ and $\mathbf{G}$ matrices are also extended to the sizes $(N + L) \times (N + L)$ as in the third schema (Figure 2.3).

Substituting the vector $\boldsymbol{\alpha} = \mathbf{F}^{-1}\mathbf{b}$ back into equation (2.41), one can obtain

$$\mathbf{C}(k_1\dot{\boldsymbol{u}} + k_2\ddot{\mathbf{u}}) + \mathbf{Hu} = \mathbf{Gq} - \mathbf{C}(\mathbf{b_0} + \mathbf{B_1}\mathbf{p}(\mathbf{u})) \tag{2.43}$$

where

$$\mathbf{C} = -(\mathbf{H}\hat{\mathbf{U}} - \mathbf{G}\hat{\mathbf{Q}})\mathbf{F}^{-1} \tag{2.44}$$

and $\mathbf{H}$, $\mathbf{G}$, $\hat{\mathbf{U}}$, $\hat{\mathbf{Q}}$, $\mathbf{C}$ are $(N + L) \times (N + L)$ matrices and $\mathbf{u}$ and $\mathbf{q}$ are $(N + L) \times 1$ vectors with N and L being the number of boundary and interior nodes, respectively. The $(N + L) \times 1$ vector $\boldsymbol{p}\,(\mathbf{u})$ is formed by evaluating $\boldsymbol{p}\,(\mathbf{u})$ at (x_i, y_i, t) $(i = 1, 2, ..., N + L)$ using a previously known solution vector $\boldsymbol{u}$.

2.2 The Dual Reciprocity Boundary Element Method Solution of Nonlinear Reaction-Diffusion Equation

The equation governing the nonlinear reaction-diffusion problem can be expressed as

$$\dot{u} = \nu\nabla^2 u + p(u) \qquad\qquad (2.45)$$

in a two-dimensional bounded domain Ω in $\mathbb{R}^2$ with the boundary Γ and ν is a nonzero constant (diffusivity constant).

Equation (2.45) subjects to the initial condition

$$u(x,y,0) = u_0(x,y) \qquad\qquad (x,y) \in \Omega \qquad\qquad (2.46)$$

and to the mixed type boundary conditions

$$\beta(x,y,t)u + \gamma(x,y,t)q = 0 \qquad\qquad (x,y) \in \Gamma, \ t > 0 \qquad (2.47)$$

where $q = \dfrac{\partial u}{\partial n}$, n being the outward normal to the boundary and $u_0(x,y)$, $\beta(x,y,t)$ and $\gamma(x,y,t) \neq 0$ are given functions.

If we put nonlinear reaction-diffusion equation in the form of Poisson equation, the nonhomogenity term b takes the form (taking $k_1 = 1/\nu$, $k_2 = 0$, $b_0(x,y) = 0$, $b_1(x,y) = -1/\nu$ in equation (2.38).)

$$b = \frac{1}{\nu}(\dot{u} - p(u)) \qquad\qquad (2.48)$$

Using a similar procedure as in Section 2.1.4 leads to the $(N+L) \times (N+L)$ system of matrix-vector equations

$$\mathbf{Hu} - \mathbf{Gq} = \frac{1}{\nu}(\mathbf{H\hat{U}} - \mathbf{G\hat{Q}})\boldsymbol{\alpha} \qquad\qquad (2.49)$$

where

$$\boldsymbol{\alpha} = \mathbf{F}^{-1}\mathbf{b} = \mathbf{F}^{-1}(\dot{\mathbf{u}} - \mathbf{p}(\mathbf{u})). \qquad\qquad (2.50)$$

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Substitution of $\boldsymbol{\alpha}$ in (2.49) gives

$$\mathbf{Hu} - \mathbf{Gq} = \frac{1}{\nu}(\mathbf{H\hat{U}} - \mathbf{G\hat{Q}})\mathbf{F}^{-1}(\dot{\mathbf{u}} - \mathbf{p(u)}). \tag{2.51}$$

Equation (2.51) can be rewritten to have

$$\mathbf{C\dot{u}} + \mathbf{Hu} = \mathbf{Gq} + \mathbf{Cp} \tag{2.52}$$

with

$$\mathbf{C} = -\frac{1}{\nu}(\mathbf{H\hat{U}} - \mathbf{G\hat{Q}})\mathbf{F}^{-1}. \tag{2.53}$$

The mixed type boundary conditions (2.47) are made use of to obtain the following system of ODE

$$\mathbf{C\dot{u}} + \mathbf{\bar{H}u} = \mathbf{Cp} \tag{2.54}$$

where

$$\mathbf{\bar{H}} = \mathbf{H} + \mathbf{GD} \tag{2.55}$$

with a diagonal matrix $\mathbf{D}$ defined as

$$\mathbf{D}_{ii} = \begin{cases} \dfrac{\beta_i}{\gamma_i} & i = 1, ..., N \\[2em] 0 & i = N+1, ..., N+L. \end{cases} \tag{2.56}$$

In equation (2.56) β_i and γ_i denote the values of the functions β and γ at the node i, respectively.

2.3 The Dual Reciprocity Boundary Element Method Solution of Nonlinear Wave Equation in an Infinite Region

The nonlinear scalar exterior wave equation can be described as

$$\ddot{u} = c^2 \nabla^2 u + p(u) \tag{2.57}$$

in a two dimensional infinite domain Ω in $\mathbb{R}^2$ which is the outside of an obstacle with boundary Γ_0, c is the wave speed, $u(x, y, t)$ is the unknown wave function and $p(u)$ is the nonlinear term.

Equation (2.57) is supplied with the Dirichlet and Neumann type boundary conditions

$$u(x, y, t) = \bar{u}(x, y, t) \quad (x, y) \in \Gamma_1, \quad t > 0$$

$$\tag{2.58}$$

$$q = \frac{\partial u}{\partial n} = \bar{q}(x, y, t) \quad (x, y) \in \Gamma_2, \quad t > 0$$

and with the initial conditions

$$u(x, y, 0) = u_0(x, y) \quad (x, y) \in \Omega$$

$$\tag{2.59}$$

$$\dot{u}(x, y, 0) = u_1(x, y) \quad (x, y) \in \Omega$$

for obtaining a well-defined problem. Here $\bar{u}$, $\bar{q}$ are given functions of space and time, and u_0, u_1 are given functions of space, n is the inward normal to the boundary $\Gamma_0 = \Gamma_1 + \Gamma_2$.

The nonhomogenity for the nonlinear wave equation now is in the form (taking $k_1 = 0$, $k_2 = 1/c^2$, $b_0(x, y) = 0$, $b_1(x, y) = -1/c^2$ in equation (2.38).)

$$b = \frac{1}{c^2}(\ddot{u} - p(u)). \tag{2.60}$$

With a similar procedure given in Section 2.1.4 the boundary integral equation for the problem (2.57- 2.59) can be obtained as

$$c^2(c_i u_i + (\int_{\Gamma_0} uq^* d\Gamma_0 - \int_{\Gamma_0} u^* q d\Gamma_0) + (\int_{\Gamma_\infty} uq^* d\Gamma_\infty - \int_{\Gamma_\infty} qu^* d\Gamma_\infty)) =$$

$$- \int_\Omega (\ddot{u} - p(u))u^* d\Omega$$

$$(2.61)$$

where Γ_0 is the boundary of the obstacle, which is the inner boundary of the exterior region Ω and Γ_∞ is the infinitely distant circular boundary. i is a point either on Γ_0 or in the exterior region.

As is indicated in Section 2.1.3, the choice of the interpolation functions f for unbounded domains can not be free. The first two integrals over the infinitely remote boundary on the left-hand side of equation (2.61) are zero. For a transient elastic wave propagation analysis this statement is verified by considering the behaviour of potential $u(x,t)$ and its normal derivative $q(x,t)$ beyond the wave front. In this case waves from infinity can not interfare in the analysis, because of causality principle [21].

The boundary condition can be restricted only to the boundary Γ_0, if the following condition is satisfied

$$\lim_{\xi \to \infty} \int_{\Gamma_\infty} (\hat{u}q^* - \hat{q}u^*) d\Gamma_\infty = 0 \qquad (2.62)$$

where ξ is the radius of the infinite circular region. For this, the radial basis functions should be chosen properly as described in Section 2.1.3. With rational and exponential radial basis functions given in (2.34) and (2.35) respectively, the boundary of the region can be taken as Γ_0. The nonhomogenity b given with (2.60) can be approximated with one of these radial basis functions given by equations (2.34) or (2.35) in the form

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$$b \approx \sum_{j=1}^{N+L} \alpha_j(t) f_j = \sum_{j=1}^{N+L} \alpha_j(t)(\nabla^2 \hat{u}_j). \tag{2.63}$$

When this approximation is substituted into the boundary integral equation (2.61), one has boundary integrals on both sides over the boundary Γ_0, i.e.,

$$c^2 \left(c_i u_i + \int_{\Gamma_0} u q^* d\Gamma_0 - \int_{\Gamma_0} u^* q d\Gamma_0 \right) =$$

$$\sum_{j=1}^{N+L} \alpha_j(t) \left(c_i \hat{u}_{ij} + \int_{\Gamma_0} q^* \hat{u}_j d\Gamma_0 - \int_{\Gamma_0} u^* \hat{q}_j d\Gamma_0 \right)$$

$$i = 1, ..., N + L$$

$$\tag{2.64}$$

where $\hat{q}_j = \dfrac{\partial \hat{u}_j}{\partial n}$, n being the inward normal to the boundary Γ_0. The point i is one of the inner boundary (Γ_0) node or one of these L scattered exterior node.

This equation can be written in matrix-vector form as

$$\mathbf{H}\mathbf{u} - \mathbf{G}\mathbf{q} = \frac{1}{c^2}(\mathbf{H}\hat{\mathbf{U}} - \mathbf{G}\hat{\mathbf{Q}})\boldsymbol{\alpha} \tag{2.65}$$

with the $(N+L) \times (N+L)$ matrices $\mathbf{H}$, $\mathbf{G}$, $\hat{\mathbf{U}}$, $\hat{\mathbf{Q}}$ and the $(N+L) \times 1$ vectors $\mathbf{u}$, $\mathbf{q}$ and $\boldsymbol{\alpha}$, which are obtained in a similar manner as in Section 2.1.4. The vector $\boldsymbol{\alpha} = \boldsymbol{F}^{-1}\mathbf{b}$ is now

$$\boldsymbol{\alpha} = \mathbf{F}^{-1}\mathbf{b} = \mathbf{F}^{-1}(\ddot{\mathbf{u}} - \mathbf{p}(\mathbf{u})). \tag{2.66}$$

Finally, the DRBEM formulation for the nonlinear exterior wave equation is obtained as

$$\mathbf{C}\ddot{\boldsymbol{u}} + \mathbf{H}\mathbf{u} = \mathbf{G}\mathbf{q} + \mathbf{C}\mathbf{p} \tag{2.67}$$

where

$$\mathbf{C} = -\frac{1}{c^2}(\mathbf{H}\hat{\mathbf{U}} - \mathbf{G}\hat{\mathbf{Q}})\mathbf{F}^{-1}. \tag{2.68}$$

2.4 Time Integration Methods

In this section, several time integration schemes (FDM, LSM, FEM) are applied to the system of ordinary differential equations (2.54) and (2.67) which are obtained after DRBEM discretization of the nonlinear reaction-diffusion and wave equations with the nonhomogenities (2.48) and (2.60), respectively.

2.4.1 FDM for the Time Discretization of the DRBEM Solution of Nonlinear Reaction-Diffusion Equation

The time dependent system of ODEs (2.54) can be written in the form

$$\dot{\mathbf{u}} = \bar{\bar{\mathbf{H}}}\mathbf{u} + \mathbf{p} \tag{2.69}$$

where $\bar{\bar{\mathbf{H}}} = -\mathbf{C}^{-1}\bar{\mathbf{H}}$ and $\mathbf{p}$ is the vector containing the nonlinearity at the discretized points.

The time derivative in this equation can be discretized explicitly or implicitly using low order finite difference schemes. We will employ a two-level explicit time integration scheme (Euler scheme)[20]

$$\dot{\mathbf{u}} = \frac{1}{\Delta t}(\mathbf{u}^{m+1} - \mathbf{u}^m) \tag{2.70}$$

where superscript m indicates the time level and Δt is the time step. Then equation (2.69) takes the form

$$\frac{1}{\Delta t}(\mathbf{u}^{m+1} - \mathbf{u}^m) = \bar{\bar{\mathbf{H}}}\mathbf{u}^m + \mathbf{p}(\mathbf{u}^m). \tag{2.71}$$

Since this is an explicit scheme, the stability problems can be encountered and Δt must be taken carefully. A relaxation procedure is employed to the right-hand side of (2.71) with a parameter $0 \leq \mu \leq 1$ for the unknown $\mathbf{u}$ in the form

$$\mathbf{u} = (1 - \mu)\mathbf{u}^m + \mu\mathbf{u}^{m+1} \tag{2.72}$$

positioning the values of $\mathbf{u}$ between the time levels m and $(m+1)$. Then equation (2.71) is written as

$$(\mathbf{I} - \mu\Delta t\bar{\bar{\mathbf{H}}})\mathbf{u}^{m+1} = (\mathbf{I} + \Delta t(1 - \mu)\bar{\bar{\mathbf{H}}})\mathbf{u}^m + \Delta t\mathbf{p}(\mathbf{u}^m). \tag{2.73}$$

This system gives the solution iteratively, using the values from m-th time level for the solution at $(m + 1)$-st time level. The nonlinearity $\mathbf{p}(\mathbf{u})$ is approximated only at the time level t^m in order to obtain a linear system of equations at the end.

2.4.2 FDM for the Time Discretization of the DRBEM Solution of Nonlinear Wave Equation in an Exterior Region

Equation (2.67) which is the DRBEM discretized form of nonlinear exterior wave equation can be written in the form

$$\ddot{\mathbf{u}} = \hat{\mathbf{H}}\mathbf{u} + \hat{\mathbf{G}}\mathbf{q} + \mathbf{p}(\mathbf{u}) \tag{2.74}$$

with $\ddot{\mathbf{u}}$ denoting the second order time derivative, $\mathbf{q} = \dfrac{\partial \mathbf{u}}{\partial \mathbf{n}}$, n being the inward normal to the obstacle boundary Γ_0, $\hat{\mathbf{H}} = -\mathbf{C}^{-1}\mathbf{H}$ and $\hat{\mathbf{G}} = \mathbf{C}^{-1}\mathbf{G}$. All the matrices in equation (2.74) are $(N + L) \times (N + L)$ and the vectors are of size $(N + L) \times 1$ where N is the number of boundary nodes on the obstacle boundary and L is the number of nodes in the exterior domain Ω.

Employing central difference for $\ddot{\mathbf{u}}$ i.e.,

$$\ddot{\mathbf{u}} = \frac{1}{\Delta t^2}(\mathbf{u}^{m+1} - 2\mathbf{u}^m + \mathbf{u}^{m-1}) \tag{2.75}$$

gives

$$\frac{1}{\Delta t^2}(\mathbf{u}^{m+1} - 2\mathbf{u}^m + \mathbf{u}^{m-1}) = \hat{\mathbf{H}}\mathbf{u}^m + \hat{\mathbf{G}}\mathbf{q}^{m+1} + \mathbf{p}(\mathbf{u}^m). \tag{2.76}$$

Employing a relaxation procedure in the form of equation (2.72) to equation (2.76) the solution is obtained iteratively from

$$(\mathbf{I} - \Delta t^2 \mu \hat{\mathbf{H}})\mathbf{u}^{m+1} = (2\mathbf{I} + \Delta t^2(1-\mu)\hat{\mathbf{H}})\mathbf{u}^m - \mathbf{u}^{m-1} + \Delta t^2 \hat{\mathbf{G}}\mathbf{q}^{m+1} + \Delta t^2 \mathbf{p}^m \tag{2.77}$$

where $\mathbf{p}^m = \mathbf{p}(\mathbf{u}^m)$.

Equation (2.77) gives the solution iteratively for $m = 1, 2, ...$. For $m = 0$ one should make use of the initial condition (i.e. equation (2.59)) in terms of the time derivative of the solution using the backward difference formula

$$\dot{\mathbf{u}}|_{t=0} = \frac{1}{\Delta t}(\mathbf{u}^0 - \mathbf{u}^{-1}) \tag{2.78}$$

and this leads to the matrix-vector equations for $m = 0$

$$(\mathbf{I} - \Delta t^2 \mu \hat{\mathbf{H}})\mathbf{u}^1 = (\mathbf{I} + \Delta t^2(1-\mu))\hat{\mathbf{H}}\mathbf{u}_0 + \Delta t \mathbf{u}_1 + \Delta t^2 \hat{\mathbf{G}}\mathbf{q}^1 + \Delta t^2 \mathbf{p}^0 \tag{2.79}$$

where $\mathbf{u}_0$, $\mathbf{u}_1$ and $\mathbf{p}^0$ are the vectors of length $(N + L) \times 1$ containing the initial conditions given in equation (2.59) and the nonlinearity, respectively. The solution then is obtained iteratively from equation (2.77) for $m = 1, 2, 3, ...$ In all steps, the nonlinearity is evaluated at the m-th (previous) time level and a linear system of equations are solved for the solution.

In solving the system (2.77) the unknowns $\mathbf{u}^{m+1}$ and $\mathbf{q}^{m+1}$ on the boundary are switched such that on the partition Γ_1, $\mathbf{q}^{m+1}$ and on the partition Γ_2, $\mathbf{u}^{m+1}$

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stay as unknowns, since they are given as boundary conditions on the other partitions.

2.4.3 LSM for the Time Discretization of the DRBEM Solution of Nonlinear Reaction-Diffusion Equation

In this section, a least squares method is applied to the time domain for the solution of the nonlinear reaction-diffusion equation which has been discretized spatially using DRBEM in Section 2.2.

The solution vector $\mathbf{u}$ of length $(N + L) \times 1$ of the system of ODEs given in equation (2.54) can be approximated in a typical element of length Δt [26]

$$\mathbf{u} \approx \phi_1(t)\mathbf{u}^m + \phi_2(t)\mathbf{u}^{m+1} \tag{2.80}$$

where superscripts m and $(m + 1)$ denote the time levels and ϕ_1, ϕ_2 are linear interpolation functions defined by

$$\phi_1(t) = \frac{t^{m+1} - t}{\Delta t}, \quad \phi_2(t) = \frac{t - t^m}{\Delta t}. \tag{2.81}$$

The residual vector is obtained on each time element by substituting the approximation (2.80) in equation (2.54), i.e.,

$$\mathbf{r}(t) = \mathbf{C}\dot{\mathbf{u}} + \bar{\mathbf{H}}\mathbf{u} - \mathbf{C}\mathbf{p}(\mathbf{u}). \tag{2.82}$$

The square of the error over the time element constructs the error functional Π, i.e.,

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$$\Pi = \int_{t^m}^{t^{m+1}} \mathbf{r}^T \mathbf{r} dt$$

or $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ (2.83)

$$\Pi = \int_{t^m}^{t^{m+1}} (\mathbf{C}\dot{\mathbf{u}} + \bar{\mathbf{H}}\mathbf{u} - \mathbf{C}\mathbf{p}(\mathbf{u}))^T (\mathbf{C}\dot{\mathbf{u}} + \bar{\mathbf{H}}\mathbf{u} - \mathbf{C}\mathbf{p}(\mathbf{u})) dt$$

over the m-th time element with the initial point t^m and the end point t^{m+1} (Figure 2.4). Introducing a new variable $\xi = \dfrac{t - t^m}{\Delta t}$ transforms the integrals over $[0,1]$

$$\Pi = \Delta t \int_0^1 (\mathbf{C}\dot{\mathbf{u}} + \bar{\mathbf{H}}\mathbf{u} - \mathbf{C}\mathbf{p}(\mathbf{u}))^T (\mathbf{C}\dot{\mathbf{u}} + \bar{\mathbf{H}}\mathbf{u} - \mathbf{C}\mathbf{p}(\mathbf{u})) d\xi. \qquad (2.84)$$
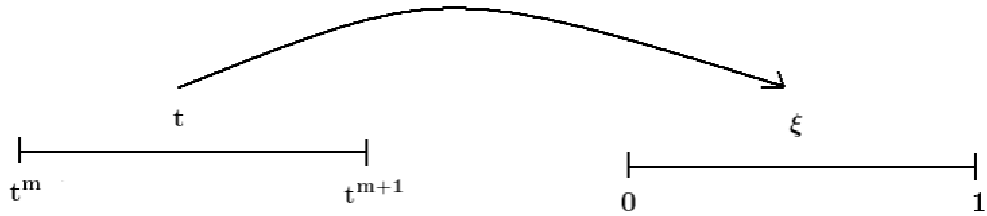

Figure 2.4:   A typical time element

The error functional Π can be calculated using the approximation (2.80) and its derivative $\dot{\mathbf{u}}$, i.e.,

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$$\dot{\mathbf{u}} = \dot{\phi}_1(t)\mathbf{u}^m + \dot{\phi}_2(t)\mathbf{u}^{m+1} \tag{2.85}$$

where

$$\dot{\phi}_1 = \frac{d\phi_1}{dt} = \frac{d\phi_1}{d\xi}\frac{d\xi}{dt} = -\frac{1}{\Delta t}$$

$$\dot{\phi}_2 = \frac{d\phi_1}{dt} = \frac{d\phi_2}{d\xi}\frac{d\xi}{dt} = \frac{1}{\Delta t}. \tag{2.86}$$

The desired recurrence relation between the m-th and $(m+1)$-st time levels is found by minimizing the error functional with respect to the unknown vector $\boldsymbol{u}^{m+1}$ in the following form,

$$\mathbf{A}\mathbf{u}^{m+1} = \mathbf{B_1}\mathbf{u}^m + \mathbf{B_2}\mathbf{p}^m \tag{2.87}$$

where

$$\mathbf{A} = \frac{1}{\Delta t^2}\mathbf{C}^T\mathbf{C} + \frac{1}{2\Delta t}(\mathbf{C}^T\bar{\mathbf{H}} + \bar{\mathbf{H}}^T\mathbf{C}) + \frac{1}{3}\bar{\mathbf{H}}^T\bar{\mathbf{H}}$$

$$\mathbf{B_1} = \frac{1}{\Delta t^2}\mathbf{C}^T\mathbf{C} - \frac{1}{2\Delta t}(\mathbf{C}^T\bar{\mathbf{H}} - \bar{\mathbf{H}}^T\mathbf{C}) - \frac{1}{6}\bar{\mathbf{H}}^T\bar{\mathbf{H}} \tag{2.88}$$

$$\mathbf{B_2} = \frac{1}{\Delta t}\mathbf{C}^T\mathbf{C} + \frac{1}{2}\bar{\mathbf{H}}^T\mathbf{C}$$

with the $(N+L) \times (N+L)$ matrices $\bar{\boldsymbol{H}}$ and $\boldsymbol{C}$ given in equations (2.55) and (2.44), respectively.

2.4.4 LSM for the Time Discretization of the DRBEM Solution of Nonlinear Wave Equation in an Exterior Region

In Section 2.3 the DRBEM solution of nonlinear wave equation in an exterior region is given as a system of second order ODEs in time (equation (2.67)). Space

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discretization is performed on the obstacle boundary of the exterior region Ω and at the points of the region itself. There, the system of ODEs is given as

$$\mathbf{C\ddot{u} + Hu = Gq + Cp} \tag{2.89}$$

with the matrix $\mathbf{C} = -\dfrac{1}{c^2}(\mathbf{H\hat{U} - G\hat{Q})F}^{-1}$ depending on the DRBEM matrices $\mathbf{H}, \ \mathbf{\hat{U}}, \mathbf{\hat{Q}}, \ \mathbf{F}$ given in Sections 2.1.2 and 2.1.3.

For the LSM discretization of the second order time derivative on the left-hand side of equation (2.89) the quadratic time element $\Omega_t^e = [t^{m-1}, t^{m+1}]$ is considered instead of the linear ones due to the second order time derivative.

The time dependent vectors $\boldsymbol{u}$ and $\boldsymbol{q}$ in equation (2.89), which have the discretized values at the $(N + L)$ DRBEM collocation points, can be approximated on a typical quadratic time element as [26]

$$
\begin{aligned}
\mathbf{u} &\approx \phi_{m-1}\mathbf{u}^{m-1} + \phi_m\mathbf{u}^m + \phi_{m+1}\mathbf{u}^{m+1} \\
\mathbf{q} &\approx \phi_{m-1}\mathbf{q}^{m-1} + \phi_m\mathbf{q}^m + \phi_{m+1}\mathbf{q}^{m+1}
\end{aligned} \tag{2.90}
$$

where

$$
\begin{aligned}
\phi_{m-1} &= \frac{1}{2\Delta t^2}(t - t^m)(t - t^{m+1}), \\[2mm]
\phi_m &= \frac{1}{\Delta t^2}(t^{m+1} - t)(t - t^{m-1}), \\[2mm]
\phi_{m+1} &= \frac{1}{2\Delta t^2}(t - t^m)(t - t^{m-1}).
\end{aligned} \tag{2.91}
$$

The error functional Π is constructed by using the residual vector

$$\mathbf{r = C\ddot{u} + Hu - Gq - Cp} \tag{2.92}$$

as

$$\Pi = \int_{t^{m-1}}^{t^{m+1}} \mathbf{r}^T \mathbf{r}\, dt \qquad (2.93)$$

over the m-th time element with the initial point t^{m-1} and the terminal point t^{m+1}. Introducing the variable $\xi = \dfrac{t - t^m}{\Delta t}$ again transforms the integral

$$\Pi = \Delta t \int_{-1}^{1} (\mathbf{C\ddot{u}} + \mathbf{Hu} - \mathbf{Gq} - \mathbf{Cp})^T (\mathbf{C\ddot{u}} + \mathbf{Hu} - \mathbf{Gq} - \mathbf{Cp})\, d\xi \qquad (2.94)$$

with the quadratic interpolation functions in terms of ξ as

$$\phi_{-1}(\xi) = \frac{1}{2}\xi(\xi - 1), \quad \phi_0(\xi) = (1 - \xi)(1 + \xi), \quad \phi_1(\xi) = \frac{1}{2}\xi(\xi + 1). \qquad (2.95)$$

The error functional Π can be calculated using the approximation vectors (2.90) and their derivatives which can be written

$$\ddot{\mathbf{u}} = \ddot{\phi}_{-1}\mathbf{u}^{m-1} + \ddot{\phi}_0\mathbf{u}^m + \ddot{\phi}_1\mathbf{u}^{m+1}$$

$$\ddot{\mathbf{q}} = \ddot{\phi}_{-1}\mathbf{q}^{m-1} + \ddot{\phi}_0\mathbf{q}^m + \ddot{\phi}_1\mathbf{q}^{m+1}$$

$$(2.96)$$

where

$$\ddot{\phi}_{-1} = \frac{1}{\Delta t^2}, \quad \ddot{\phi}_0 = -\frac{2}{\Delta t^2}, \quad \ddot{\phi}_1 = \frac{1}{\Delta t^2}. \qquad (2.97)$$

For the LSM solution procedure, one should minimize the error functional Π with respect to the unknown vectors $\mathbf{u}^{m+1}$ and $\mathbf{q}^{m+1}$. Thus, on the first part of the boundary Γ_1, Π is minimized with respect to $\mathbf{q}^{m+1}$, since the boundary conditions are of Dirichlet type and it is going to be minimized with respect to $\mathbf{u}^{m+1}$ on the second part of the boundary and for the nodes in the exterior region Ω. By equating the gradient vectors to zero

$$\frac{\partial \Pi}{\partial \mathbf{q}^{m+1}} = 0 \quad \text{on} \quad \Gamma_1$$

$$\tag{2.98}$$

$$\frac{\partial \Pi}{\partial \mathbf{u}^{m+1}} = 0 \quad \text{on} \quad \Gamma_2 \quad \text{and in} \quad \Omega$$

one has the final form of the linear system of equations in the form

$$\mathbf{A}\mathbf{q}^{m+1} = \mathbf{B_1}\mathbf{u}^{m-1} + \mathbf{B_2}\mathbf{u}^m + \mathbf{B_3}\mathbf{u}^{m+1} + \mathbf{B_4}\mathbf{q}^{m-1} + \mathbf{B_5}\mathbf{q}^m + \mathbf{B_6}\mathbf{p}^m$$

$$\tag{2.99}$$

$$\bar{\mathbf{A}}\mathbf{u}^{m+1} = \bar{\mathbf{B}}_1\mathbf{u}^{m-1} + \bar{\mathbf{B}}_2\mathbf{u}^m + \bar{\mathbf{B}}_3\mathbf{q}^{m+1} + \bar{\mathbf{B}}_4\mathbf{q}^{m-1} + \bar{\mathbf{B}}_5\mathbf{q}^m + \bar{\mathbf{B}}_6\mathbf{p}^m$$

on Γ_1, and on Γ_2 and in Ω respectively. The matrices in equation (2.99) are given in the form of the DRBEM matrices as

$$\mathbf{A} = \frac{4}{15}\mathbf{G}^T\mathbf{G}$$

$$\mathbf{B_1} = \frac{1}{3\Delta t^2}\mathbf{G}^T\mathbf{C} - \frac{1}{15}\mathbf{G}^T\mathbf{H}$$

$$\mathbf{B_2} = -\frac{2}{3\Delta t^2}\mathbf{G}^T\mathbf{C} + \frac{2}{15}\mathbf{G}^T\mathbf{H}$$

$$\tag{2.100}$$

$$\mathbf{B_3} = \frac{1}{3\Delta t^2}\mathbf{G}^T\mathbf{C} + \frac{4}{15}\mathbf{G}^T\mathbf{H}$$

$$\mathbf{B_4} = \frac{1}{15}\mathbf{G}^T\mathbf{G}$$

$$\mathbf{B_5} = -\frac{2}{15}\mathbf{G}^T\mathbf{G}$$

$$\mathbf{B_6} = -\frac{1}{3}\mathbf{G}^T\mathbf{C}$$

$$\bar{\mathbf{A}} = -\frac{1}{3\Delta t^2}\mathbf{C}^T\mathbf{H} - \frac{1}{3\Delta t^2}\mathbf{H}^T\mathbf{C} - \frac{2}{\Delta t^4}\mathbf{C}^T\mathbf{C} - \frac{4}{15}\mathbf{H}^T\mathbf{H}$$

$$\bar{\mathbf{B}}_1 = \frac{2}{\Delta t^4}\mathbf{C}^T\mathbf{C} + \frac{1}{3\Delta t^2}\mathbf{H}^T\mathbf{C} + \frac{1}{3\Delta t^2}\mathbf{C}^T\mathbf{H} - \frac{1}{15}\mathbf{H}^T\mathbf{H}$$

$$\bar{\mathbf{B}}_2 = -\frac{4}{\Delta t^4}\mathbf{C}^T\mathbf{C} - \frac{2}{3\Delta t^2}\mathbf{H}^T\mathbf{C} + \frac{4}{3\Delta t^2}\mathbf{C}^T\mathbf{H} + \frac{2}{15}\mathbf{H}^T\mathbf{H}$$

$$\bar{\mathbf{B}}_3 = -\frac{1}{3\Delta t^2}\mathbf{C}^T\mathbf{G} - \frac{4}{15}\mathbf{H}^T\mathbf{G}$$

$$\bar{\mathbf{B}}_4 = -\frac{1}{3\Delta t^2}\mathbf{C}^T\mathbf{G} + \frac{1}{15}\mathbf{H}^T\mathbf{G}$$

$$\bar{\mathbf{B}}_5 = -\frac{4}{3\Delta t^2}\mathbf{C}^T\mathbf{G} - \frac{2}{15}\mathbf{H}^T\mathbf{G}$$

$$\bar{\mathbf{B}}_6 = -\frac{1}{3}\mathbf{H}^T\mathbf{C} - \frac{2}{\Delta t^2}\mathbf{C}^T\mathbf{C}$$

2.4.5 FEM for the Time Discretization of the DRBEM Solution of Nonlinear Reaction-Diffusion Equation

In Sections 2.4.1-2.4.4 the FDM and the LSM are applied to the system of ODEs, which are obtained after the DRBEM discretization to spatial derivatives of the nonlinear reaction-diffusion and wave equations. In all these applications the representitave time level $[t^m, t^{m+1}]$ or $[t^{m-1}, t^{m+1}]$ are taken and the solution is obtained iteratively between the time levels m and $(m+1)$ or $(m-1)$ and $(m+1)$.

For the FEM discretization of the time derivative, a partition of the time domain $\Omega_m = ((m-1)T, mT]$ $m > 0$ is taken and this domain Ω_m is divided into M finite elements and the solution is obtained at once in this domain without an iteration.

The method is described with the first partition of the time domain $\Omega_1 = (0, T]$. The time domain Ω_1 is divided into a number of finite elements M each of which has length Δt, with two nodes at the ends of the elements.

For a typical element with the starting point t^1 and end point t^2, the linear shape functions are defined as,

$$\psi_1 = \frac{t^2 - t}{\Delta t}, \quad \psi_2 = \frac{t - t^1}{\Delta t}. \tag{2.101}$$

With the help of these shape functions, the approximate solution denoted by $\mathbf{u}_e^h$ for the unknown vector $\mathbf{u}_e$ is defined as [70]

$$\mathbf{u}_e^h(t) = \sum_{j=1}^{2} \mathbf{u}_e^j \psi_j(t) \tag{2.102}$$

where $\mathbf{u}_e^j$ is the value of $\mathbf{u}_e^h$ at the node t^j $(j = 1, 2)$ for the element e. $\mathbf{u}_e$ is the discretized unknown vector obtained by using DRBEM for the time element $'e'$.

For the FEM discretization of the time derivative of nonlinear reaction-diffusion equation, the system of ODEs resulting from the DRBEM discretization is considered (equation (2.69))

$$\dot{\mathbf{u}} = \bar{\bar{\mathbf{H}}}\mathbf{u} + \mathbf{p} \tag{2.103}$$

where $\bar{\bar{\mathbf{H}}} = -\mathbf{C}^{-1}\bar{\mathbf{H}}$, $\mathbf{C} = -\frac{1}{\nu}(\mathbf{H}\hat{\mathbf{U}} - \mathbf{G}\hat{\mathbf{Q}})\mathbf{F}^{-1}$ with the nonlinear vector $\mathbf{p}$.

In order to obtain the corresponding variational statement for the nonlinear reaction-diffusion equation, one should multiply the equation (2.103) by ψ_k $(k = 1, 2)$ and integrate by parts i.e,

$$\int_{t^1}^{t^2} \mathbf{u}_e^h \dot{\psi}_k dt + \bar{\bar{\mathbf{H}}} \int_{t^1}^{t^2} \mathbf{u}_e^h \psi_k dt \;=\; \mathbf{u}_e^h(t^2)\psi_k(t^2) - \mathbf{u}_e^h(t^1)\psi_k(t^1)$$

$$\tag{2.104}$$

$$- \int_{t^1}^{t^2} \mathbf{p}(\mathbf{u}(0))\psi_k(t)dt.$$

As in the previous time integration schemes, the nonlinearity is evaluated at the previous time level, in order to have a linear system of equations at the end.

After substituting the approximate solution $\mathbf{u}_e^h$, equation (2.104) can be written as a linear system of equations of the form

$$\begin{bmatrix} s_{11} & s_{12} \\ & \\ s_{21} & s_{22} \end{bmatrix} \begin{Bmatrix} (\mathbf{u}_e^h)_1 \\ \\ (\mathbf{u}_e^h)_2 \end{Bmatrix} = \begin{Bmatrix} (\mathbf{g}_e)_1 \\ \\ (\mathbf{g}_e)_2 \end{Bmatrix} \tag{2.105}$$

where each entry of the matrix in (2.105) is an $(N + L) \times (N + L)$ matrix s_{kj} $(k, j = 1, 2)$ of element $'e'$ and each entry of the vectors in (2.105) is $(N + L) \times 1$ vector for the points t^k $(k = 1, 2)$ given by,

$$s_{kj} \;=\; \left(\int_{t^1}^{t^2} \dot{\psi}_k \psi_j dt \right) \mathbf{I} + \left(\int_{t^1}^{t^2} \psi_k \psi_j dt \right) \bar{\bar{\mathbf{H}}}$$

$$\tag{2.106}$$

$$(\mathbf{g}_e)_k \;=\; \psi_k(t^2)\mathbf{u}_e^h(t^2) - \psi_k(t^1)\mathbf{u}_e^h(t^1) - \left(\int_{t^1}^{t^2} \mathbf{p}(\mathbf{u}(0))\psi_k dt \right)$$

for $k, j = 1, 2$ where $\mathbf{I}$ is the identity matrix.

After the assembly procedure [70], which is obtained by adding up the contributions coming from each element to obtain the whole system of equations, one obtains the whole $(N + L)\, M \times (N + L)\, M$ system of equations, for the representative time element $[0, T]$ in the form,

$$\mathbf{S}_f \mathbf{u}_f = \mathbf{g}_f \tag{2.107}$$

with the unknown vector $\mathbf{u}_f$ with M vector blocks of length $(N + L)$. Each block contains the solution for the time levels $t = \{t : t = d\Delta t, d = 0, 1, ..., M\}$. $\mathbf{S}_f$ and $\mathbf{g}_f$ are the assembled matrix and vector, respectively, for system of equations (2.105) by using the element definitions given in (2.106).

After finding the solution for the time interval $(0, T]$, the same procedure can be applied for the interval $(T, 2T]$ by using the values for $t = T$ as initial values. Therefore, the solution can be obtained recursively between the partitions $((m-1)T, mT]$, for $m > 0$ integer.

2.5 System of Nonlinear Reaction-Diffusion Equations

In this and in the sections 2.6.2 and 2.6.3 the system of nonlinear reaction diffusion equations of the form

$$\dot{u} = \nu_1 \nabla^2 u + p_1(u, v) + h_1(x, y, t)$$

(2.108)

$$\dot{v} = \nu_2 \nabla^2 v + p_2(u, v) + h_2(x, y, t)$$

in an open bounded domain $\Omega \subset \mathbb{R}^2$ is considered. The system is supplied with the initial conditions

$$u(x, y, 0) = u_0(x, y)$$
$$(x, y) \in \Omega \qquad (2.109)$$
$$v(x, y, 0) = v_0(x, y)$$

and with the mixed type boundary conditions

$$\beta_1(x, y, t) u + \gamma_1(x, y, t) q_1 = 0$$
$$(x, y) \in \Gamma, \quad t > 0 \qquad (2.110)$$
$$\beta_2(x, y, t) v + \gamma_2(x, y, t) q_2 = 0$$

where $q_1 = \dfrac{\partial u}{\partial n}$, $q_2 = \dfrac{\partial v}{\partial n}$, n being the outward normal to the boundary Γ and $u_0\,(x,y)$, $v_0\,(x,y)$, $\beta_1\,(x,y,t)$, $\beta_2\,(x,y,t)$, $\gamma_1\,(x,y,t)$ and $\gamma_2\,(x,y,t)$ are given functions.

In equation (2.108), ν_1, ν_2 are nonzero constants; h_1, h_2 are known functions of time and position and p_1 and p_2 are the nonlinear functions of u and v.

In order to solve the system of nonlinear reaction-diffusion equations, the space derivatives of both systems are discretized using the DRBEM, which is described for a single nonlinear reaction-diffusion equation in Section 2.2. The nonhomogenities for the system of nonlinear reaction-diffusion equations are given now

$$b_1 = \frac{1}{\nu_1}(\dot{u} - p_1\,(u,v) - h_1\,(x,y,t))$$

$$b_2 = \frac{1}{\nu_2}(\dot{v} - p_2\,(u,v) - h_2\,(x,y,t)).$$

(2.111)

Following the same procedure explained in Section 2.2 we obtain two $(N+L) \times (N+L)$ systems of time dependent ODEs (in matrix-vector form)

$$\mathbf{Hu} - \mathbf{Gq_1} = \frac{1}{\nu_1}(\mathbf{H\hat{U}} - \mathbf{G\hat{Q}})\mathbf{F}^{-1}(\dot{\mathbf{u}} - \mathbf{p_1}(\mathbf{u},\mathbf{v}) - \mathbf{h_1})$$

$$\mathbf{Hv} - \mathbf{Gq_2} = \frac{1}{\nu_2}(\mathbf{H\hat{U}} - \mathbf{G\hat{Q}})\mathbf{F}^{-1}(\dot{\mathbf{v}} - \mathbf{p_2}(\mathbf{u},\mathbf{v}) - \mathbf{h_2}).$$

(2.112)

We rewrite in the form

$$\mathbf{C_1\dot{u}} + \mathbf{Hu} = \mathbf{Gq_1} + \mathbf{C_1p_1} + \mathbf{C_1h_1}$$

$$\mathbf{C_2\dot{v}} + \mathbf{Hv} = \mathbf{Gq_2} + \mathbf{C_2p_2} + \mathbf{C_2h_2}$$

(2.113)

with

$$\mathbf{C_i} = -\frac{1}{\nu_i}(\mathbf{H\hat{U}} - \mathbf{G\hat{Q}})\mathbf{F}^{-1} \qquad (2.114)$$

for $i = 1, 2$.

The mixed type boundary conditions (2.110) are made use of to obtain the following systems of ODEs

$$\mathbf{C_1\dot{u}} + \mathbf{\bar{H}_1 u} = \mathbf{C_1 p_1} + \mathbf{C_1 h_1}$$

$$\qquad (2.115)$$

$$\mathbf{C_2\dot{v}} + \mathbf{\bar{H}_2 v} = \mathbf{C_2 p_2} + \mathbf{C_2 h_2}$$

where

$$\mathbf{\bar{H}_i} = \mathbf{H} + \mathbf{GD_i} \qquad (2.116)$$

with a diagonal matrix $\boldsymbol{D_i}$ defined as

$$(\mathbf{D_i})_{jj} = \begin{cases} \dfrac{(\beta_i)_j}{(\gamma_i)_j} & j = 1, ..., N \\ \\ 0 & j = N+1, ..., N+L \end{cases} \qquad (2.117)$$

for $i = 1, 2$.

In equation (2.117) $(\beta_i)_j$ and $(\gamma_i)_j$ denote the values of the functions β_i and γ_i at the node j, respectively.

The system of ODEs (2.115) discretized at the DRBEM collocation points is also solved by using three different time algorithms FDM, LSM and FEM in order to obtain accurate results.

The FDM can be applied as in Section 2.4.1 to obtain

$$(\mathbf{I} - \mu_1 \Delta t \bar{\bar{\mathbf{H}}}_{\mathbf{1}}) \mathbf{u}^{m+1} = (\mathbf{I} + \Delta t (1 - \mu_1) \bar{\bar{\mathbf{H}}}_{\mathbf{1}}) \mathbf{u}^m + \Delta t (\mathbf{p}_1^{m,m} + \mathbf{h_1}^{m+1})$$

$$(\mathbf{I} - \mu_2 \Delta t \bar{\bar{\mathbf{H}}}_{\mathbf{2}}) \mathbf{v}^{m+1} = (\mathbf{I} + \Delta t (1 - \mu_2) \bar{\bar{\mathbf{H}}}_{\mathbf{2}}) \mathbf{v}^m + \Delta t (\mathbf{p_2}^{m,m+1} + \mathbf{h_2}^{m+1})$$

$$(2.118)$$

where $\bar{\bar{\mathbf{H}}}_{\mathbf{1}} = -\mathbf{C_1}^{-1} \bar{\mathbf{H}}_{\mathbf{1}}$, $\bar{\bar{\mathbf{H}}}_{\mathbf{2}} = -\mathbf{C_2}^{-1} \bar{\mathbf{H}}_{\mathbf{2}}$ and μ_1, μ_2 are the relaxation parameters varying between 0 and 1 for the solutions $\mathbf{u}$ and $\mathbf{v}$, respectively. In equation (2.118) $\mathbf{p_{i+1}}^{m,m+i} = \mathbf{p_{i+1}}(\mathbf{u}^m, \mathbf{v}^{m+i})$ denotes the vectors containing the nonlinearity for $i = 0, 1$.

The LSM can be applied to the equations in (2.115) as in the case of single reaction-diffusion equation which is explained in Section 2.4.3 to have

$$\mathbf{A} \mathbf{u}^{m+1} = \mathbf{B_1} \mathbf{u}^m + \mathbf{B_2} (\mathbf{p_1}^{m,m} + \mathbf{h_1}^{m+1})$$

$$(2.119)$$

$$\bar{\mathbf{A}} \mathbf{v}^{m+1} = \bar{\mathbf{B}}_{\mathbf{1}} \mathbf{v}^m + \bar{\mathbf{B}}_{\mathbf{2}} (\mathbf{p_2}^{m,m+1} + \mathbf{h_2}^{m+1})$$

where

$$\mathbf{A} = \frac{1}{\Delta t^2} \mathbf{C_1}^T \mathbf{C_1} + \frac{1}{2\Delta t} (\mathbf{C_1}^T \bar{\mathbf{H}}_{\mathbf{1}} + \bar{\mathbf{H}}_{\mathbf{1}}^T \mathbf{C_1}) + \frac{1}{3} \bar{\mathbf{H}}_{\mathbf{1}}^T \bar{\mathbf{H}}_{\mathbf{1}}$$

$$\mathbf{B_1} = \frac{1}{\Delta t^2} \mathbf{C_1}^T \mathbf{C_1} - \frac{1}{2\Delta t} (\mathbf{C_1}^T \bar{\mathbf{H}}_{\mathbf{1}} - \bar{\mathbf{H}}_{\mathbf{1}}^T \mathbf{C_1}) - \frac{1}{6} \bar{\mathbf{H}}_{\mathbf{1}}^T \bar{\mathbf{H}}_{\mathbf{1}}$$

$$\mathbf{B_2} = \frac{1}{\Delta t} \mathbf{C_1}^T \mathbf{C_1} + \frac{1}{2} \bar{\mathbf{H}}_{\mathbf{1}}^T \mathbf{C_1}$$

$$(2.120)$$

$$\bar{\mathbf{A}} = \frac{1}{\Delta t^2} \mathbf{C_2}^T \mathbf{C_2} + \frac{1}{2\Delta t} (\mathbf{C_2}^T \bar{\mathbf{H}}_{\mathbf{2}} + \bar{\mathbf{H}}_{\mathbf{2}}^T \mathbf{C_2}) + \frac{1}{3} \bar{\mathbf{H}}_{\mathbf{2}}^T \bar{\mathbf{H}}_{\mathbf{2}}$$

$$\bar{\mathbf{B}}_{\mathbf{1}} = \frac{1}{\Delta t^2} \mathbf{C_2}^T \mathbf{C_2} - \frac{1}{2\Delta t} (\mathbf{C_2}^T \bar{\mathbf{H}}_{\mathbf{2}} - \bar{\mathbf{H}}_{\mathbf{2}}^T \mathbf{C_2}) - \frac{1}{6} \bar{\mathbf{H}}_{\mathbf{2}}^T \bar{\mathbf{H}}_{\mathbf{2}}$$

$$\bar{\mathbf{B}}_{\mathbf{2}} = \frac{1}{\Delta t} \mathbf{C_2}^T \mathbf{C_2} + \frac{1}{2} \bar{\mathbf{H}}_{\mathbf{2}}^T \mathbf{C_2}.$$

Taking the FEM formulation for the single nonlinear reaction-diffusion equation into consideration (Section 2.4.5), one can write the FEM solution of the systems

of ODEs (2.115) for a typical time element with the starting point t^1 and the end point t^2 as

$$\begin{bmatrix} s_{11} & s_{12} \\ \\ s_{21} & s_{22} \end{bmatrix} \left\{ \begin{array}{c} (\mathbf{u}_e^h)_1 \\ \\ (\mathbf{u}_e^h)_2 \end{array} \right\} = \left\{ \begin{array}{c} (\bar{\mathbf{g}}_e)_1 \\ \\ (\bar{\mathbf{g}}_e)_2 \end{array} \right\}$$

$$\begin{bmatrix} \bar{s}_{11} & \bar{s}_{12} \\ \\ \bar{s}_{21} & \bar{s}_{22} \end{bmatrix} \left\{ \begin{array}{c} (\mathbf{v}_e^h)_1 \\ \\ (\mathbf{v}_e^h)_2 \end{array} \right\} = \left\{ \begin{array}{c} (\bar{\bar{\mathbf{g}}}_e)_1 \\ \\ (\bar{\bar{\mathbf{g}}}_e)_2 \end{array} \right\}$$

(2.121)

where

$$\mathbf{s_{kj}} = (\int_{t^1}^{t^2} \dot{\psi}_k \psi_j dt)\mathbf{I} + (\int_{t^1}^{t^2} \psi_k \psi_j dt)\bar{\bar{\mathbf{H}}}_1$$

$$(\bar{\mathbf{g}}_e)_k = \psi_k(t^2)\mathbf{u}_e^h(t^2) - \psi_k(t^1)\mathbf{u}_e^h(t^1) - (\int_{t^1}^{t^2} (\mathbf{p_1}(\mathbf{u}(t^1), \mathbf{v}(t^1)) + \mathbf{h_1}(t^2))\psi_k dt)$$

$$\bar{\mathbf{s}}_{\mathbf{kj}} = (\int_{t^1}^{t^2} \dot{\psi}_k \psi_j dt)\mathbf{I} + (\int_{t^1}^{t^2} \psi_k \psi_j dt)\bar{\bar{\mathbf{H}}}_2$$

$$(\bar{\bar{\mathbf{g}}}_e)_k = \psi_k(t^2)\mathbf{v}_e^h(t^2) - \psi_k(t^1)\mathbf{v}_e^h(t^1) - (\int_{t^1}^{t^2} (\mathbf{p_2}(\mathbf{u}(t^2), \mathbf{v}(t^1)) + \mathbf{h_2}(t^2))\psi_k dt).$$

(2.122)

With the approximation vectors $\mathbf{u}_e^h$ and $\mathbf{v}_e^h$ similar to equation (2.102) the discretized unknown vectors $\mathbf{u}_e$ and $\mathbf{v}_e$ are obtained by using DRBEM for the time element 'e', respectively.

The assembly procedure leads to the following $(N + L)M \times (N + L)M$ system of matrix-vector equations in the form

$$(\mathbf{S_1})_f \bar{\mathbf{u}}_f = \bar{\mathbf{g}}_f$$

$$(2.123)$$

$$(\mathbf{S_2})_f \bar{\mathbf{v}}_f = \bar{\bar{\mathbf{g}}}_f$$

for the unknown vectors $\bar{\mathbf{u}}_f$ and $\bar{\mathbf{v}}_f$ with vector blocks of length $(N+L)$ containing the solution at the time levels $t = \{t : t = d\Delta t, d = 0, 1, ..., M\}$. $(\mathbf{S_1})_f$, $(\mathbf{S_2})_f$ and $\bar{\mathbf{g}}_f$, $\bar{\bar{\mathbf{g}}}_f$ are the assembled matrices and vectors for the element equations (2.121), respectively.

In all time integration schemes the nonlinearities are taken in the previous step for the first equation and the values of $\boldsymbol{u}$ found are used in the second nonlinearity for obtaining $\mathbf{v}$.

2.6 Numerical Results

In this section, the numerical solution of the nonlinear reaction-diffusion equation as well as the system of nonlinear reaction-diffusion equations, and the nonlinear wave equation are considered. The equations are discretized by the DRBEM spatially. As the temporal discretization method, which is applied to the system of ODEs obtained after the DRBEM discretization of the space derivatives, three different methods (FDM, LSM and FEM) are used for the nonlinear reaction-diffusion equations, and two different methods (FDM and LSM) are used for the nonlinear wave equation. The above mentioned time integration methods are aimed to use for obtaining accurate and computationally efficient results. Several numbers of constant boundary elements (N) and time steps (Δt) are tested to find the best solution for each test problem. The comparison between the time integration methods is made in terms of maximum absolute error, whenever the exact solution is available.

The problems considered in this section are (1) Nonlinear reaction-diffusion problem, (2) System of nonlinear reaction-diffusion equations, (3) Nonlinear reaction-diffusion Brusselator system (4) Nonlinear exterior wave equation.

For these test problems, the maximum absolute error τ_m for the m-th time level t^m which is defined in the form

$$\tau_m = \max_{1 \le i \le (N+L)} |u_{exact}(x_i, y_i, t^m) - u_{num}(x_i, y_i, t^m)| \tag{2.124}$$

is used to measure the quality of the numerical solution, whenever the exact solution is available (Problems 2.6.1 and 2.6.2). For the other problems the expected behaviour of the solutions are checked.

In equation (2.124) (x_i, y_i) is one of the DRBEM collocation point either on the boundary or in the domain, $u_{exact}(x_i, y_i, t^m)$ and $u_{num}(x_i, y_i, t^m)$ denote the exact and numerical solutions obtained by one of the above mentioned time integration methods (FDM, LSM or FEM) combined with DRBEM at (x_i, y_i) for the m-th time level, respectively.

In the case that the exact solution is not available (Problem 2.6.3 and 2.6.4), the known behaviour of the solution is seen to be satisfied by the numerical solutions obtained with the mentioned time integration methods.

2.6.1   Nonlinear Reaction-Diffusion Problem

The solution of the following nonlinear reaction-diffusion equation

$$\dot{u} = \frac{1}{2}\nabla^2 u + u^2(1-u) \tag{2.125}$$

is considered in the unit square $\Omega = \{(x,y) \mid 0 \le x \le 1, \ 0 \le y \le 1\}$ for $t \ge 0$. Initial and the mixed type boundary conditions are taken appropriate with the exact solution [48]

$$u(x, y, t) = \frac{1}{1 + e^{p(x+y-pt)}} \quad \text{where} \quad p = \frac{1}{\sqrt{2}}. \tag{2.126}$$

In the DRBEM dicretization of the square region, we use several number of (as 12, 20, 40, 60, 80) constant elements on the boundary and as can be seen from

Figure 2.5, $N = 40$ is found to be the suitable number of freedom in terms of maximum absolute error.

Since we use an explicit FDM for time derivative discretization, stability problems may occur and usually very small time increments are needed. Therefore, the number of iterations may be quite large causing a computationally expensive scheme for reaching the steady-state solution. For this reason, we propose a relaxation procedure between two time levels. But the choice of the relaxation parameter μ is also important and it is found by trial and error. For this problem we found the optimal value of the relaxation parameter as 0.8.
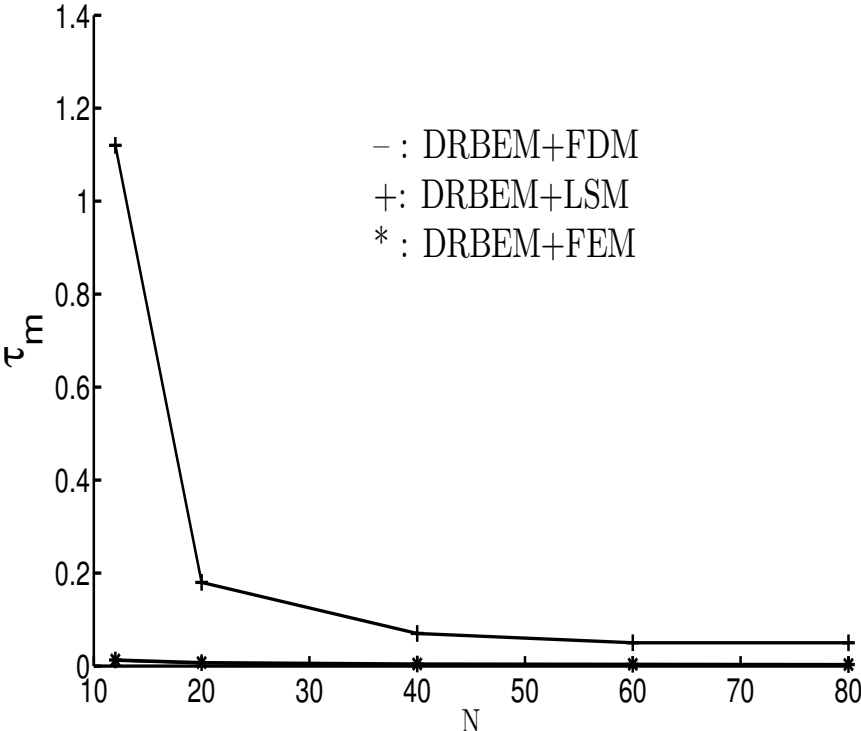
Figure 2.5:   Maximum absolute error depending on the number of boundary elements at $t = 2$ for problem 2.6.1

The problem is also solved using the combinations of DRBEM with LSM and FEM. As the time increment we have seen that $\Delta t = 0.01$ is a better choice for the FDM and FEM whereas LSM needs only $\Delta t = 0.1$ to achieve an accuracy about 10^{-3} for small time levels (up to $t = 2.0$) (Figures 2.6(a)-2.6(c)).The same is observed in [25] that the smaller the time increment is, the larger the error in LSM.
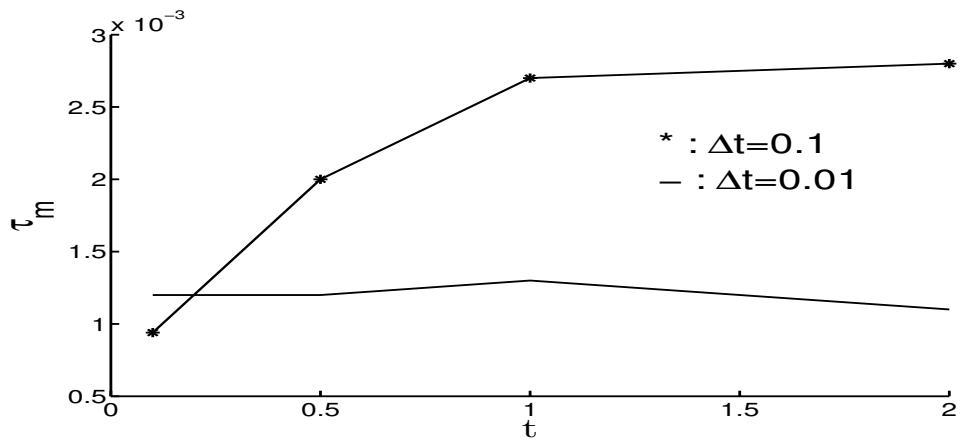
(a) DQM+FDM
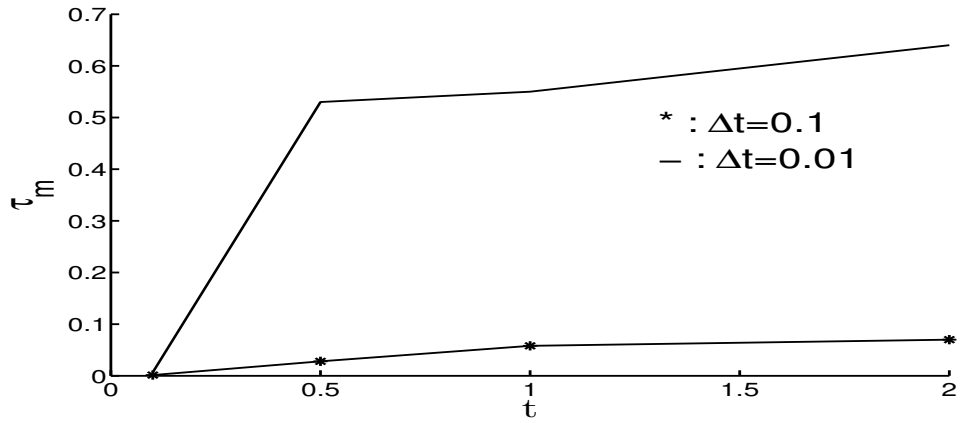
(b) DQM+LSM
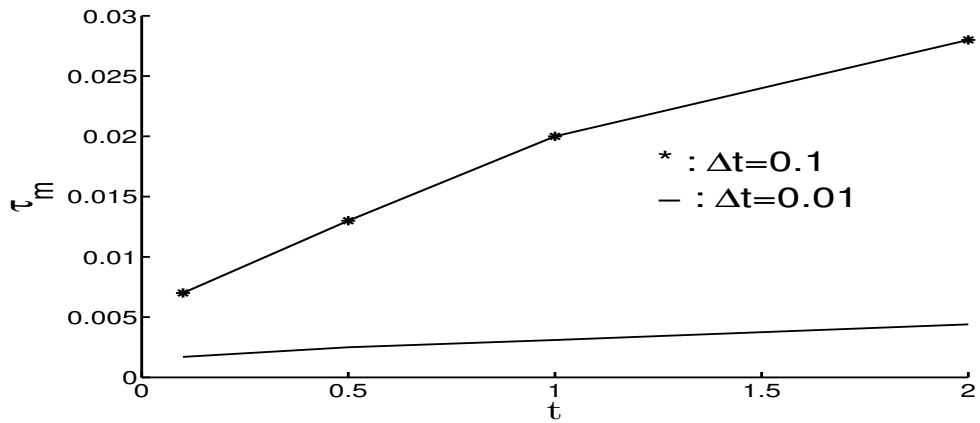
(c) DQM+FEM

Figure 2.6:   Maximum absolute errors with different time steps for problem 2.6.1

To measure the quality of the approximate solutions with those three time integration methods we use the maximum absolute error τ_m given in (2.124).

The results in terms of these maximum absolute errors for small time levels as well as the time levels leading to steady-state are presented in Tables 2.1 and 2.2 for the points on the line $x = \dfrac{1}{2}$.

In Table 2.1, the maximum absolute errors at small time levels are presented. We see from this table that the methods give the same accuracy for very small time levels like $t = 0.01$ and $t = 0.1$ when $\Delta t = 0.01$ and $\Delta t = 0.1$ are used in FDM, FEM and LSM, respectively. The difference between the methods becomes visible starting from the time $t = 0.5$. We observe that FDM with the optimal value of the relaxation parameter and FEM give better results than the results with LSM. For larger time levels through steady-state FDM and FEM have almost the same accuracy and they are both better than LSM (Table 2.2).

Table 2.1: Maximum absolute errors for Problem 2.6.1 at small time levels

Method	$t = 0.01$	$t = 0.1$	$t = 0.5$	$t = 2.0$
FDM	$1.7{\times}10^{-3}$	$1.2{\times}10^{-3}$	$1.2{\times}10^{-3}$	$1.1{\times}10^{-3}$
LSM	$4.4{\times}10^{-3}$	$1.4{\times}10^{-3}$	$2.8{\times}10^{-2}$	$6.9{\times}10^{-2}$
FEM	$1.4{\times}10^{-3}$	$1.7{\times}10^{-3}$	$2.5{\times}10^{-3}$	4.4×10^{-3}

Table 2.2: Maximum absolute errors for Problem 2.6.1 at increasing time levels

Method	$t = 8.0$	$t = 12.0$	$t = 16.0$	$t = 20.0$
FDM	$4.5{\times}10^{-4}$	$3.4{\times}10^{-5}$	$4.8{\times}10^{-6}$	$5.7{\times}10^{-7}$
LSM	$6.6{\times}10^{-2}$	$9.5{\times}10^{-3}$	$1.2{\times}10^{-3}$	$1.6{\times}10^{-4}$
FEM	$6.0{\times}10^{-4}$	$1.7{\times}10^{-4}$	$2.5{\times}10^{-5}$	3.4×10^{-6}

Figures 2.7 and 2.8 show the agreement of the solutions with the exact solution on the line $x = \dfrac{1}{2}$ with $L = 20$ interior nodes at several time levels. From these figures one can see that the agreement of the solutions with the exact solution obtained by FDM and FEM time integrations is much better than obtained by LSM time integration. At the steady-state all the methods coincide.
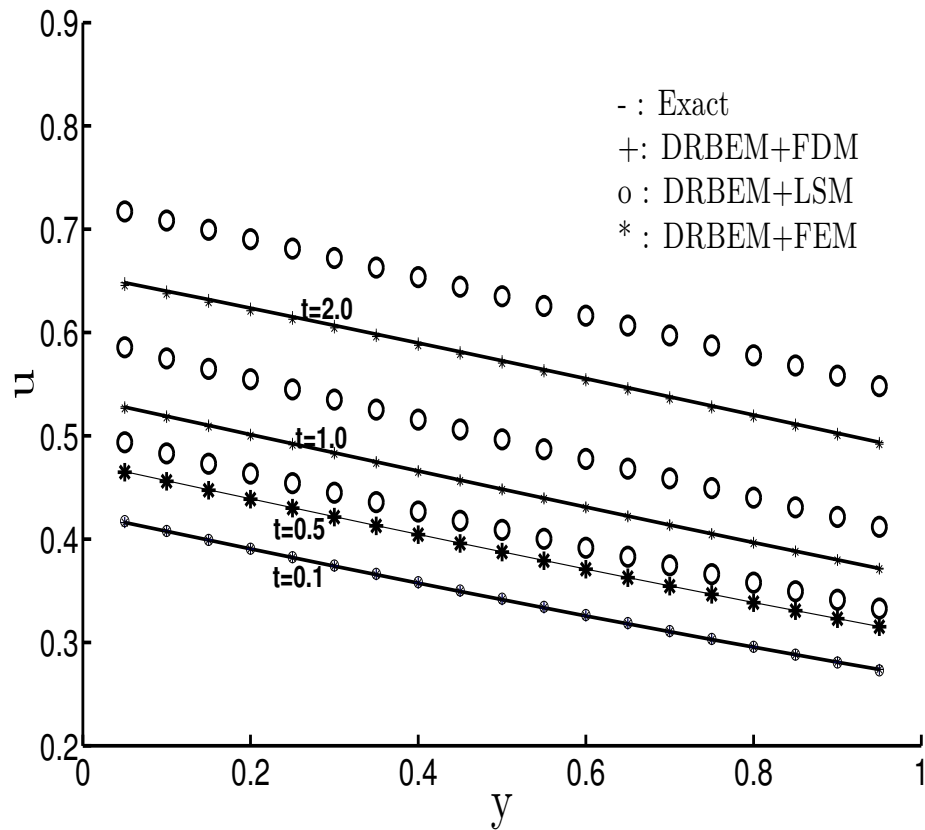
Figure 2.7:   Solutions at small time levels for problem 2.6.1
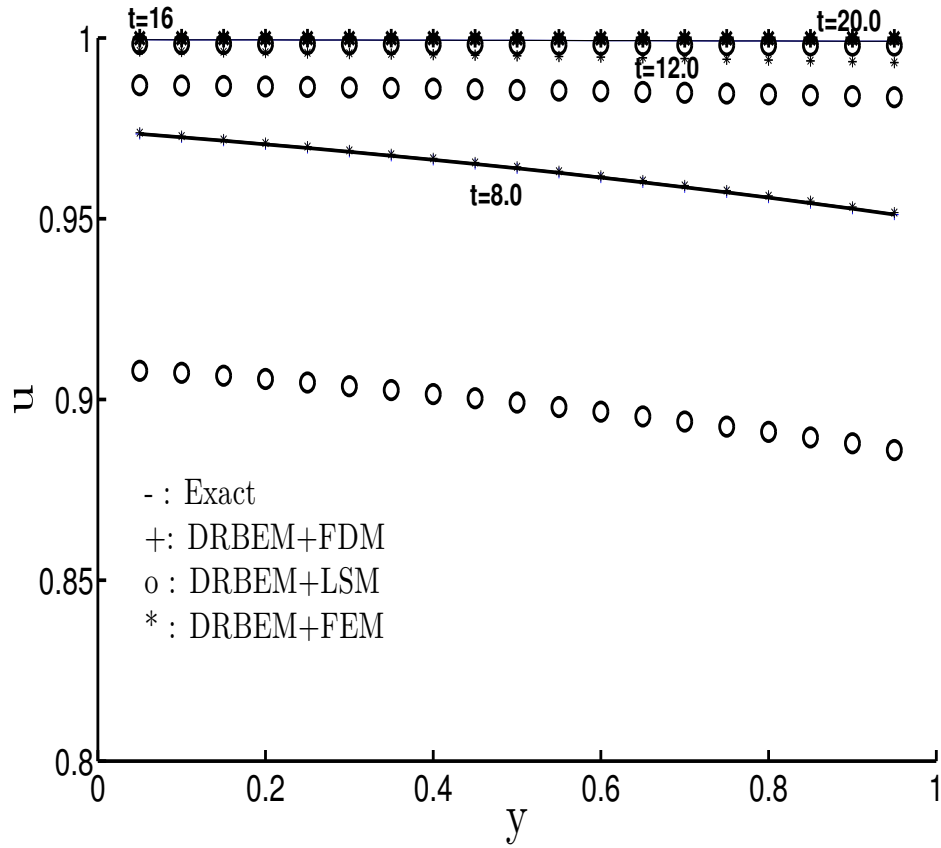
Figure 2.8:   Solutions of problem 2.6.1 at steady state

In Figure 2.9, one can also see that, the maximum absolute errors for the DRBEM solution with the combination of FDM or FEM are almost the same which is less than the maximum absolute error obtained by LSM even when $\Delta t = 0.1$ is used for the time increment. Also, at steady-state each maximum absolute error tends to zero.
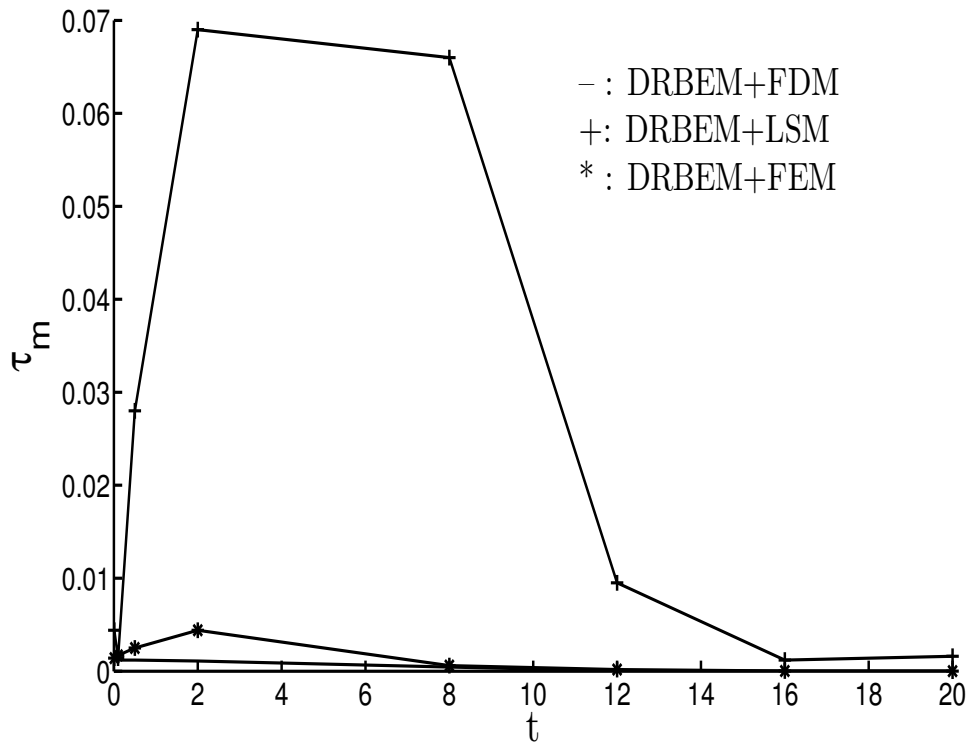
Figure 2.9:   Maximum absolute errors for problem 2.6.1 at several times

As a result the combinations DRBEM+FDM and DRBEM+FEM are preferred for this initial and boundary value problem defined by the nonlinear reaction-diffusion equation (2.125). Although LSM uses larger time increment the accuracy is still lower then the accuracies obtained by FDM and FEM.

2.6.2   Nonlinear Reaction-Diffusion System

We consider solving the system [51]

$$\dot{u} = \nabla^2 u + u^2(1 - v^2) + h_1(x, y, t)$$

$$(2.127)$$

$$\dot{v} = \nabla^2 v + v^2(1 - u^2) + h_2(x, y, t)$$

in $\Omega = \{(x, y) \mid 0 \le x \le 1, \ 0 \le y \le 1\}$ for $t \ge 0$.

The functions $h_1(x, y, t)$, $h_2(x, y, t)$, the Neumann type boundary conditions and the initial condition are selected to accommodate the exact solution which is given in [51]

$$u(x, y, t) = \exp(-t) \sin x \sin y$$

$$(2.128)$$

$$v(x, y, t) = \exp(-2t) \sin 2x \sin 2y.$$

$N = 80$ boundary nodes and $L = 20$ interior nodes are used in DRBEM for obtaining the agreement with the exact solution. We take the interior nodes on the line $x = \dfrac{1}{2}$. It is observed that the relaxation parameter in FDM must be taken greater than or equal to 0.7 for both unknowns to achieve a preassigned accuracy at all transient levels.

Our previous observation for the time increment is also valid for Problem 2.6.2 that we need to take $\Delta t = 0.01$ for FDM and for each time block $[t^{iM}, t^{(i+1)M}]$ in FEM at the transient levels. The same time step does not give results in LSM, we need to take larger time step as $\Delta t = 0.1$. Through steady-state all three integration schemes give almost the same accuracy especially for the first component of the solution.

Tables 2.3 and 2.4 show the maximum absolute errors for the first and second components of the solution, respectively. For this system of nonlinear reaction-diffusion equations FDM with a proper value of relaxation parameter seems to give better accuracy for the first component of the solution. For the second component there is an accuracy drop in the results obtained by FDM whereas

LSM and FEM give almost the same accuracy.

Table 2.3: Maximum absolute errors for the first component of the solution of Problem 2.6.2

Method	t=0.1	t=0.5	t=1.0	t=1.5
FDM	3.4×10^{-3}	4.9×10^{-3}	6.2×10^{-3}	7.4×10^{-3}
LSM	1.2	4.5×10^{-1}	2.0×10^{-1}	1.4×10^{-1}
FEM	6.3×10^{-1}	4.2×10^{-1}	2.6×10^{-1}	1.6×10^{-1}

Method	t=2.0	t=3.0	t=5.0
FDM	8.2×10^{-3}	9.0×10^{-3}	9.2×10^{-3}
LSM	9.1×10^{-2}	3.5×10^{-2}	4.8×10^{-3}
FEM	9.4×10^{-2}	3.5×10^{-2}	4.7×10^{-3}

Table 2.4: Maximum absolute errors for the second component of the solution of Problem 2.6.2

Method	t=0.1	t=0.5	t=1.0	t=1.5
FDM	4.0×10^{-2}	1.1×10^{-1}	1.4×10^{-1}	1.4×10^{-1}
LSM	2.4	6.1×10^{-1}	1.8×10^{-1}	9.4×10^{-2}
FEM	7.4×10^{-1}	3.3×10^{-1}	1.2×10^{-1}	4.5×10^{-2}

Method	t=2.0	t=3.0	t=5.0
FDM	1.4×10^{-1}	1.2×10^{-1}	9.9×10^{-2}
LSM	4.0×10^{-2}	6.3×10^{-3}	1.2×10^{-4}
FEM	1.7×10^{-2}	2.3×10^{-3}	4.1×10^{-5}

2.6.3 Nonlinear Reaction-Diffusion Brusselator System

The nonlinear reaction-diffusion Brusselator system is considered which is in the form

$$\dot{u} = \frac{1}{500} \nabla^2 u + 1 + u^2 v - \frac{3}{2} u$$

$$\dot{v} = \frac{1}{500} \nabla^2 v + \frac{1}{2} u - u^2 v$$

(2.129)

in the unit square $\Omega = \{(x, y) \mid 0 \le x \le 1, \ 0 \le y \le 1\}$ for $t \ge 0$.

Equation (2.129) is subjected to the initial conditions

$$u(x, y, 0) = \frac{1}{2} x^2 - \frac{1}{3} x^3$$

$$v(x, y, 0) = \frac{1}{2} y^2 - \frac{1}{3} y^3$$

$$(x, y) \in \Omega$$

(2.130)

and the boundary conditions are

$$\left(\frac{\partial u}{\partial n}, \frac{\partial v}{\partial n} \right) = (0, 0) \qquad (x, y) \in \Gamma, \quad t > 0.$$

(2.131)

There is no exact solution given to this problem. It is reported in [49, 52] that the solution (u, v) of the system (2.129) tends to $(1, 1/2)$ for increasing t.

One can see from Figures 2.10 and 2.11 that the DRBEM solutions obtained with all three time integration schemes coincide especially at the steady-state. The time step $\Delta t = 0.1$ is seen to be enough to catch the behaviour of the solution.

In [52], they use DRBEM with a predictor-corrector approach in time in solving the same problem, and they used at least $N=64$ boundary nodes in order to catch the behaviour of the solution. In our calculations we have used only $N = 8$ constant boundary elements to catch the behaviour of the solution and this number is very small comparing to the number used in [52].
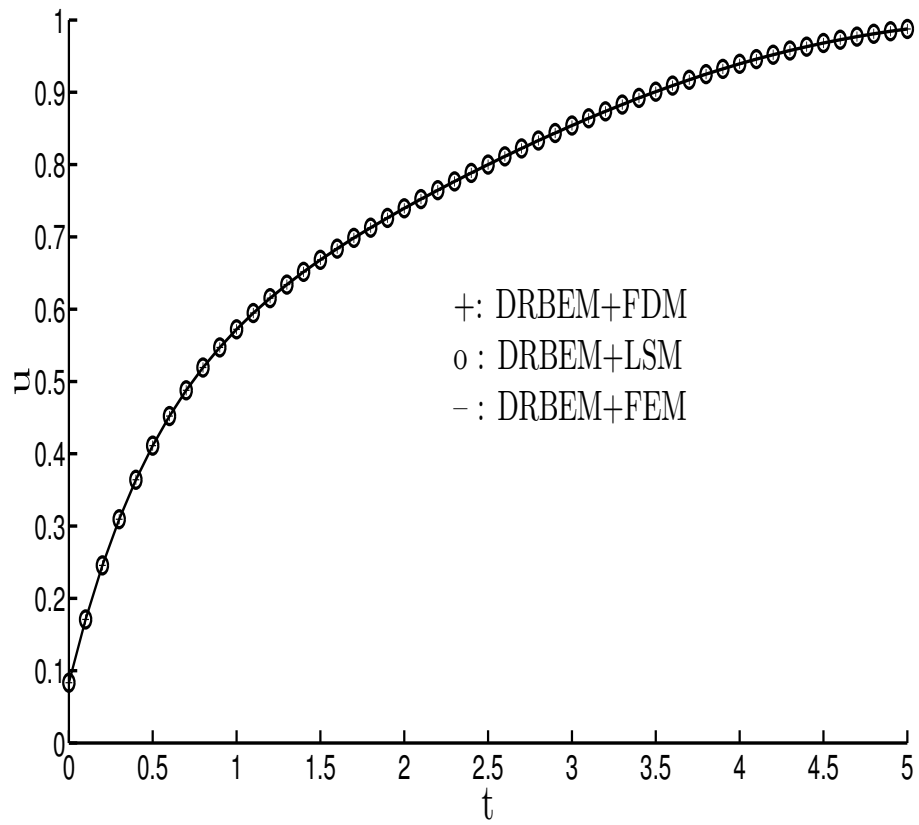
Figure 2.10:   Graph of the first component of the solution for problem 2.6.3
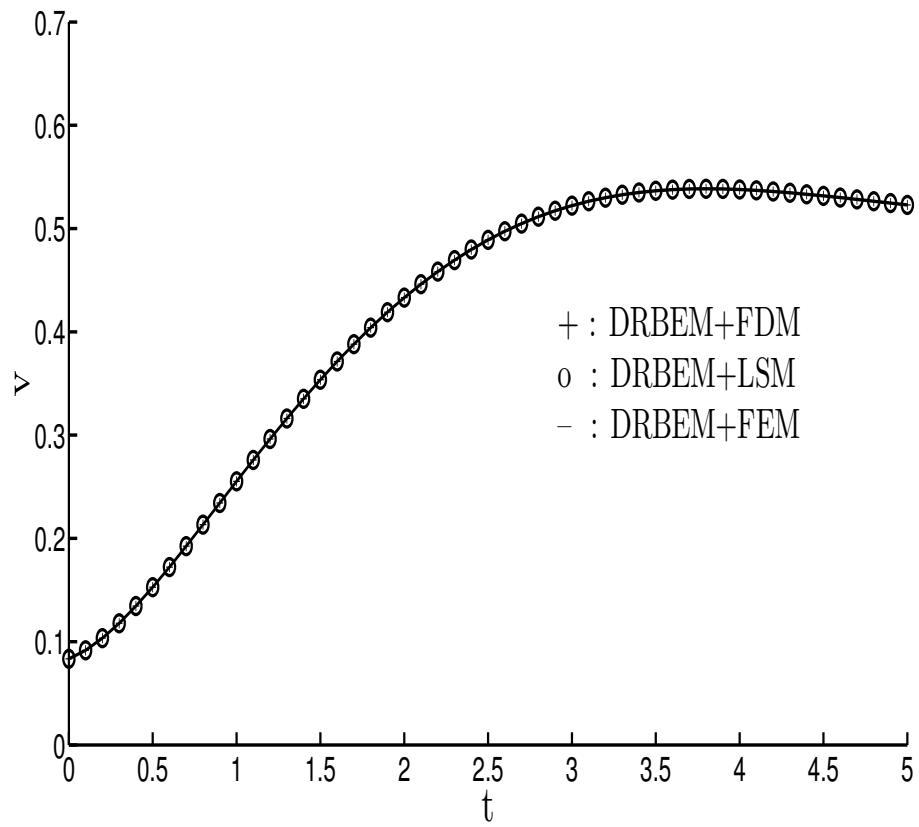
Figure 2.11:   Graph of the second component of the solution for problem 2.6.3

The level curves of the solutions u and v are given at $t = 0, 1, 2$ and 5 in the Figures 2.12-2.18 for observing the consistency of the solution as t increases. In order to draw these level curves we define a regular mesh $(0.1 \leq x \leq 0.9, \quad 0.1 \leq y \leq 0.9)$ with 81 interior points (L). It can be seen from these figures that the DRBEM solution has the same behaviour with all these three time integration schemes, i.e., (u, v) tends to $(1, 1/2)$ smoothly as t increases.
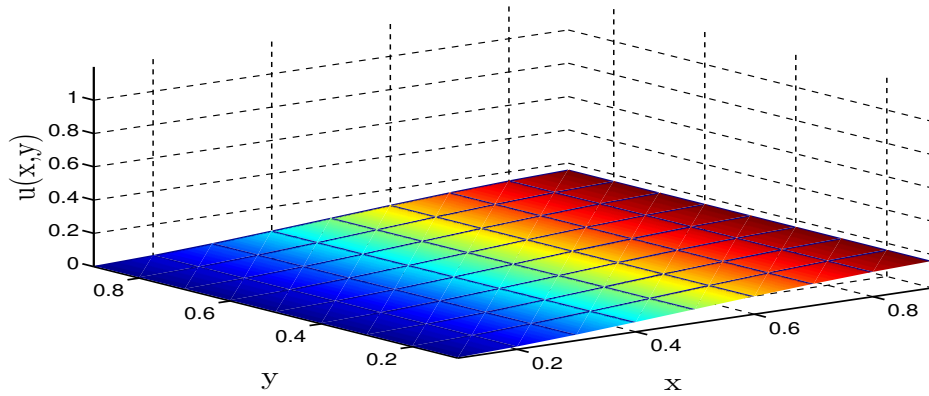
(a) u at $t = 0$
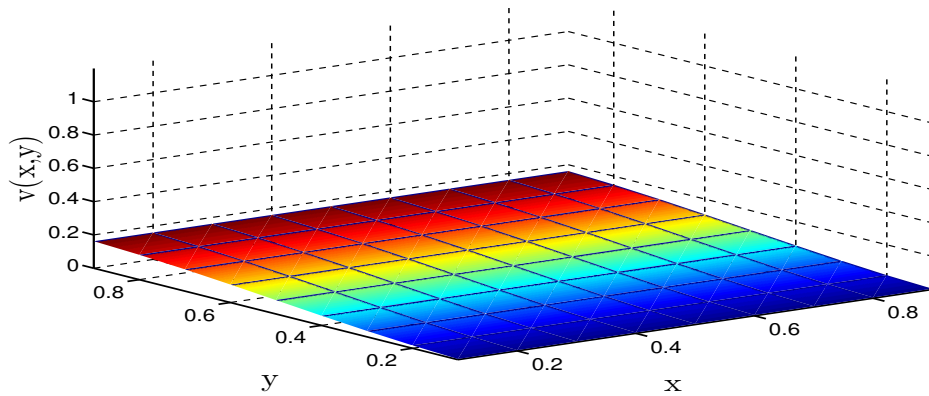
(b) v at $t = 0$

Figure 2.12: u and v at $t = 0$ for Problem 2.6.3
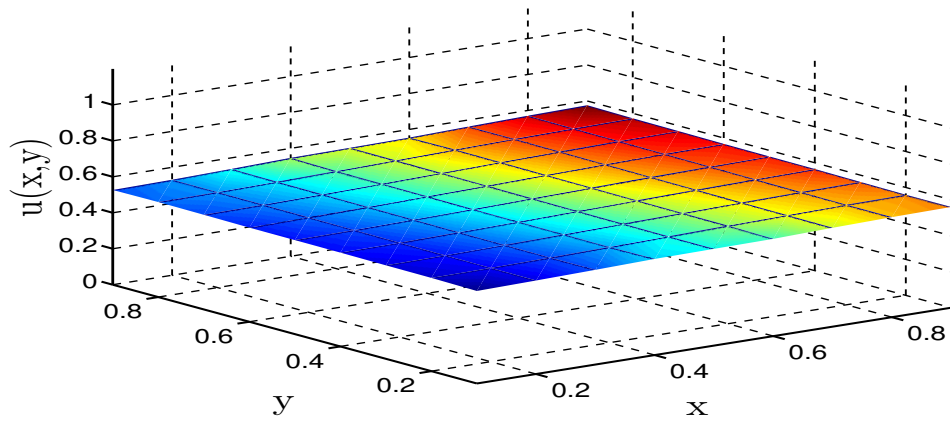
(a) DRBEM+FDM
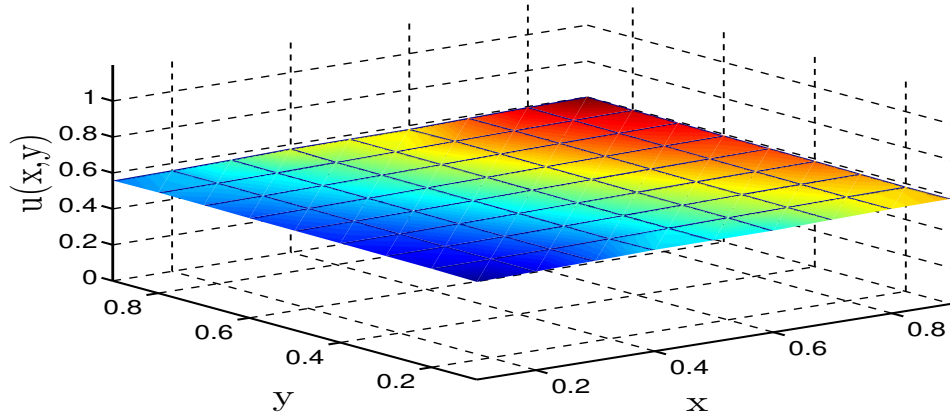
(b) DRBEM+LSM

(c) DRBEM+FEM

Figure 2.13: u at $t = 1$ for Problem 2.6.3

(a) DRBEM+FDM

(b) DRBEM+LSM

(c) DRBEM+FEM

Figure 2.14: u at $t = 2$ for Problem 2.6.3
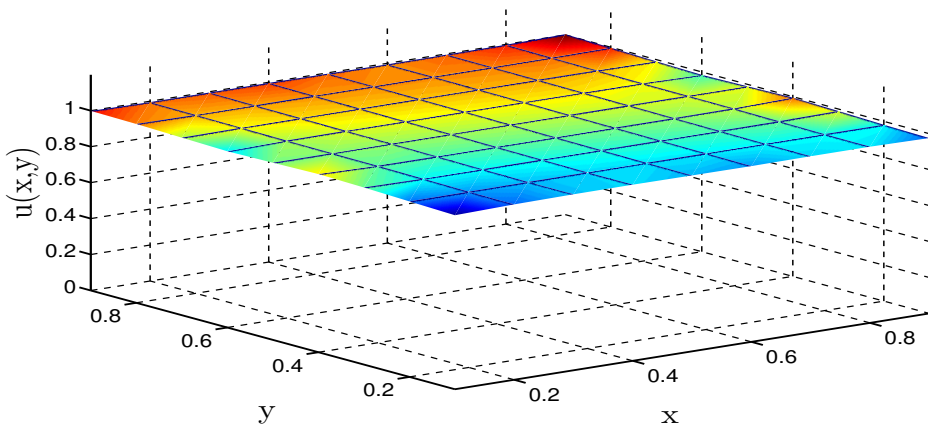
(a) DRBEM+FDM
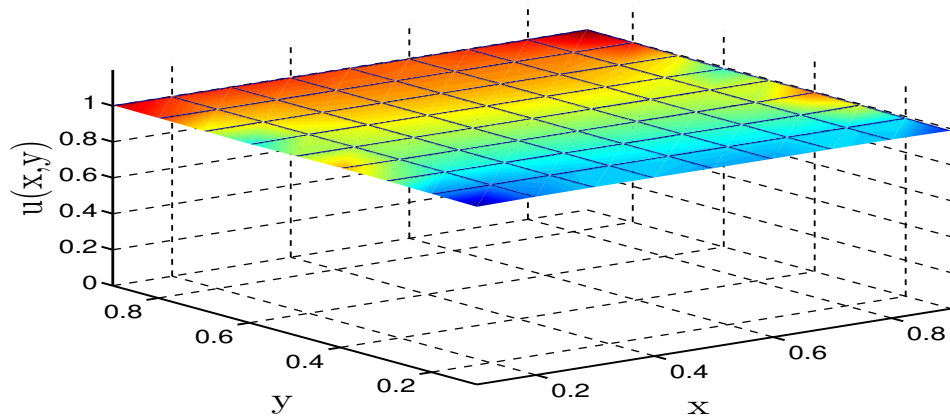
(b) DRBEM+LSM

(c) DRBEM+FEM

Figure 2.15: u at $t = 5$ for Problem 2.6.3

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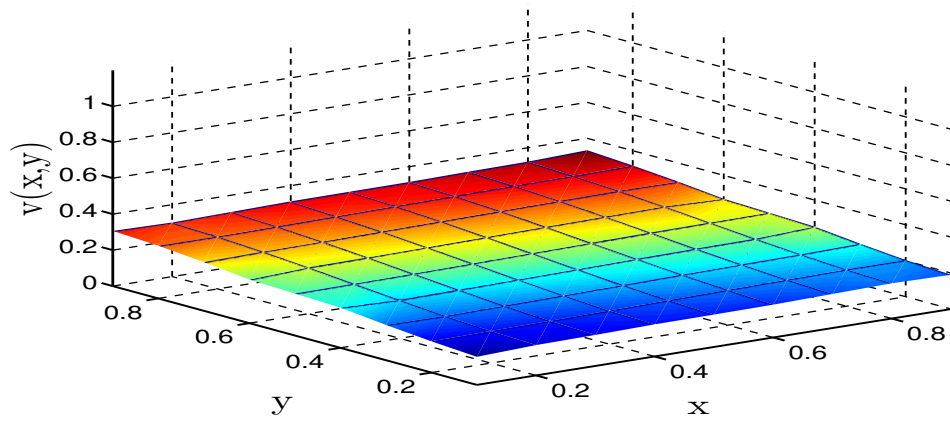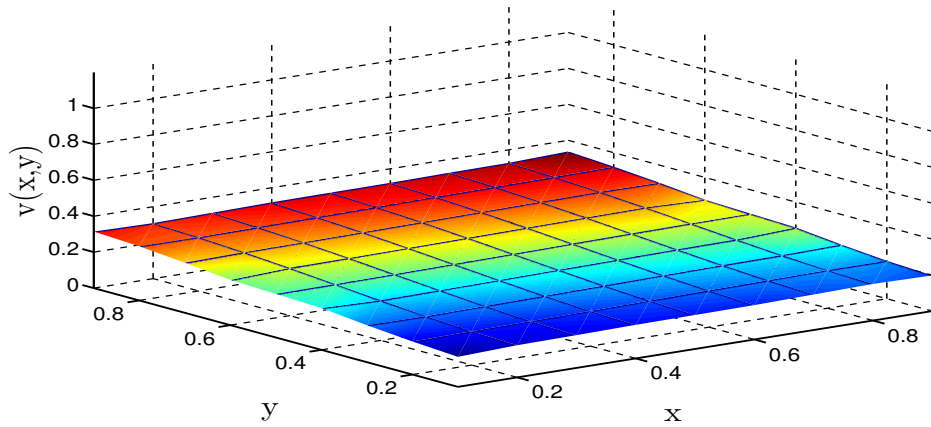
(a) DRBEM+FDM
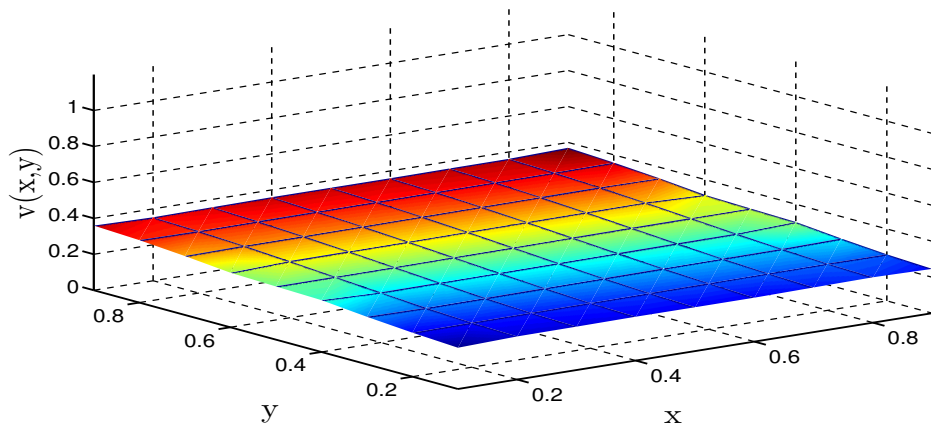
(b) DRBEM+LSM

(c) DRBEM+FEM

Figure 2.16: v at $t = 1$ for Problem 2.6.3
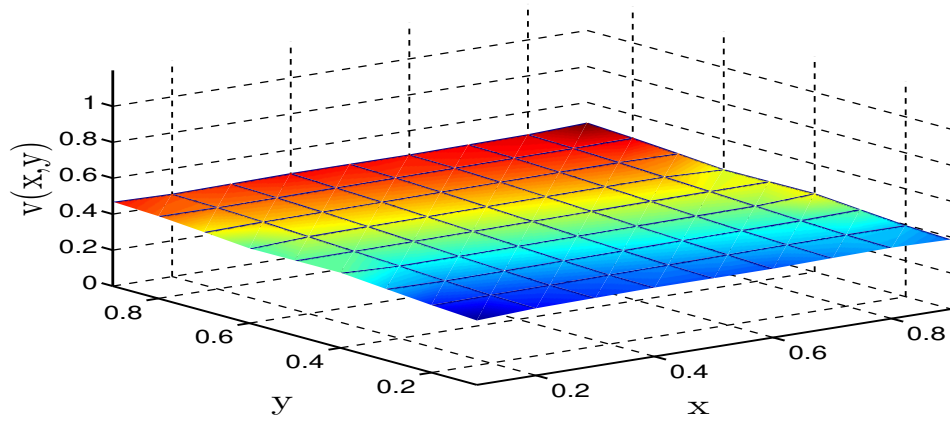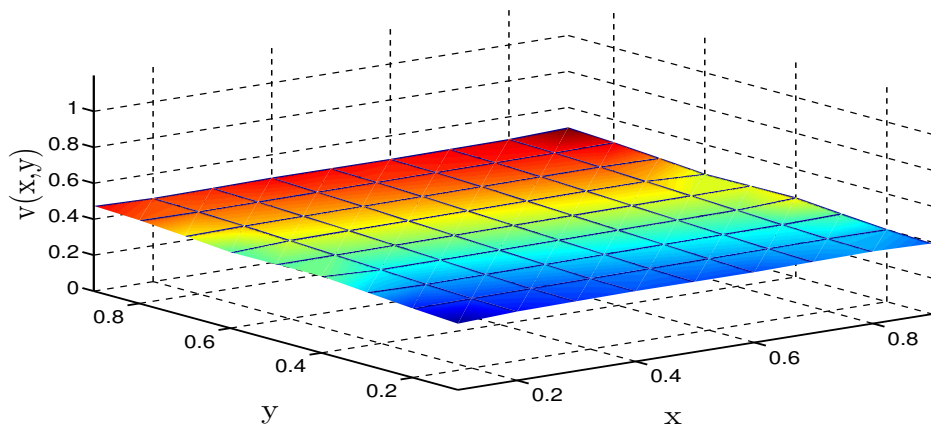
(a) DRBEM+FDM
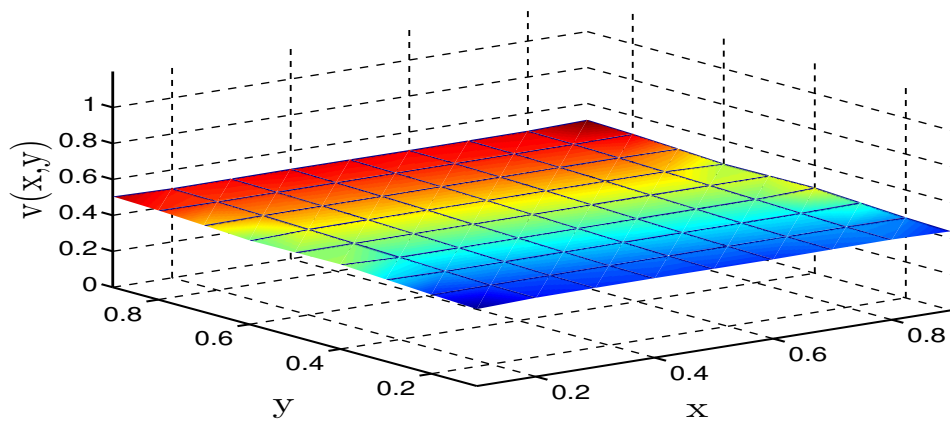
(b) DRBEM+LSM

(c) DRBEM+FEM

Figure 2.17: v at $t = 2$ for Problem 2.6.3
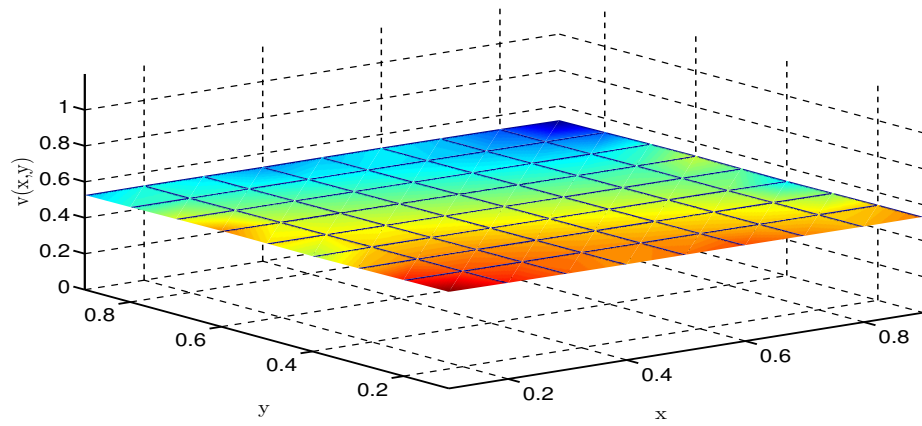
(a) DRBEM+FDM
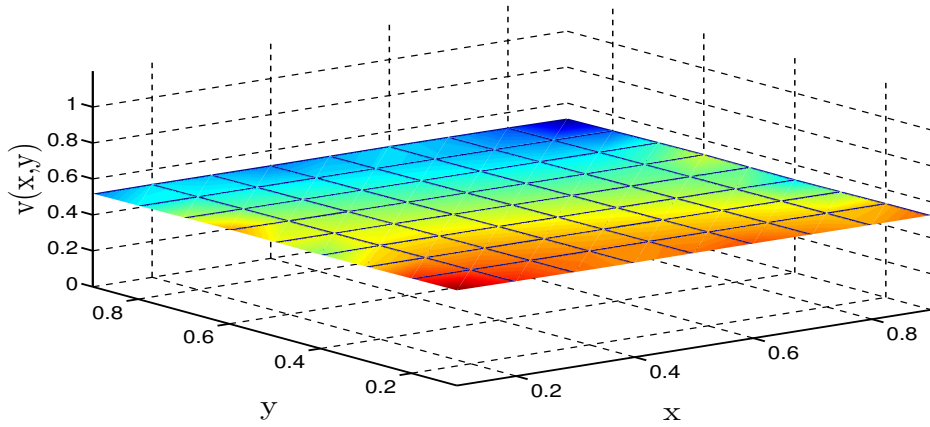
(b) DRBEM+LSM
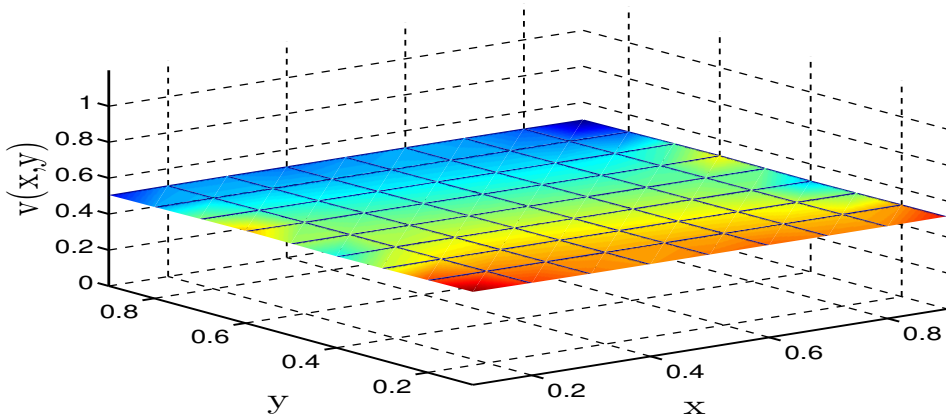
(c) DRBEM+FEM

Figure 2.18: v at $t = 5$ for Problem 2.6.3
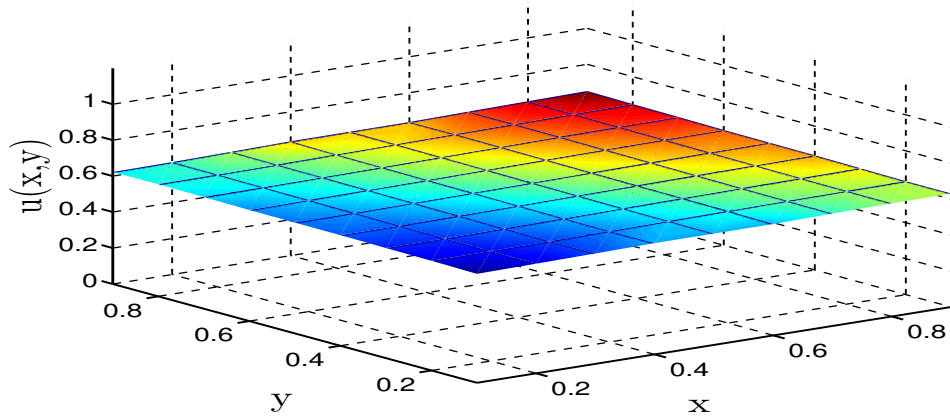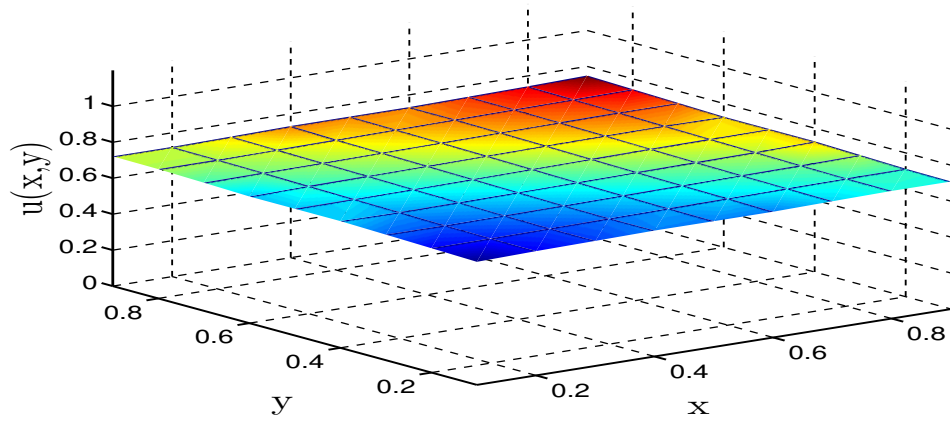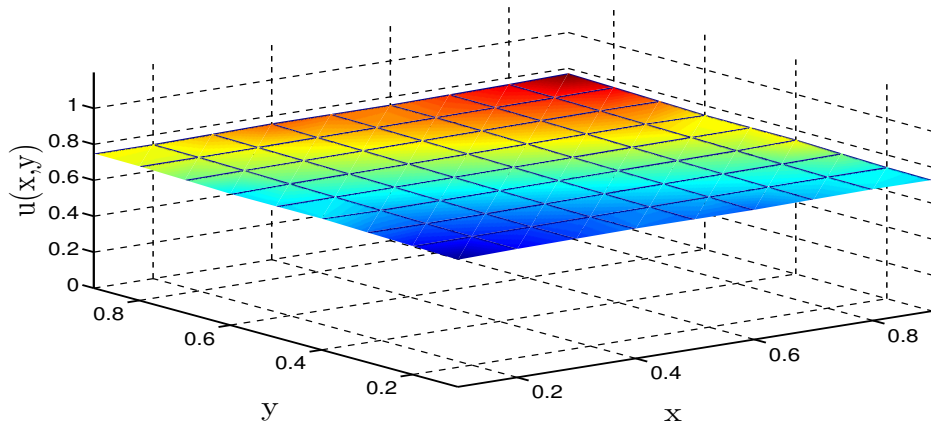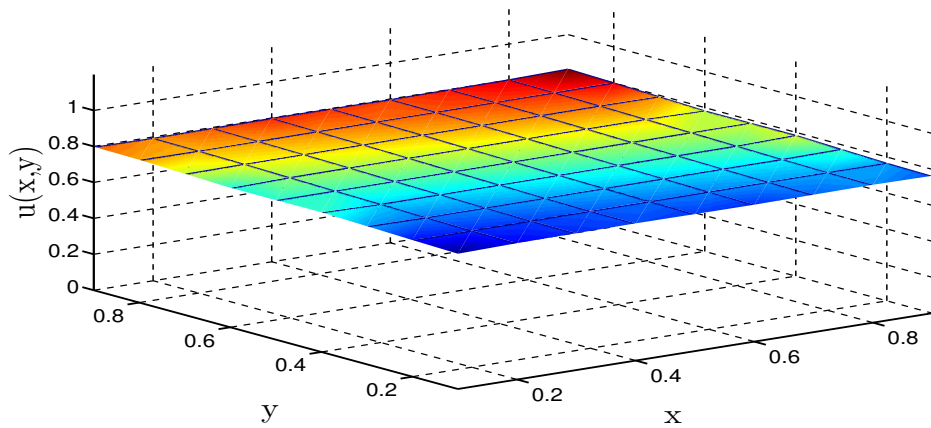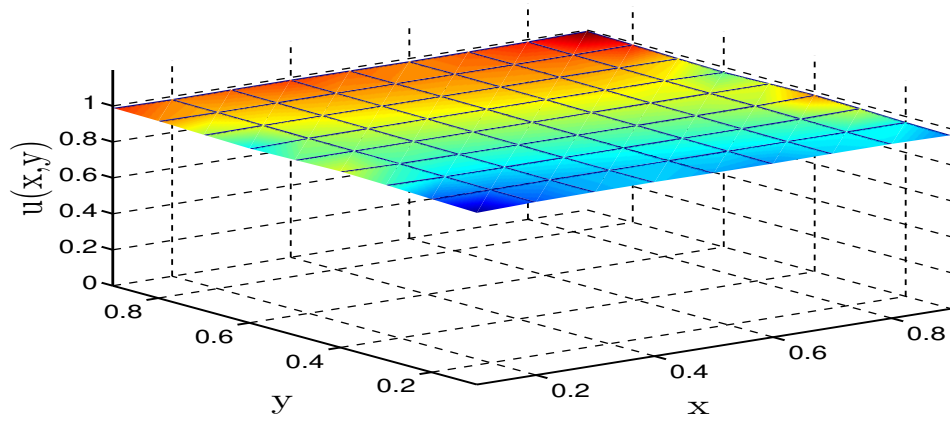
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2.6.4 Nonlinear Exterior Wave Problem

We consider the nonlinear exterior wave equation

$$\ddot{u} = c^2 \nabla^2 u + qu^2 \qquad\qquad (2.132)$$

in a two-dimensional infinite domain which is the outside of an obstacle (a circle) with radius $r = 0.25$ [56]. The wave speed c is taken as 200 and three different values of the nonnegative constant q ($q = 0$, $q = 2000$, $q = 5000$) are examined.

The homogeneous initial values $u|_{t=0}$ and $\dot{u}|_{t=0}$ are taken throughout the infinite domain. On the obstacle boundary Γ_0, u is prescribed as $u = 1$. Thus, the obstacle is at rest as $t \to 0^-$ and starts to radiate cylindrical waves as $t \to 0^+$ [56].

The solution is expected to oscillate for the linear case ($q = 0$), and it blows up for the nonlinear cases ($q = 2000$ and $q = 5000$), [56].

Three different types of radial basis functions ($f(r) = 1 + r$, $f(r) = \dfrac{2 - r}{(1 + r)^4}$ and $f(r) = e^{-r^2}$) are used in the calculations. The number of boundary elements (constant) used is $N = 120$. The solution is computed along straight lines radiating from $r = 0.25$ to $r = 0.5$.

For the DRBEM+FDM solution it is observed that the relaxation parameter gains more importance comparing to the parabolic problems (Problems 2.6.1-2.6.3). It is hard to find a proper value of the relaxation parameter which works for every nonlinear function and for all times. It can be seen from Figures 2.19(a), 2.20(a), 2.21(a) that the DRBEM+FDM solution for $q = 0$ with different radial basis functions oscillate for increasing t. For the cases $q = 2000$ and $q = 5000$ (Figures 2.19(b), 2.20(b), 2.21(b); 2.19(c), 2.20(c), 2.21(c)) the DRBEM+FDM solution has an unlimited growth. It is also noticed that the solution starts to grow at an earlier time level for the stronger nonlinearity with $q = 5000$. The time increment Δt is taken as $\Delta t = 0.01$ for all values of q.

In DRBEM+FDM solution procedure it is possible to use the radial basis function $f = 1 + r$ with the help of relaxation parameter, although it is not suitable for infinite regions. However, the computations are not extended to the points further than $r = 0.5$.

It is also noted that the relaxation parameter for the nonlinear wave equation is required to be less than 0.5, whereas for the nonlinear reaction-diffusion equation it has to be taken greater than 0.7.

For the DRBEM+LSM solution, it is noticed that the usage of the linear radial basis function does not give results due to the fact that the linear radial basis functions are not suitable for the exterior regions. This difficulty is overcome by the usage of a relaxation parameter for the DRBEM+FDM solution. In Figures 2.22 and 2.23, the expected behaviour, i.e., the solution oscillates in the linear case and has an unlimited growth for the nonlinear cases, is seen to be satisfied with the corresponding radial basis functions $f(r) = \dfrac{(2-r)}{(r+1)^4}$ and $f(r) = e^{-r^2}$. In the linear case $(q = 0)$, for all time levels Δt may be taken as 0.01. However, for increasing times and for the nonlinear cases Δt should be chosen in between 0.01 and 0.15. The same is also observed in the nonlinear reaction-diffusion problems as LSM needs larger time increment.

(a) q=0
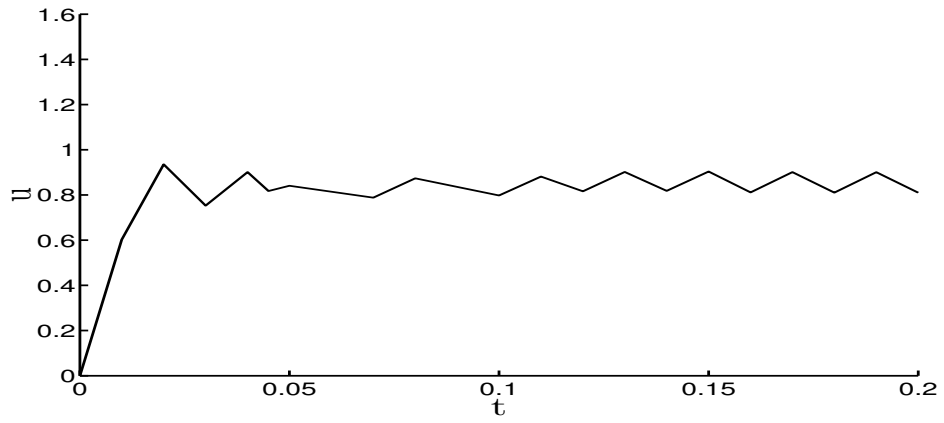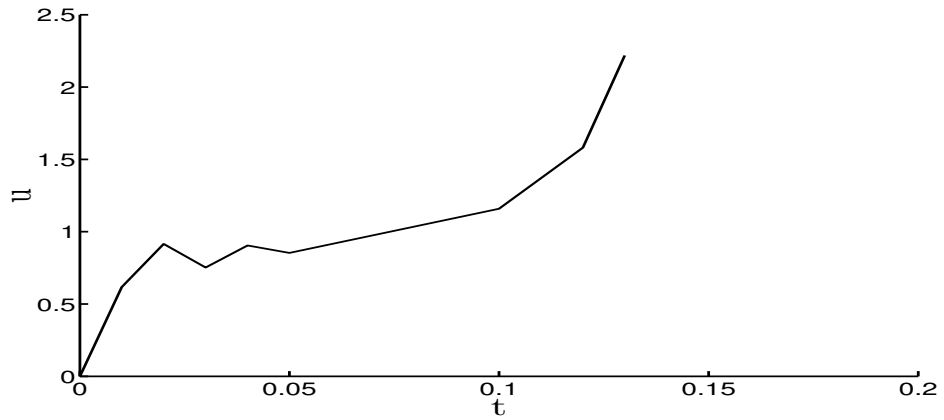
(b) q=2000
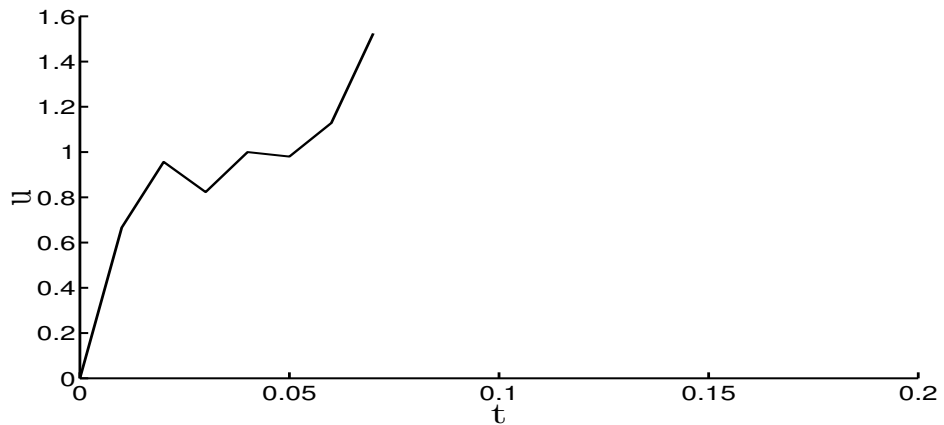
(c) q=5000

Figure 2.19:   DRBEM+FDM solution of Problem 2.6.4 with $f(r) = 1 + r$ with different nonlinearities
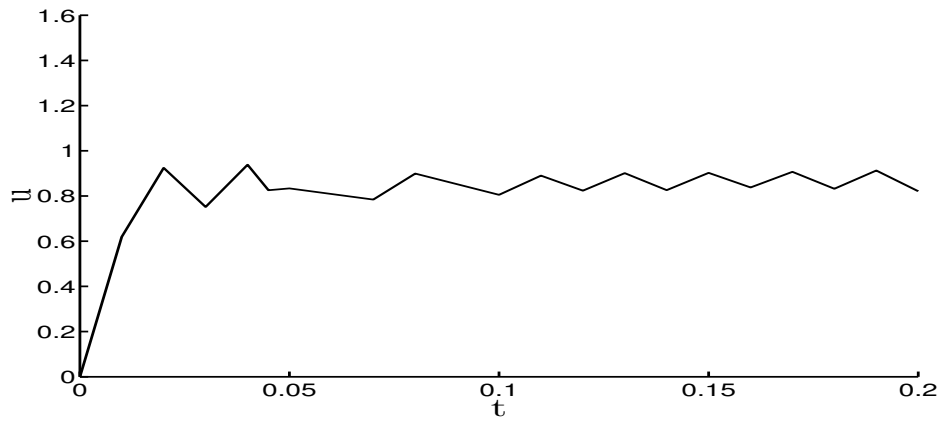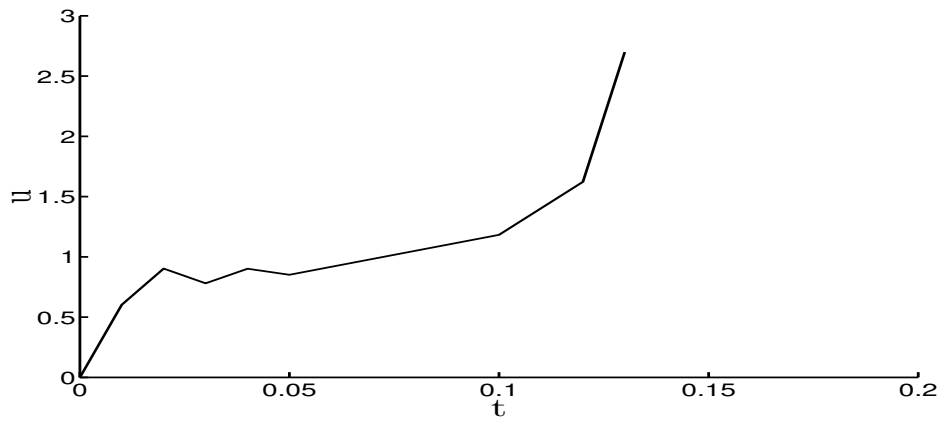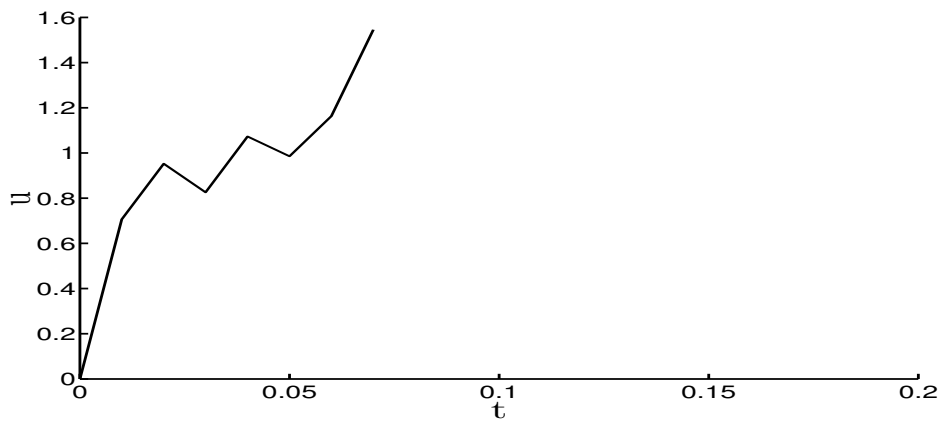
Figure 2.20: DRBEM+FDM solution of Problem 2.6.4 with $f(r) = \dfrac{(2-r)}{(r+1)^4}$ with different nonlinearities

(a) q=0
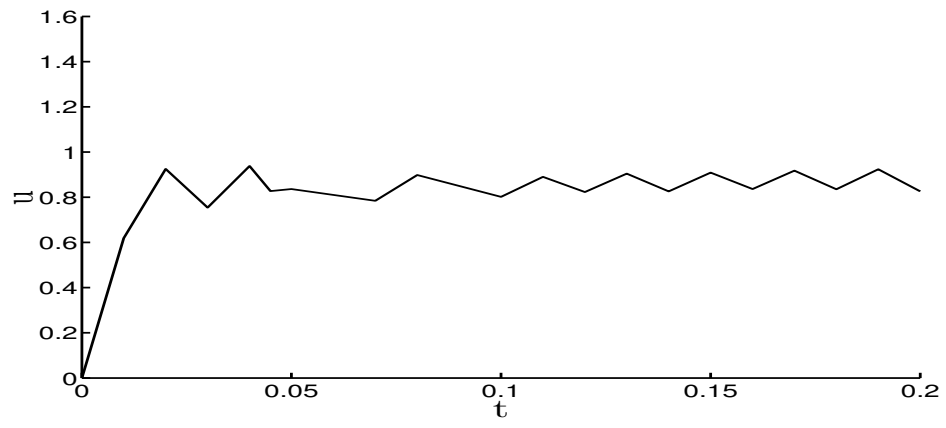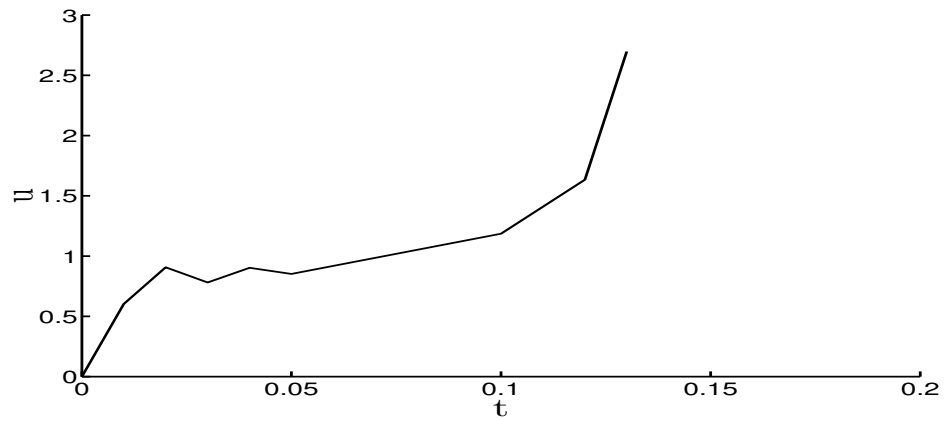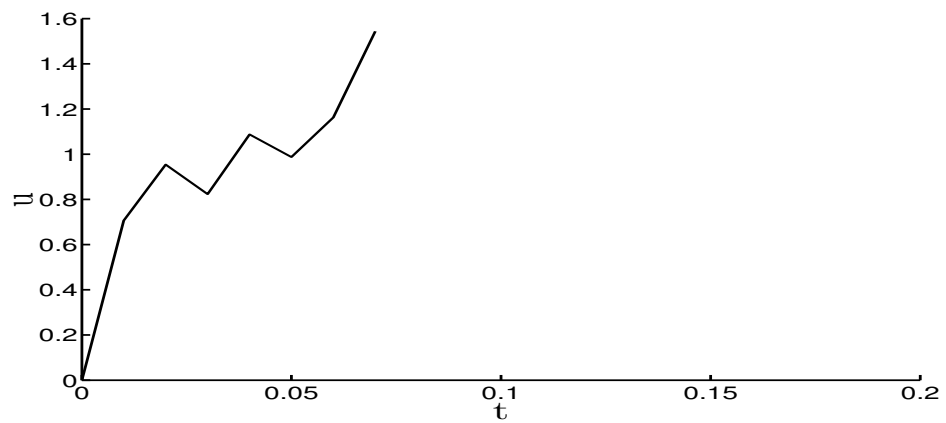
(b) q=2000

(c) q=5000

Figure 2.21: DRBEM+FDM solution of Problem 2.6.4 with $f(r) = e^{-r^2}$ with different nonlinearities
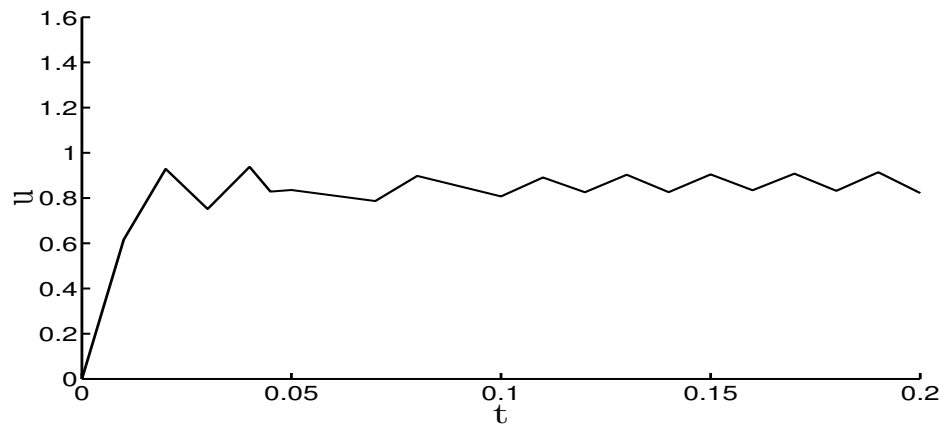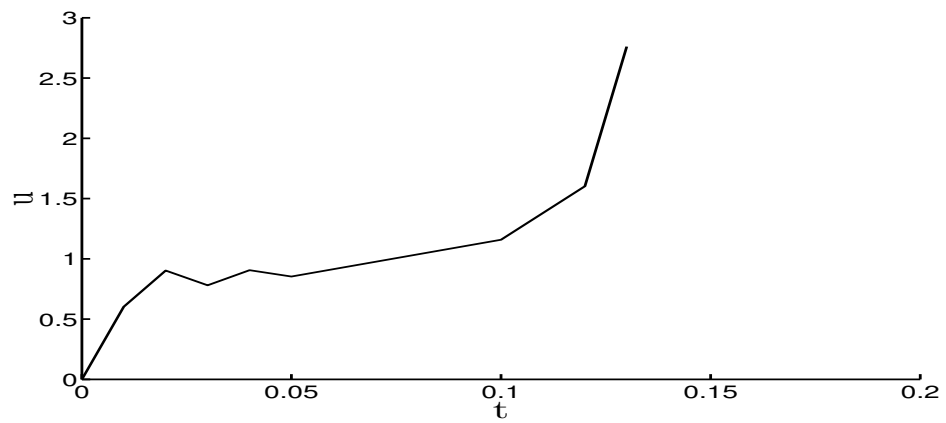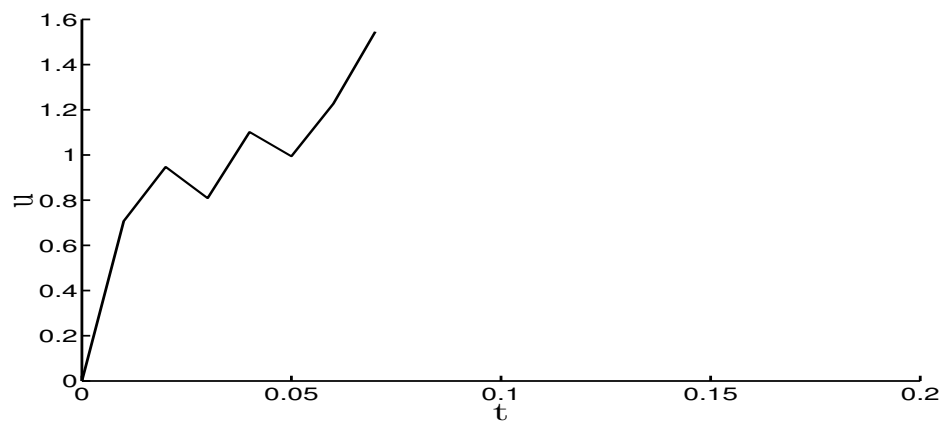
Figure 2.22: DRBEM+LSM solution of Problem 2.6.4 with $f(r) = \dfrac{(2-r)}{(r+1)^4}$ with different nonlinearities

(a) q=0
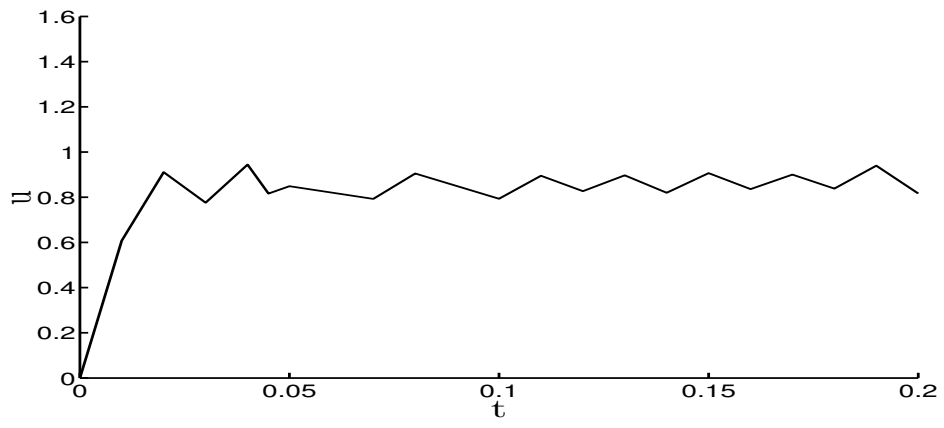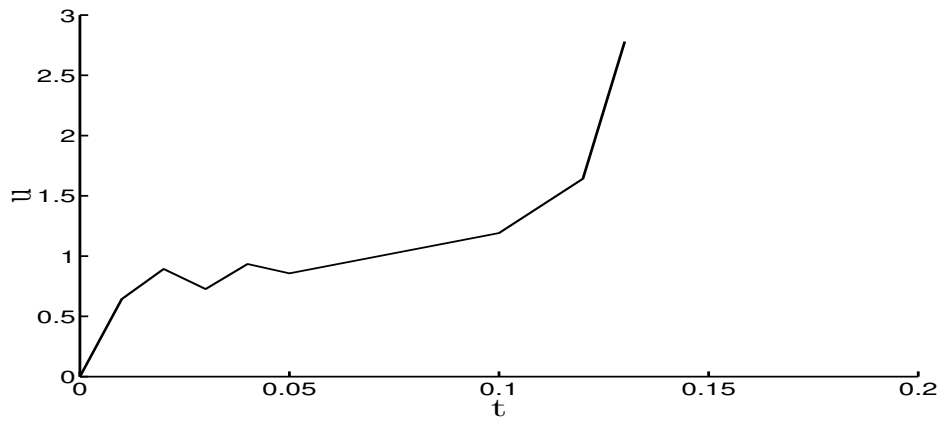
(b) q=2000
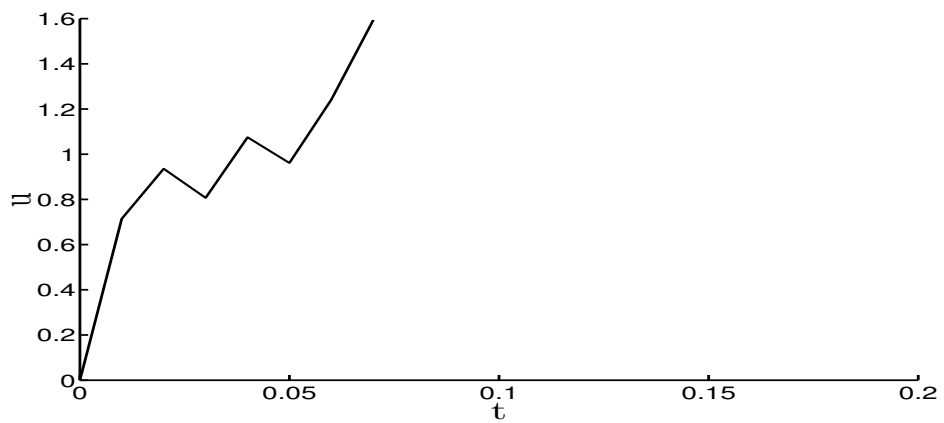
(c) q=5000

Figure 2.23: DRBEM+LSM solution of Problem 2.6.4 with $f(r) = e^{-r^2}$ with different nonlinearities

In this chapter, the initial and boundary value problems defined by the nonlinear reaction-diffusion and wave equations have been solved. In the latter case the problem is defined in an exterior region. The DRBEM is used as the spatial discretization. DRBEM discretizes boundary of the problem only and it solves the problems defined in an exterior region discretizing only the inner boundary of the region. Thus, as a discretization method, DRBEM is a suitable method for such exterior problems. Following the DRBEM discretization of the space derivatives, the obtained system of ordinary differential equations with respect to time, is solved using three different time integration methods, FDM, LSM and FEM. The comparison among the methods is made.

The DRBEM+FDM and DRBEM+FEM solution procedures give better accuracy compared to the DRBEM+LSM solution procedure, for the boundary and initial value problems defined by the nonlinear reaction-diffusion equation and system of nonlinear reaction-diffusion equations. It is possible to use LSM time integration method with larger time steps but still there is an accuracy drop in terms of maximum absolute error. Although, the DRBEM+FDM and DRBEM+FEM solutions have almost the same accuracy (in terms of maximum absolute error for the problems that have exact solution), FEM is accepted as the method of choice since FDM solutions depend on the relaxation parameter. For the problems which the exact solutions are not known the expected behaviour of the solution is caught by all the methods.

For the solution of exterior wave equation, several radial basis functions (linear, exponential, rational) are used for the DRBEM application. As the time integration method FDM and LSM are used. It is known that the linear radial basis functions are not suitable to the nature of the problem. One needs such radial basis functions that vanish for the far enough boundary. It is observed that, the difficulty of using linear radial basis functions is overcome with the help of relaxation parameter in FDM to obtain the solution at the points not very far from the obstacle. The DRBEM is applied with exponential and rational basis functions when LSM time integration is used. In the computations the expected behaviour of the solution is seen to be satisfied by both methods.

CHAPTER 3

THE DIFFERENTIAL QUADRATURE METHOD SOLUTION OF NONLINEAR REACTION-DIFFUSION AND WAVE EQUATIONS

In this chapter, numerical solutions of nonlinear reaction-diffusion and wave equations are going to be presented. The spatial derivatives are discretized by applying the differential quadrature method. And the obtained systems of initial value problems are solved using three different time integration schemes, FDM, LSM and FEM.

The differential quadrature method [14] approximates the solution of a partial differential equation using a high order polynomial approximation or using Fourier series expansion (in case the solution is known to be periodic). The polynomial based differential quadrature method is going to be applied for nonlinear reaction-diffusion and wave equations explaining in detail the first and second order derivative approximations in Section 3.1. The DQM formulations for the nonlinear reaction-diffusion and the wave equations are given in Sections 3.2 and 3.3, respectively. Then, the time dependent initial value problems resulting from the DQM discretization in space are solved using three different time integration schemes (FDM, LSM, FEM) which are explained in Sections 3.4 and 3.5. The applications of the proposed methods are considered in Section 3.6 by solving several test problems.

3.1 The Differential Quadrature Method

In this section, the differential quadrature method based on polynomial approximation is explained following the reference [14]. The method depends on the high order polynomial approximation of a smooth solution and its derivatives of a given partial differential equation, and based on the Weirstrass' first Theorem which is stated as follows:

Weierstrass' first Theorem Let $f(x)$ be a real valued continuous function defined in the closed interval $[a, b]$. Then there exists a sequence of polynomials $P_n(x)$ which converges to $f(x)$ uniformly as n goes to infinity, i.e. for every $\epsilon > 0$, there exists a polynomial $P_n(x)$ of degree $n = n(\epsilon)$ such that the inequality

$$|f(x) - P_n(x)| \leq \epsilon$$

holds through the interval $[a, b]$.

Thus, if $u(x)$ represents a smooth solution of a PDE, then it can be accurately approximated by a high degree polynomial, say degree $N - 1$. It is shown in [14] that this approximated polynomial constitutes an N-dimensional linear vector space V_N with the operation of vector addition and scalar multiplication. This approximation can be expressed as

$$u(x) \approx P_{N-1}(x) = \sum_{k=0}^{N-1} d_k x^k \tag{3.1}$$

where d_k's are constants.

For the numerical solution of a PDE, one needs to find out the functional values at the desired nodal points. Assuming that there are N nodal points in the closed interval $[a, b]$ with coordinates $a = x_1, x_2, ..., x_N = b$ and the functional value at a nodal point x_i is $u(x_i)$, the constants d_k can be determined from the following equation system

$$\begin{cases} d_0 + d_1 x_1 + d_2 x_1^2 + ... + d_{N-1} x_1^{N-1} = u(x_1) \\[3mm] d_0 + d_1 x_2 + d_2 x_2^2 + ... + d_{N-1} x_2^{N-1} = u(x_2) \\[3mm] .... \\[3mm] d_0 + d_1 x_N + d_2 x_N^2 + ... + d_{N-1} x_N^{N-1} = u(x_N). \end{cases} \qquad (3.2)$$

The coefficient matrix of the system (3.2) is Vandermonde matrix, which is known to be nonsingular. Thus, equation (3.2) has a unique solution for constants $d_0, d_1, d_2..., d_{N-1}$. Once the constants are determined, the approximated polynomial is obtained. For the case, in which N is large the system is highly ill-conditioned and its inversion is very difficult, and it is hard to determine the constants $d_0, d_1, d_2, ..., d_{N-1}$.

As is shown in [14], there exist many sets of base vectors in the linear vector space V_N of approximated polynomial $P_{N-1}(x)$. In this case, the vectors of this vector space are polynomials which are called the base polynomials. In this section, the base polynomials are set as the Lagrange interpolation polynomials for the application of the differential quadrature method (Shu's general approach [14]). For simplicity the k-th degree Lagrange interpolation polynomial is written in the form

$$l_k(x) = \frac{N(x, x_k)}{M^{(1)}(x_k)} \qquad (3.3)$$

with

$$M(x) = (x - x_1)(x - x_2)...(x - x_N) = N(x, x_k)(x - x_k)$$

$$M^{(1)}(x_k) = (x_k - x_1)...(x_k - x_{k-1})(x_k - x_{k+1})...(x_k - x_N) = \prod_{i=1, i \neq k}^{N} (x_k - x_i)$$

$$N(x_k, x_j) = M^{(1)}(x_k)\delta_{kj}$$

$$(3.4)$$

where δ_{kj} is the Kronecker delta function and $k = 1, 2, ..., N$.

The k-th degree Lagrange polynomial $l_k(x)$ in equation (3.3) possesses the property

$$l_k(x_i) = \begin{cases} 1, & \text{when} \quad k = i \\ \\ 0, & \text{otherwise.} \end{cases} \qquad (3.5)$$

When the Lagrange polynomials $l_k(x)$ in (3.3) are used in the approximation polynomial $P_{N-1}(x)$, this gives together with the property (3.5)

$$u(x) \approx P_N(x) = \sum_{i=1}^{N} u(x_i)l_i(x). \qquad (3.6)$$

Assuming that the solution u is sufficiently smooth over the interval $[a, b]$, i.e. m times continuously differentiable, its $m-$th order derivative $\dfrac{\partial^m u}{\partial x^m}$ at any grid point can be approximated as

$$\frac{\partial^m u}{\partial x^m}|_{x=x_i} = \sum_{j=1}^{N} w_{ij}^{(m)} u(x_j), \quad i \neq j \quad i = 1, 2, ..., N \qquad (3.7)$$

where the weighting coefficients $w_{ij}^{(m)}$ for $m = 1$ are given in the form

$$w_{ij}^{(1)} = \frac{N^{(1)}(x_i, x_j)}{M^{(1)}(x_j)}, \qquad i \neq j. \tag{3.8}$$

Differentiating the first equation given in (3.4), $w_{ij}^{(1)}$ can be rewritten as

$$w_{ij}^{(1)} = \frac{M^{(1)}(x_i)}{(x_i - x_j)M^{(1)}(x_j)}, \qquad i \neq j. \tag{3.9}$$

The weighting coefficients $w_{ii}^{(1)}$ are calculated according to the property of a linear vector space, if one set of base polynomials satisfies a linear operator, so does another set of base polynomials. Thus, the equation system for determination of $w_{ij}^{(1)}$ derived from the Lagrange interpolation polynomials in (3.6) should be equivalent to that derived from another set of base polynomials x^{k-1} ($k = 1, 2, ..., N$), in (3.1). Therefore $w_{ij}^{(1)}$ satisfies the following equation which is obtained by the base polynomial x^{k-1} when $k = 1$

$$\sum_{j=1}^{N} w_{ij}^{(1)} = 0 \quad \text{or} \quad w_{ii}^{(1)} = -\sum_{j=1, j\neq i}^{N} w_{ij}^{(1)}. \tag{3.10}$$

By using Shu's general approach, i.e., polynomial approximation and the linear vector space analysis, the second order weighting coefficients $w_{ij}^{(2)}$ can be obtained in terms of first order weighting coefficients as

$$w_{ij}^{(2)} = 2w_{ij}^{(1)}(w_{ii}^{(1)} - \frac{1}{x_i - x_j}) \quad \text{for} \ \ i \neq j$$

$$\tag{3.11}$$

$$w_{ii}^{(2)} = -\sum_{j=1, j\neq i}^{N} w_{ij}^{(2)}.$$

Shu's general approach can be applied for finding the recurrence relation formulation for higher order derivatives for $m = 2, 3, ..., N - 1$

$$w_{ij}^{(m)} = m(w_{ij}^{(1)} w_{ii}^{(m-1)} - \frac{w_{ij}^{(m-1)}}{x_i - x_j}), \qquad i \neq j$$

(3.12)

$$w_{ii}^{(m)} = - \sum_{j=1, j\neq i}^{N} w_{ij}^{(m)}$$

with $i, j = 1, 2, ..., N$.

In the other existing numerical methods, it is often preferred to use the uniform mesh, due to its practical use. However, for the DQM discretization, it is demonstrated in [14] that, the use of the nonuniform mesh in the PDQ approach gives rise to more stable numerical results. Thus, in this study also, the Chebyshev-Gauss-Lobatto (CGL) points are used to discretize the spatial domain as a nonuniform mesh which clusters close to the end points.

To define the CGL points one should use the Chebyshev polynomial of degree k which is defined by

$$T_k(x) = \cos k\theta, \quad \theta = \arccos x.$$

(3.13)

The Chebyshev-Gauss-Lobatto points are chosen as the roots of $|T_N(x)| = 1$, which are given by

$$x_i = \cos(i\pi/N), \quad i = 0, 1, ..., N.$$

(3.14)

Equation (3.14) is valid for the interval $[-1, 1]$. For a general domain $[a, b]$, the following transformation

$$x = \frac{(b-a)}{2}(1 - \xi) + a$$

(3.15)

can be used to map the interval $[a, b]$ in the x-domain onto the interval $[-1, 1]$ in the ξ-domain.

3.1.1 DQM for the Equation $\nabla^2 u = b(\mathbf{x}, t, p(u), \dot{u}, \ddot{u})$

In this section, the application of the DQM to the equations of the type

$$\nabla^2 u = b(\mathbf{x}, t, p(u), \dot{u}, \ddot{u}) \tag{3.16}$$

with

$$b = b_0(\mathbf{x}, t) + b_1(\mathbf{x}, t)p(u) + k_1\dot{u} + k_2\ddot{u} \tag{3.17}$$

is considered. In equation (3.17) b_0 and b_1 are functions of position and time, k_1 and k_2 are constants and $p(u)$ is the nonlinear function which is given in terms of the unknown u. Here $\mathbf{x}$ denotes the position vector either in one- or two-space dimensions.

DQM Formulation in one-space Dimension

In one-space dimension equation (3.16) takes the form

$$\frac{\partial^2 u}{\partial x^2} = b_0(x, t) + b_1(x, t)p(u) + k_1\dot{u} + k_2\ddot{u}. \tag{3.18}$$

Assuming that N grid points are taken in the computational domain $[a, b]$, the DQM formulation for equation (3.18) at any grid point $x = x_i$ $(i = 1, 2, ..., N)$ can be obtained using the derivative approximation (3.7) with $m = 2$ and the weighting coefficients for second order derivatives (equation (3.11))

$$\sum_{k=1}^{N} w_{ik}^{(2)} u(x_k, t) = b_0(x_i, t) + b_1(x_i, t)p(u(x_i, t)) + k_1\dot{u}|_{x=x_i} + k_2\ddot{u}|_{x=x_i} \tag{3.19}$$
$$i = 1, 2, ..., N.$$

Writing in matrix-vector form, this formulation leads to a system of $N \times N$ ODEs, i.e.,

$$\mathbf{Bu} = \mathbf{b_0} + \mathbf{B_1 p} + k_1 \dot{\mathbf{u}} + k_2 \ddot{\mathbf{u}} \tag{3.20}$$

where $\mathbf{B}$ is the $N \times N$ matrix containing the second order weighting coefficients, $\mathbf{u}$, $\dot{\mathbf{u}}$ and $\ddot{\mathbf{u}}$ are the $N \times 1$ vectors containing the unknown and its first and second order time derivatives, at the grid points, respectively, $\mathbf{b_0}$ and $\mathbf{p}$ are the vectors of length N containing the function values of b_0 and the nonlinearity, respectively, at the grid points. $\mathbf{B_1}$ is the $N \times N$ diagonal matrix with the diagonals containing the function b_1 at x_i for $i = 1, 2, ..., N$.

DQM Formulation in two-space Dimensions

In two space dimensions equation (3.16) is written as

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = b_0(x, y, t) + b_1(x, y, t)p(u) + k_1 \dot{u} + k_2 \ddot{u}. \tag{3.21}$$

If one takes N_x grid points in x-direction and N_y grid points in y-direction in the computational rectangular domain $[a_1, b_1] \times [a_2, b_2]$, the DQM discretization for equation (3.21) with the second order weighting coefficients (3.11) in x- and y- directions leads to

$$\sum_{k=1}^{N_x} w_{ik}^{(2)} u(x_k, y_j, t) + \sum_{k=1}^{N_y} \bar{w}_{jk}^{(2)} u(x_i, y_k, t) = b_0(x_i, y_j, t) + b_1(x_i, y_j, t)p(u)$$
$$+ k_1 \dot{u}(x_i, y_j, t) + k_2 \ddot{u}(x_i, y_j, t) \tag{3.22}$$

for $i = 1, 2, ..., N_x$ and $j = 1, 2, ..., N_y$.

Then, the system is rearranged as an $N_x \times N_y$ system of matrices

$$\mathbf{B_x U} + \mathbf{U B_y}^T = \mathbf{B_0} + \tilde{\mathbf{P}} + \dot{\mathbf{U}} + \ddot{\mathbf{U}} \tag{3.23}$$

where $\mathbf{B_x}$ is an $N_x \times N_x$ matrix and $\mathbf{B_y}$ is an $N_y \times N_y$ matrix containing the second order weighting coefficients in x- and y-directions, respectively. $\mathbf{U}$ is

the $N_x \times N_y$ matrix containing $u(x_i, y_j)$ as the ij-th entry, $\mathbf{B_0}$, $\tilde{\mathbf{P}}$, $\dot{\mathbf{U}}$ and $\ddot{\mathbf{U}}$ are the $N_x \times N_y$ matrices containing $b_0(x_i, y_j)$, $b_1(x_i, y_j)p(x_i, y_j)$, $k_1\dot{u}(x_i, y_j)$ and $k_2\ddot{u}(x_i, y_j)$, respectively as the ij-th entry.

3.2 The Differential Quadrature Method Solution of Nonlinear Reaction-Diffusion Equation

In this section, two kinds of problems governed by the nonlinear reaction-diffusion equation

$$\dot{u} = \nu\nabla^2 u + p(u) \tag{3.24}$$

will be considered. In equation (3.24) ∇^2 is the Laplacian operator either in one- or two-space dimensions, u is the unknown function with the first order time derivative $\dot{u}$ and $p(u)$ is the nonlinear function.

The first problem considered is the one-dimensional Cauchy problem which will be presented in Section 3.2.1. In solving Cauchy problems one tackles difficulty of having no boundary conditions. At this stage, we make use of DQM which may also be applied without any boundary conditions.

Next, in Section 3.2.2, the two-dimensional initial and boundary value problem is solved which has been also solved using DRBEM in Chapter 2. In DRBEM only the boundary discretization is necessery together with some needed interior points, which is computationally less expensive comparing to the other discretization methods. Although, the DQM is a domain discretization method the solution can be obtained with a very small number of freedom. In Section 3.6, it is observed that this number is even less than the one used in Chapter 2 with DRBEM.

3.2.1 The DQM Solution of the one-dimensional Cauchy Problem for Nonlinear Reaction-Diffusion Equation

The one-dimensional Cauchy problem governed by the nonlinear reaction-diffusion equation

$$\begin{cases} \dot{u} = \nu \left(\dfrac{\partial^2 u}{\partial x^2} \right) + p\left(u\right) & x \in \mathbb{R}, \quad t > 0 \\[3mm] u\left(x, 0\right) = u_0\left(x\right) & x \in \mathbb{R} \end{cases} \tag{3.25}$$

is discretized in space using DQM. For the Fisher type equation the nonlinear function $p\left(u\right)$ satisfies the conditions

$$\begin{cases} p\left(0\right) = p\left(1\right) = 0, \quad p'\left(0\right) > 0 > p'\left(1\right) \\[3mm] p\left(0\right) > 0, \quad 1 > u > 0 \end{cases} \tag{3.26}$$

and ν is a nonzero constant, u_0 is a given function of position. This problem together with the properties (3.26) shows a model describing the interaction between reaction mechanism and diffusion transportation corresponding to some physical and biological systems [71].

When the nonlinear reaction-diffusion equation (3.25) is compared with the general form (3.16) (taking $k_1 = \dfrac{1}{\nu}$, $k_2 = 0$, $b_0\left(x\right) = 0$, $b_1\left(x\right) = -\dfrac{1}{\nu}$) the function b will take the form

$$b = \frac{1}{\nu}\dot{u} - \frac{1}{\nu}p\left(u\right). \tag{3.27}$$

Assuming that $I = [a, b]$ $(a, \ b \in \mathbb{R})$ is taken as the computational domain with N CGL points, one has the $N \times N$ system of ODEs from the DQM formulation (Equation (3.20), i.e.,

$$\dot{\mathbf{u}} = \nu \mathbf{B} \mathbf{u} + \mathbf{p}\left(\mathbf{u}\right). \tag{3.28}$$

3.2.2 The DQM Solution of the two-dimensional Initial and Boundary Value Problem for Nonlinear Reaction-Diffusion Equation

The initial and boundary value problem for the nonlinear reaction-diffusion equation is given by

$$
\begin{cases}
\dot{u} = \nu \left(\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} \right) + p\left(u\right) & (x,y) \in \Omega, \quad t > 0 \\[2ex]
u\left(x,y,0\right) = u_0\left(x,y\right) & (x,y) \in \Omega \\[2ex]
\beta\left(x,y,t\right) u + \gamma\left(x,y,t\right) q = 0 & (x,y) \in \Gamma, \quad t > 0
\end{cases}
\tag{3.29}
$$

where $q = \dfrac{\partial u}{\partial n}$, n being the outward normal to the boundary. $u_0\left(x,y\right)$ is a given function in a rectangular domain $\Omega = \{(a_1, b_1) \times (a_2, b_2): \quad a_1, \quad b_1, \quad a_2, \quad b_2 \in \mathbb{R}\}$ with boundary Γ. $\beta\left(x,y,t\right)$ and $\gamma\left(x,y,t\right)$ are given functions in $\Gamma \times [0,T]$.

The problem (3.29) is written in the form of general equation (3.21) by taking $b_0 = 0, \quad b_1 = -\dfrac{1}{\nu}, \quad k_1 = \dfrac{1}{\nu}$ and $k_2 = 0$ as

$$\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = \frac{1}{\nu} \dot{u} - \frac{1}{\nu} p. \tag{3.30}$$

We discretize the rectangular domain Ω using N_x CGL points in x-direction and N_y CGL points in y-direction , which makes totally $N_x N_y$ discretization points in the domain of the problem.

The mixed type boundary condition in problem (3.29)

$$\beta(x_i, y_j, t)u(x_i, y_j, t) + \gamma(x_i, y_j, t)q(x_i, y_j, t) = 0$$

or equivalently

$$\beta(x_i, y_j, t)u(x_i, y_j, t) + \gamma(x_i, y_j, t)(\frac{\partial u}{\partial x}\frac{\partial x}{\partial n} + \frac{\partial u}{\partial y}\frac{\partial y}{\partial n})|_{(x_i, y_j, t)} = 0$$

(3.31)

is also discretized by using DQM approximation for the derivatives

$$\frac{\partial u}{\partial x}(x_i, y_j, t) = \sum_{k=1}^{N_x} w_{ik}^{(1)}u(x_k, y_j, t)$$

and

$$\frac{\partial u}{\partial y}(x_i, y_j, t) = \sum_{k=1}^{N_y} \bar{w}_{jk}^{(1)}u(x_i, y_k, t)$$

(3.32)

for $(x_i, y_j) \in \Gamma$, i.e. with $i = 1, N_x, \quad j = 1, 2, ..., N_y$ and $j = 1, N_y$, $i = 1, 2, ..., N_x$.

The nonlinear reaction-diffusion equation (3.30) is discretized for the interior points, i.e., for $i = 2, ... N_x - 1$ and $j = 2, ... N_y - 1$

$$\dot{u}(x_i, y_j, t) - p(u(x_i, y_j, t)) = \nu(w_{i1}^{(2)}u(x_1, y_j, t) + w_{iN_x}^{(2)}u(x_{N_x}, y_j, t)+$$

$$\sum_{k=2}^{N_x-1} w_{ik}^{(2)}u(x_k, y_j, t)) + \nu(\bar{w}_{j1}^{(2)}u(x_i, y_1, t) + \bar{w}_{jN_y}^{(2)}u(x_i, y_{N_y}, t) + \sum_{k=2}^{N_y-1} \bar{w}_{jk}^{(2)}u(x_i, y_k, t))$$

(3.33)

where the four terms outside of the summations come from the computed u_{ij} values on the boundary (from equations (3.31) and (3.32)).

Thus, the discretized equations (3.31) with (3.32) for the boundary condition together with (3.33) for the differential equation itself lead to the following equation system

$$\dot{\mathbf{U}} = \mathbf{B_x}\mathbf{U} + \mathbf{U}\mathbf{B_y}^T + \mathbf{P} \tag{3.34}$$

with the $(N_x - 2) \times (N_x - 2)$ matrix $\mathbf{B_x}$ and $(N_y - 2) \times (N_y - 2)$ matrix $\mathbf{B_y}$ containing the second order weighting coefficients in x- and y-directions times the diffusivity constant ν at interior nodes, respectively. $\mathbf{U}$, $\dot{\mathbf{U}}$ denote the $(N_x - 2) \times (N_y - 2)$ matrices containing $u(x_i, y_j)$, $\dot{u}(x_i, y_j)$ as the ij-th entry for $i = 2, 3, ..., N_x - 2$, $j = 2, 3, ..., N_y - 2$. Also the $(N_x - 2) \times (N_y - 2)$ matrix $\mathbf{P}$ contains the nonlinearity and the terms coming from the boundary.

3.3 The Differential Quadrature Method Solution of Nonlinear Wave Equation

This section contains the differential quadrature solution of the nonlinear wave equation

$$\ddot{u} = c^2 \nabla^2 u + p\left(u\right) \tag{3.35}$$

where ∇^2 is the Laplacian operator in one- or two-space dimensions, u is the unknown function with the second order time derivative $\ddot{u}$, $p\left(u\right)$ is the nonlinear function and c is the nonzero wave speed.

As in the previous section, first the DQM solution of the Cauchy problem will be considered which gives the opportunity of having solution without boundary conditions. It is followed by the solution of two-dimensional initial and boundary value problem for the nonlinear wave equation.

3.3.1 The DQM Solution of the one-dimensional Cauchy Problem for Nonlinear Wave Equation

The Cauchy problem for the one-dimensional nonlinear wave equation can be described as

$$
\begin{cases}
\ddot{u} = c^2 u_{xx} + p\left(u\right) & x \in \mathbb{R}, \quad t > 0 \\
\\
u\left(x, 0\right) = u_0\left(x\right) & x \in \mathbb{R} \\
\\
\dot{u}\left(x, 0\right) = u_1\left(x\right) & x \in \mathbb{R}
\end{cases}
\tag{3.36}
$$

with the nonzero wave speed c and the nonlinear function $p\left(u\right)$ for the unknown u. The functions u_0 and u_1 are the known functions of position.

Now, the general form (3.17) of the nonhomogenity b takes the form (by taking $b_0\left(x, t\right) = 0, \quad b_1\left(x, t\right) = -\dfrac{1}{c^2}, \quad k_1 = 0, \quad k_2 = \dfrac{1}{c^2}$)

$$
b = \frac{1}{c^2}\ddot{u} - \frac{1}{c^2}p\left(u\right).
\tag{3.37}
$$

With a similar procedure given in Section 3.1.1 the spatial discretization for the problem (3.36) by using DQM is obtained in matrix-vector form of length N

$$
\ddot{\mathbf{u}} = c^2 \mathbf{B} \mathbf{u} + \mathbf{p}\left(\mathbf{u}\right)
\tag{3.38}
$$

where $\mathbf{B}$ matrix contains the second order weighting coefficients and the vectors $\mathbf{u}$, $\ddot{\mathbf{u}}$, $\mathbf{p(u)}$ contain discretized values of the solution, its second order time derivative and the nonlinearity, respectively.

3.3.2 The DQM Solution of the two-dimensional Initial and Boundary Value Problem for Nonlinear Wave Equation

The initial and boundary value problem for the nonlinear wave equation is given by

$$
\begin{cases}
\ddot{u} = c^2 \left(\dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} \right) + p\left(u\right) & \left(x, y\right) \in \Omega, \ \ t > 0 \\[2em]
u\left(x, y, 0\right) = u_0\left(x, y\right) & \left(x, y\right) \in \Omega \\[2em]
\dot{u}\left(x, y, 0\right) = u_1\left(x, y\right) & \left(x, y\right) \in \Omega \\[2em]
\beta\left(x, y, t\right) u + \gamma\left(x, y, t\right) q = 0 & \left(x, y\right) \in \Gamma, \ \ t > 0
\end{cases}
\tag{3.39}
$$

where $q = \dfrac{\partial u}{\partial n}$, n being the outward normal to the boundary. $u_0\left(x, y\right)$ and $u_1\left(x, y\right)$ are given functions in a rectangular domain $\Omega = \{\left(a_1, b_1\right) \times \left(a_2, b_2\right) : \ a_1,$ $b_1, \ a_2, \ b_2 \in \mathbb{R}\}$ with boundary Γ. $\beta\left(x, y, t\right)$ and $\gamma\left(x, y, t\right)$ are given functions in $\Gamma \times [0, T]$.

When the problem is matched with the general form (3.21) by taking $b_0 = 0$, $b_1 = -\dfrac{1}{c^2}$, $k_1 = 0$ $k_2 = \dfrac{1}{c^2}$ as

$$
\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = \frac{1}{c^2}\ddot{u} - \frac{1}{c^2}p.
\tag{3.40}
$$

The DQM formulation for the two-dimensional initial and boundary value problem follows the same steps with the DQM discretization of the nonlinear reaction-diffusion equation which is given in Section 3.2.2. The only difference in the formulation is caused from the second order time derivative and the resulting formulation takes the form

$$
\ddot{\mathbf{U}} = \mathbf{B_x}\mathbf{U} + \mathbf{U}\mathbf{B_y}^T + \mathbf{P}
\tag{3.41}
$$

with the $\left(N_x - 2\right) \times \left(N_x - 2\right)$ matrix $\mathbf{B_x}$ and $\left(N_y - 2\right) \times \left(N_y - 2\right)$ matrix $\mathbf{B_y}$ containing the second order weighting coefficients in x- and y-directions respectively, times the square of the wave constant c at interior nodes. $\mathbf{U}$, $\ddot{\mathbf{U}}$ denote the $\left(N_x - 2\right) \times \left(N_y - 2\right)$ matrices containing $u(x_i, y_j)$, $\ddot{u}(x_i, y_j)$ as the ij-th entry for $i = 2, 3, ..., N_x - 2$, $j = 2, 3, ..., N_y - 2$. Also, the $\left(N_x - 2\right) \times \left(N_y - 2\right)$ matrix

P contains the nonlinearity and the terms coming from the boundary.

3.4 Time Integration Methods for the Nonlinear Reaction-Diffusion Equation

The time integration methods given in Chapter 2 (FDM, LSM and FEM) are also used for the solution of system of ordinary differential equations in time resulting from the DQM discretization of the nonlinear reaction-diffusion equation.

3.4.1 FDM for the Time Discretization of the DQM Solution of one-dimensional Cauchy Problem

The time dependent system of ODEs obtained after the DQM discretization of the nonlinear reaction-diffusion equation (Equation (3.28)) can be written in the form

$$\dot{\mathbf{u}} = \tilde{\mathbf{B}}\mathbf{u} + \mathbf{p}(\mathbf{u}) \tag{3.42}$$

where $\mathbf{p}$ is the $N \times 1$ vector containing the nonlinearity, $\tilde{\mathbf{B}}$ denotes the $N \times N$ matrix containing the second order weighting coefficients in x-direction times the diffusivity constant ν. This equation is similar to equation (2.69) when the DQM matrix $\tilde{\mathbf{B}}$ is replaced by the DRBEM matrix $\bar{\bar{\mathbf{H}}}$.

Thus, as in Section 2.4.1, the time derivative can be discretized using the Euler scheme [20] to have

$$\frac{1}{\Delta t}(\mathbf{u}^{m+1} - \mathbf{u}^m) = \tilde{\mathbf{B}}\mathbf{u}^m + \mathbf{p}(\mathbf{u^m}) \tag{3.43}$$

where m denotes the time level, Δt is the time increment and $\mathbf{p}\,(\mathbf{u^m})$ is the vector of length N containing the nonlinearity. Since Euler scheme is an explicit method, a relaxation procedure with a parameter $0 \leq \mu \leq 1$ for the unknown $\mathbf{u}$ in the form

$$\mathbf{u} = (1 - \mu)\,\mathbf{u}^m + \mu\mathbf{u}^{m+1} \tag{3.44}$$

is employed to the right-hand side of equation (3.43) in order to avoid the stability problems and this leads to

$$(\mathbf{I} - \mu\Delta t\tilde{\mathbf{B}})\mathbf{u}^{m+1} = (\mathbf{I} + \Delta t(1 - \mu)\tilde{\mathbf{B}})\mathbf{u}^m + \Delta t\mathbf{p}(\mathbf{u}^m). \tag{3.45}$$

Equation (3.45) contains an $N \times N$ system of linear equations which gives the solution vector $\mathbf{u}$ at $(m + 1)$-st time level in terms of the solution at m-th level. In the solution procedure, the nonlinearity $\mathbf{p}$ is approximated at m-th time level t^m in order to have a linear system of equations.

3.4.2   FDM for the Time Discretization of the DQM Solution of Initial and Boundary Value Problem

The $(N_x - 2) \times (N_y - 2)$ system of equations obtained after the DQM solution of two-dimensional initial and boundary value problem (3.34) is discretized by using FDM for the time derivative as

$$\frac{1}{\Delta t}(\mathbf{U}^{m+1} - \mathbf{U}^m) = \mathbf{B_x}\mathbf{U}^m + \mathbf{U}^m\mathbf{B_y}^T + \mathbf{P}^m \tag{3.46}$$

where $\mathbf{P}^m$ denotes the vector evaluated at the m-th time level. For the boundary nodes, equation (3.31) is used together with the DQM discretized form of the derivatives given in equation (3.32).

Since, this is a rectangular system, it is hard to arrange the system dimension if the relaxation procedure is applied from the begining. Thus, we first find $\mathbf{U}^{m+1}$ from equation (3.46) then we apply the relaxation procedure in the form

$$\mathbf{U}^{m+1} = (1 - \mu)\mathbf{U}^m + \mu\mathbf{U}^{m+1} \tag{3.47}$$

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for $0 \leq \mu \leq 1$.

3.4.3 LSM for the Time Discretization of the DQM Solution of one-dimensional Cauchy Problem

The DQM solution of the one-dimensional nonlinear reaction-diffusion equation (equation (3.42)) can be approximated

$$\mathbf{u} \approx \phi_1(t)\,\mathbf{u}^m + \phi_2(t)\,\mathbf{u}^{m+1} \tag{3.48}$$

for a typical time element of length Δt between m and $(m+1)$-st time levels. The linear interpolation functions $\phi_1, \quad \phi_2$ are defined in Section 2.4.3 with equation (2.81).

The residual vector $\mathbf{r}$ is obtained by substituting the approximation vector $\mathbf{u}$ from equation (3.48) in equation (3.42)

$$\mathbf{r}(t) = \dot{\mathbf{u}} - \tilde{\mathbf{B}}\mathbf{u} - \mathbf{p}(\mathbf{u}). \tag{3.49}$$

The error functional $\mathbf{\Pi}$ is constructed by taking the square of the error over each time element m for m=0,1,2,... i.e. [25],

$$\Pi = \int_{t^m}^{t^{m+1}} \mathbf{r}^T \mathbf{r}\, dt$$
$$\text{or} \tag{3.50}$$
$$\Pi = \int_{t^m}^{t^{m+1}} (\dot{\mathbf{u}} - \tilde{\mathbf{B}}\mathbf{u} - \mathbf{p}(\mathbf{u}))^T (\dot{\mathbf{u}} - \tilde{\mathbf{B}}\mathbf{u} - \mathbf{p}(\mathbf{u}))\, dt.$$

Setting up a new variable $\xi = \dfrac{t - t^m}{\Delta t}$ transforms the integrals to the ones over $[0, 1]$

$$\Pi = \Delta t \int_0^1 (\dot{\mathbf{u}} - \tilde{\mathbf{B}}\mathbf{u} - \mathbf{p}(\mathbf{u}))^T (\dot{\mathbf{u}} - \tilde{\mathbf{B}}\mathbf{u} - \mathbf{p}(\mathbf{u}))\, d\xi. \tag{3.51}$$

The error functional can be calculated after substituting the approximation for the unknown $\mathbf{u}$, and the approximation for the derivative of the solution which is obtained by taking the derivative of the approximation (3.48) (also given by equations (2.85) and (2.86) in Section 2.4.3).

The desired recurrence relation is obtained by minimizing the error functional with respect to u^{m+1} in the form

$$\mathbf{A}\mathbf{u}^{m+1} = \mathbf{B_1}\mathbf{u}^m + \mathbf{B_2}\mathbf{p}^m \tag{3.52}$$

where

$$
\begin{aligned}
\mathbf{A} &= \frac{1}{\Delta t^2}\mathbf{I} - \frac{1}{2\Delta t}(\tilde{\mathbf{B}} + \tilde{\mathbf{B}}^T) + \frac{1}{3}\tilde{\mathbf{B}}^T\tilde{\mathbf{B}} \\[2mm]
\mathbf{B_1} &= \frac{1}{\Delta t^2}\mathbf{I} + \frac{1}{2\Delta t}(\tilde{\mathbf{B}} - \tilde{\mathbf{B}}^T) - \frac{1}{6}\tilde{\mathbf{B}}^T\tilde{\mathbf{B}} \\[2mm]
\mathbf{B_2} &= \frac{1}{\Delta t}\mathbf{I} - \frac{1}{2}\tilde{\mathbf{B}}^T.
\end{aligned}
\tag{3.53}
$$

3.4.4 LSM for the Time Discretization of the DQM Solution of Initial and Boundary Value Problem

In this section, we consider the LSM solution of equation (3.34) which is the system of ODEs in time resulting from the DQM discretization of two-dimensional initial and boundary value problem. First, we reorganize the $(N_x - 2) \times (N_y - 2)$ system (3.34) which contains products of matrices in the form of matrix-vector equations of length $(N_x - 2)(N_y - 2)$, assuming that N_x grid points are taken in x-direction and N_y grid points are taken in y-direction. The reason for this transformation is to apply LSM to a matrix-vector system. For this, CGL points are renumbered only in the interior of the region. Boundary values are separately inserted. (Discretization of the domain and the reorganization can be seen in Figure 3.1)
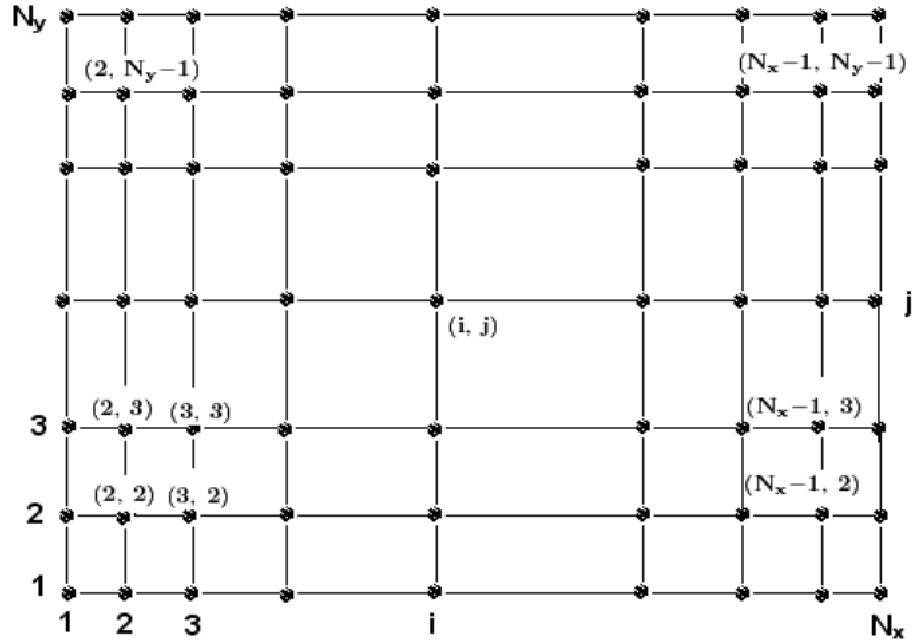
(a) Discretization of the domain with the CGL points
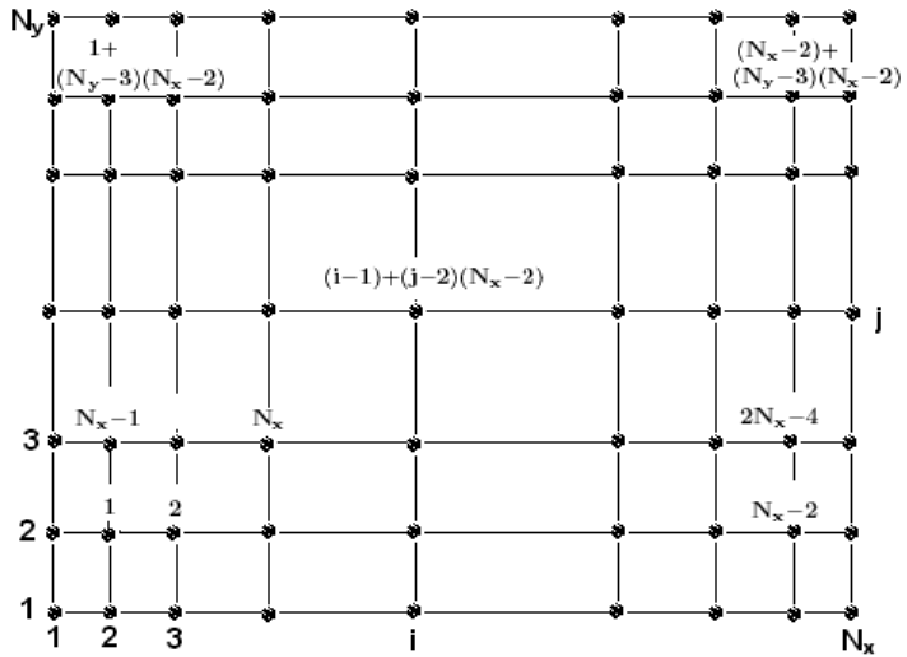
(b) Renumberred CGL points

Figure 3.1: Discretization of the domain with CGL points and renumberred form using CGL points

Rewriting the system (3.34) in matrix-vector form leads to $(N_x - 2)(N_y - 2)$ matrix-vector equations of the form

$$\dot{\tilde{\mathbf{u}}} = (\tilde{\mathbf{B}}_{\mathbf{x}} + \tilde{\mathbf{B}}_{\mathbf{y}})\tilde{\mathbf{u}} + \tilde{\mathbf{p}} \qquad (3.54)$$

where $\tilde{\mathbf{u}} = \left(u_{22}, u_{32}, ..., u_{(N_x-1)2}, u_{23}, ..., u_{(N_x-1)3}, ..., u_{2(N_y-1)}, ..., u_{(N_x-1)(N_y-1)}\right)^T$,
$\tilde{\mathbf{p}} = \left(p_{22}, p_{32}, ..., p_{(N_x-1)2}, p_{23}, ..., p_{(N_x-1)3}, ..., p_{2(N_y-1)}, ..., p_{(N_x-1)(N_y-1)}\right)^T$. Here u_{ij}'s and p_{ij}'s are the entries of the matrices $\mathbf{U}$ and $\mathbf{P}$, respectively.

The matrices $\tilde{\mathbf{B}}_{\mathbf{x}}$, $\tilde{\mathbf{B}}_{\mathbf{y}}$ are expressed as

$$\tilde{\mathbf{B}}_{\mathbf{x}} = \begin{bmatrix} \boldsymbol{B_x} & & & & \\ & \boldsymbol{B_x} & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \cdot \\ & & & & & \boldsymbol{B_x} \end{bmatrix} \qquad (3.55)$$

where $\boldsymbol{B_x}$ is the $(N_x - 2) \times (N_x - 2)$ matrix of second order weighting coefficients,

$$\tilde{\mathbf{B}}_{\mathbf{y}} = \begin{bmatrix} (\boldsymbol{B_y})_{11} & (\boldsymbol{B_y})_{12} & ... & (\boldsymbol{B_y})_{1(N_y-2)} \\ (\boldsymbol{B_y})_{21} & (\boldsymbol{B_y})_{22} & ... & (\boldsymbol{B_y})_{2(N_y-2)} \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ (\boldsymbol{B_y})_{(N_y-2)1} & (\boldsymbol{B_y})_{(N_y-2)2} & ... & (\boldsymbol{B_y})_{(N_y-2)(N_y-2)} \end{bmatrix} \qquad (3.56)$$

with $(N_x - 2) \times (N_x - 2)$ diagonal matrix

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$$(\mathbf{B_y})_{ij} = \begin{bmatrix} (b_y)_{(i+1)(j+1)} & & & & & \\ & (b_y)_{(i+1)(j+1)} & & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & & & (b_y)_{(i+1)(j+1)} \end{bmatrix}. \qquad (3.57)$$

Here $(b_y)_{(i+1)(j+1)}$ are the ij-th entry of the matrix $\mathbf{B_y}$ containing the second order coefficients times the diffusivity constant in y-direction.

Thus, the corresponding matrix-vector equations for the DQM solution of the two-dimensional initial and boundary value problem, defined by the nonlinear reaction-diffusion equation, is obtained as

$$\dot{\tilde{\mathbf{u}}} = \mathbf{B}'\tilde{\mathbf{u}} + \tilde{\mathbf{p}} \qquad (3.58)$$

where $\mathbf{B}' = \tilde{\mathbf{B}}_{\mathbf{x}} + \tilde{\mathbf{B}}_{\mathbf{y}}$.

Then, the application of LSM to the system of ODEs (3.58) with the solution vector $\tilde{\mathbf{u}}$ of length $(N_x - 2)(N_y - 2)$ follows the same lines as to obtain a similar system (3.52) for the one-dimensional nonlinear reaction-diffusion equation . The $N_x \times N_x$ matrix $\tilde{\mathbf{B}}$ in (3.53) is replaced by the $(N_x - 2)(N_y - 2) \times (N_x - 2)(N_y - 2)$ matrix $\mathbf{B}'$.

3.4.5 FEM for the Time Discretization of the DQM Solution of one-dimensional Cauchy Problem

In this section, the time dependent system of ODEs, obtained after the DQM discretization of the one-dimensional Cauchy problem, defined by the nonlinear reaction-diffusion equation (Equation (3.42)), is solved using FEM. For this time discretization method, a partition Ω_m in time, $\Omega_m = ((m - 1)T, mT]$ $m > 0$, is taken and the domain Ω_m is divided into M finite elements. Thus, the solution

is obtained at once in this domain without an iteration as is done in Section 2.4.5.

For the solution procedure, the first partition of the time domain ($\Omega_1 = (0, T]$) is divided into M time elements each of length Δt, with two nodes at the end of each element. The approximate solution denoted by $\mathbf{u}_e^h$ is defined as [70]

$$\mathbf{u}_e^h(t) = \sum_{j=1}^{2} \mathbf{u}_e^j \psi_j(t) \tag{3.59}$$

where $\mathbf{u}_e^j$ is the value of $\mathbf{u}_e^h$ at the node t^j $(j = 1, 2)$ for the element $'e'$. $\mathbf{u}_e$ is the discretized unknown vector obtained by using DQM for the time element $'e'$ with the linear shape functions defined in Chapter 2 (Equations (2.101)).

The corresponding variational statement is obtained after the multiplication of the system (3.42) by the shape functions ψ_k $(k = 1, 2)$, and integration by parts i.e,

$$\int_{t^1}^{t^2} \mathbf{u}_e^h \dot{\psi}_k dt + \tilde{\mathbf{B}} \int_{t^1}^{t^2} \mathbf{u}_e^h \psi_k dt = \mathbf{u}_e^h(t^2)\psi_k(t^2) - \mathbf{u}_e^h(t^1)\psi_k(t^1)$$
$$\tag{3.60}$$
$$- \int_{t^1}^{t^2} \mathbf{p}(\mathbf{u}(0)) \psi_k(t)dt$$

with $\tilde{\mathbf{B}} = \nu \mathbf{B}$.

Substitution of the approximate solution $\mathbf{u}_e^h$ given in equation (3.59) to equation (3.60) gives the solution as a linear system of equations of the form

$$\begin{bmatrix} s_{11} & s_{12} \\ \\ s_{21} & s_{22} \end{bmatrix} \left\{ \begin{array}{c} (\mathbf{u}_e^h)_1 \\ \\ (\mathbf{u}_e^h)_2 \end{array} \right\} = \left\{ \begin{array}{c} (\mathbf{g}_e)_1 \\ \\ (\mathbf{g}_e)_2 \end{array} \right\} \tag{3.61}$$

where each entry of the matrix in (3.61) is an $N \times N$ matrix s_{kj} $(k, j = 1, 2)$ for element $'e'$ and each entry of the vectors in (3.61) is $N \times 1$ vector for the points

$t^k \ (k = 1, 2)$

$$s_{kj} = (\int_{t^1}^{t^2} \dot{\psi}_k \psi_j dt) \boldsymbol{I} + (\int_{t^1}^{t^2} \psi_k \psi_j dt) \tilde{\boldsymbol{B}}$$

(3.62)

$$(\mathbf{g}_e)_k = \psi_k(t^2) \boldsymbol{u}_e^h(t^2) - \psi_k(t^1) \boldsymbol{u}_e^h(t^1) - (\int_{t^1}^{t^2} \mathbf{p}\,(\mathbf{u}(0)) \psi_k dt)$$

for $k, j = 1, 2$ where $\mathbf{I}$ is the identity matrix.

After the assembly procedure [70], the whole $NM \times NM$ system of equations for the representative time element $(0, T]$ is obtained as

$$\mathbf{S}_f \bar{\mathbf{u}}_f = \mathbf{g}_f$$

(3.63)

with the unknown vector $\bar{\mathbf{u}}_f$ with M vector blocks of length N. Each block contains the solution for the time levels $t = \{t : t = d\Delta t, \ d = 0, 1, ..., M\}$. $\mathbf{S}_f$ and $\mathbf{g}_f$ are the assembled matrix and vector, respectively, for the system of equations (3.61).

The solution is continued to the m-th partition $((m-1)T, mT\,]$, $m > 0$, m integer), repeating the same procedure described here for the first partition, and using the values obtained for the last node of $(m-1)$-st partition.

3.4.6 FEM for the Time Discretization of the DQM Solution of Initial and Boundary Value Problem

For the time discretization of the DQM solution of the two-dimensional nonlinear reaction-diffusion equation by FEM, the matrix-vector formulation obtained in Section 3.4.4 is used, i.e.,

$$\dot{\tilde{\mathbf{u}}} = \mathbf{B}' \tilde{\mathbf{u}} + \tilde{\mathbf{p}}.$$

(3.64)

To find the solution, the time domain Ω_m is divided into M finite elements as

is done in the previous section and the same steps are followed..

Therefore, the resulting system of linear equations for a typical element $'e'$ will be obtained as

$$\begin{bmatrix} \tilde{s}_{11} & \tilde{s}_{12} \\[2ex] \tilde{s}_{21} & \tilde{s}_{22} \end{bmatrix} \left\{ \begin{array}{c} (\tilde{\mathbf{u}}_e^h)_1 \\[2ex] (\tilde{\mathbf{u}}_e^h)_2 \end{array} \right\} = \left\{ \begin{array}{c} (\tilde{\mathbf{g}}_e)_1 \\[2ex] (\tilde{\mathbf{g}}_e)_2 \end{array} \right\} \tag{3.65}$$

where each entry of the matrix in (3.65) is an $(N_x-2)(N_y-2) \times (N_x-2)(N_y-2)$ matrix $\tilde{s}_{kj}$ $(k,j=1,2)$ for element $'e'$ and each entry of the vectors in (3.65) is $(N_x-2)(N_y-2) \times 1$ vector for the points t^k $(k=1,2)$

$$\begin{aligned} \tilde{s}_{kj} &= \left(\int_{t^1}^{t^2} \dot{\psi}_k \psi_j dt \right) \boldsymbol{I} + \left(\int_{t^1}^{t^2} \psi_k \psi_j dt \right) \boldsymbol{B}' \\[3ex] (\tilde{\mathbf{g}}_e)_k &= \psi_k(t^2) \tilde{\boldsymbol{u}}_e^h(t^2) - \psi_k(t^1) \tilde{\boldsymbol{u}}_e^h(t^1) - \left(\int_{t^1}^{t^2} \mathbf{p}(\tilde{\mathbf{u}}(0)) \psi_k dt \right) \end{aligned} \tag{3.66}$$

for $k,j = 1,2$ and $\mathbf{I}$ is the identity matrix.

Then, the assembly procedure will give the whole $(N_x-2)(N_y-2)M \times (N_x-2)(N_y-2)M$ system of equations for the first partition of time $(0,T]$ as

$$\tilde{\mathbf{S}}_f \tilde{\mathbf{u}}_f = \tilde{\mathbf{g}}_f. \tag{3.67}$$

The unknown vector $\tilde{\mathbf{u}}_f$ is with M vector blocks each of which has length $(N_x-2)(N_y-2)$ for each element of the time domain Ω_m, and the assembled matrix $\tilde{\mathbf{S}}_f$, the assembled vector $\tilde{\mathbf{g}}_f$ are obtained from the assembly of the system (3.65).

Then, the above described solution procedure may be continued up to the desired time level, using the values found from the previous step as the initial data.

3.5 Time Integration Methods for the Nonlinear Wave Equation

In this Section the system of ODEs obtained from the DQM discretization of nonlinear wave equation will be discretized using FDM, LSM and FEM. The systems (3.38) and (3.41) of second order ordinary differential equations with respect to time for the nonlinear wave equations in one- and two-space dimensions, respectively, can be written in the following form

$$\ddot{\tilde{\mathbf{u}}} = \tilde{\mathbf{B}}\tilde{\mathbf{u}} + \tilde{\mathbf{p}}\left(\tilde{\mathbf{u}}\right). \tag{3.68}$$

For the one-dimensional problem (3.38) $\tilde{\mathbf{u}} = \mathbf{u}$, $\tilde{\mathbf{p}} = \mathbf{p}$ and $\tilde{\mathbf{B}} = c^2\mathbf{B}$ with the $N \times N$ matrix $\mathbf{B}$ containing the second order DQM weighting coefficients and the nonlinear function $\mathbf{p}$ in terms of the unknown $\mathbf{u}$.

In order to obtain equation (3.68) for the two-dimensional case the reformulation described in Section 3.4.4 is once more used. Thus, in equation (3.68) $\tilde{\mathbf{u}}$ and $\tilde{\mathbf{p}}$ are the vectors of length $(N_x - 2)(N_y - 2)$ containing the entries of the matrices $\mathbf{U}$ and $\mathbf{P}$ which are provided for the DQM solution of the two-dimensional wave equation by equation (3.41), and the vectors are given in the form

$$\tilde{\mathbf{u}} = \left(u_{22}, u_{32}, ..., u_{(N_x-1)2}, u_{23}, ..., u_{(N_x-1)3}, ..., u_{2(N_y-1)}, ..., u_{(N_x-1)(N_y-1)}\right)^T,$$
$$\tilde{\mathbf{p}} = \left(p_{22}, p_{32}, ..., p_{(N_x-1)2}, p_{23}, ..., p_{(N_x-1)3}, ..., p_{2(N_y-1)}, ..., p_{(N_x-1)(N_y-1)}\right)^T$$
$$\tag{3.69}$$

and $\tilde{\mathbf{B}} = \tilde{\mathbf{B}}_{\mathbf{x}} + \tilde{\mathbf{B}}_{\mathbf{y}}$ which are defined with the block matrices in equations (3.55) and (3.56). The matrices $\tilde{\mathbf{B}}_{\mathbf{x}}$ and $\tilde{\mathbf{B}}_{\mathbf{y}}$ contain the matrices $\mathbf{B}_{\mathbf{x}}$ and $\mathbf{B}_{\mathbf{y}}$ which have the second order weighting coefficients times square of the wave speed c (the diffusivity constant ν in the nonlinear reaction-diffusion equation case).

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3.5.1 FDM for the Time Discretization of the DQM Solution of the Nonlinear Wave Equation

In order to solve the second order time dependent system of ordinary differential equations (3.68) using FDM the central difference formula is applied, i.e.,

$$\frac{1}{\Delta t^2}(\tilde{\mathbf{u}}^{m+1} - 2\tilde{\mathbf{u}}^m + 2\tilde{\mathbf{u}}^{m-1}) = \tilde{\mathbf{B}}\tilde{\mathbf{u}}^m + \mathbf{p}(\tilde{\mathbf{u}}^{\mathbf{m}}). \tag{3.70}$$

Since central difference is an explicit scheme, a relaxation procedure given in (3.44) is employed to the right-hand side of equation (3.70) to have,

$$(\mathbf{I} - \Delta t^2 \mu \tilde{\mathbf{B}})\tilde{\mathbf{u}}^{m+1} = (2\mathbf{I} + \Delta t^2 (1-\mu)\tilde{\mathbf{B}})\tilde{\mathbf{u}}^m - \tilde{\mathbf{u}}^{m-1} + \Delta t^2 \tilde{\mathbf{p}}(\tilde{\mathbf{u}}^m). \tag{3.71}$$

This is an iterative procedure to find the values at $(m+1)$-st level using previously obtained two consecutive level solutions. However, one still needs the value of $\tilde{\mathbf{u}}^{-1}$ in order to find $\tilde{\mathbf{u}}^1$. To this end, the second initial condition, given in terms of the first order time derivative in problems (3.36) and (3.39) for the one- and two-dimensional cases, is made use of with its backward difference approximation

$$\frac{\partial \tilde{u}}{\partial t}\Big|_{t=0} = \frac{\tilde{u}^0 - \tilde{u}^{-1}}{\Delta t} \qquad \text{or} \qquad \tilde{u}^{-1} = \tilde{u}_0 - \Delta t \frac{\partial \tilde{u}}{\partial t}\Big|_{t=0}. \tag{3.72}$$

Thus, equation (3.71) together with equation (3.72) produces the following system of equations to be solved for $m = 1$ as

$$(\mathbf{I} - \Delta t^2 \mu \tilde{\mathbf{B}})\tilde{\mathbf{u}}^1 = (\mathbf{I} + \Delta t^2 (1-\mu)\tilde{\mathbf{B}})\tilde{\mathbf{u}}_0 + \Delta t \tilde{\mathbf{u}}_1 + \Delta t^2 \tilde{\mathbf{p}}(\tilde{\mathbf{u}}^0) \tag{3.73}$$

where $\tilde{\mathbf{u}}_0$ and $\tilde{\mathbf{u}}_1$ denote the vectors of length N containing the initial conditions $u_0(x)$ and $u_1(x)$ of problem (3.36) or the vector of length $(N_x - 2)(N_y - 2)$ containing the initial conditions $u_0(x, y)$ and $u_1(x, y)$ of problem (3.39) at the grid points for the one- and two-dimensional problems, respectively.

Thus, using equation (3.73) for the first step and equation (3.71) for $m = 1, 2, ...$ iteratively, one is able to find the solution at the desired time level.

3.5.2 LSM for the Time Discretization of the DQM Solution of the Nonlinear Wave Equation

Solution of the second order time dependent system of ordinary differential equations resulting from the DQM discretization of nonlinear wave equation can be approximated by the quadratic interpolation functions (defined in Section 2 with the equation (2.91))

$$\tilde{\mathbf{u}} = \phi_{-1}\tilde{\mathbf{u}}^{m-1} + \phi_0\tilde{\mathbf{u}}^m + \phi_1\tilde{\mathbf{u}}^{m+1} \tag{3.74}$$

over the m-th time element with the initial point t^{m-1} and the terminal point t^{m+1}.

The error functional over the m-th time element, which is obtained in terms of the residual vector $\mathbf{r}$ as in the previous sections, leads to

$$\Pi = \int_{t^{m-1}}^{t^{m+1}} \mathbf{r}^T\mathbf{r}\,dt = \Delta t \int_{-1}^{1} (\ddot{\tilde{\mathbf{u}}} - \tilde{\mathbf{B}}\tilde{\mathbf{u}} - \tilde{\mathbf{p}})^T(\ddot{\tilde{\mathbf{u}}} - \tilde{\mathbf{B}}\tilde{\mathbf{u}} - \tilde{\mathbf{p}})\,d\xi \tag{3.75}$$

with the appropriate transformation ($\xi = \dfrac{t - t^m}{\Delta t}$) (The transformed quadratic interpolation functions are given by equation (2.95)).

The second derivatives of the quadratic interpolation functions are replaced in (3.74) by using the definitions (2.97) as

$$\ddot{\tilde{\mathbf{u}}} = \ddot{\phi}_{-1}\tilde{\mathbf{u}}^{m-1} + \ddot{\phi}_0\tilde{\mathbf{u}}^m + \ddot{\phi}_1\tilde{\mathbf{u}}^{m+1} = \frac{1}{\Delta t^2}\tilde{\mathbf{u}}^{m-1} - \frac{2}{\Delta t^2}\tilde{\mathbf{u}}^m + \frac{1}{\Delta t^2}\tilde{\mathbf{u}}^{m+1}. \tag{3.76}$$

One should minimize the error functional Π with respect to $\tilde{\mathbf{u}}^{\mathbf{m+1}}$ to obtain the final system of linear equations

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$$\mathbf{A_1}\tilde{\mathbf{u}}^{m+1} = \mathbf{A_2}\tilde{\mathbf{u}}^{m-1} + \mathbf{A_3}\tilde{\mathbf{u}}^m + \mathbf{A_4}\tilde{\mathbf{p}}^m \tag{3.77}$$

with the matrices

$$\mathbf{A_1} = -\frac{2}{\Delta t^4}\mathbf{I} + \frac{1}{3\Delta t^2}(\tilde{\mathbf{B}} + \tilde{\mathbf{B}}^T) - \frac{4}{15}\tilde{\mathbf{B}}^T\tilde{\mathbf{B}}$$

$$\mathbf{A_2} = \frac{2}{\Delta t^4}\mathbf{I} - \frac{1}{3\Delta t^2}(\tilde{\mathbf{B}} + \tilde{\mathbf{B}}^T) - \frac{1}{15}\tilde{\mathbf{B}}^T\tilde{\mathbf{B}}$$

$$\mathbf{A_3} = -\frac{4}{\Delta t^4}\mathbf{I} + \frac{2}{3\Delta t^2}(\tilde{\mathbf{B}}^T - 2\tilde{\mathbf{B}}) + \frac{2}{15}\tilde{\mathbf{B}}^T\tilde{\mathbf{B}} \tag{3.78}$$

$$\mathbf{A_4} = -\frac{2}{\Delta t^2}\mathbf{I} + \frac{1}{3}\tilde{\mathbf{B}}^T.$$

Equation (3.77) is used to obtain the solution for $m = 1, 2, ...$ iteratively. For $m = 0$, one should make use of the initial condition given in terms of the first order time derivative of the solution at $t = 0$. The approximation (3.74) is differentiated with respect to $'t'$ and evaluated at $t = 0$, i.e.,

$$\frac{\partial\tilde{\mathbf{u}}}{\partial t}\Big|_{t=0} = \dot{\phi}_{-1}\tilde{\mathbf{u}}^{-1} + \dot{\phi}_0\tilde{\mathbf{u}}^0 + \dot{\phi}_1\tilde{\mathbf{u}}^1 \tag{3.79}$$

which gives,

$$\tilde{\mathbf{u}}^{-1} = \tilde{\mathbf{u}}^1 - 2\Delta t\left(\frac{\partial\tilde{\mathbf{u}}}{\partial t}\Big|_{t=0}\right). \tag{3.80}$$

Thus, this approximation is used in equation (3.77) to obtain the iteration step for $m = 0$,

$$\left(\mathbf{A_1} - \mathbf{A_2}\right)\tilde{\mathbf{u}}^1 = \mathbf{A_3}\tilde{\mathbf{u}}^0 - 2\Delta t\mathbf{A_2}\dot{\tilde{\mathbf{u}}}^0 + \mathbf{A_4}\tilde{\mathbf{p}}^0 \tag{3.81}$$

where the matrices $\mathbf{A_1}$, $\mathbf{A_2}$, $\mathbf{A_3}$, $\mathbf{A_4}$ are defined in equation (3.78).

3.5.3 FEM for the Time Discretization of the DQM Solution of the Nonlinear Wave Equation

The FEM solution of the ODEs resulting from the DQM discretization of non-linear wave equation is going to be described for the first partition of the time domain $\Omega_1 = (0, T]$ initially, then the same procedure can be followed for the other partitions. Each partition is divided into M finite elements each of which has length Δt, with two nodes at the end points.

The unknown vector $\tilde{\mathbf{u}}_e$ for the element $'e'$ of the first partititon Ω_1 is approximated by $\tilde{\mathbf{u}}_e^h$ as

$$\tilde{\mathbf{u}}_e^h(t) = \sum_{j=1}^{2} \tilde{\mathbf{u}}_e^j \psi_j(t) \tag{3.82}$$

where $\tilde{\mathbf{u}}_e^j$ is the value of $\tilde{\mathbf{u}}_e^h$ at the node t^j $(j = 1, 2)$ and ψ_j's are the linear shape functions defined by the equation (2.101).

The variational statement is obtained after multiplying the equation (3.68) by the shape function ψ_k $(k = 1, 2)$, and integrating by parts as

$$\int_{t^1}^{t^2} \frac{\partial \tilde{\mathbf{u}}_e^h}{\partial t} \dot{\psi}_k dt + \tilde{\mathbf{B}} \int_{t^1}^{t^2} \tilde{\mathbf{u}}_e^h \psi_k dt = \frac{\partial \tilde{\mathbf{u}}_e^h}{\partial t}(t^2)\psi_k(t^2) - \frac{\partial \tilde{\mathbf{u}}_e^h}{\partial t}(t^1)\psi_k(t^1)$$
$$- \int_{t^1}^{t^2} \tilde{\mathbf{p}}(\tilde{\mathbf{u}}(0))\psi_k(t)dt \tag{3.83}$$

where the solution $\tilde{\mathbf{u}}$ is taken at $t = 0$ for the evaluation of the nonlinear function for the first partition.

Then, the linear system of equations are obtained after substituting the approximate solution (3.82) in (3.83) and performing the integrals, as

$$\begin{bmatrix} \tilde{\mathbf{s}}_{11} & \tilde{\mathbf{s}}_{12} \\ \\ \tilde{\mathbf{s}}_{21} & \tilde{\mathbf{s}}_{22} \end{bmatrix} \left\{ \begin{array}{c} (\tilde{\mathbf{u}}_e^h)_1 \\ \\ (\tilde{\mathbf{u}}_e^h)_2 \end{array} \right\} = \left\{ \begin{array}{c} (\tilde{\mathbf{g}}_e)_1 \\ \\ (\tilde{\mathbf{g}}_e)_2 \end{array} \right\} \tag{3.84}$$

where

$$\begin{aligned} \tilde{\mathbf{s}}_{\mathbf{kj}} &= (\int_{t^1}^{t^2} \dot{\psi}_k \dot{\psi}_j dt)\mathbf{I} + (\int_{t^1}^{t^2} \psi_k \psi_j dt)\tilde{\mathbf{B}} \\ \\ (\tilde{\mathbf{g}}_e)_k &= \psi_k(t^2)\frac{\partial \tilde{\mathbf{u}}_e^h}{\partial t}(t^2) - \psi_k(t^1)\frac{\partial \tilde{\mathbf{u}}_e^h}{\partial t}(t^1) - \int_{t^1}^{t^2} \tilde{\mathbf{p}}(\tilde{\mathbf{u}}(0))\psi_k dt \end{aligned} \tag{3.85}$$

for $k = 1, 2$.

A similar assembly procedure is applied to have the whole system of equations for the partition $[0, T]$. However, this time we need the value of $\frac{\partial \tilde{\mathbf{u}}}{\partial t}$ at $t = T$ as the last entry of the load vector and likewise to the previous time integration schemes, it is approximated by using the approximation (3.82).

The final assembled system

$$\tilde{\mathbf{S}}_{\mathbf{w}}\tilde{\mathbf{u}}_{\mathbf{w}} = \tilde{\mathbf{g}}_{\mathbf{w}} \tag{3.86}$$

is obtained for the unknown $\tilde{\mathbf{u}}_{\mathbf{w}}$ with M blocks each of length N and $(N_x - 2)(N_y - 2)$ for the one- and two-dimensional problems respectively. Each block contains the solution $\tilde{\mathbf{u}}$ for the time levels $t = d\Delta t, d = 0, 1, ..., M$. The matrix $\tilde{\mathbf{S}}_{\mathbf{w}}$ and the vector $\tilde{\mathbf{g}}_{\mathbf{w}}$ are the assembled forms of $\tilde{\mathbf{s}}_{\mathbf{kj}}$ and $(\tilde{\mathbf{g}}_{\mathbf{e}})_k$, respectively.

3.6   Numerical Results

In this section, the numerical solutions of the Cauchy problems and the boundary-initial value problems defined by one-dimensional and two-dimensional nonlinear reaction-diffusion and wave equations are solved, respectively. The spatial discretization is done by using the DQM which approximates the solution and its spatial derivatives using high degree polynomials. The DQM is known to give very good accuracy with a considerably small number of mesh points. Then, the obtained system of ODEs in time are discretized with the temporal discretization

methods as FDM, LSM and FEM. For each problem several number of DQM points N or $(N_x - 2)(N_y - 2)$ (depending on the dimension of the problem) and time steps Δt are tested to find the best solution in terms of maximum absolute errors.

The problems considered in this section are (1) Fisher equation, (2) Generalized Fisher equation, (3) Nonlinear equation of Fisher type with $p(u) = 6u(1 - u)$, (4) Nonlinear reaction-diffusion equation with $p(u) = u(1 - u)(u - 1)$, (5) Two-dimensional nonlinear reaction-diffusion equation, (6) Nonlinear wave equation with $p(u) = \frac{3}{2}(u^3 - u)$, (7) Nonlinear wave equation with $p(u) = u^2 - u - u^3$, (8) Two-dimensional nonlinear wave equation.

For these test problems, the maximum absolute error τ_m for the m-th time level which is defined in the form

$$\tau_m = \max_{1 \leq i \leq N_x, 1 \leq j \leq N_y} |u_{exact}(x_i, y_j, t^m) - u_{num}(x_i, y_j, t^m)| \qquad (3.87)$$

is used to measure the quality of the numerical solution.

The calculations for the test problems are performed using the Chebyshev-Gauss-Lobatto points which are giving rise to more stable results [14].

As the computational domain $[-1, 1]$ is taken for the Cauchy Problems (Problem 3.6.1-3.6.4 and 3.6.6, 3.6.7). The problems are solved with very small number of discretization points, which is one of the main advantage of the DQM. The other advantage, which we make use of in our problems is that, the method does not need any boundary condition to evaluate the solution, which is not the case for the other discretization methods. However, for boundary value problems (Problems 3.6.5 and 3.6.8), we have better accuracy comparing to one-dimensional initial value-problems. Thus, having boundary conditions leads to more accurate results.

3.6.1 Fisher Equation

The Cauchy problem for the nonlinear reaction-diffusion equation

$$
\begin{cases}
\dot{u} = \dfrac{\partial^2 u}{\partial x^2} + u(1-u) & x \in (-\infty, \infty), \quad t > 0 \\[2mm]
u(x,0) = \dfrac{1}{4}[(1 - \tanh(\dfrac{x}{2\sqrt{6}}))^2 & x \in (-\infty, \infty)
\end{cases}
\tag{3.88}
$$

is considered which is called Fisher equation. Problem (3.88) is proposed as a model for the propagation of an advantageous gene in a population [1].

The exact solution to this problem is [71]

$$
u(x,t) = \frac{1}{4}[1 - \tanh[(\frac{1}{2\sqrt{6}})(x - 5\sqrt{6}t)]^2 .
\tag{3.89}
$$

Several time steps (between 0.001 and 0.1) are tested. It is noted that the accuracy remains the same for all time steps and thus $\Delta t = 0.1$ is preferred in the calculations since a larger time step leads to small number of iterations to achieve steady-state solution.

As is noted in Section 3.1, for large number of discretization points the Vandermonde system becomes ill-conditioned. However, it is seen that, $N = 5$ is enough to obtain the solution with 7 digits accuracy at steady-state when FDM or FEM is used for the time discretization. But, $N = 5$ is seen to be not enough for obtaining the LSM solution for the times $t > 0.5$ and one needs more discretization points ($N = 21$) in DQM. In either case, ($N = 5$, $N = 21$) the number of freedom is very small comparing to the other discretization methods, which makes the DQM solution computationally less expensive than the other methods.

The comparison between the methods can be observed from Table 3.1. The relaxation parameter μ seems to be not very much effective on accuracy for this Cauchy problem. (The results corresponding to FDM in Table 3.1 are obtained

with $\mu = 0.7$.) One can also see that FDM and FEM time integration schemes give the same accuracy which is higher than the one obtained by LSM. One should take into account that FDM and LSM need more iterations comparing to FEM, which makes the solution procedure computationally expensive. Thus, the combination of DQM in space- FEM in time solution procedure is preferred for this problem.

Table 3.1: Maximum absolute errors for Problem 3.6.1

| Method	$t = 0.01$	$t = 0.1$	$t = 0.5$	$t = 2.0$	$t = 20.0$
FDM	7.6×10^{-6}	5.5×10^{-4}	2.6×10^{-3}	8.8×10^{-3}	2.1×10^{-7}
LSM($N = 5$)	6.0×10^{-5}	6.6×10^{-3}	7.6×10^{-1}	——	——
LSM($N = 21$)	2.7×10^{-4}	3.1×10^{-3}	1.7×10^{-2}	3.0×10^{-2}	2.1×10^{-6}
FEM	6.4×10^{-6}	5.3×10^{-4}	8.9×10^{-3}	8.7×10^{-3}	2.0×10^{-7}

From equation (3.89), it can be easily observed that the exact solution possesses the property

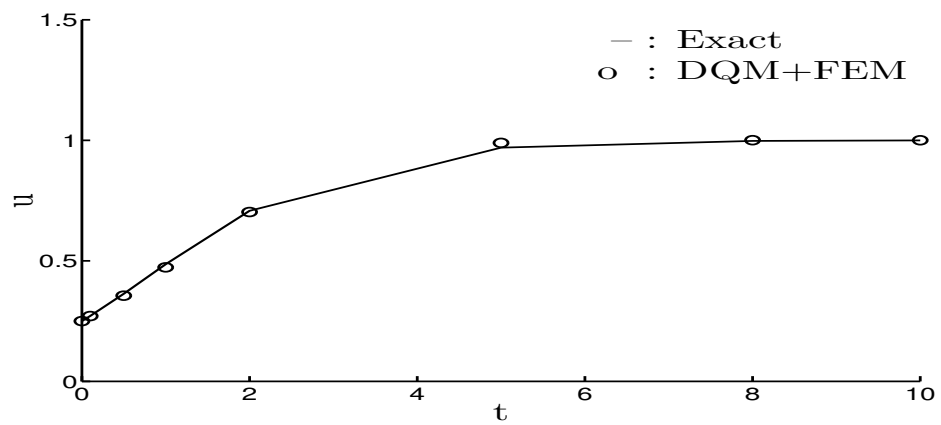$$\lim_{t \to -\infty} u(x, t) = 0, \quad \lim_{t \to \infty} u(x, t) = 1. \tag{3.90}$$

In Figure 3.2, the exact solution and the solutions obtained by the proposed methods are given at several time levels at the point $x = 0$. It can be observed from the figures that the behaviour of the exact solution (Equation (3.90)) is caught by all the methods.
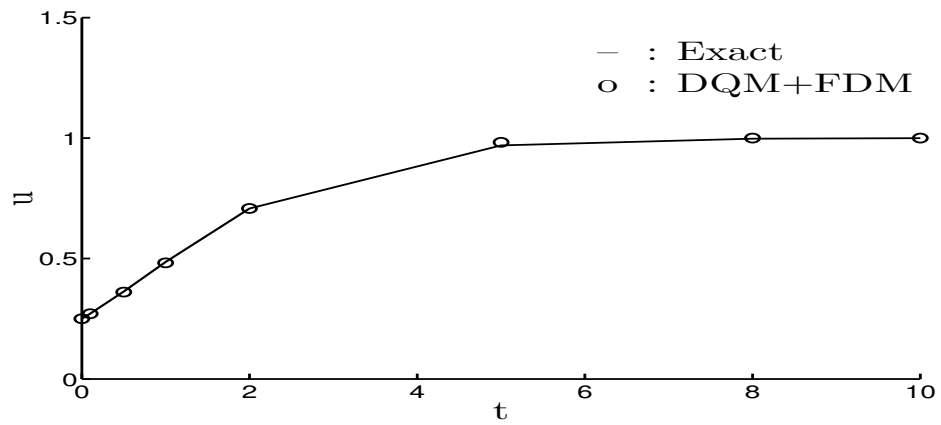
(a) DQM+FDM
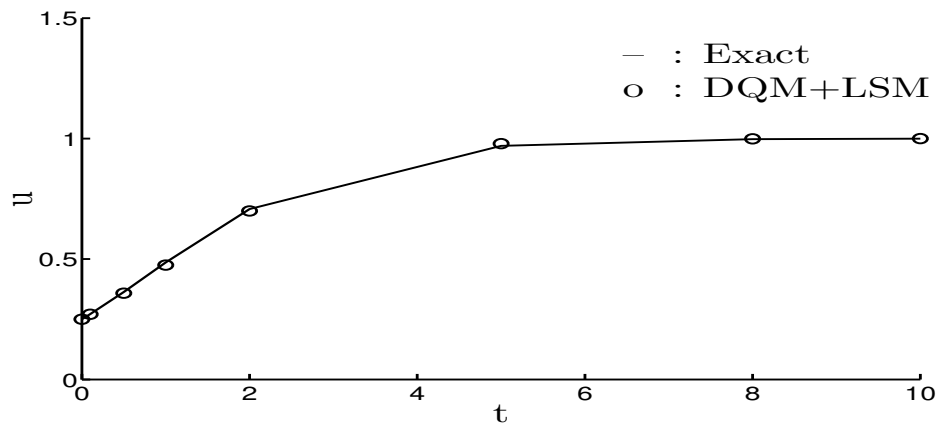
(b) DQM+LSM

(c) DQM+FEM

Figure 3.2: Behaviour of numerical solutions of Problem 3.6.1 at $x = 0$ for increasing time levels

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3.6.2 Generalized Fisher Equation

The nonlinear reaction-diffusion equation with $\nu = 1$ and $p(u) = u(1 - u^{\alpha})$ is called generalized Fisher equation. In this example, the generalized Fisher equation for $\alpha = 6$, i.e.,

$$\begin{cases} \dot{u} = \dfrac{\partial^2 u}{\partial x^2} + u(1 - u^6) & x \in (-\infty, \infty), \quad t > 0 \\[3mm] u(x, 0) = \dfrac{1}{(1 + e^{(3/2)x})^{1/3}} & x \in (-\infty, \infty) \end{cases} \tag{3.91}$$

is solved. The exact solution to this problem is given in [71] as

$$u(x, t) = \left(\frac{1}{2} \tanh\left[-\frac{3}{4}\left(x - \frac{5}{2}t\right)\right] + \frac{1}{2}\right)^{1/3}. \tag{3.92}$$

The maximum absolute errors are given in Table 3.2 at various time levels up to steady-state with $N = 5$ DQM discretization points for all time integration methods, and also with $N = 21$ for the LSM. There, the superiority of FDM and FEM over LSM can be observed in terms of accuracy. For the small time levels the methods coincide. But the LSM does not work well for the times tending to steady-state. Thus, one should increase the number of discretization points in DQM to $N = 21$ to obtain the solution with LSM also at steady-state. Even in this case, there are two digits accuracy drop in the solution at steady-state with LSM.

Table 3.2: Maximum absolute errors for Problem 3.6.2

| Method	$t = 0.01$	$t = 2.0$	$t = 5.0$
FDM	2.9×10^{-4}	7.4×10^{-4}	1.0×10^{-8}
LSM($N = 5$)	3.0×10^{-4}	1.0	7.3×10^{-1}
LSM($N = 21$)	1.0×10^{-3}	8.0×10^{-4}	5.3×10^{-6}
FEM	2.8×10^{-4}	7.8×10^{-4}	1.1×10^{-8}

Among the several time steps between 0.001 and 0.1, $\Delta t = 0.01$ is found to be the suitable choice in obtaining solutions for all time levels. As in the previous problem the accuracy is almost the same with FDM and FEM but it drops in LSM. It can be concluded that a higher order nonlinear function results with a need of smaller time increment.

For the solution of generalized Fisher equation the same property ($\lim_{t \to -\infty} u(x,t) = 0$, $\lim_{t \to \infty} u(x,t) = 1$) as in the case of Fisher equation (Problem 3.6.1) is valid. In Figure 3.3, the exact and the DQM solutions are given at $x = 0$ at increasing times. It can be also seen that the steady-state is achieved at an earlier time (at $t = 1$) comparing to the Fisher equation, which is the effect of stronger nonlinearity.
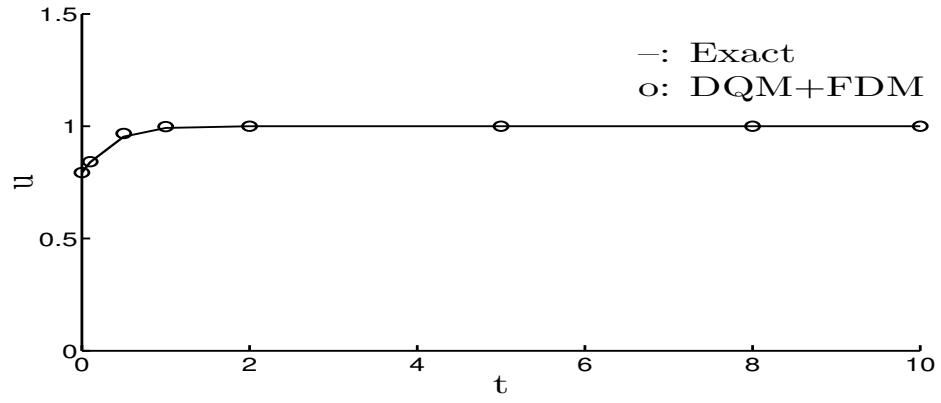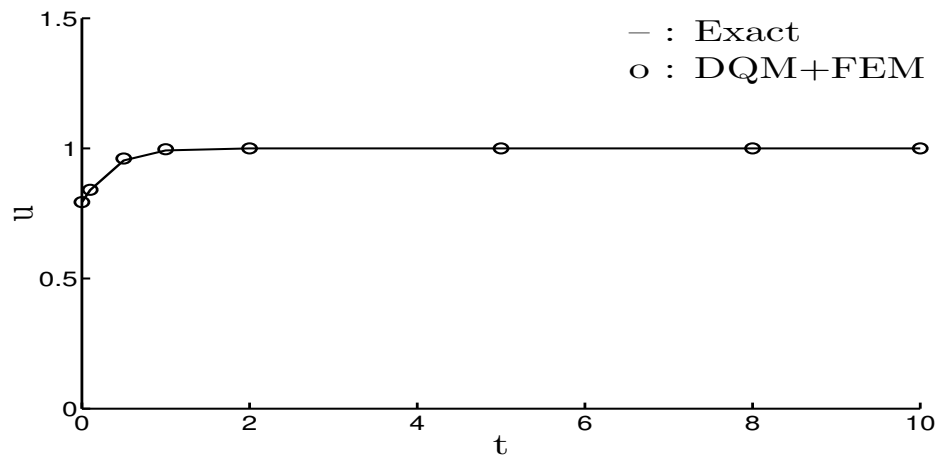
(a) DQM+FDM
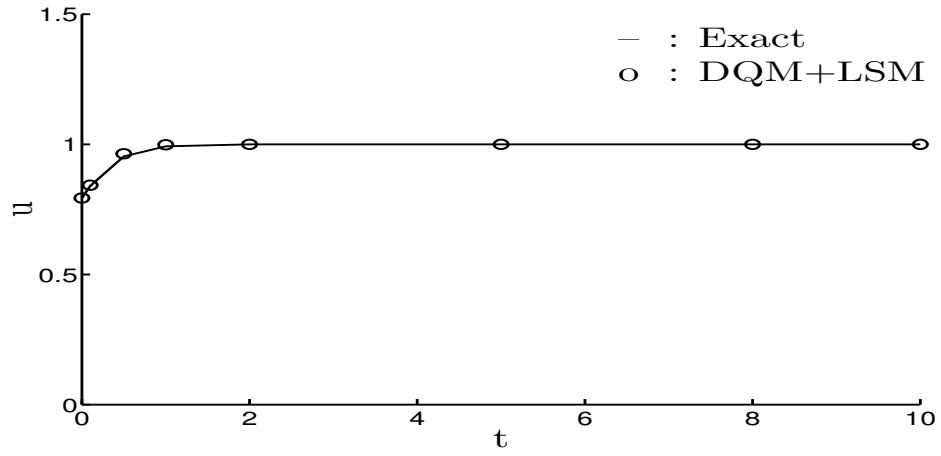
(b) DQM+LSM

(c) DQM+FEM

Figure 3.3:   Behaviour of numerical solutions of Problem 3.6.2 at $x = 0$ for increasing time levels

3.6.3 Nonlinear Equation of Fisher type with $p(u) = 6u(1 - u)$

The following Cauchy problem for the nonlinear reaction-diffusion equation

$$
\begin{cases}
\dot{u} = \dfrac{\partial^2 u}{\partial x^2} + 6u(1 - u) & x \in (-\infty, \infty), \quad t > 0 \\[3mm]
u(x, 0) = \dfrac{1}{(1 + e^x)^2} & x \in (-\infty, \infty)
\end{cases}
\tag{3.93}
$$

has the effects of linear diffusion via $\dfrac{\partial^2 u}{\partial x^2}$ with the nonlinear reaction $6u(1 - u)$. The exact solution to this problem is stated as

$$
u(x, t) = \frac{1}{(1 + e^{x - 5t})^2}
\tag{3.94}
$$

in [72].

In Table 3.3, the same observations are valid with the Problem 3.6.2 that the approximate solutions obtained with the time integration methods FDM and FEM are better than the solutions obtained with LSM in terms of accuracy and the number of discretization points.

Table 3.3: Maximum absolute errors for Problem 3.6.3

Method	$t = 0.01$	$t = 2.0$	$t = 5.0$
FDM	2.9×10^{-4}	3.0×10^{-4}	8.0×10^{-11}
LSM($N = 5$)	3.6×10^{-4}	1.48	1.48
LSM($N = 21$)	1.4×10^{-3}	1.9×10^{-4}	7.0×10^{-6}
FEM	2.9×10^{-4}	2.8×10^{-4}	7.6×10^{-11}

The computations are carried out by taking $\Delta t = 0.01$. As in the previous test problem, one needs smaller time increment since the nonlinearity is stronger than the nonlinearity in the Fisher equation. Also LSM needs more DQM discretization points.

Figure 3.4 shows the agreement between the exact solution and the proposed numerical solutions at $x = 0$ with respect to time levels. As in the previous problem, the steady-state is arrived at an earlier time comparing to the Fisher equation, but the solution is increasing with a higher rate comparing to Problem 3.6.2 at small time levels.
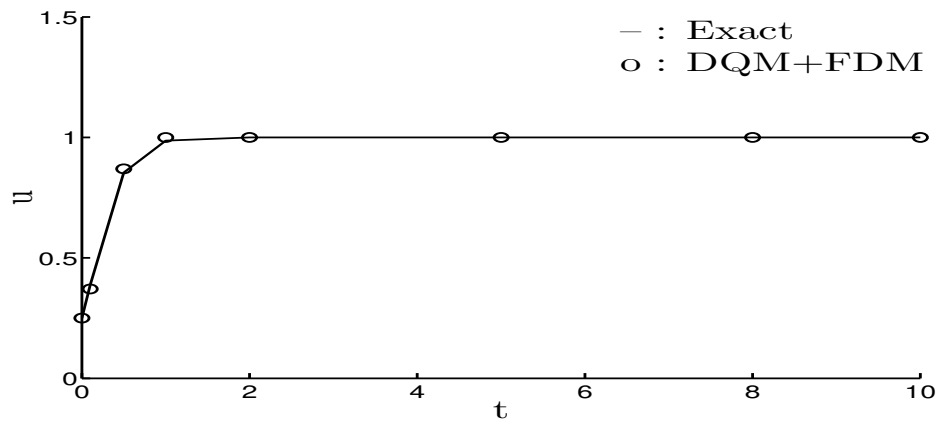
(a) DQM+FDM
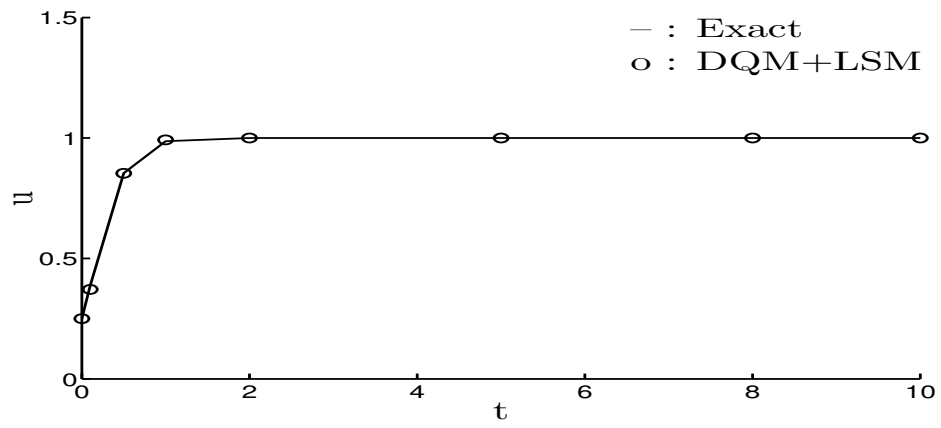
(b) DQM+LSM
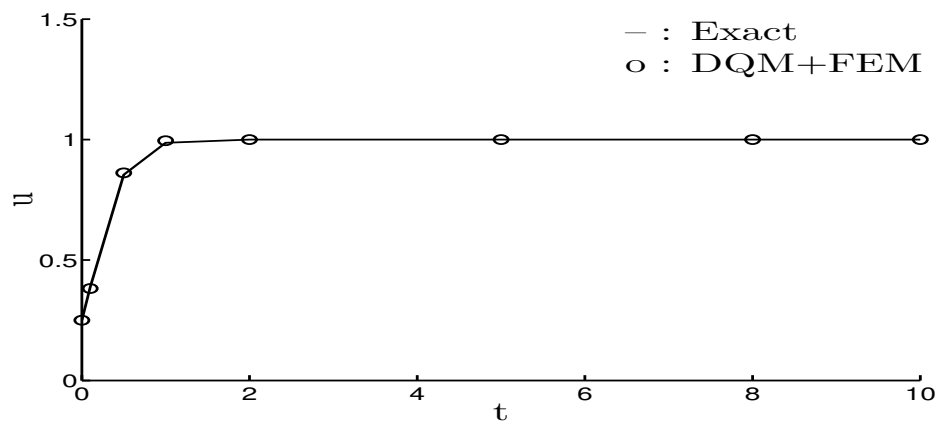
(c) DQM+FEM

Figure 3.4:   Behaviour of numerical solutions of Problem 3.6.3 at $x = 0$ for increasing time levels

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3.6.4 Nonlinear Reaction-Diffusion Equation with $p(u) = u(1-u)(u-1)$

The Cauchy problem defined by the nonlinear reaction-diffusion equation with the nonlinearity $p(u) = u(1-u)(u-1)$

$$\begin{cases} \dot{u} = \dfrac{\partial^2 u}{\partial x^2} + u(1-u)(u-1) & x \in (-\infty, \infty), \quad t > 0 \\[4mm] u(x,0) = \dfrac{1}{2} + \dfrac{1}{2}\tanh\dfrac{\sqrt{2}}{4}x & x \in (-\infty, \infty) \end{cases} \qquad (3.95)$$

is solved. The exact solution to this problem is stated as

$$u(x,t) = \dfrac{1}{2} + \dfrac{1}{2}\tanh(\dfrac{\sqrt{2}}{4}x - \dfrac{1}{4}t) \qquad (3.96)$$

in [72].

The maximum absolute errors for the problem in this section are shown in Table 3.4 by using $\Delta t = 0.1$. They justify our previous observations obtained in the problems 3.6.1-3.6.3. The LSM needs $N = 21$ discretization points in DQM and it achieves lower accuracy at small time levels although through steady-state all three methods have equal accuracy. Thus, the combination of DQM in space-FEM in time solution procedure is preferred.

Table 3.4: Maximum absolute errors for Problem 3.6.4

Method	$t = 0.01$	$t = 0.5$	$t = 1.0$	$t = 6.0$	$t = 20.0$
FDM	3.9×10^{-5}	7.3×10^{-3}	3.3×10^{-2}	9.5×10^{-2}	9.2×10^{-5}
LSM ($N = 5$)	8.2×10^{-5}	3.422	—	—	—
LSM($N = 21$)	3.8×10^{-4}	2.1×10^{-2}	4.1×10^{-2}	5.8×10^{-2}	9.4×10^{-5}
FEM	3.6×10^{-5}	5.7×10^{-3}	2.5×10^{-2}	8.2×10^{-2}	9.2×10^{-5}

Figure 3.5 shows that the solution reaches steady-state which is zero for increasing time levels. The agreement with the exact solution is also observed.
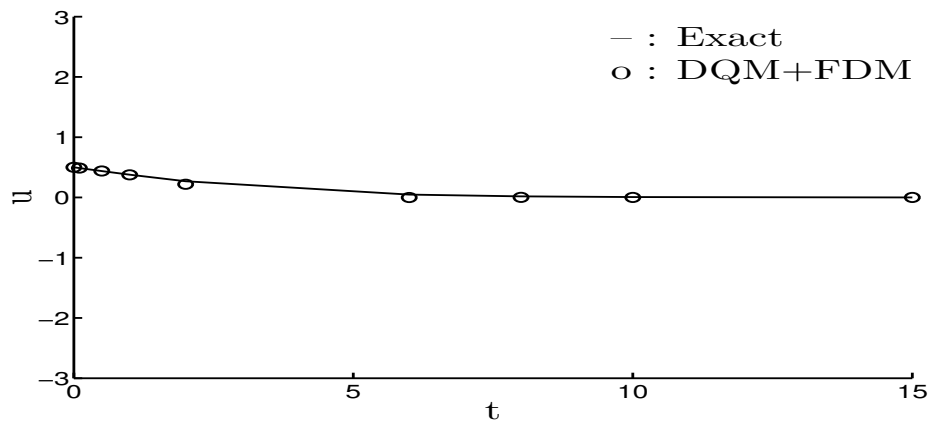
(a) DQM+FDM
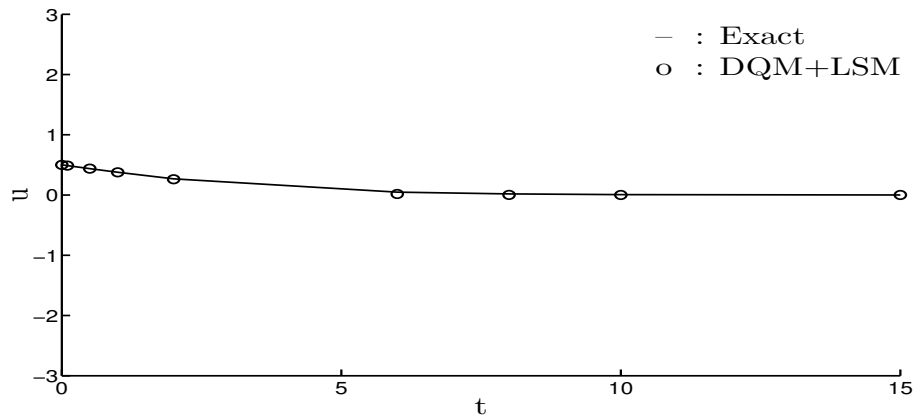
(b) DQM+LSM

(c) DQM+FEM

Figure 3.5: Numerical solutions of Problem 3.6.4 at $x = 0$ for increasing time levels

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3.6.5 Two-dimensional Nonlinear Reaction-Diffusion Equation

The two-dimensional initial and boundary value problem for the nonlinear reaction diffusion equation

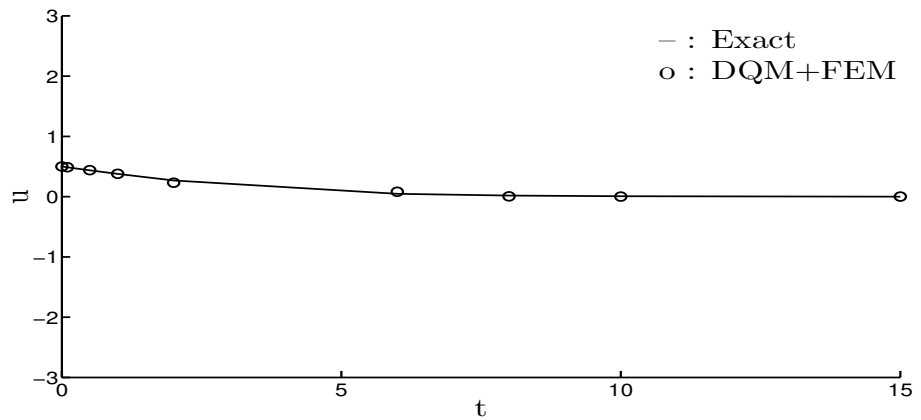$$\dot{u} = \frac{1}{2}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + u^2\left(1 - u\right) \tag{3.97}$$

is considered in a square region $\Omega = \{(x, y) \mid 0 \le x \le 1, \ 0 \le y \le 1\}$. The initial and Dirichlet type boundary conditions are taken appropriate with the exact solution [48]

$$u(x, y, t) = \frac{1}{1 + e^{p(x+y-pt)}} \quad \text{where} \quad p = \frac{1}{\sqrt{2}}. \tag{3.98}$$

For this boundary value problem the DQM discretization is performed by taking only five points in each direction ($N_x = N_y = 5$). It is possible to obtain solution even with a very small number of Chebyshev-Gauss-Lobatto points .

The time step $\Delta t = 0.01$ is found to be a suitable choice for all the time integration methods but in FDM the relaxation parameter μ needs the value 0.9. FEM and FDM give almost the same accuracy. In LSM the accuracy drop is noticed through steady-state. The advantage of using relaxation parameter in FDM is realized for initial and boundary value problems as in the DRBEM solution in Chapter 2. However, the dependence to the relaxation parameter is stronger for DRBEM solution (for $\mu < 0.7$ one cannot obtain the solution). In the DQM, the solution can still be obtained for small values of μ but the accuracy drops.

Figure 3.6 shows maximum absolute errors with respect to values of relaxation parameter μ at $t = 5$. It can be seen that as μ increases we obtain better accuracy.
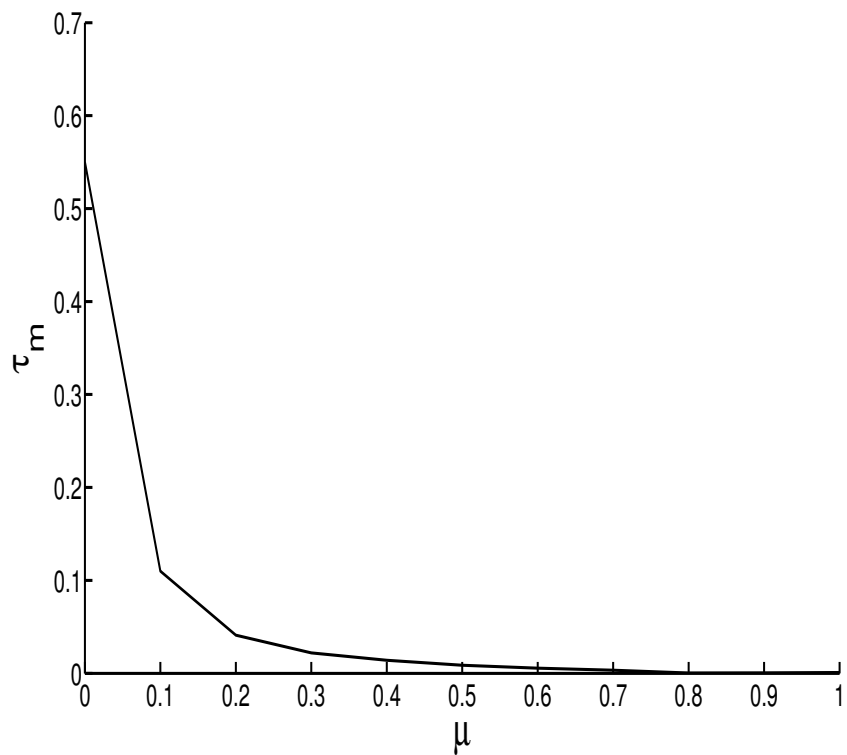
Figure 3.6: Maximum absolute errors of the DQM+FDM solution at $t = 5$ for Problem 3.6.5 with different relaxation parameters

In Figure 3.7 we present the exact solution and the DQM solutions obtained by FDM, LSM and FEM time integration methods at $t = 12$. LSM time discretization gives still oscillations although FDM and FEM already reach steady-state solution.
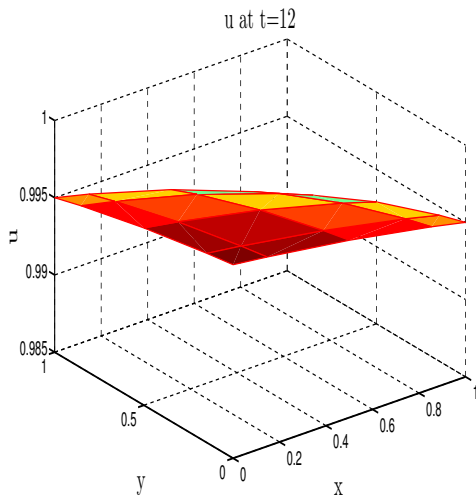
(a) Exact solution
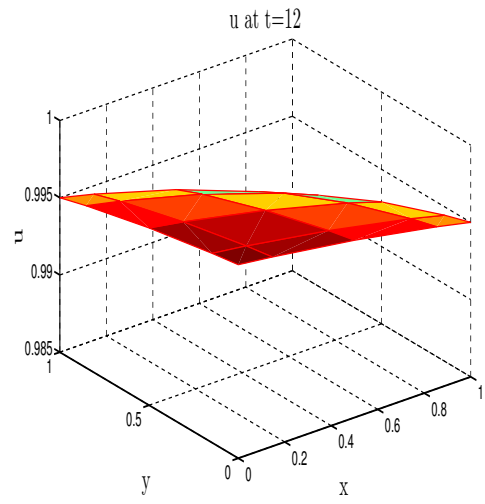
(b) DQM+FDM
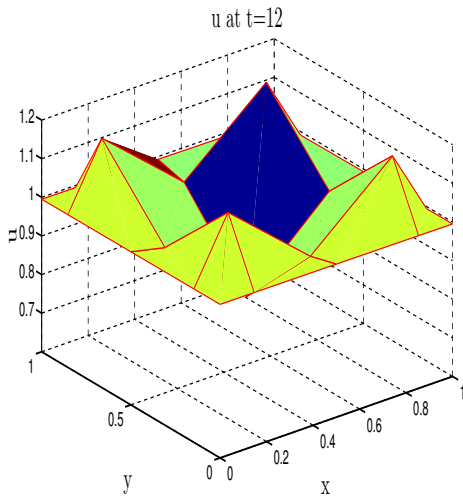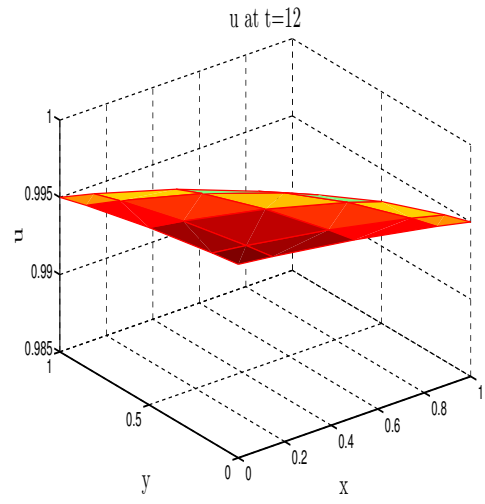
(c) DQM+LSM

(d) DQM+FEM

Figure 3.7:   Solutions of Problem 3.6.5 at $t = 12$

In Table 3.5, one can see the maximum absolute errors obtained with the DQM+FDM, DQM+LSM and DQM+FEM solutions at several time levels starting from small ones reaching to steady-state. In order to obtain these results 5 grid points are used in each direction which is very small comparing to the solution obtained by DRBEM in Chapter 2. The FEM is the method of choice for time integration in DQM solution of initial and boundary value problems in terms of accuracy since it is a direct method compared to FDM.

Table 3.5: Maximum absolute errors for Problem 3.6.5

| Method	$t = 0.01$	$t = 0.1$	$t = 2.0$	$t = 5.0$	$t = 20.0$
FDM	3.2×10^{-4}	6.4×10^{-4}	8.1×10^{-4}	4.8×10^{-4}	4.8×10^{-7}
LSM	3.2×10^{-2}	8.7×10^{-2}	1.3×10^{-1}	1.9×10^{-1}	2.2×10^{-1}
FEM	9.6×10^{-4}	1.4×10^{-3}	1.3×10^{-3}	7.6×10^{-4}	6.5×10^{-7}

3.6.6 Nonlinear Wave Equation with $p(u) = \dfrac{3}{2}(u^3 - u)$

The Cauchy problem defined by the nonlinear wave equation

$$
\begin{cases}
\dfrac{\partial^2 u}{\partial t^2} = \dfrac{1}{2}\dfrac{\partial^2 u}{\partial x^2} + \dfrac{3}{2}(u^3 - u) & x \in (-\infty, \infty), \ \ t > 0 \\[3mm]
u(x, 0) = \tanh x & x \in (-\infty, \infty) \\[3mm]
\dot{u}(x, 0) = -\operatorname{sech}^2 x & x \in (-\infty, \infty)
\end{cases}
\tag{3.99}
$$

is solved with the combination of DQM and three time integration methods FDM, LSM and FEM.

The exact solution of this equation is given in [73] as

$$u(x,t) = \tanh(x - t). \tag{3.100}$$

As in the Cauchy problems with reaction-diffusion equations, the relaxation parameter is not much effective in FDM. The time step $\Delta t \leq 0.01$ can be used in all the time integration methods. Higher values than this cause significant accuracy drop.

In Table 3.6 the maximum absolute errors of the DQM solutions with three time integration methods are given. For obtaining the solutions only $N = 8$ discretization points (CGL) are used in DQM. It can be observed from the table that LSM achieves considerable accuracy increase for small time levels contrary to Cauchy problems with reaction-diffusion equation.

For higher time levels all the time integration methods exhibit accuracy drop. This may be due to the oscillatory behaviour of the wave equation. The FEM time discretization does not give the expected accuracy as FDM and LSM. Thus, LSM appears to be the suitable time integration method for Cauchy problems defined by nonlinear wave equation.

Table 3.6: Maximum absolute errors for Problem 3.6.6

Method	$t = 0.01$	$t = 0.1$	$t = 0.5$	$t = 1.0$
FDM	$3.8{\times}10^{-5}$	$4.1{\times}10^{-4}$	$6.0{\times}10^{-3}$	$4.8{\times}10^{-2}$
LSM	$7.6{\times}10^{-7}$	$8.1{\times}10^{-5}$	$4.2{\times}10^{-3}$	$4.2{\times}10^{-2}$
FEM	$9.7{\times}10^{-3}$	$9.8{\times}10^{-2}$	$4.9{\times}10^{-1}$	$9.3{\times}10^{-1}$

3.6.7 Nonlinear Wave Equation with $p(u) = u^2 - u - u^3$

Another Cauchy problem defined by the nonlinear wave equation

$$\ddot{u} = \frac{\partial^2 u}{\partial x^2} + u^2 - u - u^3 \tag{3.101}$$

is considered. The initial conditions are taken appropriate with the exact solution [72]

$$u(x,t) = \frac{3}{2}(1 + \tanh[\frac{1}{\sqrt{3}}(x - \frac{t}{2})])^{-1/2}. \tag{3.102}$$

The DQM solution with $N = 8$ CGL discretization points and the previously mentioned time integration methods (FDM, LSM, FEM) are used and the maximum absolute errors are given in Table 3.7. $\Delta t = 0.1$ is found to be suitable time increment for all methods. It can be concluded that Cauchy problems defined by nonlinear wave equation are better solved with the combination of DQM and LSM, especially for small time levels.

Table 3.7: Maximum absolute errors for Problem 3.6.7

Method	$t = 0.01$	$t = 0.1$	$t = 0.5$	$t = 1.0$
FDM	1.1×10^{-4}	1.1×10^{-2}	1.9×10^{-1}	7.4×10^{-1}
LSM	5.8×10^{-5}	5.8×10^{-3}	9.9×10^{-2}	9.9×10^{-1}
FEM	2.4×10^{-3}	9.7×10^{-3}	8.3×10^{-2}	2.0×10^{-1}

3.6.8 Two-dimensional Nonlinear Wave Equation

The two-dimensional initial and boundary value problem for the nonlinear wave equation

$$\ddot{u} = \frac{1}{2}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + u^5 \tag{3.103}$$

is considered in the square region $\Omega = \{(x,y) \mid 5 \le x \le 10, \ 5 \le y \le 10\}$. The initial and Dirichlet type boundary conditions are taken consistent with the exact solution [72] defined by

$$u(x,y,t) = \frac{1}{2}(\frac{x^2}{4} + \frac{y^2}{4} - \frac{t^2}{4})^{-1/4} \tag{3.104}$$

which is defined for $x^2 + y^2 > t^2$.

For the DQM discretization of this problem, we use 5 CGL grid points in each direction, thus totally 25 nodes in the region. As the time step, it is found that $\Delta t = 0.01$ is the suitable choice for all time integration methods.

In Table 3.8, one can see the maximum absolute errors for the DQM solution of the problem, obtained with FDM, LSM and FEM time integration methods at several time levels. In this problem we are limited by the condition $x^2 + y^2 > t^2$, thus, we stop our calculations at $t = 5$ before this condition is satisfied. The superiority of LSM is kept over the other time integration methods at all time levels also for the two-dimensional nonlinear wave equation as in the case of the one-dimensional problem. It is noted that, for the boundary-value problem the accuracy is better comparing to the one-dimensional Cauchy problems which is due to lack of boundary conditions. The accuracy also drops at high values of time.

Table 3.8: Maximum absolute errors for Problem 3.6.8

Method	$t = 0.01$	$t = 0.1$	$t = 0.5$	$t = 2.0$	$t = 5.0$
FDM	1.9×10^{-8}	4.9×10^{-6}	2.0×10^{-4}	3.5×10^{-3}	2.6×10^{-2}
LSM	4.5×10^{-9}	4.6×10^{-7}	1.2×10^{-5}	8.3×10^{-5}	2.1×10^{-4}
FEM	2.3×10^{-2}	1.9×10^{-3}	1.9×10^{-3}	2.1×10^{-3}	4.7×10^{-3}

In Figure 3.8 the agreement of the exact solution with our solutions at several time levels at the point $(7.5, 7.5)$ is observed. The superiority of DQM+LSM solution is noted in these figures. Moreover, the harmony between the behaviours of the solutions with the exact solution is seen to be maintained in Figure 3.9 at the fixed time level $t = 2$.
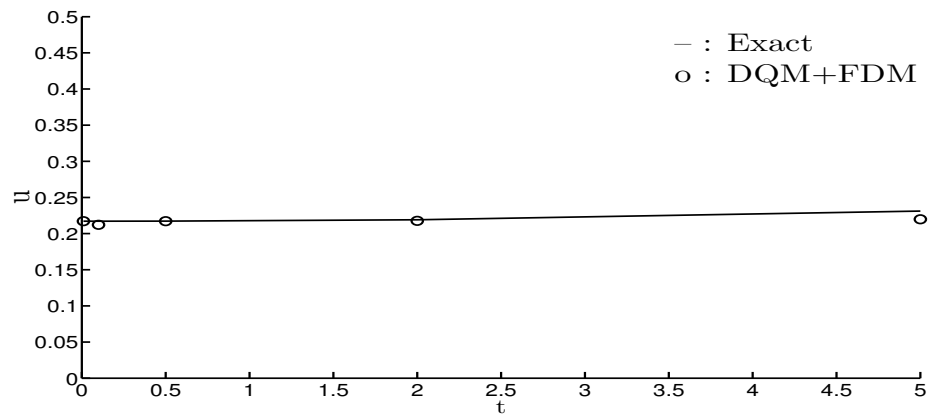
(a) DQM+FDM
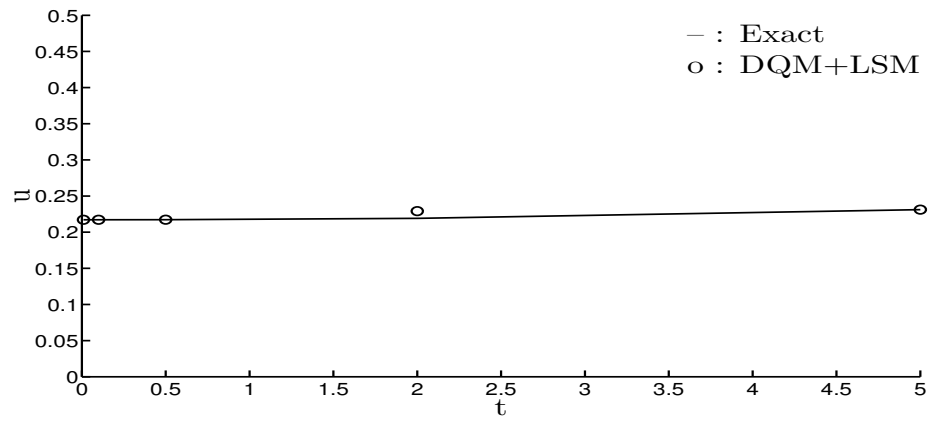
(b) DQM+LSM
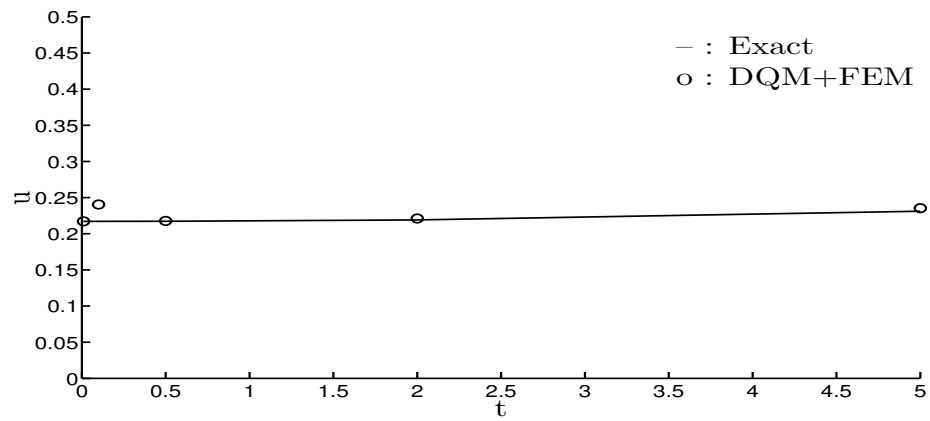
(c) DQM+FEM

Figure 3.8:   Solutions of Problem 3.6.8 for several time levels at the point $(7.5, 7.5)$
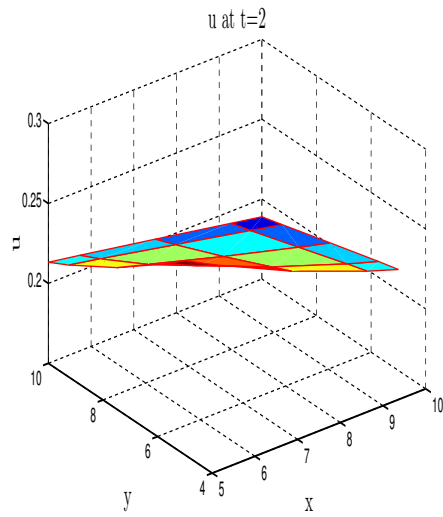
(a) Exact solution
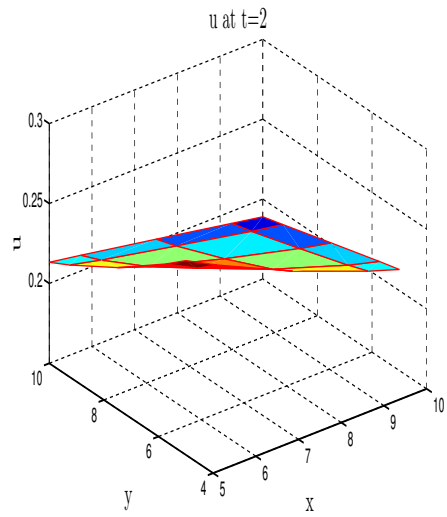
(b) DQM+FDM
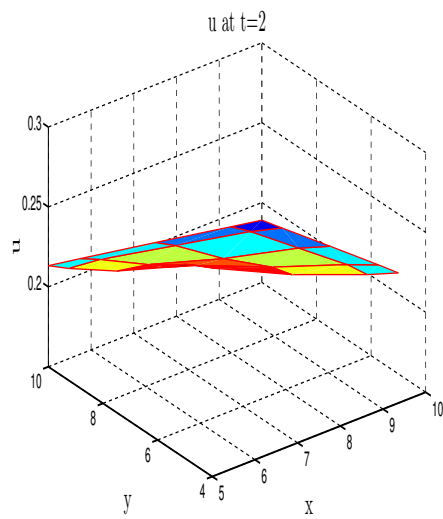
(c) DQM+LSM
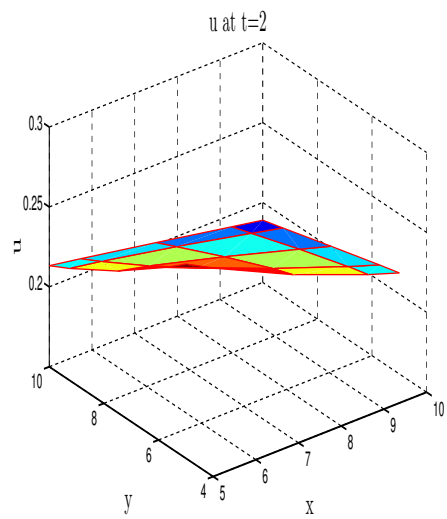
(d) DQM+FEM

Figure 3.9:   Solutions of Problem 3.6.8 at $t = 2$

In this chapter, the Cauchy problems, and initial and boundary value problems defined by the nonlinear reaction-diffusion and wave equations are solved by using DQM in space and with three different discretization methods (FDM, LSM and FEM) in time.

The resulting ordinary differential equations in time can be expressed in the form

$$\frac{\partial^i \mathbf{u}}{\partial t^i} = \tilde{\mathbf{A}} \mathbf{u} + \tilde{\mathbf{b}} \tag{3.105}$$

after the DQM application and the linearization (i.e. taking the nonlinearity always in the previous level). Here $i = 1$ or $i = 2$ corresponds to nonlinear reaction-diffusion or wave equations, respectively. Clearly, $\tilde{\mathbf{A}}$ depends on the spatial discretization DQM. In [14], it has been shown that for a stable DQM solution of diffusion type equations, the real part of eigenvalues of $\tilde{\mathbf{A}}$ should be negative or zero. For the problems considered in the thesis, it is checked that the matrix $\tilde{\mathbf{A}}$ has eigenvalues with negative real parts. For the nonlinear wave equation numerical instabilities may still occur for large values of time. However, using CGL nonuniform gridpoints increases the accuracy even the number of points is small [74].

For the Cauchy problems considered, the effect of relaxation parameter in using FDM is not that pronounced. But for initial and boundary problems it achieves a significant accuracy increase.

In the Cauchy problems defined by nonlinear reaction-diffusion equations we are able to use quite large time steps in all the time integration methods. As a result both FDM and FEM are the methods of choice giving more accuracy than LSM (LSM needs more DQM discretization points to achieve the same accuracy with FDM and FEM). The combination of DQM in space-FEM in time solution procedure is preferred for the Cauchy problems.

For the two-dimensional initial and boundary value problems defined by the nonlinear reaction-diffusion equation, the positive effect of the relaxation parameter

is realized in terms of accuracy. With the proper choice of relaxation parameter both FDM and FEM are suitable time integration methods which can be used with quite large time steps. As a direct method FEM is preffered to FDM.

In the Cauchy problems defined by the nonlinear wave equations, FDM and LSM give almost the same accuracy whereas there is a certain accuracy drop in FEM, when the same time step is used. As in the case of one-dimensional Cauchy problems defined by reaction-diffusion equation the relaxation parameter in FDM is not that important. Still the combination of DQM and LSM appears to be much suitable and it does not need very small time increment.

For the two-dimensional initial and boundary value problems defined by the nonlinear wave equation the same observations are obtained as in the Cauchy problems. The DQM with FDM and LSM give almost the same accuracy in terms of maximum absolute errors. And as a direct method DQM with LSM is the method of choice.

CHAPTER 4

CONCLUSION

This thesis is devoted to the numerical solutions of nonlinear reaction-diffusion and wave equations.

First, the numerical solutions of the initial and boundary value problems defined by the nonlinear reaction-diffusion and exterior wave equations are presented. The dual reciprocity boundary element method (DRBEM) is used to discretize the spatial partial derivatives. To do so, fundamental solution of Laplace equation is used; the nonlinearity and the first and second order time derivatives in the nonlinear reaction-diffusion and wave equations, respectively, are taken as the nonhomogenity. The DRBEM is preferred, since it is suitable for the infinite regions and gives the flexibility of using fundamental solution which corresponds to a simpler part of the original equation (in the thesis the Laplace equation). The right-hand side is approximated using the linear radial basis functions in the solution of nonlinear reaction-diffusion equation. For the nonlinear wave equation defined in the exterior of an obstacle three different kinds of radial basis functions are used; linear, rational and exponential. The latter two types are known to be suitable for the problems defined in infinite domains. The DRBEM application to the space derivatives ends up with a system of initial value problems in time which is first and second order for the nonlinear reaction-diffusion and wave equations, respectively. To solve these system of ordinary differential equations (ODE), three different time integration methods are used, finite difference method (FDM), least squares method (LSM) and finite element method (FEM). The comparison among the methods is made in each case in terms of

accuracy. An explicit FDM (Euler Method) is used. Since explicit methods may lead to unstable results and need very small time increments, a relaxation procedure, which is a linear approximation in time for the variation of the solution, is used for the solution. In all time integration methods the nonlinearity is taken in the previous time step, and thus the application of the above mentioned time integration methods results with a system of linear algebraic equations. The FDM and LSM give the solution at the required time level iteratively whereas FEM does not need any iteration, and gives the solution at once. However, since we solve the nonlinear problems and the linearization is made by taking the non-linearity in the previous time level, we prefer to divide the whole time interval into time blocks, and solve the system in each block using the information from the previous block.

The methods are tested with the initial and boundary value problems defined by the nonlinear reaction-diffusion as well as the system of nonlinear reaction-diffusion equations, and the nonlinear wave equations. The first test problem (The nonlinear reaction-diffusion equation) shows that the solutions obtained with the combinations of DRBEM and FDM, DRBEM and FEM reach almost the same accuracy at steady-state, which is higher than the one obtained by the DRBEM and LSM solution. In the previous studies and also in the thesis it is observed that comparing to the FDM and FEM, LSM needs larger time increment. However, for the same (larger) value of the time increment the superiority of the FDM and FEM are still preserved. Since FDM needs the optimal value of the relaxation parameter to obtain the best accuracy and needs more iteration, FEM is found to be the method of choice. The application to the system of nonlinear reaction-diffusion equations also supports the superiority of FEM over the other time integration methods. The last two test problems in this chapter do not have exact solutions. The third problem is the well-known Brusselator system given in terms of nonlinear reaction-diffusion equations, and the expected behaviour of the solution is seen to be satisfied by all the time integration methods combined with DRBEM. The last problem is defined in the exterior of a circle and the suitability of the DRBEM to the infinite domains is made use of. The FDM and LSM are used as the time integration methods.

The linear radial basis functions are once more seen to be not suitable for the infinite domains, and it can only be used by the FDM with the optimal value of relaxation parameter for points not very far from the obstacle. The oscillatory and the blow up behaviours for the linear and nonlinear cases, respectively, are caught by both methods.

In the second part of the thesis, the solutions of the one-dimensional Cauchy problems, and the two-dimensional initial and boundary value problems defined by the nonlinear reaction-diffusion equations are presented by using differential quadrature method (DQM). The DQM is preferred for the one-dimensional Cauchy problems since it may be used without the need of boundary conditions. The DQM has also the advantage of giving accurate results with a very small number of discretization points comparing to other methods. For the discretization of the domain the Chebyshev-Gauss-Lobatto (CGL) points are used which are known to lead more stable results comparing to uniform meshes. The obtained system of initial value problems in time are then solved using the same time integration schemes (FDM, LSM and FEM). The nonlinearity is taken at the previous time level in each case to obtain a linear system of equations.

In the applications, several test problems for the one-dimensional Cauchy problems and initial and boundary value problems defined by the nonlinear reaction-diffusion, and the wave equations are used to be able to have accurate results and for the comparison of the methods. The results for the test problems for the Cauchy problems defined by the nonlinear reaction-diffusion equations show that the relaxation parameter in using FDM is not that pronounced. It gains importance for the initial and boundary value problems. It is observed that as the nonlinearity gets stronger, the methods need smaller time increments to achieve the prescribed accuracies. The results show that FDM and FEM are the methods of choice with almost the same accuracy for these kinds of problems. Even though the effect of the relaxation parameter is not as that much strong as in the DRBEM solution, the relaxation parameter effects the accuracy of the DQM solutions in the case of two-dimensional initial and boundary value problems. For the DQM solution of the two-dimensional nonlinear reaction-diffusion equation with the mentioned time integration methods the FDM and FEM are

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found to have almost the same accuracy, which is higher than the accuracy obtained with LSM. The results support our previous observations for these kinds of problems, namely for the nonlinear reaction-diffusion equations the time integration method FEM is found to be the method of choice in terms of accuracy. Note that the FEM does not need any parameter to determine for obtaining the solution, and needs less iterations (the iteration is just made among the time blocks).

For the one-dimensional Cauchy problems as well as the two-dimensional initial and boundary value problems defined by the nonlinear wave equations, the superiority of the time integration methods is completely different, and FEM looses its attractiveness for these kind of problems. FDM and LSM are seen to be superior in terms of accuracy comparing to FEM. Thus, as a direct method, needing no parameter, LSM time integration scheme, is found to be the method of choice for the problems defined by the nonlinear wave equations.

This thesis gives the DRBEM and DQM solutions of nonlinear reaction-diffusion and nonlinear wave equations when each method is combined with FDM, LSM and FEM time integration schemes. These methods for solving time dependent system of ODEs are deeply compared in terms of accuracy. The combinations of these solution procedures are the original contributions for solving IBVPs defined by nonlinear reaction-diffusion and nonlinear wave equations.

The thesis involves nonlinearities in reaction-diffusion and wave equations in terms of added functions of solutions to the equations. The DRBEM and DQM solution procedures are not directly applicable when the nonlinearity is included in the diffusion operator. Future researches and studies should concentrate on these type of nonlinearities, and use the advantages of DRBEM and DQM.

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CURRICULUM VITAE

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Foreign Languages: English (advance), German (intermediate)

2. Education

M. Sc. 2002-2005 Middle East Technical University, Department of Mathematics, Thesis Title: 'Solution of Nonlinear Diffusion Equation Using Dual Reciprocity Boundary Element Method and Relaxation Type Time Integration Scheme'

B.S. 1998-2002 Ankara University, Department of Mathematics

High School İncirli (Foreign Language Intensive) High School

3. Work Experience

2002-present Research Assistant in the Department of Mathematics, Middle East Technical University

4. Foreign Institute Experience

04.2006-06.2007 Visiting Research Fellow, University of Stuttgart

5. Awards

- DAAD (Deutsche Akademische Austausche Dienst (German Academic Exchange Service)) Sandwich Programme, 06.2006-03.2007.

- TÜBİTAK (Türkiye Bilimsel ve Teknolojik Araştırma Kurumu (The Scientific and Technological Research Council of Turkey)) for 4 months for the research in Stuttgart University (04.2006- 06.2007) under Foreign Country Research Fellowship.

- Travel grant for the IABEM Conference, July 10-12, 2006, Graz, Austria.

- TÜBİTAK Financial Award for the Scientific Activities in Foreign Countries (For the International Conference on Boundary Element Techniques).

6.Refereeing

1. Reviewer at 'Engineering Analysis with Boundary Elements'

7. International Conferences

1. G. Meral, *Solution of the nonlinear diffusion equation using the dual reciprocity boundary element method and the relaxation type time integration scheme*, Proc. of BEM/MRM 27-th world conference on Boundary Elements and other Mesh Reduction Methods, Boundary Elements XXVII, WIT Press, pp: 133-140, Orlando Florida, USA, March 15-17, 2005.

2. G. Meral, *Solution of the nonlinear scalar exterior wave equation using the dual reciprocity boundary element method*, in Proc. of International Association for Boundary Element Methods 2006 Conference, , pp: 237-240, Graz Austria, July 10-12, 2006.

3. G. Meral, M. Tezer-Sezgin, *Solution of nonlinear reaction-diffusion equation by using dual reciprocity boundary element method with finite difference or least squares method*, Proc. of International Conference on Boundary Element Techniques IX, Advances in Boundary Element Techniques IX, EC Ltd., pp:317-322,

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8. Publications

1. G. Meral, *Solution of the nonlinear diffusion equation using the dual reciprocity boundary element method and the relaxation type time integration scheme*, WIT Transaction on Modelling and Simulation On-line Journal, **39**, 133-140, 2005.

2. G. Meral, M. Tezer-Sezgin, *Differential quadrature solution of nonlinear reaction-diffusion equation with relaxation type time integration*, International Journal of Computer Mathematics, **86**(3), 451-463, 2009.

3. G. Meral, M. Tezer-Sezgin, *The differential quadrature solution of nonlinear reaction-diffusion and wave equations using several time integration schemes*, ,Communications in Numerical Methods in Engineering, revised version is submitted.

4. G. Meral, M. Tezer-Sezgin, *The DRBEM solution of nonlinear reaction-diffusion equations by using several time integration schemes*, Applied Numerical Mathematics, submitted.