

ADAMA SCIENCE AND TECHNOLOGY UNIVERSITY

SCHOOL OF APPLIED NATURAL SCIENCE

APPLIED MATHEMATICS PROGRAM

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RESEARCH ON

POLYNOMIAL BASED DIFFERENTIAL QUADRATURE METHOD FOR
THE SOLUTION OF TIME DEPENDENT DIFFUSION EQUATION

By: ABDO KEDIR

ADVISOR: LAMI GUTA (Ph.D)

ADAMA, ETHIOPIA

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Abstract

The Differential Quadrature method is a powerful numerical method for the solution of partial differential equation that arise in various fields of mathematics, engineering, and physics. This thesis presents the differential quadrature method for solving time dependent diffusion problems. Differential Quadrature Method discretizes the space derivative giving a system of ordinary differential equation with respect to time. fourth order Runge-Kutta method is employed for solving this system. stability of discretized differential quadrature equation are determined and step size are arranged accordingly.

The method is applied to two problems and the solution are presented in terms of graph comparing with the exact solution.

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CHAPTER ONE

1 Introduction

The numerical solution of partial differential equation plays a considerable role in the area of engineering. The differential quadrature method is a numerical method which can satisfy the diffusion equation. Differential quadrature is characterized by approximating the derivative of function using weighted sum of functions value on a set of selected discrete points.

The main goal of this chapter is to provide a description (overview) of the study. The second chapter is review of related literature, which describes how deep the researcher gets information on the issues. The third chapter discusses about the method and procedure which gives a brief overview of the thesis and shows how the researcher interprets the information and goes to his conclusion. The fourth chapter deals with discretization of the method and doing two examples. The fifth chapter comes with conclusion of the research.

A short description of this thesis is presented in four chapters. The first chapter contains background of the study, statement of the problem, objective of the study, delimitation, limitation and hypothesis of the study.

1.1 background of the study

The time dependent diffusion equation in two-dimension has second order derivatives and first order time derivative. The Polynomial based Differential Quadrature method is applied for the discretization of space derivative of the unknown function u . Discretization with respect to time will be performed by using fourth order Runge-Kutta Method. The diffusion equation in two dimension

$$\frac{\partial u(x, y, t)}{\partial t} = \frac{\partial^2 u(x, y, t)}{\partial x^2} + \frac{\partial^2 u(x, y, t)}{\partial y^2} \quad (1)$$

With initial condition $u(x, y, 0) = u_0(x, y)$

and the Dirichlet and Neumann type boundary condition will be implemented

The equation can be discretized using polynomial based differential quadrature method. As we saw the diffusion equation in the above equation, the solution needs both boundary and initial conditions. Finding the exact solution for some practical problems may be very crucial, but unfortunately it may not be possible in some cases to find such solutions. If such cases exist, one must need

to find the approximate solution using different methods. From these different methods, numerical method is the one that is very important (W.reektenwald (2002)). From several techniques of finding numerical solutions to solve transient diffusion equation the Differential Quadrature (DQ) method can obtain very accurate numerical result using a considerably small number of grid point and hence requiring relatively little computational effort. It will be shown in this thesis that the polynomial based differential quadrature method is an efficient approach to solve the transient diffusion problem. In this thesis, the partial differential equation will be replaced by a discrete approximation. The word discrete means the numerical solution is approximated at a finite number of points from the given physical domain. The discrete approximation results in a set of algebraic equations that are evaluated (solved) for the values of the discrete unknowns (Douglas NA(1998)). In the diffusion equation, there are two types of derivatives. These are derivative with respect to space and derivative with respect to time. The difference schemes (explicit and Rung-Kutta) are applied to solve such derivative.

1.2 Statement of the problem

polynomial based differential quadrature method is used to solve several ODEs of BVPs. Even though there exist several methods (Holsapple.R(2003)), for solving BVP. In this thesis we shall focus on the solution of diffusion equation using polynomial based differential quadrature.

- Is the Runge -Kutta scheme effective method to get a numerical solution for problems of diffusion equation?
- Is the polynomial based differential quadrature stable?
- Is the method consistent and specific to the diffusion equation?

1.3 Objectives of the study

1.3.1 General objectives

The general objectives of this research is to find the numerical solution of diffusion equation by using polynomial based differential quadrature method.

1.3.2 Specific objectives

The specific objectives of this thesis are

- To solve diffusion equation approximately using polynomial based differential quadrature method.
- To show the stability and consistency of discretized differential quadrature method.
- To determine the function with respect to time by using RKM.

1.4 Significance of the study

The main purpose of this study is to enhance numerical method which can give us better approximate solution of the diffusion equation. Moreover, This research report may be used as additional reference for similar work in the university.

1.5 Delimitation /scope/ of the study

This study is mainly delimited to the solution of time dependent diffusion equation using polynomial based differential quadrature.

1.6 Limitation of the study

The limitation of the study are :-

- Time constraint
- Shortage of materials
- Lack of enough reference books in the area
- Lack of internet service on work place

CHAPTER TWO

2 Review of related Literature

The differential quadrature method (DQM) is a numerical technique used to solve the initial and boundary value problem. It was developed by late Richard Bellman and his associate in the early 70s (Bert;Wang,(1993,1994,1997)) and since then ,the technique has been successfully employed in a variety of problem in engineering and physical science. Hence attracted many researchers attention in recent years. The method has been projected by its proponent as a potential alternative to the conventional numerical solution technique such as the finite difference and finite element (Bellman and Casti (1996)). In seeking an efficient discretization technique to obtain accurate numerical solution using a considerably small number of grid points,(Bellman,R.Kashef,and Casti(1972)) introduced the method of DQ where a partial derivative of a function with respect to a coordinate direction is expressed as a linear weighted sum of all the functional values at all grid point along the direction (Bellmann,1986)) suggested two method to determine the weighting coefficient of the first derivative. The first method solves an algebraic equation system. The second uses a simple algebraic formulation ,but with the coordinates of grid points chosen as a root of the Legendre polynomials. Unfortunately, when the order of the algebraic equation system is large, its matrix is ill conditioned Thus, it is difficult to obtain the weighting coefficients. The differential Quaderature method (DQM)(Bellman,R.Kashef,and Casti(1972))is an effective numerical technique to be used as global finite difference scheme or generalized collocation method.The study of DQM has been mainly focused on how to select grid point,how to impose initial or boundary condition,how to determine weighting coefficient,and convergence of solution.The relevant and representative publications are reviewed below in turn since DQM is applied to the discretization of spatial and temporal domains in the present work. The exteremum point of Legender polynomial in the domain $[-1,1]$ (Bert,Wang and Striz(1993))and the so-called Gauss-Lobatto-Chebyshev point (Shu and Richard(1992)) where taken as unequally alingned node points, and the latter has been widely accepted by far. The efficient way to deal with boundary conditions are formulating weighting matrix(Tamsir;Sirvastava;Jiwari;Malik;Berta,(2016,1996)) except δ method (Shu,Richard;Bert,Jang,(1992,1988))and modifying the weighting coefficient point (Malik;Bert;Wang,(1996,1993)) ading boundary degree of freedom

(Chen;Striz;Bert,(1997)) employing differential quadrature Element method(DQEM) (Wang;Huizhi,(1997)),etc, The initial condition can be applied via some representative ways,including expressing initial condition as Differential Quadrature (DQ) analog equation as sampling point (Bert;Wang;Fung,Shu(1993,2001,1997)) modifying DQ rule (Fung;Eftekhari;Jafari (2001,2013)) modifying trial function (Wu;Liu,(1999,2000))and modifying weighting coefficient matrix (Tank,Chen,Jawari, (2001,2016)). Notably, the advantage of modified DQ rule method is the accuracy of state variable at the end of time interval, and its accuracy can be improved up to $2n$ order by using only $n+1$ sampling point with unconditional stability and non-dissipation. However, the power of the displacement polynomials is the same with that of the velocity, which violates the differential relation between displacement and velocity (Fung,(2001,2002)). Xing and Guo changed coefficient matrix and generalized load vector to simplify the imposition of initial conditions(Xing;Guo,(2012)). As for the weighting coefficient,Quan and Chang obtained the first and second order explicit weighting coefficient by differentiating Lagrange polynomial(Quan,(1989)).Shu and Richards derived high order weighting coefficients from recursion formula(Shu,Richard,(1992)). In addition,Bert and Wang pointed out that DQM convergence speed is equal to that of fourier series solution,while faster than that resulting from Ritz method; moreover,DQM is much simpler than fourier series,which is easily implemented by coding and applicable to static and dynamic structural analysis (Bert;Wang;String,(1994)). The differential quadrature method is crucial step to the conventional integral quadrature method, approximates the derivative of a function at any location by a linear summation of all the functional values along mesh(grid) line. The main procedure in the differential quadrature application lies in the determination of weighting coefficient by other researchers. As a result, the differential quadrature method emerged as a powerful numerical discretization tool in the past decades,(Shu and Chew,(1997)). To further improve the computation of (Quan,(1997)) applied Lagrange interpolated polynomial as a test function and obtained explicit formulation to calculate the weighting coefficient for the discretization of first and second order derivatives. The technique of differential quadrature method for the solution of two-dimensional partial differential equation is extended by (Lam,(1993)) to encompass problem with arbitrary geometry. He compared the result of thermal and torsional problems with the other solution and showed reasonably good accuracy. In this thesis, DQM will be applied to time dependent diffusion equation in two dimensional space. The diffusion

equation is supplemented with Dirichlet or Dirichlet-Neumann type boundary condition together with an initial condition forming an initial and boundary value problem in two dimension space. Time dependent boundary condition as well as time dependent coefficient in the equation will also discussed and accompanied with sample problem. Differential quadrature technique approximate the derivative of a function at a grid point by a linear weighted summation of all the functional values. Derivative with respect to space variables are discretized using DQM giving a system of ordinary differential equation for the time derivative. We used fourth order explicit Rung-Kutta Method for discretizing time derivative since its stability region is larger comparing the other time integration method and simple for the computations. This DQM and the order RK method combination gives very good numerical technique for solving time dependent diffusion problems. Stability criteria are also controlled with several time increment t and number of grid point N in space region. Implicit RK method is not preferred because of its complexity in the computation.

CHAPTER THREE

3 Methods and Procedures

In this part the researcher tries to consider the study design, study sight, period and source of information, study procedure, instrumentation and administration.

3.1 Design

The design of this study is application of DQM and discretize the space derivatives giving a system of ordinary differential equation with respect to time and the fourth order Runge- kutta Method (RKM) is employed for solving the system.

3.2 Procedure of the study

1. Application of Differential Quadrature method in two dimensional case and choice of grid point is done.
2. Implementation of Dirichlet and Neumann type boundary condition to final system of ordinary differential equation is presented.
3. Discretization of time derivative by using fourth order Runge- kutta method is introduced .
4. Stability analysis of ODE
5. Application of Differential Quadrature method for diffusion equation type problem is implemented and graphically solution is presented.

Are the procedure of the thesis.

3.3 Study Sight

The study is done in Adama science and Technology University.

3.4 Data Collection

The researcher collect the necessary data (information) from different reference:-

- Articles and research papers.

- Journals
- Reference books.
- Down load materials from internet etc. on this study.

CHAPTER FOUR

4 Differential Quadrature Method For Diffusion Equation

In this chapter I present the combined application of differential quadrature method and the fourth order Runge-Kutta method (RKM) to the solution of time dependent diffusion equation. The governing equation for the solution of transient diffusion problems can be expressed as

$$\frac{\partial u(x, y, t)}{\partial t} = \nabla^2 u(x, y, t), \quad (x, y) \in \Omega \quad (2)$$

with initial condition

$$u(x, y, 0) = u_0(x, y) \quad (3)$$

and the dirichlet and Neumann boundary conditions are given by

$$u(x, y, t) = \bar{u}(x, y, t), \quad (x, y) \in \Gamma_u \quad (4)$$

$$q(x, y, t) = \frac{\partial \bar{u}(x, y, t)}{\partial n} = \bar{q}(x, y, t), \quad (x, y) \in \Gamma_q \quad (5)$$

$$q(x, y, t) = -h(x, y, t)(u(x, y, t) - u_r(x, y, t)), \quad (x, y) \in \Gamma_r \quad (6)$$

where a variable domain $\Omega \in R^2$, is bounded by a piecewise smooth boundary $\Gamma = \Gamma_u + \Gamma_q + \Gamma_r$ here $q = \frac{\partial u}{\partial n}$, n is the unit out ward normal, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ is Laplace operator. the function $\bar{u}(x, y, t)$, $\bar{q}(x, y, t)$, $h(x, y, t)$ and $u_r(x, y, t)$ are given function of (x, y, t) and the initial condition $u_0(x, y)$ is a given function of space variable (x, y) .

The transient diffusion equation

$$\frac{\partial u}{\partial t} = \nabla^2 u \quad (7)$$

can be considered in general form

$$\nabla^2 u = b(x, y, t, u, u_t) \quad (8)$$

where (x, y) represent the spatial coordinates, u is the dependent unknown solution. t is the time and u_t denotes the time derivative of u . There are many available numerical discretization techniques to solve transient diffusion equation

such as the finite element method, finite volume method and finite difference method. when we compare to these lower order numerical method, the differential quadrature method can obtain vary accurate Numerical result using a considerable small number of grid points and hence requiring relatively little computational effort. Differential Quadrature method is applied to equation (8) containing Laplace Operator. Since right hand side function b contains also the time derivative of u . the resulting system of equation will contain u_t . Therefore, the time derivatives will be discretized by one of the explicit scheme which is the fourth order Rung-kutta method in this thesis.

4.1 Differential Quaderature Method

The differential quadrature method was presented by R.E Bellmann and his associate in early 1970's and it is a numerical discretization technique for the approximation of derivatives. In seeking an efficient discretization technique to obtain accurate numerical solution using a considerably small number of grid point, Bellmann (1971,1972) introduced the method of differential quadrature, where a partial derivative of a function with respect to a coordinate direction is expressed as a linear weighted sum of all the functional values at all grid point along that direction. The key to differential quadrature method is to determine the weighting coefficient for the discretization of a derivative of any order. A major breakthrough in computing the weighting coefficient was made by Shu and Richard(1990) in which all the current methods for determination of the weighting coefficient are generalized under the analysis of a high order polynomial approximation and analysis of a linear vector space. According to Shus the weighting coefficient of the first order derivatives are determined by a simple algebraic formulation without any restriction on choice of grid points, whereas the weighting coefficient of second and higher order derivatives are determined by a recurrence relationship, clearly, all the work is based on the polynomial approximation and accordingly, the related differential quadrature method can be considered as the polynomial based Differential Quadrature. Recently Shu and Chew (1997) and Shu and Xue (1997) have developed some simple algebraic formulation to compute the weighting coefficient of the first and second order derivatives in the Differential Quadrature approach. When the function or the solution of a partial differential equation is approximated by a Fourier Series expansion. These formulation are different from PDQ and the approach can be

termed as the Fourier Expansion Based Differential Quadrature method.

Depending on the feature of the problem the solution of a partial differential equation can be approximated by a polynomial of high degree or by the Fourier Series expansion. The FDQ approach is more suitable for harmonic behaviors such as the Helmholtz equation. Since transient diffusion equation does not have this kind of behavior. The polynomial based differential quadrature method is used in this thesis.

4.1.1 Two Dimensional Differential Quadrature Method For Time Dependent Diffusion Equation

The time dependent diffusion equation in two-dimensions has second order space derivatives and first order time derivative. The PDQ method is applied for the discretization of space derivatives of the unknown function u , discretization with respect to time will be performed by using fourth order Runge Kutta method. The diffusion equation in two dimensions,

$$\frac{\partial u(x, y, t)}{\partial t} = \frac{\partial^2 u(x, y, t)}{\partial x^2} + \frac{\partial^2 u(x, y, t)}{\partial y^2} \quad (9)$$

can be discretized by using first PDQ method as

$$\frac{\partial u(x_i, y_j, t)}{\partial t} = \sum_{K=1}^N A_{ik}^{(2)} u_{kj} + \sum_{k=1}^M B_{jk}^{(2)} u_{ik} \quad (10)$$

For $i = 1, 2, 3, \dots, N$ and $j = 1, 2, 3, \dots, M$ where N and M are the number of grid point in the x and y direction respectively, $A_{ik}^{(2)}$ and $B_{jk}^{(2)}$ are the DQ weighting coefficient of the second order derivative of u with respect to x and y respectively.

$$A_{ik}^{(2)} = 2A_{ik}^{(1)} \left(A_{ii}^{(1)} - \frac{1}{x_i - x_k} \right), i, k = 1, 2, 3, \dots, N \quad (11)$$

$$B_{jk}^{(2)} = 2B_{jk}^{(1)} \left(B_{jj}^{(1)} - \frac{1}{y_j - y_k} \right), j, k = 1, 2, 3, \dots, M \quad (12)$$

where $A_{ik}^{(1)}$, $A_{ii}^{(1)}$, $B_{jk}^{(1)}$ and $B_{jj}^{(1)}$ are

$$A_{ik}^{(1)} = a_{ik} = \frac{M^{(1)}(x_i)}{(x_i - x_k)M^{(1)}(x_k)}, i \neq k \quad (13)$$

$$A_{ii}^{(1)} = a_{ii} = \frac{M^{(2)}(x_i)}{2M^{(1)}(x_i)} \quad (14)$$

$$B_{jk}^{(1)} = \bar{a}_{jk} = \frac{M^{(1)}(y_j)}{(y_j - y_k)M^{(1)}(y_k)}, j \neq k \quad (15)$$

$$B_{jj}^{(1)} = \bar{a}_{jj} = \frac{M^{(2)}(y_j)}{2M^{(1)}(y_j)} \quad (16)$$

For the computation of diagonal enteres $A_{ii}^{(1)}, B_{jj}^{(1)}, A_{ii}^{(2)}, B_{jj}^{(2)}$ again are made use of giving

$$A_{ii}^{(1)} = \sum_{j=1}^N A_{ij}^{(1)}, A_{ii}^{(2)} = - \sum_{j=1, i \neq j}^N A_{ij}^{(2)}, i = 1, 2, \dots, N \quad (17)$$

$$B_{jj}^{(1)} = \sum_{i=1, i \neq j}^M B_{jk}^{(1)}, B_{jj}^{(2)} = - \sum_{i=1, i \neq j}^M B_{ji}^{(2)}, j = 1, 2, \dots, M \quad (18)$$

Now $\frac{\partial u}{\partial t}$ is also considered discrized as $\frac{\partial u_{ij}}{\partial t}$, thus equation (10) is a set of algebric equation which can be written in the matrix form

$$[A]u = b \quad (19)$$

Where u is a vector of unknown NM functional values at all discretized points of the region, [A] is the NM x NM coefficient matrix containing the weighting coefficient $A_{ik}^{(2)}, B_{jk}^{(2)}$ and the right hand side vector b of size NM x 1 contains first order time derivatives of the function at the same discrized points, therefore, a numerical scheme is necessary for handling this time derivatives. Equation (18) can be solved by several time integration schemes such as Eulers, modified Eulers, Runge-kutta method. Here Runge Kutta method is used since it is one step method obtained from the Taylor series expansion of u up to and including the terms involving $(\Delta t)^4$ where Δt is the step size with respect to time.

4.1.2 Choice Of Grid Point

Since the weighting coefficients $A_{ik}^{(2)}, B_{jk}^{(2)}$ and $A_{ik}^{(1)}, B_{jk}^{(1)}$ corresponding to discrization of the second and first order derivatives respectively, contain grid point x_i, y_j s the choice of this grid points becomes quite important, equally spaced grid points, due to their obvious convenience, have been in use by most investigators. However, unequally spaced grid point especially the zero of orthogonal polynomials like Legendre and Chebyshev polynomials usually give more accurate solutions than the equally spaced grid points.

The natural choice for the grid points is the equally spaced point which is given by

$$x_i = \frac{i-1}{N-1}a; i = 1, 2, 3, \dots, N \quad (20)$$

$$y_j = \frac{j-1}{M-1}b; j = 1, 2, 3, \dots, M \quad (21)$$

In the x and y directions respectively for a region $[0,a] \times [0,b]$, for this uniform grid point with step size Δx and Δy in x and y direction respectively, one can obtain

$$x_k - x_i = (k - i)\Delta x, y_k - y_j = (k - j)\Delta y$$

$$M^{(1)}(x_i) = (-1)^{N-1}(\Delta x)^{N-1}(i-1)!(N-i)!; i = 1, 2, 3, \dots N$$

$$M^{(1)}(y_j) = (-1)^{M-1}(\Delta y)^{M-1}(j-1)!(M-j)!; j = 1, 2, 3, \dots M$$

and the coefficients for the first order derivative reduce to

$$A_{ij}^{(1)} = (-1)^{i+j} \frac{(i-1)!(N-1)}{(i-j)(j-1)!(N-j)!}; i, j = 1, 2, \dots N, i \neq j$$

$$B_{ij}^{(1)} = (-1)^{i+j} \frac{(i-1)!(M-1)}{\Delta y(i-j)(j-1)!(M-j)!}; i, j = 1, 2, 3, \dots M, i \neq j$$

The so called Chebyshev-gauss-Lobatto point distribution offer a better choice and have found consistently better than the equally spaced, Legendre and Chebyshev points in a variety of problems (Bert and Malik,1996). These points are the Chebyshev collocation points which are the root of $|T_N(x)| = 1$ and given by (Shu,(2000))

$$x_k = \cos\left(\frac{k-1}{N-1}\pi\right), 1 \leq k \leq N$$

for an interval $[-1, 1]$ for a region on $[a, b]$

$$x_i = \frac{1}{2}\left[1 - \cos\left(\frac{i-1}{N-1}\pi\right)\right]a, i = 1, 2, 3, \dots N \quad (22)$$

and

$$y_j = \frac{1}{2}\left[1 - \cos\left(\frac{j-1}{M-1}\pi\right)\right]b, j = 1, 2, 3, \dots M \quad (23)$$

in x and y direction, respectively.

For Chebyshev-Gauss-Lobatto point we have (in x direction)

$$M^{(1)}(x_i) = (-1)^{i+1}N^2$$

$$M^{(2)}(x_i) = (-1)^i N^2 \frac{x_i}{1-x_i^2}$$

And the corresponding weighting coefficient simplify greatly and Chebyshev-Gauss-Lobatto is used since it gives the real part of all the PDQ matrix eigenvalues strictly negative, this is the condition of obtaining stable solution (Shu,(2000)) for the system of ordinary differential equations.

4.1.3 Implementation of Boundary Condition

The insertion of Dirichlet type boundary conditions is straightforward since these known values contribute to the right hand side vector in the system (19). If the boundary condition involves normal derivatives of the unknown function u then these derivatives can also be approximated by the DQM.

Dirichlet Type Boundary Condition

Since the solution at the boundary grid points is known the equation (10) should only be applied

at the interior points to impose the Dirichlet type boundary condition ,Thus the equation (10) can be rewritten as

$$\frac{\partial u_{ij}}{\partial t} - S_{ij} = \sum_{k=2}^{N-1} A_{ik}^{(2)} u_{kj} + \sum_{k=2}^{M-1} B_{jk}^{(2)} u_{ik} \quad (24)$$

where $2 \leq i \leq N-1, 2 \leq j \leq M-1$ and

$S_{ij} = (A_{i1}^{(2)} u_{1j} + A_{iN}^{(2)} u_{Nj} + B_{j1}^{(2)} u_{i1} + B_{jM}^{(2)} u_{iM})$ equation(4.24) is a set of DQ algebraic equation which can be written in matrix form.

$$[A]u = b - S \quad (25)$$

u is a vector of unknown functional values at all the interior point given by

$$u = [u_{22}, u_{23} \dots u_{2,M-1}, u_{32} \dots u_{3M-1}, \dots u_{N-1,2} \dots u_{N-1,M-1}]^T$$

And b is a vector still containing discretized time derivative of u and s vector contains known values of u at the boundary grid points. The size of the matrix [A] is $(N-2)(M-2) \times (N-2)(M-2)$. Equation (24) can be solved by using iterative method for discrete time derivative values of u after the time derivative is discretized. As mentioned before the fourth order Runge-Kutta method is used for discretizing the time derivative u.

Neumann Type Boundary Condition

For the Neumann condition the normal derivatives on the boundary should also be discretized by polynomial based differential quadrature method

The normal derivative of u can be written as

$$\frac{\partial u}{\partial n} = \frac{\partial u}{\partial x} n_x + \frac{\partial u}{\partial y} n_y \quad (26)$$

Now

$$\frac{\partial u_{ij}}{\partial x} = \sum_{k=1}^N A_{ik}^{(1)} u_{kj}, i = 1, 2, 3 \dots N \quad (27)$$

And

$$\frac{\partial u_{ij}}{\partial y} = \sum_{k=1}^M B_{jk}^{(1)} u_{ik}, j = 1, 2, 3 \dots M \quad (28)$$

where $A_{ik}^{(1)}$ and $B_{jk}^{(1)}$ are the weighting coefficient with respect to x and y direction and obtained. Thus

$$A_{ik}^{(1)} = \frac{M^{(1)}(x_i)}{(x_i - x_k)M^{(1)}(x_k)}, i \neq k \quad (29)$$

$$A_{ii}^{(1)} = \frac{M^{(2)}(x_i)}{2M^{(1)}(x_i)} \quad (30)$$

$$B_{jk}^{(1)} = \frac{M^{(1)}(y_j)}{(y_j - y_k)(M^{(1)}(y_k))} \quad (31)$$

$$B_{jj}^{(1)} = \frac{M^{(2)}(y_j)}{2M^{(1)}(y_j)} \quad (32)$$

Assuming $\partial u N_j / \partial x = c_j (j = 1, 2, \dots, M)$ and $\partial u N_j / \partial y = 0$ any given on one part of the boundary, we can write

$$\frac{\partial u N_j}{\partial x} = \sum_{k=1}^N A_{NK}^{(1)} u_{kj} = c_j \quad (33)$$

Rewrite equation (4.33)

$$A_{NN}^{(1)} u_{Nj} + \sum_{k=1}^{N-1} A_{Nk}^{(1)} u_{kj} = c_j \quad (34)$$

$$u_{Nj} = \frac{1}{A_{NN}^{(1)}} (c_j - \sum_{k=1}^{N-1} A_{Nk}^{(1)} u_{kj}), j = 1, 2, 3, \dots, M \quad (35)$$

These M equation for the unknown u_{Nj} , ($j = 1, 2, M$) are going to be added to the DQ system of equations (4.10) which is written for $i \neq N, j = 1, 2, M$ for the case of Neumann type of boundary condition $\frac{\partial u N_j}{\partial x} = c_j$ on $x = x_N$, ($i = N$ case) When normal boundary condition are implemented at all the related grid points. The final system of DQ equations will be again in the form of equation (25) $[A] \{u\} = \{b\} - \{S\}$

Where the vectors b and s still contain the discretized time derivatives of u and known values of u at the boundary grid points respectively.

Thus, equation found by discretizing the normal derivatives of u on the boundary are updated using interior u values which are not known yet, This problem is handled during the iteration performed in the Runge-Kutta method since initial u values are given.

The mixed type boundary conditions which are combinations of the Dirichlet and Neumann conditions are implemented in a similar fashion.

4.2 Runge-Kutta Method

The fourth order explicit Runge-Kutta method is applied to discretize time derivative in the resulting system of algebraic equation (24). RKM is one step method for solving initial value problem. Our time dependent diffusion problem is an initial and boundary value problem, therefore, the resulting algebraic system of equation (24) can originally be considered as an initial value problem in the form (a set of ordinary differential equation in time).

$$\{b\} = \frac{d\{u\}}{dt} = [A] \{u\} + \{s\} \quad (36)$$

Where u is the unknown vector of values at the interior grid points, s is the vector containing known boundary conditions and [A] is the weighting coefficient matrix. The fourth order explicit RKM is going to be explained for ordinary differential equation (initial value problem) in the form.

$$\dot{u} = f(t, u)$$

$$U(t_0) = u_0$$

And then modified for our system of equations. One step method for solving $\dot{u} = f(t, u)$ require

only a knowledge of the numerical solution in order to compute the next value u_{n+1} . This has advantages over the p step multistep methods that use several past values $u_1 \dots u_p$ that have to be calculated by another method.

The best known one-step method are the Runge-Kutta methods. They are fairly simple to program and their truncation error can be controlled more than for the multistep methods. (Atkinson.(1978)).

The most simple one step method is based on Taylor series expansion

$$\dot{u} = f(t, u), u(x, y, t_0) = U_0 \quad (37)$$

Expanding $U(x, y, t_1)$ about t_0 using Taylor's theorem

$$U(x, y, t_1) = U(x, y, t_0) + \Delta t \dot{U}(x, y, t_0) + \dots + \frac{(\Delta t)^r}{r!} U^{(r)}(x, y, t_0) + \frac{(\Delta t)^{r+1}}{(r+1)!} U^{(r+1)}(\xi) \quad (38)$$

For some $t_0 \leq \xi_0 \leq t_1$, dropping the remainder term, we have an approximation for $U(x, y, t_1)$ provided that we can calculate $\dot{U}, \dots U^{(r)}(x, y, t_0)$, differentiate

$\dot{U}(x, y, t_0) = f(t, U)$ to obtain

$$\ddot{U}(x, y, t) = f_t(t, U(x, y, t)) + f_U(t, U(x, y, t), \dot{U}(x, y, t))$$

$$\ddot{U} = f_t + f_U f$$

And proceed similarly to obtain the higher order derivatives $U^{(r)}(x, y, t_0)$ of $U(x, y, t)$. Although the Taylor series method can give excellent results, the derivatives can be very difficult to calculate and very time consuming to evaluate. To avoid differentiation of $f(t, u)$, one can use the Runge-Kutta formulas.

Runge-Kutta method are closely related to the Taylor series expansion of $U(x, y, t)$ in equation (38). but differentiation of f are not necessary in the method. All Runge kutta method will be written in the form

$$u_{n+1} = U_n + \Delta t F(t_n, u_n, \Delta t : f), n \geq 0 \quad (39)$$

we want

$$F(t, U(x, y, t), \Delta t : f) \approx U(x, y, t) = f(t, U(x, y, t))$$

For all small values of Δt , the truncation error for equation (39) is defined as

$$T_{n+1}(U) = U(x, y, t_{n+1}) - U(x, y, t_n) - \Delta t F(t_n, U(x, y, t_n), \Delta t : f) n \geq 0 \quad (40)$$

The derivative of a formula for truncation error is linked to the derivatives of these methods and these will also be true when considering Runge-Kutta methods of a higher order. The derivation of Runge-Kutta method will be introduced by deriving a family of second order formulas (Butcher,(2003)).

we suppose F has the general form

$$F(t, u, \Delta t : f) = \gamma_1 f(t, u) \gamma_2 f(t + \alpha \Delta t, u + \alpha \Delta t f(t, u)) \quad (41)$$

in which the three constant $\gamma_1, \gamma_2, \alpha$ are to be determined

When the Taylor's theorem for function of two variables is used to expand the second term on the right hand side of equation (40), through the second derivative terms, we obtain

$$F(t, u, \Delta t : f) = \gamma_1 f(t, u) + \gamma_2 [f(t, u) + \Delta t(\alpha f_{t+u} + (\Delta t)^2(\frac{1}{2}\alpha^2 f_u f + \alpha f_{tu} f + \frac{1}{2}\alpha^2 f^2 f_{uu}))] + o((\Delta t)^3) \quad (42)$$

also one needs derivatives of

$$\begin{aligned} \dot{U}(x, y, t_0) &= f(t, U(x, y, t)) \\ \ddot{U} &= f_t + f_u f \end{aligned}$$

$$U^{(3)} = f_{tt} + 2f_{tu}f^2 + f_{uu}f^2 + f_u f_t + f_u^2 f \quad (43)$$

For the truncation error

$$\begin{aligned} T_{n+1}(U) &= U(x, y, t_{n+1}) - U(x, y, t_n) - hF(t_n, U(x, y, t_n), \Delta t : f) \\ &= \Delta t U(x, y, t_0) + \frac{(\Delta t)^2}{2} U(x, y, t_n) + \frac{(\Delta t)^3}{6} U^{(3)}(x, y, t_n) \\ &+ o(\Delta t)^4 - \Delta t F(t_n, U(x, y, t_n), \Delta t : f) \end{aligned}$$

substitution from equation (4.42) and Equation (4.43) and collecting together, we obtain

$$\begin{aligned} T_{n+1}(U) &= \Delta t[1 - \gamma_1 - \gamma_2]f + (\Delta t)^2[(\frac{1}{2} - \gamma_2\alpha)f_t + (\frac{1}{2} - \gamma_2\alpha)f_u f] \\ &+ (\Delta t)^3[(\frac{1}{6} - \frac{1}{2}\gamma_2\alpha^2)f_{tt} + (\frac{1}{3} - \gamma_2\alpha^2)f_{tu}f \\ &+ (\frac{1}{6} - \frac{1}{2}\gamma_2\alpha^2)f_u f_u^2 + \frac{1}{6}f_u f_t + \frac{1}{6}f_u^2 f] + o((\Delta t)^4) \end{aligned} \quad (44)$$

where all derivatives are evaluated at (t_n, U_n)

We want to make truncation error converge to zero as rapidly as possible. The coefficient of $(t)^3$ cannot be zero in general, if f is allowed to vary arbitrarily. The requirement that the coefficients of t and $(t)^2$ be zero leads to

$$\gamma_1 + \gamma_2 = 1, \gamma_2\alpha = 1/2 \quad (45)$$

we observe that Equation (4.45) reduce to $\gamma_2 = 1/2\alpha$ and $\gamma_1(1 - (1/2\alpha))$. that there are infinitely many solutions for the parameters is a peculiarity of Range-Kutta Methods. For example, one choice is $\alpha = 1/2$, giving sequence

$$y_{n+1} = y_n + \Delta t f(t_n + \frac{\Delta t}{2}, u_n + \frac{\Delta t}{2} f(t_n, u_n)), n \geq 0$$

which is usually called the modified Euler's Method. Another choice is $\alpha = 2/3$ which leads to second order Runge-kutta method

$$y_{n+1} = y_n + \frac{\Delta t}{4}[f(t_n, u_n) + 3f(t_n + \frac{2}{3}\Delta t, u_n + \frac{2}{3}\Delta t f(t_n, u_n))] n \geq 0 \quad (46)$$

higher order formulas can be created, although the algebraic becomes very complicated, Assume a formula for $F(t, u, : f)$ of the form

$$F(t, u, \Delta t : f) = \sum_{j=1}^m \gamma_j - j k_j$$

$$k_1 = f(t, u)$$

$$k_j = f(t + \alpha_j \Delta t, u + \Delta t \sum_{i=1}^{j-1} \beta_{ji} k_i) \quad (47)$$

where $0 \leq \alpha_j \leq 1$ and $\alpha_j = \sum_{i=1}^{j-1} \beta_{ji}$

The coefficients can be chosen to make the leading terms in the truncation error equal to zero, just as was done with equation (44) and equation (45). using. Equation (47), one can obtain m-stage Runge-Kutta method to solve $u = f(t, u)$. higher order Runge-Kutta method are more accurate than lower order. But it is unknown that m and order k must satisfy $m \geq k$ for an m-stage kth order method. For a given value of m, there are many choices for the weights γ_j in equation (4.46) and for the parameters α_j and β_{ji} for $m = 4$, a very popular four stage. 4th order Runge- Kutta method is

$$U_{n+1} = U_n + \frac{\Delta t}{6} [K_1 + 2K_2 + 2K_3 + K_4] \quad (48)$$

where

$$K_1 = f(t_n, u_n)$$

$$K_2 = f(t_n + \frac{1}{2}\Delta t, u_n + \frac{1}{2}\Delta t K_1)$$

$$K_3 = f(t_n + \frac{1}{2}\Delta t, u_n + \frac{1}{2}\Delta t K_2)$$

$$K_4 = f(t_n + \Delta t, u_n + \Delta t K_3)$$

For the transient diffusion equation consider in this thesis, the DQ discretized set of ordinary differential equation (equation 25)

$$[A] \{u\} + \{S\} = \{b\} = \frac{d\{u\}}{dt} \quad (49)$$

Are solved now by using 4th order Runge-Kutta Method (equation (4.48)). thus, we can easily write by taking $[A]u + S$ as the vector function $f(t, u)$ in the same initial value problem $\dot{U} = f(t, u)$ so

$$f(t, u) = [A] \{u\} + \{S\} \quad (50)$$

Thus the fourth order Runge-Kutta method gives for the transient diffusion equation the following vector equation

$$\{u_{n+1}\} = \{u_n\} + \frac{\Delta t}{6} [\{K_1\} + 2\{K_2\} + 2\{K_3\} + \{K_4\}] \quad (51)$$

where

$$\{K_1\} = [A] \{u_n\} + \{S\}$$

$$\{K_2\} = [A] \left\{ u_n + \frac{\Delta t}{2} \{K_1\} \right\} + \{S\}$$

$$\{K_3\} = [A] \left\{ u_n + \frac{\Delta t}{2} \{K_2\} \right\} + \{S\}$$

$$\{K_4\} = [A] \{u_n + \Delta t \{K_3\}\} + \{S\}$$

Now the stability of the numerical scheme (4.51) in applying the system (4.25) has to be considered for obtaining converged numerical solution to the transient diffusion equation.

4.3 Stability of Discretized Differential Quadrature Equation

From the application of PDQ method to the transient diffusion equation we obtained the set of ordinary differential equation(25)

$$[A] \{u\} = \{b\} - \{S\}$$

The stability analysis of this equation is based on the eigenvalue distribution of the DQ discretization matrix $[A]$. If $[A]$ has eigenvalues λ_i and the corresponding eigenvectors $\xi_i (i = 1, 2, \dots, k)$ being the size of matrix $[A]$ the similarity transformation reduce the system of the form

$$\frac{d\{u\}}{dt} = [D] \{U\} + \{S\} \quad (52)$$

Here the diagonal matrix $[D]$ is formed from the eigenvalue and from a non singular matrix $[P]$ containing the eigenvector as columns

$$[D] = [P]^{-1} [A] [P] \quad (53)$$

$$\{U\} = [P]^{-1} \{u\} \quad (54)$$

$$\{S\} = [P]^{-1} \{S\} \quad (55)$$

Since $[D]$ is a diagonal matrix equation (52) is an uncoupled set of ordinary differential equation considering the i^{th} equation of (52)

$$\frac{dU_i}{dt} = \lambda_i U_i + S_i \quad (56)$$

The solution is given by

$$U_i = (U_i(0) + \frac{S_i}{\lambda_i}) e^{\lambda_i t} - \frac{S_i}{\lambda_i} \quad (57)$$

Thus the solution $\{u\}$ of the system (4.25) can be obtained as

$$\{u\} = [P] \{U\} = \sum_{i=1}^k U_i \xi_i = \sum_{i=1}^k [U_i(0) e^{\lambda_i t} + \frac{S_i}{\lambda_i} (e^{\lambda_i t} - 1)] \xi_i \quad (58)$$

clearly, the stability solution of $\{u\}$ when $t \rightarrow \infty$ requires

$$Re(\lambda_i) < 0 \text{ for all } i \quad (59)$$

where $Re(\lambda_i)$ denotes the real part of λ_i , This is the stability condition for the system (25)

when single step method is applied to the system of ordinary differential equation. it is absolutely stable if

$$|E_i(\lambda_i \Delta t)| < 1, \quad i = 1, 2, 3, \dots, k$$

where $Re(\lambda_i) < 0$ and $E_i(\lambda_i)$ denotes the growth factor for each diagonal elements of $E(D\Delta t)$ for approximating the matrix $exp(D\Delta t)$.

Fourth order RKM has the region of absolute stability (Butcher, (2003)).

$$-2.78 < \lambda_i \Delta t < 0 \text{ for real } \lambda_i \quad (60)$$

$$0 < |\lambda_i \Delta t| < 2^{(3/2)} \text{ for pure imaginary } \lambda_i \quad (61)$$

Test problem 1

The Dirichlet problem is defined as

$$\frac{\partial u(x, y, t)}{\partial t} - \nabla^2 u(x, y, t) = 0 \quad (x, y) \in (-1, 1) \quad (62)$$

with initial condition

$$u(x, y, 0) = u_0(x, y) = 1 \quad (63)$$

and the Dirichlet boundary conditions are given by

$$u(x, y, t) = 0 \quad x, y = (-1, 1). \quad (64)$$

The analytical solution is (Tanaka and Chen (2001))

$$u(x, y, t) = v(x, t)v(y, t) \text{ where } v(z, t) = \frac{4}{z} \sum_{i=0}^{\infty} \frac{(-1)^i}{2i+1} \cos\left(\frac{2i+1}{2}\pi z\right) e^{[-(2i+1)^2 \frac{\pi^2 t}{4}]} \quad (65)$$

This problem is solved by using several number of grid point and compared with analytical solution for finding the suitable number of grid points. We employed $N = 5, N = 7, N = 9$ and $N = 13$ Chebyshev-Gauss-Lobatto grid points in one direction in the Differential Quadrature Method for comparing with analytical solution. The number of grid points N_x and N_y respectively for x and y direction are taken as equal to N and grid step size $\Delta x = \Delta y = h$. Since we use Chebyshev-Gauss-Lobatto grid point the resulting polynomial based differential quadrature set of ordinary differential equation (equation 24) are stable in the sense that all the eigen values of weighting coefficient matrix $[A]$ are real and negative for both Dirichlet and Neumann boundary condition. Also absolute stability region for the fourth order RKM is $-2.78 < \lambda_i \Delta t < 0, i = 1, 2, \dots, k$ where k is the size of the matrix $[A]$. Therefore choice of h and Δt plays an important role for stability of the overall numerical scheme employed for solving transient diffusion equation. While the refinement of h improves the result for PDQ part (discretization of Laplace operator part), Δt in RKM must also be decreased since the eigenvalue are getting large in magnitude for small h . For the number of grid points $N = 5, 7$ the time step Δt was taken to be 0.01 first and the approximated solution agree with the exact solution at the time level $t = 1.0$ as can be seen from Figure 4.1 and 4.2. When the number of grid point N is increased (h decreased) to get smoother contour of the potential at the same time level, we need smaller time steps. Thus for $N = 9$ and 13, we have taken $\Delta t = 0.001$ since the maximum eigenvalue in magnitude is about 20×10^3 for $N = 10$ (Shu, (2000)) and obtained very well agreement with the exact solution. Figure 4.3, 4.4, 4.5 show potential values at $t = 1.0$ from both DQM and exact solution u . Figure 4.6 represent both solution at the time level $t = 2.0$ and Figure 4.7 shows the very well agreement of the potential with the exact solution for several values of Δt . Smaller Δt values provide the same accuracy but since it requires more computational time, $\Delta t = 0.0001$ values are suitable for most of Dirichlet problems. Since the solution obtained with $N = 13$ is already very accurate there is no need for this problem to increase N . Increasing N will increase the size of the coefficient matrix and this will be costly in terms of computation since in the Runge-Kutta Method we have matrix vector multiplications four times in each time step.

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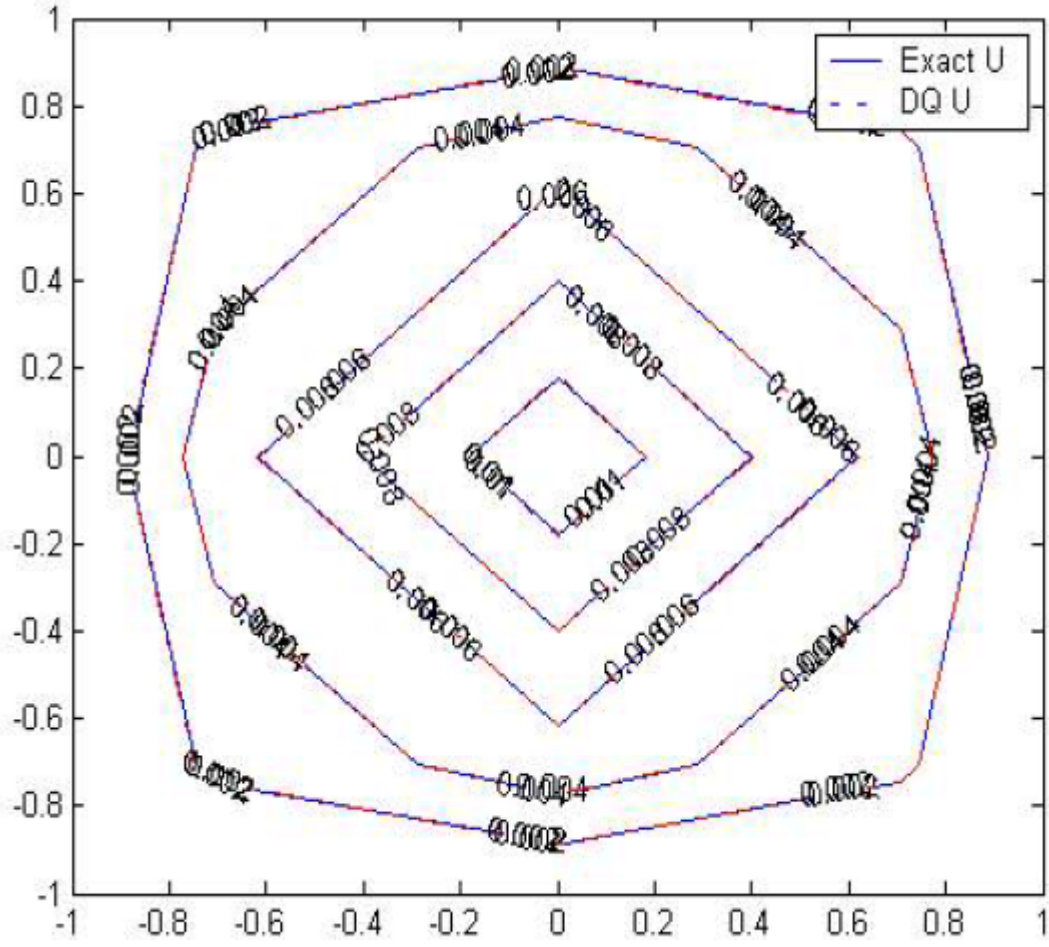


Figure 1: At $t=1.0$ with $N=5$ grid points, $\Delta t = 0.01$

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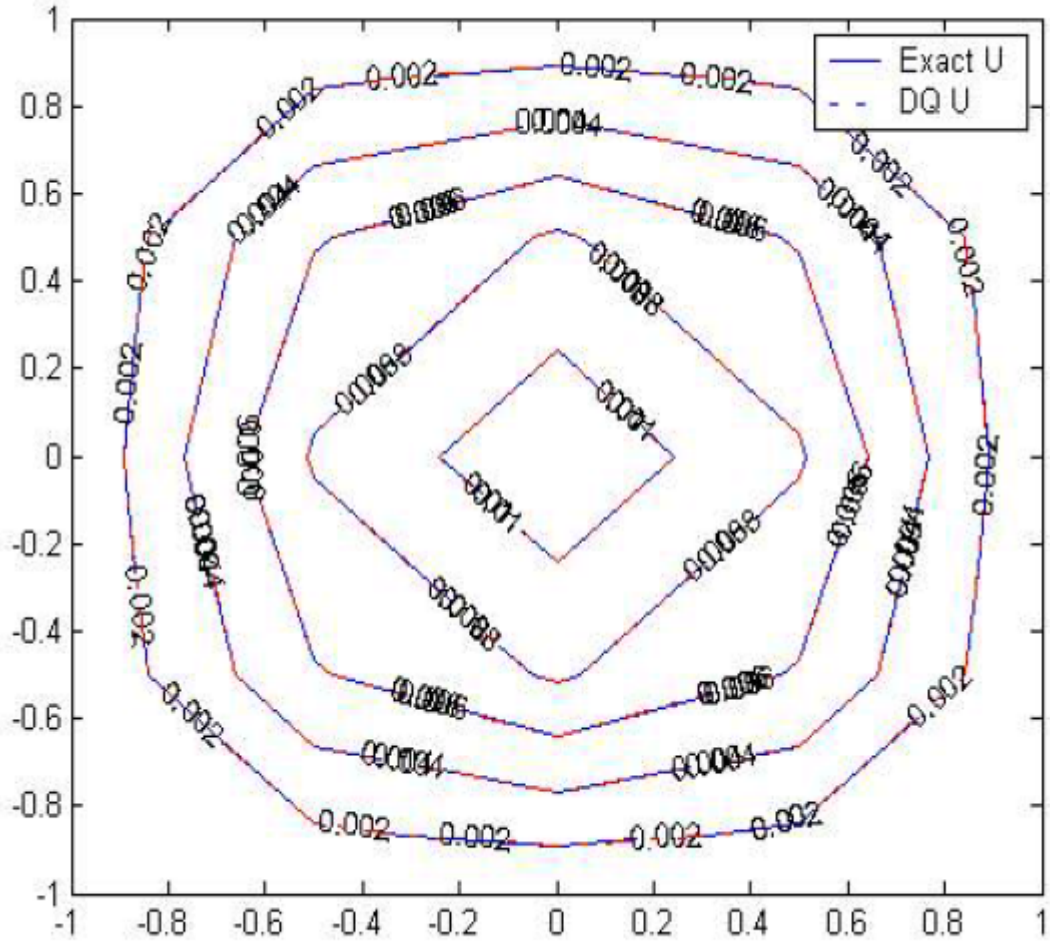


Figure 2: At $t=1.0$ with $N=7$ grid point, $\Delta t = 0.01$

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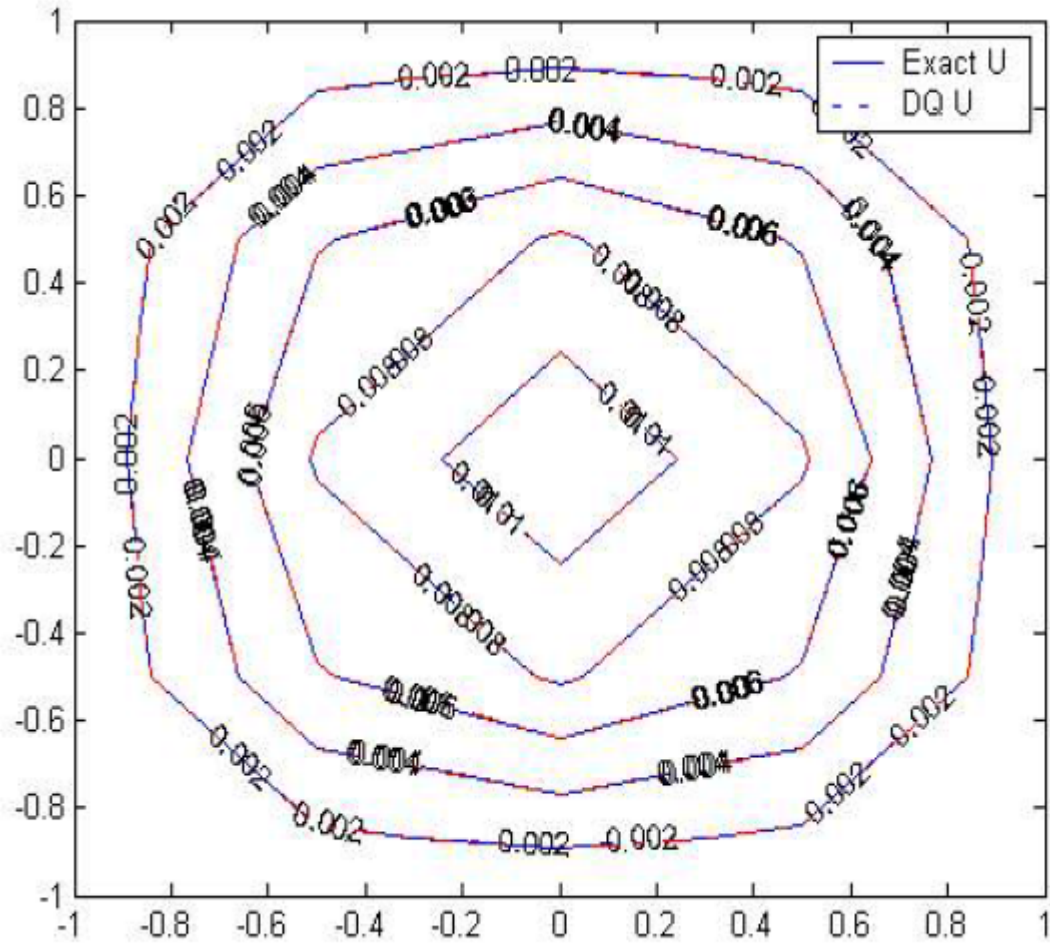
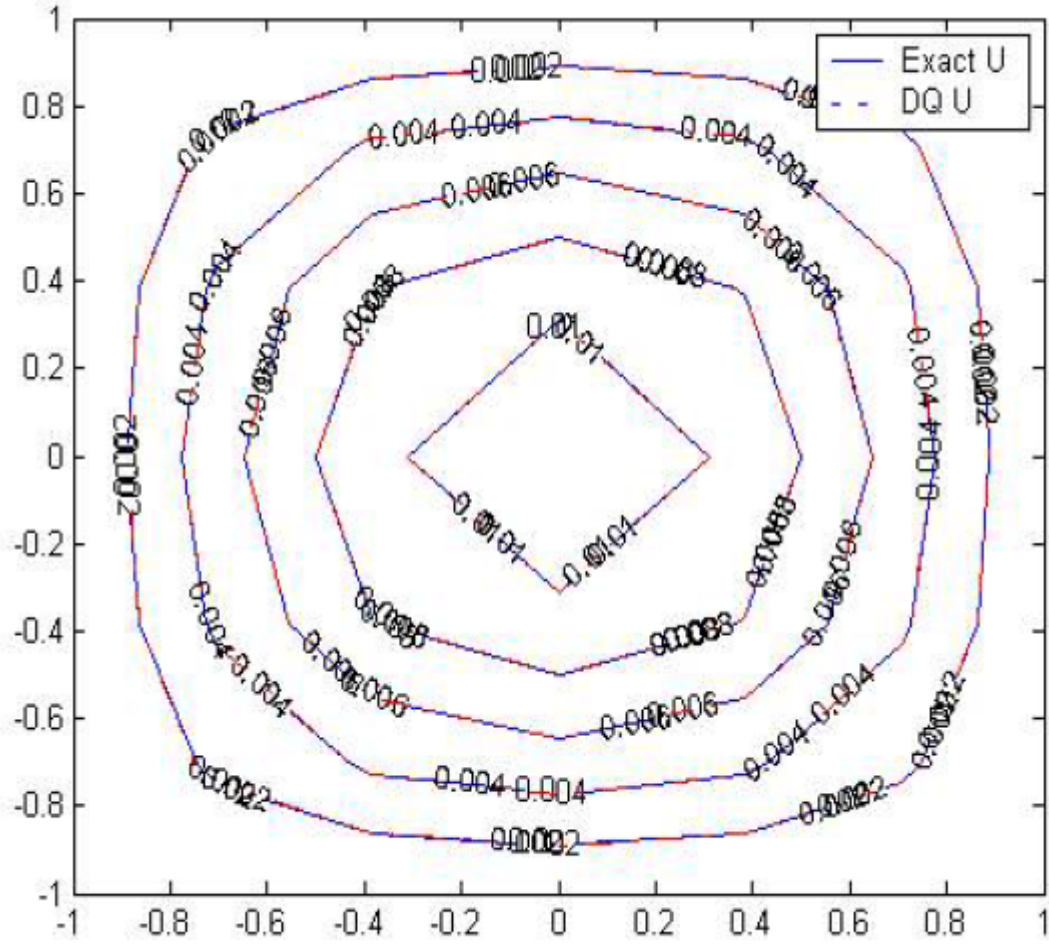


Figure 3: At $t=1.0$ with $N=7$ gridpoint, $\Delta t = 0.001$

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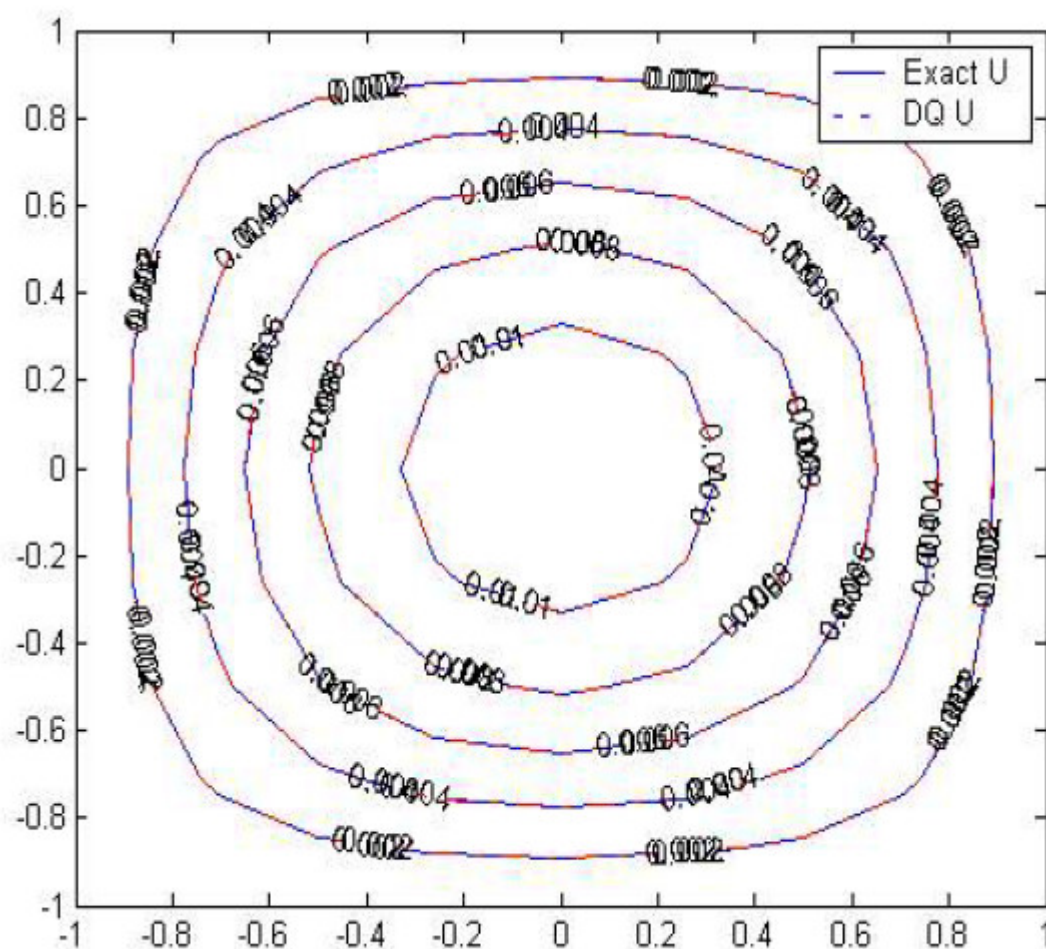


Figure 5: At $t=1.0$ with $N=13$ gridpoint, $\Delta t = 0.001$

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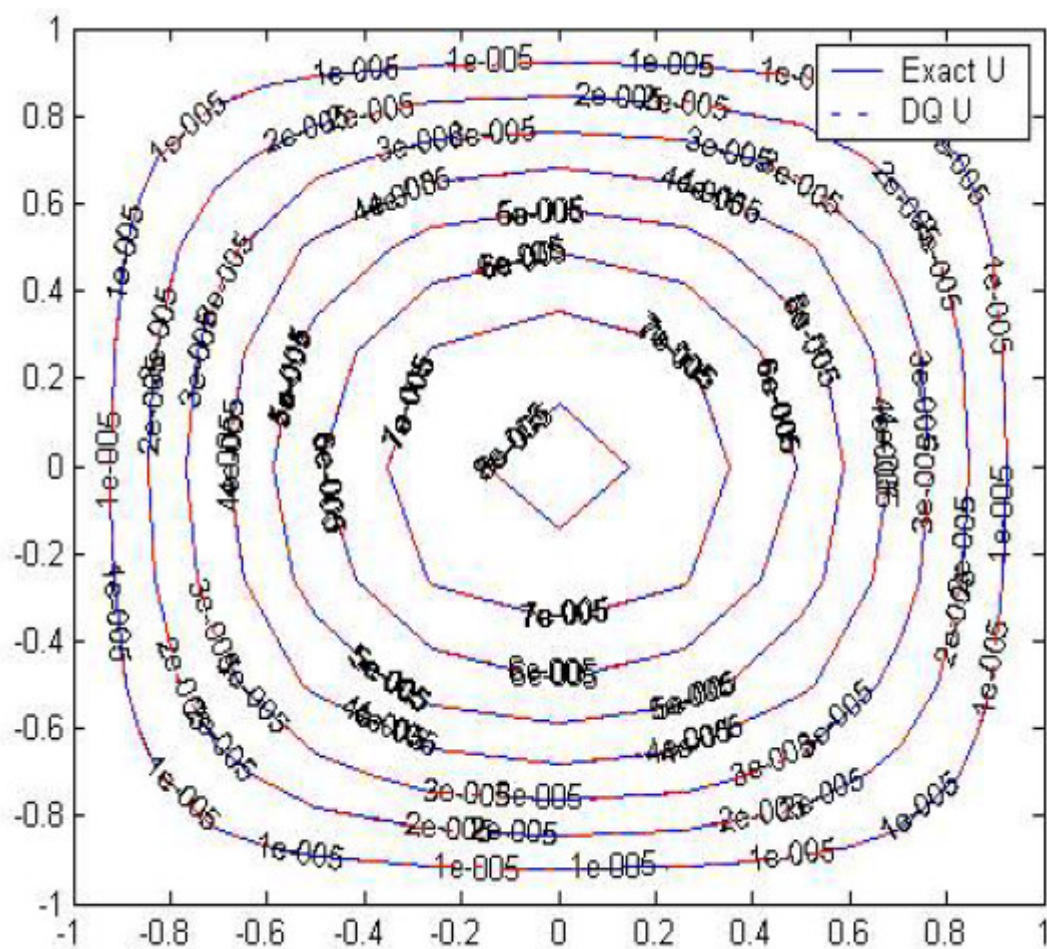


Figure 6: At $t=2.0$ with $N=13$ gridpoint, $\Delta t = 0.001$

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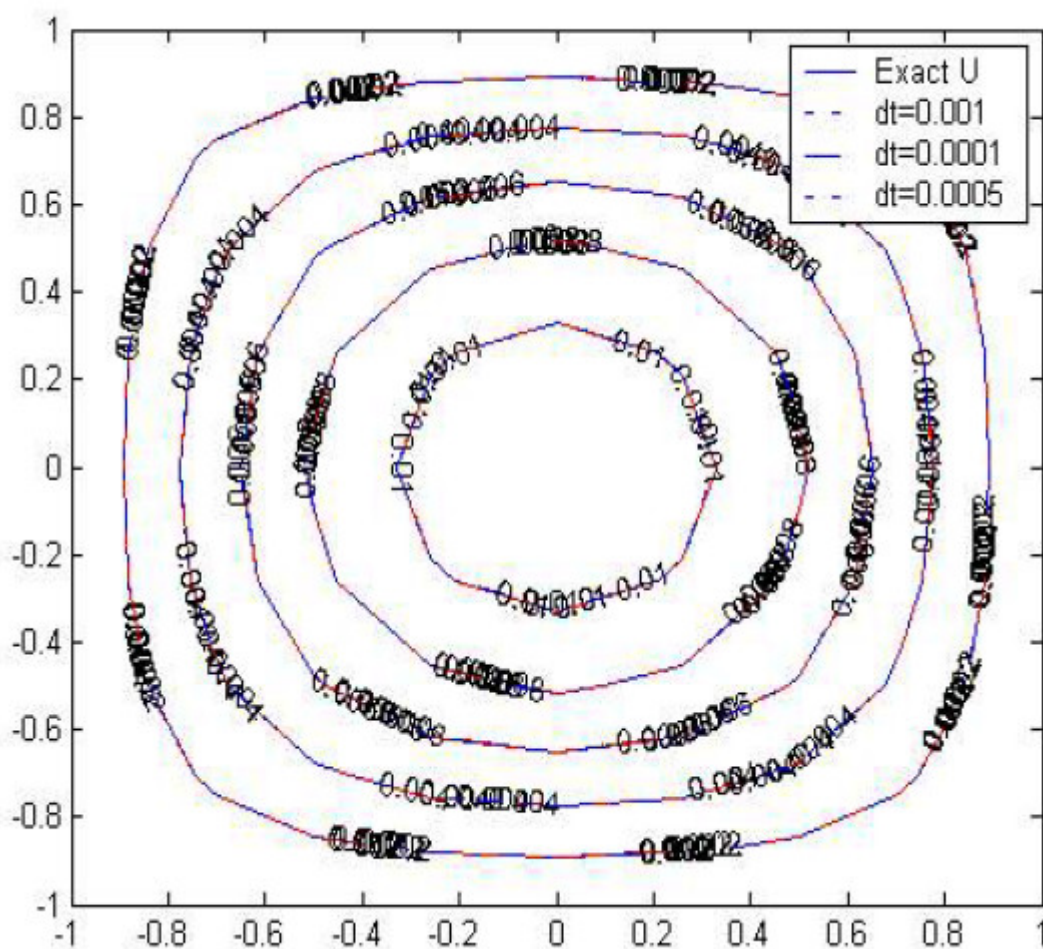


Figure 7: At $t=1.0$ with $N=13$ grid point

The following problem are Dirichlet-Neumann problems that on some boundaries normal derivative q of the potential u is given and another still Dirichlet condition are specified.
problem 2

This case is a reduced form of the Dirichlet problem 1 and thus holds the same analytical solution formulas. The problem is a Dirichlet-Neumann problem

$$\frac{\partial u(x, y, t)}{\partial t} - \nabla^2 u(x, y, t) = 0 \quad (x, y) \in (0, 1) \quad (66)$$

with the initial condition

$$u(x, y, t) = u_0(x, y) = 1 \quad (67)$$

The Dirichlet boundary condition are given by

$$u(1, y, t) = 0, \quad u(x, 1, t) = 0 \quad (68)$$

and the Neumann boundary conditions are specified as

$$q(0, y, t) = 0, \quad q(x, 0, t) = 0 \quad (69)$$

The analytical solution is given by the equation (4.4),(4.5) in problem 1 as

$$u(x, y, t) = v(x, t)v(y, t) \quad (70)$$

where

$$v(z, t) = \frac{4}{\pi} \sum_{i=0}^{\infty} \frac{(-1)^i}{2i+1} \cos\left(\frac{2i+1}{2}\pi z\right) e^{-(2i+1)^2 \frac{\pi^2 t}{4}} \quad (71)$$

For Dirichlet-Neumann problem defined in the region $(x, y) \in [0, 1] \times [0, 1]$ has two homogenous Dirichlet and two homogenous Neumann type boundary condition with unity initial condition. For this problem Neumann condition are also discretized to the final system of equation. The number of discretization point $N = 10$ was suitable for obtaining potential contours. Figure 4.8 gives potential at $t = 0.1$ with $\Delta t = 0.001$ obtained by using $N = 13$ grid points. Figure 4.9 and 4.10 present solution of the problem at the time level $t = 0.1$ with $\Delta t = 0.001$ and $\Delta t = 0.0001$ respectively and by using $N = 10$. As can be seen smaller Δt gives better accuracy for this Dirichlet-Neumann problem. This may be due to the behavior of mixed boundary conditions since the maximum eigenvalue in magnitude also vary with h . we continue with $N = 10$ grid points since it gives almost the same accuracy with $N = 13$ for the other computations in solving Dirichlet-Neumann diffusion problems for computational cost.

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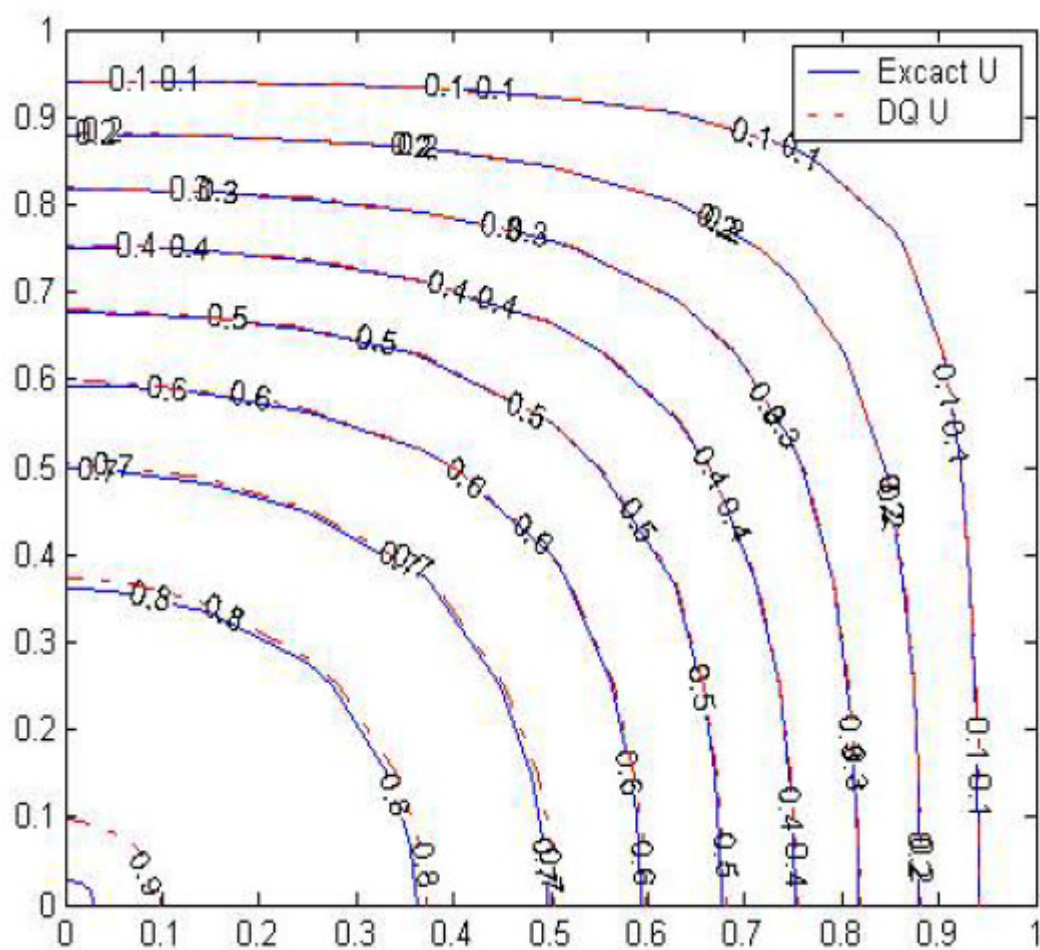


Figure 8: At $t=0.1$ with $N=13$ grid points, $\Delta t = 0.001$

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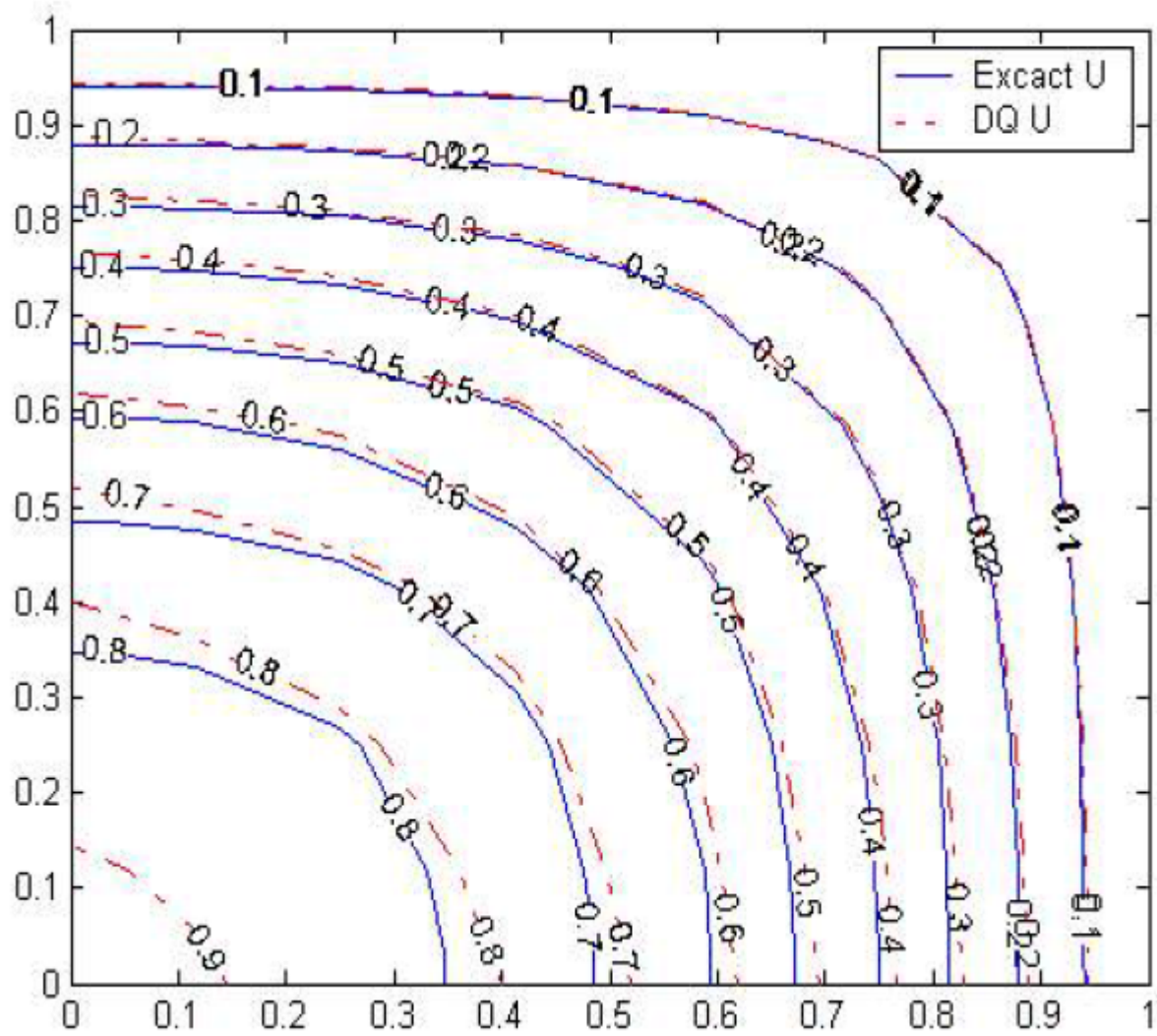


Figure 9: At $t=0.1$ with $N=10$ grid point, $\Delta t = 0.001$

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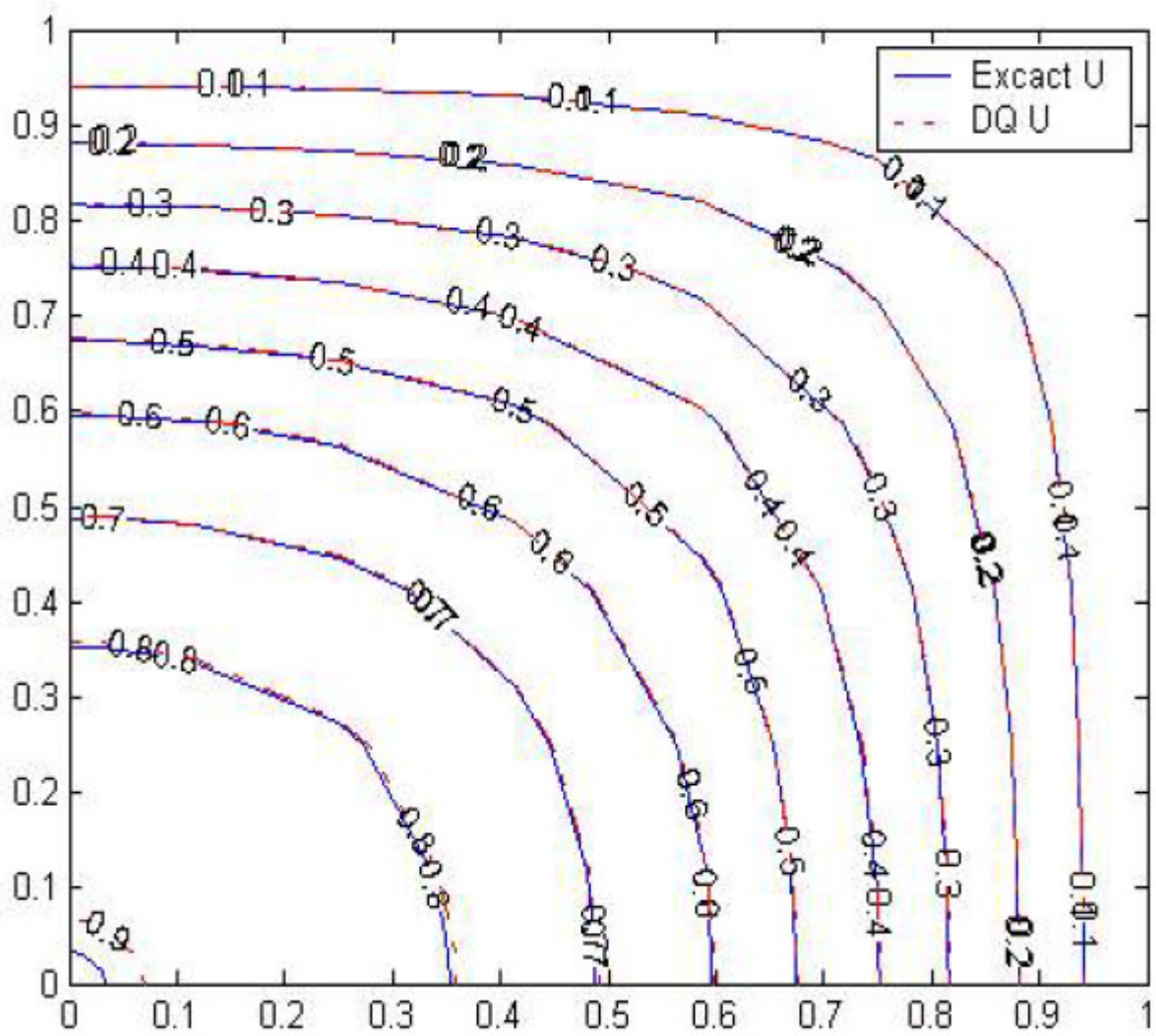


Figure 10: At $t=0.1$ with $N=10$ grid points, $\Delta t = 0.0001$

CHAPTER FIVE

5 CONCLUSION

In this thesis the Differential Quadrature method is accompanied with the fourth order Runge-kutta Method for solving time dependent diffusion equation. Derivatives in space direction are discretized with DQM while time derivative is discretized by using 4th order RKM. The combination of this two methods performs very well since the resulting system of ordinary differential equation is stable for Dirichlet and Dirichlet-Neumann type of boundary conditions and the explicit 4th order RKM has quite a large stability region as well as practical to use.

The numerical procedure presented is applied to Dirichlet and Dirichlet-Neumann type problems. The solution depends on the choice of step size Δt and h in time and space directions respectively since they have to satisfy the stability criteria of RKM. Thus, results are obtained and presented in terms of contours for several values of Δt and h (for several values of number of grid points).

Time dependent coefficient in the equation and time dependent boundary conditions are also implemented in the method and applied to two problems.

When the results are compared with the exact solutions, the high accuracy, efficiency and the stability of the method is observed.

For the DQM discretization, we did not require more than $N = 13$ number of grid points in space directions since with $N = 13$ we obtained very well accuracy. Thus, DQM has the advantage that it gives accurate numerical results using a considerably small number of grid points as compared to the other numerical method.

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