NUMERICAL SOLUTION OF ONE-DIMENSIONAL HEAT EQUATION USING RADIAL BASIS FUNCTIONS

A Thesis Submitted to the Department of Mathematics, Jimma University in partial Fulfillment for the Requirements of the Degree of Masters of Science in Mathematics (Numerical Analysis)

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DECLARATION

I undersigned declare that this thesis entitled "**Numerical solution of one dimensional heat equation using Radial basis functions"** is my own original work and it has not been submitted for the award of any academic degree or the like in any other institution or university, and that all the sources I have used or quoted have been indicated and acknowledged as complete references.

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ABSTRACT

In this thesis, inverse Multiquadric Radial basis functions for solving 1D heat equation is presented. First, the solution domain is discretized and the derivative involving the spatial variable is replaced by the sum of the weighting coefficients times functional values at each grid points along the spatial variable. Then, the resulting first order linear ordinary differential equation is solved by ode 45. To validate the applicability of the present method, one model example is considered and solved for different shape parameter 'c'. Numerical results are presented in tables in terms of root mean square $\left(E^2\right)$*, maximum absolute error* (E^∞) *and condition number of the system matrix. The numerical results presented in tables and graphs show that, the present method approximates the exact solution very well and is superior over the method presented by Dehghan and Tatari, 2010.*

Keywords: Radial Basis; Inverse multiquadric; heat equation; condition number; shape parameter.

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CHAPTER ONE

1. INTRODUCTION

1.1 Background of the Study

Mathematical modeling of most physical systems leads to linear/nonlinear partial differential equations (PDEs) in various fields of science. PDEs have enormous applications compared to ordinary differential equations (ODEs), to mention some of these: in dynamical system, electricity, heat transfer, electromagnetic theory, quantum mechanics and so on (Erwin, 2006). Although PDEs have a wide range of applications to real world problems in science and engineering, the majority of PDEs do not have analytical solutions. Therefore, the approximation solution via numerical methods comes into place.

Numerical methods were widely used for solving the partial differential equations (PDEs).Mesh-based numerical methods such as finite difference method (FDM), finite element method (FEM), boundary element method (BEM) have shown their efficiency in solving the PDEs over the past few decades(Watson,2017). These methods require a mesh to connect nodes inside the computational domain or boundary. Complications of these methods include a slow rate of convergence, spatial dependence, instability, low accuracy, and difficulty of implementation in complex geometries (Watson, 2017). But scientists in the field of computational mathematics are trying to develop numerical methods by using modern computers. One of this is a differential quadrature method (DQM).

A Differential Quadrature (DQ) is a numerical method for evaluating derivatives of a sufficiently smooth function (Bellman and Casti, 1971). The DQM are able to produce the accurate result using only a small number of grid points. They are mesh-based method. Furthermore, the distribution of the nodes has limitations, and they must be clustered near the boundary limiting its usefulness (Waston, 2017). However, mesh-less approximation techniques using radial basis functions (RBFs) have been developed over the last several decades. These methods are easy to implement, highly accurate, and truly mesh-less and avoids troublesome mesh generation for high-dimensional problems (Waston, 2017).

Over recent decades, mehless methods using RBFs have evolved, and a number of different techniques have been developed for solving partial differential equations. Such as Kansa method, method of approximate particular solutions, method of fundamental solutions, singular boundary method. In addition to these well-known methods, the radial basis function differential quadrature method (RBF-DQ) is significant and effective method. Bellman et al., (1972) first proposed the differential quadrature (DQ) method when searching for a method that only required a few grid points in order to obtain accurate numerical results. Borrowing from integral the quadrature where an integral on a closed domain is approximated by a linear combination of functional values at all nodes, the differential quadrature approximates a derivative of a function with respect to a coordinate direction. Shu and Wu (2002) combined this differential quadrature method with radial basis functions and referred to it as the RBF-DQ method. This method is simple to implement, ensures non-singularity, and is appropriate for both linear and non-linear problems.

In the past few years a new technique for the numerical solution of (PDEs) has gained prominence in the scientific community: the method of Radial basis functions (RBFs). RBFs are conceptually similar to both the finite difference method (FDM) and the finite element method (FEM). However, unlike the FEM which interpolates the solution using low-order piecewise-continuous polynomials or the FDM which approximates the derivatives of the equations by finite quotients, RBFs use globally-defined splines to approximate the PDE solution and its derivatives (Trefethen, 2000).

RBFs were conceived independently by Hardy and Duchon during the 1970's as effective multidimensional scattered interpolation method. During the 1990's, Kansa demonstrated how RBF can be combined with the classic method of collocation for the numerical solution of a variety of elliptic, parabolic and hyperbolic PDEs (Kansa, 1990). Since then, there have been a myriad of applications on RBFs in scientific community (both for interpolation and numerical solution to PDEs) ranging from artificial neutral networks to spacecraft design, from air pollution modeling to aerial photography, from medical imaging to hydrodynamics.

RBFs are so popular because of :(1) they are natively high-dimensional, making them easy to construct in any number of dimensions; (2) they are very accurate, with convergence rates increasing with the dimensionality of the problem; (3) they are mesh-free, requiring only an arbitrary set of nodes rather than a full mesh, like FDM or FEM, to compute approximate solution; (4) they produce smooth approximations not only for the unknown function but also for its derivatives(Buhmann, 2003); finally, (5) they can be applied to sophisticated free-boundary and convection dominated problems. Predictably, RBFs also have some disadvantages: because of their global nature they generate full and sometimes ill-conditioned matrices during intermediate steps in their calculation. Nevertheless, if there are handled appropriately, RBFs offer an accurate and robust numerical solution method for variety of PDEs (Hon and Kansa, 2000).

In a meshless (meshfree) method a set of scattered nodes is used instead of meshing the domain of the problem. The use of radial basis functions as a meshless method for numerical solution of PDEs is based on the collocation method. Because of the collocation technique, this method does not need to evaluate any integral. The main advantage of numerical methods, which use radial basis functions over traditional techniques, is the meshless property of these methods. The radial basis functions method is used actively for solving PDEs.

Due to the wide range application of the one dimensional linear parabolic equation, several numerical methods have been developed. Most of the researchers have studied the numerical solutions of 1D Heat Equation. Heat equation mainly in one dimension had been studied by many authors. A comparative study between the traditional separation of variables method and Adomain method for heat equation had been examined by (Chan and Gorguis, 2008). Dehghan and Mohebbi (2010) presented a fourth-order compact finite difference approximation and cubic C^1-spline collocation method for the solution with fourth-order accuracy in both space and time variables. Dabral et al., (2011) propose B-spline finite element method to get numerical solution of one dimensional heat equation. Haidari et al., (2012) used Chebyshev wavelets methods for obtaining a numerical solution of the one-dimensional heat equation. They applied different wavelet families and the wavelet coefficients were calculated by the Galerkin or collocation method. Generally, they developed Chebyshev wavelet method with operational matrices of integration for solution of one dimensional heat equation with Dirichlet boundary conditions which is fast, mathematically simple and guarantees the necessary accuracy for a relatively small number of grid points. Thus these indicate that the method is not accurate for a relative large number of grid points and is difficult to apply for high dimensions geometric spaces. Kalyanil and Rao (2013) solved 1D heat equation by using double interpolation. They used finite difference method for double interpolation method to solve 1D heat equation, but the method gives better accuracy only for small step length and is difficult to compute the solution in complex computational domain. Benyam (2015) presented numerical solutions of a one dimensional heat Equation together with initial condition and Dirichlet boundary conditions of the form: $u_t = \alpha^2 u_{xx}$. He presented computation of the numerical solutions by using two methods, Finite difference and Finite element methods. The finite elements are implemented by Crank-Nicolson method. This method does not always converge to the exact solutions for large number of step length, because, both method are dependent on the step length of grid points. He get the accurate approximation solution with the length of time-step k=0.001 on $0 < t < 1$. Recently, Ezekiel et al., (2017) solved heat equation via C by using Finite-Difference approximations. In this approximation, size of the mesh is significantly arrive to an accurate solution when using finite difference method, the smaller the size of the mesh the closer is the numerical result to the exact solution. So that the accuracy of the predictions method is dependent on mesh spacing and time step, because of the step-length and time step they used to solve heat equation are respectively h=0.2 and k =0.006.

However, still the accuracy of the methods need attention. Because of the treatment method used to solve the heat equation is not trivial distributions and the solution depends on mesh size in case of mesh dependent method.

Even though the accuracy of the aforementioned methods are promising, they require large memory and long computational time. Besides, the methods are not suitable for higher dimensional problems and problems involving complex geometries. So, the treatment of the mesh-size presents severe difficulties that have to be addressed to ensure accurate solution. Dehghan and Tatari (2010) solved parabolic partial differential equations using radial basis functions and application to the heat equation. They used the Gaussian radial basis functions for obtaining solution of 1D heat equation. Even though the method is capable of approximating the heat equation, it fails to produce the solution for relatively small value of shape parameters: 0.5, 1, and 2.

Besides, the accuracy of the solution should be enhanced further. To this end, the aim of this thesis is to develop the method that is capable of producing a solution of one-dimension heat equation for any shape parameter and approximate the exact solution very well.

1.2 Objectives of the Study

1.2.1 General Objective

The general objective of this study is to formulate the numerical method for one dimensional Heat equation.

1.2.2 Specific Objectives

The specific objectives of this study are:

- ✓ To solve one-dimensional heat equation using inverse multiquadric radial basis functions.
- ✓ To compare the solution obtained with existing methods.
- ✓ To describe the advantage of the present method over other methods.

1.3 Significance of the Study

The outcomes of this study may have the following importance:

- ➢ To find an alternative solutions for one dimensional Heat equation.
- ➢ It will be used as reference material for anyone who works on this area.

1.4 Delimitation of the Study

This study is delimited to Inverse Multiquadraic radial basis function DQ method for solving 1D Heat equation given in the form of:

$$\frac{\partial u(x,t)}{\partial t} = a\frac{\partial^2 u(x,t)}{\partial x^2}, \quad (x,t) \in (0,1)x(0,T] \tag{1.1}$$

subject to initial condition

$$u(x,t=0) = f(x), \; 0 \le x \le 1 \tag{1.2}$$

and boundary conditions

$$\begin{cases} u(0,t) = g_0(t) \\ u(1,t) = g_1(t) \end{cases}, \qquad 0 \le t \le T \tag{1.3}$$

where $a > 0$ is the diffusive (viscous) coefficient and $f(x)$, $g_0(t)$ and $g_1(t)$ are smooth functions on the given domain.

CHAPTER TWO

2. REVIEW OF RELATED LITERATURE

2.1 One Dimensional Heat Equation

Definition 2.1.1 Heat is the energy transferred from one body to another body due to a difference in temperature. It is a form of energy that exists in any materials.

The one-dimensional in the description of the differential equation refers to the fact that we are considering only one spatial dimension. There are two methods used to solve for the rate of heat flow through an object. The first method is derived from the properties of the object. The second method is derived by measuring the rate of heat flow through the boundaries of the object (Azmi, 2009).

The partial differential equation (1.1) is used to model one-dimensional temperature evolution. In the one-dimensional heat equation given in the form of (1.1), u represents temperature measured along a 1D homogeneous rod x. Th constant (a) is called the diffusion coefficient, representing the thermal diffusivity of the material making up the rod.

The equation (1.1) is also called the diffusion equation because it also models chemical diffusion process of one substance or gas into another. The most important features of this equation are the second spatial derivative u_{xx} and the first derivative with respect to time u_t. The heat equation models the spread (transfers) of the heat from regions of high concentration to regions of lower concentration. The diffusion coefficient governs the rate of heat transfer.

The heat equation is derived from Fourier's law and conservation of energy (Cannon, 1984). By Fourier's law, the flow rate of energy per-unit surface area is proportional to the negative temperature gradient across the surface area (Bernatz, 2010). In one dimension, the gradient is an ordinary spatial derivative, and so Fourier's law is $q = -\kappa u_x$.

The heat equation is used to determine the change in the function u over time. One of the interesting properties of the heat equation is the maximum principle which says that the maximum value of u is either in time than the region of concern or on the edge of the region of concern.This essentially saying that temperature comes either from some source or from earlier in time because heat permeates but is not created from nothingness. This is a property of parabolic partial differential equations. Another interesting property is that even if u has a discontinuity at an initial time $t = t_0$, the temperature becomes smooth as soon as $t > t_0$.

Similar to the case of ordinary differential equations, the 1D heat equation has infinitely many solutions, and extra conditions are needed to pin down a particular solution. The solution of this equation is a function $u(x,t)$ which is defined for values of space and time on the given domain and satisfies boundary conditions. The solution is not defined in a closed domain but advances in an open ended region from initial values, satisfying the prescribed boundary conditions (Mayers and Morton, 2005).

In general, the study of pressure waves in a fluid, propagation of heat and unsteady state problems lead to parabolic type of equations. In contrast to the heat equation, the steady state constant is not simply the integral of the initial condition, but also depends on some complicated way on both the viscosity parameter and the shape of initial condition. Most of the researchers have studied the numerical solutions of parabolic heat equation. Ezekiel et al., (2017) solved heat equation via C by using Finite-Difference approximations. In this approximation, size of the mesh is significantly arrive to an accurate solution when using finite difference method, the smaller the size of the mesh the closer is the numerical result to the exact solution. So that the accuracy of the predictions method is depends on mesh spacing and time step, because of the step-length and time step they used to solve heat equation are respectively h =0.2 and k =0.006. So the method has high cost generation with storage capacity. Jing and Leslie (2007) obtained the numerical solution of heat equation, Fast solver in free space. The solution of the heat equation (the diffusion equation) in free space or in unbounded regions arises as a modelling task in a variety of engineering, scientific, and financial applications. While the most commonly used approaches are based on finite difference and finite element methods, these must be coupled to artificial (non-reflecting) boundary conditions imposed on a finite computational domain in order to simulate the effect of diffusion into an infinite medium(Greengard and Li, 2007). Thus Dabral et al., (2011) develop the numerical simulation of one dimensional heat equation by B-spline function. In contrast to heat equation, the steady state constant is not simply the integral of the initial condition, but also depends in some complicated way on both the viscosity parameter and shape of the initial condition (Byrnes et al., 1995). In particular, numerical calculations have been used to suggest that Euler equations do not have unique solution (Jameson, 1991). The justification for this claim is that a very fine mesh is used in calculation, problem which arises in the quasi-static theory of thermo-elasticity (Day, 1983). Investigators like Ekolin (1991) and Liu (1999) had studied the problem and introduced finite-difference methods for solving it numerically. The numerical solution of the heat equation is discussed in many textbook. See Quarterion and Valli (2008) and Cooper (1998) for modern introduction to the theory of differential equations along with a brief coverage of numerical methods. Ames (1992), Mayers and Morton (2005) and Cooper (1998) provide a more mathematical development of finite difference methods. Fletcher (1988), (Golub and Hoffman, 1992) takes a more applied approach that also introduces implementation issues. Fletcher provides FORTRAN code for several methods. Chopra and Marwah (1982) give a numerical solution for transient thermal distribution in a slab where chemical, electrical or nuclear energy is converted into thermal energy. To describe temperature profile, Cichota et al., (2004) uses exponential sinusoidal one-dimensional analytical model demonstrating that heat equation can still be solved analytically. Monte (2000), applied a natural analytical approach for solving the one dimensional transient heat conduction in a composite slap. He studied the transient response of one dimensional multi-layered composite conducting slab to the sudden variations of the temperature of surrounding fluid. In a one dimensional hollow composite cylinder with time dependent boundary conditions, Lu (2005) gave a novel analytical method applied to the transient heat conduction equation. Now a day the numerical methods need attention, because of the treatment of the method use to solve the heat equation is not trivial distributions and the solution depends on mesh size. Besides, the accuracy of the solution should be enhanced further. To this end, the aim of this thesis is to develop the method that is capable of producing a solution of one-dimension heat equation for any shape parameter and approximate the exact solution very well.

2.2 Differential Quadrature and Radial Basis Functions Differential Quadrature Method

The differential quadrature (DQ) method is a numerical technique for solving differential equations. DQM were developed by Bellman and Casti in 1971(as sited by Zhang and Zong, 2009). The basic idea of the DQ method is that any derivative at a mesh point can be approximated by a weighted linear sum of all the functional values along a mesh line. A variety of methods have been developed based on the DQM, including the polynomial based differential quadrature (PDQ) and Fourier-expansion-based differential quadrature method (FDQM) (Zhang and Zong, 2009).

The basic idea of the DQM is to determine the weighting coefficients for any order derivatives by using a weighted sum of functional values at a set of selected grid points (Cheong, 2015). PDQM and FDQM are highly efficient method by using a small number of grid points; they are not efficient when the number of grid points is large and also sensitive to grid point distribution. While the PDQ and FDQ methods are able to obtain accurate results using only a small number of grid points, they are mesh-based methods (Watson, 2017).

To overcome the limitations for the applications of DQM, many researchers have given much effort in developing and improving mesh-free DQM. More recently, a new class of methods has surfaced called mesh-less or meshfree methods. Each class of methods offers numerous and, in many ways, complementary benefits. In the ideal case, we seek a method defined on arbitrary geometries that behaves regularly in any dimension, and avoids the cost of mesh generation. The ability to locally refine area of interests in a practical fashion is also desirable. Fortunately, mesh-free methods provide all of these properties: based wholly on a set of independent points in n-dimensional space, there is minimal cost for mesh generation, and refinement is as simple as adding new points where they are needed. A subset of mesh-free methods of particular interest to the numerical modelling community today revolves around Radial Basis Functions (RBFs). This method is called radial basis function differential quadrature method (RBF-DQM). RBF methods are based on a superposition of translates of these radially symmetric functions, providing a linearly independent but non-orthogonal basis to interpolate between nodes in n-dimensional space (Boling, 2013).

2.3 Radial Basis Function

Definition 2.3.1 A function $\phi:\Re^d \to \Re$ is called radial if there exists a univariate function $\varphi:[0,\infty)\to\Re$ such that $\phi(x)=\varphi(r)$ where $r=\|x\|$ and $\|\bullet\|$ is a norm in $\Re^d$, ($\|\bullet\|$ is typically the Euclidean norm).

Definition 2.3.2 A radial basis function, $\phi(r)$, is a one-variable, continuous function defined for $r\geq 0$ that has been radialized by composition with the Euclidean norm on $\Re^d$. RBFs may have a free parameter, the shape parameter, denoted by c.

The function φ can be called as basic function whereas ϕ can be called basis function. The reason is that one single basic function can generates all of the basis function which we have used in the expansion (Naqvi, 2013).

A RBF $\phi(r_j)=\phi\left(\|x-x_j\|_2\right)$ depends only on the distance between $x\in\Re^d$ and a fixed point, $x_j\in\Re^d$. This property implies that the RBFs $\phi(x_j)$ are radially symmetric about x_j. RBFs are a powerful tool in interpolating multivariable functions or approximating solution of partial or ordinary differential equations. The RBFs have praised in a variety of setting, where one of the chief reason for their success is their ease of implementation in multivariate scattered data approximation. In the last decade, RBF meshless method has become a viable choice for solving PDEs. Kansa (1990) introduced this method for solving elliptic and parabolic PDEs. Frank and Schaback (1998) have used collocation using RBFs.

The standard radial basis functions are categorized into two major classes (Islam et al., 2009) and (Dehghan and Shokri, 2009).

Class 1.Infinitely Smooth RBFs

These basis functions are infinitely differentiable and involve a parameter, called a shape factor (such as multiquadric (MQ), inverse multiquadric (IMQ) and Gaussian (GA)) which needs to be selected so that the required accuracy of the solution is attained.

Class 2.Infinitely smooth (except at centres) RBFs

These basis functions are not infinitely differentiable. These basis functions are shape parameter free and have comparatively less accurate than basis function discussed in class1. Examples are thin plate spline.

The most popular radial basis functions are:

Name of radial basis function	$\varphi(r_j),(r \geq 0)$
Multiquadric (MQ)	$\phi(r_j) = \sqrt{r_j^{\,2} + c^2}$
Inverse multiquadric (IMQ)	$\phi(r_j) = \left(r_j^{\,2} + c^2\right)^{-\frac{1}{2}}$
Gaussian (GA)	$\phi(r_j) = \exp(-(cr_j)^2)$
Thin plate spline (TPS)	$\phi(r_j) = r_j^2 \ln(r_j)$

Table 2.1: Globally supported RBFs that generate radial basis functions

All radial basis functions given in the table 2.1 (except TPS) are parametric functions with shape (control) parameter c. They are smooth and continuously differentiable functions. Except for Multiquadric RBF, interpolation matrices of these radial basis functions are positive definite, but for Multiquadric it is conditional positive definite (Chenoweth, 2012). There are three main factors that affect the optimality of shape parameter. They are: the scale of supporting region, the number of supporting node and the distribution of supporting node. Among the three factors, the effect of nodes distribution is the most difficult to be studied since there are infinite kinds of distribution (Efranian and Kosari, 2017).

The RBFs are usually divided in to global support RBFs and local support RBFs. It is said to be global support if the $\lim_{r\to\infty}\phi(r_j) = \infty$ and local supporting if the $\lim_{r\to\infty}\phi(r_j) = 0$ (Efranian and Kosari, 2017). The global approach uses information from every center in the domain to approximate a function value or derivative at a single point. In contrast, the local method only uses a small subset of the available centers (Chenoweth, 2012).

For the given data (x_i, f_j), where $j = 1,2,3,...,N$, x_j are an element of $\Re^d$ and f_j are an element of $\Re$ then the smooth function p, defined by enforcing that $p(x_j) = f_j$.

Therefore, for any scattered set of point N with center x_j the radial basis interpolation function is given as:

$$p(x_j) = \sum_{j=1}^{N} \alpha_j \phi\left(\left\| x - x_j \right\|\right)$$

Enforcing the interpolation condition $p(x_j) = f_j$ we determine the coefficient α_j from NxN matrix for $j = 1, 2, 3, ..., N$.The choice of basis functions will determine which methods are available for solving system of interpolation and whether such a solution even exists. If the interpolation matrix is symmetric positive definite, then the linear system has a unique solution (Mongillo, 2011). Some scholars have studied the numerical solutions of parabolic PDEs by using these radial basis functions approximation method.

Ding et al., (2004) applied a global RBF-DQ method to solve partial differential equations. The numerical results of this method indicated that when the number of node is increased to a certain value, the accuracy of RBF-DQ approximation for derivative will decrease with the increase of nodes. This is because of the matrix for computing the weighting coefficients in the DQ approximation would be highly ill-conditioned when the number of number of nodes is large. To remove this difficult, a local RBF-DQ approximation for derivative is recommended. Chandhini and Sanyasiraju (2007) applied radial basis function finite difference (RBF-FD) method to solve convection-diffusion steady type equations. They used in their work that by changing the shape parameter in MQ-RBF, solution can be highly improved. Dehghan and Nikopour (2013) solved the boundary value problems using local RBF-DQ of second order. They used MQ as basis function. As the shape parameter plays a very important role in RBF, they applied two different techniques to determine the optimal shape parameter OSCP technique and OVSP method. Dehghan and Mohammadi (2015) used RBF-DQ to solve CahnHilliard equations. They used MQ as radial basis function with constant shape parameter and compared the method with global GRBF method. They show that the use of RBF-DQ reduces the ill-conditioning problem up to certain extent in GRBF method. Hashemi and Parand (2016) solved non-linear Lane-Emden type differential equations which are used in the areas of astrophysics. In their work, they tried Gaussian as a RBF and compare their result with other methods like HFC, linearization gives better result compare to other methods.

Dehghan and Tatari (2010) solved parabolic PDEs using radial basis functions. They employed Gaussian radial basis function to solve heat equation. The solution diverges for small shape parameters, namely 0.5, 1 and 2. As compared to the exact solution, the method produces less accurate solution. Consequently, this thesis aims to employ the Inverse Multiquadric radial basis function that produces convergent and more accurate solution for any shape parameter.

Chapter Three

3. Methodology

3.1 Study Site and Period

The study was conducted at Jimma University in the 2018/2019 academic year.

3.2 Study Design

This study was employed mixed design:

- Documentary review
- Numerical experimentation.

3.3 Source of Information

The sources of information for this study are: books, related articles and experimental result via MATLAB code.

3.4 Mathematical Procedures

The study followed the following mathematic procedure.

1. Describing the Problem;
2. Discretizing the solution domains;
3. Replacing and /or approximating the partial derivative involving the spatial variable by using radial basis function;
4. Determining the weighting coefficients;
5. Solving the resulting system of first order initial-value problems by using Runge-Kutta 4 solver called ode45;
6. Validating the method by using some numerical example.

CHAPTER FOUR

4. DESCRIPTION OF THE METHOD, RESULTS AND DISCUSSION

4.1 Description of the Method

Consider the one dimensional heat equation of the form:

$$\frac{\partial u(x,t)}{\partial t} = a\frac{\partial^2 u(x,t)}{\partial x^2},\ (x,t) \in (0,1)x(0,T] \tag{4.1}$$

subject to initial condition:

$$u(x,0) = f(x)\ ,\quad 0 \le x \le 1 \tag{4.2}$$

and boundary conditions

$$\begin{cases} u(0,t) = g_0(t) \\ u(1,t) = g_1(t) \end{cases},\quad 0 \le t \le T \tag{4.3}$$

where $a > 0$ is the diffusive (viscous) coefficient, and $f(x)$, $g_0(t)$ and $g_1(t)$ are known functions while $u(x,t)$ unknown function.

The computational domains $[0,1]x[0,T]$ are partitioned as a form of:

$$x_i = x_0 + ih, i = 1,2,...,M$$

$$t_j = t_0 + jk, j = 1,2,...,N$$

where h and k are mesh-size of $[0,1]$ and $[0,T]$ respectively.

4.2 Inverse Multiquadric Radial Basis Functions (IMQ-RBF)

The most popular radial basis function that is used in applications today is the Inverse Multiquadric (IMQ). The inverse multiquadric RBF was proposed by Hardy as cited by (Ding, et al., 2005) for the interpolation of topographical surfaces. IMQ-RBF are used in many applications such as multivariate function interpolation and approximation, turbulence analysis, neural networks, meteorology, solution of partial differential equations, etc.

The most popular form of inverse- multiquadric radial basis function can be given in the form of:

$$\phi(r_j) = \frac{1}{\sqrt{\left(x - x_j\right)^2 + c^2}},$$

where c is a shape parameter and $c > 0$. For time dependent problem, the inverse multiquadric function is given as:

$$\phi\left((x,t),(x_j,t)\right) = \phi\left(\left\|(x,t)-(x_j,t)\right\|\right) = \frac{1}{\sqrt{\left(x-x_j\right)^2 + c^2}}, \quad j = 1,2,...,N \tag{4.4}$$

where N is the number of grid points in the direction of spatial variable x, t is temporal variable.

The inverse multiquadric are conditionally positive definite and is completely monotonic function. The characterization of conditionally positive definite and completely monotonic function is first given by Schoenberg (1938). The generalization of Schoenberg theorem is given by (Chenoweth, 2012).

Definition 4.2.1 (Chenoweth, 2012).

A function ϕ is completely monotonic on $[0,\infty)$ if $\phi \in C[0,\infty)$, $\phi \in C^{\infty}(0,\infty)$, and $(-1)^n \phi^{(n)}(r) \geq 0$ where $r > 0$ and $n = 0,1,2,...$

Theorem 4.2.1 (Chenoweth, 2012)

Let $\phi(r) = \phi\left(\sqrt{r}\right) \in C[0,\infty)$ and $\phi(r) > 0$ for $r > 0$. Let $\phi'(r)$ be completely monotonic on $[0,\infty)$, then for any set of N distinct center x_j, $j = 1,2,3,...,N$ the NxN matrix B with entry $b_{kj} = \phi\left(\left\|x_k - x_j\right\|\right)$ is invertible. Such function is said to be a conditional positive definite.

IMQ-RBF is an example of global infinitely differentiable and conditional positive definite function. Thus, IMQ-RBF produces unique solution.

Theorem 4.2.2 (Micchell's, 1986)

For a set of N distinct data points to be approximated by the set of N approximation function ϕ and this function must be nonsingular.

Therefore, by the above definition and theorems, the interpolation matrix that obtained from IMQ-RBFs is invertible. Thus, the first and second order derivatives of inverse multiquadric function are given by:

$$\frac{\partial \phi}{\partial x} = -\frac{x - x_j}{\left[\left(x - x_j\right)^2 + c^2\right]^{\frac{3}{2}}} \tag{4.5}$$

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{2(x - x_j)^2 - c^2}{\left[\left(x - x_j\right)^2 + c^2\right]^{\frac{5}{2}}} \tag{4.6}$$

4.3 Approximating the Partial Derivatives and Determining the Weighting Coefficients

Recall that the one-dimensional heat equation is given in Eq. (4.1). The aim here is to approximate the derivative of $u(x,t)$ involving spatial variable. From primary idea of differential quadrature method, the derivative of $u_{xx}(x,t)$ can be expressed as a linear combination of functional values at each grid points. It is given as:

$$u_{xx}(x_i,t) = \sum_{j=1}^{N} w_{ij} u(x_j,t), \text{ for } i = 1, 2, ..., N. \tag{4.7}$$

where t is a temporal variable, w_{ij} are the weighting coefficients for second order derivative.

Since $u(x,t)$ is defined on one dimensional space, by properties of vector space, $u(x,t)$ can be expressed as a linear combination of inverse multiquadric radial basis function $\phi(x,t)$. Because $\phi(x,t)$ is a basis function for one dimensional space, every function define on one dimensional space can be expressed as a linear combination of these basis function using the properties of linear independence of vector in vector space. Now for any constant λ and at least one of $\lambda \neq 0$ such that

$$u(x,t) = \sum_{j=1}^{N} \lambda_j \phi(x,t) \tag{4.8}$$

Since $\phi\left((x,t),(x_j,t)\right) = \phi\left(\left\|(x,t) - (x_j,t)\right\|\right) = \frac{1}{\sqrt{(x - x_j)^2 + c^2}}$ the first and second order derivatives of Eq. (4.8) become:

$$u_x(x_i,t) = \sum_{j=1}^{N} \lambda_j \phi_x\left(\left\|x - x_j\right\|\right), \quad i = 1, 2, 3, ..., N \tag{4.9}$$

$$u_{xx}(x_i,t)=\sum_{j=1}^{N}\lambda_j\phi_{xx}\left(\left\|x-x_j\right\|\right),\ i=1,2,3,...,N \tag{4.10}$$

Substituting Eqs.(4.8) and (4.10) into Eq. (4.7), we get:

$$\sum_{j=1}^{N}\lambda_{ij}\phi_{xx}\left(\left\|x-x_j\right\|\right)=\sum_{j=1}^{N}w_{ij}\sum_{j=1}^{N}\lambda_{ij}\phi(x,t) \tag{4.11}$$

$$\phi_{xx}\left(\left\|x-x_j\right\|\right)=\sum_{j=1}^{N}w_{ij}\phi\left(\left\|x-x_j\right\|\right) \tag{4.12}$$

From Eq. (4.12) we have the following system of equations:

$$Aw=b, \tag{4.13}$$

where

$$A=\begin{bmatrix}\phi\left(\left\|x_1-x_1\right\|\right) & \phi\left(\left\|x_1-x_2\right\|\right) & \cdots & \phi\left(\left\|x_1-x_N\right\|\right)\\ \phi\left(\left\|x_2-x_1\right\|\right) & \phi\left(\left\|x_2-x_2\right\|\right) & \cdots & \phi\left(\left\|x_2-x_N\right\|\right)\\ \vdots & & \ddots & \vdots\\ \phi\left(\left\|x_N-x_1\right\|\right) & \phi\left(\left\|x_N-x_2\right\|\right) & \cdots & \phi\left(\left\|x_N-x_N\right\|\right)\end{bmatrix}$$

$$b=\begin{bmatrix}\phi_{xx}\left(\left\|x_i-x_1\right\|\right)\\ \phi_{xx}\left(\left\|x_i-x_2\right\|\right)\\ \vdots\\ \phi_{xx}\left(\left\|x_i-x_N\right\|\right)\end{bmatrix} \quad \text{and} \quad w=\begin{bmatrix}w_{i1}\\ w_{i2}\\ \vdots\\ w_{iN}\end{bmatrix}$$

The matrix A is called the interpolation matrix. The solution of the IMQ interpolation problem exist and unique, since matrix A is invertible by theorem 4.2.1 and 4.2.2. Therefore, the system of equation given in Eq. (4.13) has a unique solution.

Despite of the fact that A can be shown to be invertible for ϕ of the interest, the linear systems in Eq. (4.13) may often be very ill-conditioned, therefore, a small perturbation in initial data may produce a large amount of perturbation in the solution and it may be impossible to solve accurately using standard floating point arithmetic. Thus, we have to use more precision arithmetics than standard floating point arithmetic in our computational algorithm. The conditioning of A is measured by the conditional number defined as:

$$\kappa(A) = \|A\|_2 \, \|A^{-1}\|_2 \tag{4.14}$$

For large number of $\kappa(A)$, the system in Eq. (4.13) is ill-conditioned. This is because of the presence of shape parameter, c that affects both the condition number of the interpolation matrix A and the accuracy of the method. For a fixed number of interpolation points N, the condition number of A depends on the shape parameter c and support of the RBFs. Also, the condition number grows with N for fixed value of the shape parameter c (Dehghan and Tatari, 2010).

Despite various research works are done to develop algorithms for selecting the values of c which produces most accurate interpolation, the optimal choice of shape parameter is still an open problem. For example, Frank (1982) recommended an alternative value of $c = \frac{0.8\sqrt{N}}{D}$, where D is the diameter of the smallest circle containing the data points $\{x_j\}_{j=1}^{N}$ and N is the number of data points. Hardy (1971) suggested the value of $c = \frac{1}{0.815d}$, where $d = \frac{1}{N}\sum_{j=1}^{N} d_j$ and d_j is the distance of the j^{th} data value from its nearest neighbor. Fasshauer (1996) proposed the value $c = 2\sqrt{N}$ for interpolation in a regular domain two dimensional problem. Fasshauer later suggested a “safe” shape parameter based on Schaback’s uncertainity principle (2007), which states that it is impossible to achieve both good stability and small errors simultaneously. In this strategy, Fasshauer used the smallest value of shape parameter without MATLAB issuing a warning of ill-conditioning. While this strategy will not result in an optimal shape parameter, it does at least guarantee that the system will not be near-singular. Dehghan and Tatari (2010), used the variable shape parameter in the stability of the problem.

In this thesis a variable shape parameter is used for fixed step length to obtain better approximation. A variable shape parameter refers to using a different value of the shape parameter at each center. This results in shape parameters that are the same in each column of the interpolation matrix, A. One argument for using a variable shape parameter is that leads to more distinct entries in the RBF matrices which in turn leads to lower condition numbers.

Many RBFs are defined by a constant called the shape parameter. The choice of basis function and shape parameter have a significant impact on the accuracy of a radial basis function. From the procedure of DQ approximation of derivatives, it can be observed that the weighting coefficients are only dependent on the selected RBFs and the distribution of the supporting points in the local support (Ding et al., 2005).

Once the coefficients w_{ij} have been computed from Eq. (4.13), it is now possible to solve for u .

In fact, the IMQ-RBF is used to approximate $u_{xx}(x,t)$ by using uniform discretization grid point for spatial variable. The IMQ-RBF differential quadrature method is applied for the discretization of space derivatives of the unknown function u. The heat equation given in Eq. (4.1) can be discretization by using first IMQ-RBF differential quadrature method as

$$\frac{du_i(x_i,t)}{dt} = a\sum_{j=1}^{N} w_{ij}u(x_j,t) , \qquad i = 1(1)N \tag{4.15}$$

where N is the number of grid points in the interval of spatial variable x, w_{ij} are the weighting coefficients.

For imposing the Dirichlet boundary conditions, the Eq. (4.15) should only applied at the interior points since at the boundary grid points is known (Shu, 2000).

Thus, the Eq. (4.15) can be rewritten as

$$\frac{du_i(x_i,t)}{dt} = a\sum_{j=2}^{N-1} w_{ij}u(x_j,t) \quad , \quad 2 \le i \le N-1 \tag{4.16}$$

subjected to initial condition

$$u(x_i,0) = f(x_i)\,,\; 0 \le x_i \le 1, \tag{4.17}$$

and boundary conditions

$$\begin{cases} u_1(t) = g_1(t) \\ u_N(t) = g_2(t) \end{cases}, \quad 0 \le t \le T \tag{4.18}$$

where N is the number of grid points in the interval of spatial variable x, w_{ij} are the weighting coefficients. The resulting system of equation of ODEs in Eq. (4.16) can now be solved by using Runge-Kutta 4 solver called ode45.

4.4 Convergence Analysis

The following theorems are about the convergence theorems for the infinitely smooth RBFs:

Theorem 4.4.1 (Wendland, 2005)

Let ϕ be one of the Gaussian or (inverse) Multiquadrics. Suppose that ϕ is conditionally positive of order m. Suppose further that $\Omega \subseteq \Re$ is bounded and satisfies an interior cone condition. Denote the radial basis function interpolant to $f \in \mathrm{N}_\phi(\Omega)$ base on ϕ and $X = \{x_1,...,x_N\}$ by $s_{f,X}$. Fix $\alpha \in \mathrm{N}_0^d$. For every $l \in \mathrm{N}$ with $l \ge \max\{|\alpha|, m-1\}$ there exists constants $h_0(l), C_l > 0$ such that

$$\left| D^\alpha f(x) - D^\alpha s_{f,x} \right| \le C_l h_{x,\Omega}^{l-|\alpha|} \,|f|\, \mathrm{N}_\phi(\Omega)$$

for all $x \in \Omega$, provided that $h_{x,\Omega} \le h_0(l)$.

Theorem 4.4.2

Assume $\{x_i\}_{i=1}^{N}$ are N nodes in $\Omega \subset \Re^d$ which is convex, let: $h = \max_{x\in\Omega}\min_{1\le i\le N}\|x - x_i\|_2$

when $\phi(\eta) < c(1+|\eta|)^{-2l+d}$ for any $y(x)$ satisfies $\int \frac{\left(y(\eta)\right)^2}{\phi(\eta)} d\eta < \infty$, we have:

$$\left\|y_N^{(\alpha)} - y^{(\alpha)}\right\|_\infty < ch^{1-\alpha},$$

where $\phi(x)$ RBFs and the constant c is depends on the RBFs, d is space dimension, $y(\eta)$ and $\phi(\eta)$ are supposed to be the Fourier transforms of y and ϕ respectively, $y^{(\alpha)}$ denotes the α^{th} derivative of y, y_N is the RBFs approximation of y, $l \,\&\, \alpha$ are nonnegative integers.

A complete proof is given by Ding, et al (2004) and (Lu, 2005).

It can be seen that not only RBFs itself but also its any order derivative has a good convergence.

4.5 Criteria for Investigating the Accuracy of the Method

Here, we test the accuracy of the present method for solving one-dimensional heat equation for different shape parameters by the following error estimation techniques:

1. The maximum error is described using:

$$E^\infty = \max_{1\le k\le N}\left|U_{ex}(x_k) - u_{app}(x_k)\right|, \qquad (4.23)$$

2. The root mean square (RMS) is described using:

$$E^2 = \sqrt{\frac{1}{N}\sum_{k=1}^{N}\left|U_{ex}(x_k) - u_{app}(x_k)\right|^2}, \qquad (4.24)$$

where N is the number of collocation points U_{ex} is the exact value and u_{app} is the RBFs approximation.

Note: (1) E^{∞} measures the degree to which the numerical solution approximates the exact solution, whereas the latter measures the extent to which the condition number of the system matrix affects the numerical solution.

The larger the value E^2 means the effect of the condition number on the accuracy of the numerical solution is significant.

The smaller the value of E^2 means the effect of the condition number on the accuracy of the numerical solution is insignificant.

(2) **Trade-off (Uncertainty) principle**

The convergence results require that the fill distance is small (centers close together) and /or the shape parameter be small in order for the RBF system matrix to be well-conditioned that the shape parameter and minimum separation distance be large (centers far apart). Obviously, both situations cannot occur at the same time. This observation has been referred to as the uncertainty (trade-off) principle (Schaback, 1995). In RBF methods we cannot have both good accuracy and good conditioning at the same time.

4.6 Numerical Example

Example 1: Consider the classical heat equation (Dehghan and Tatari, 2010)

$$u_t = u_{xx}, \; 0 < x < 1, \; 0 < t \le T,$$

with initial condition

$$u(x_i, 0) = \sin(\pi x_i), \quad 0 \le x_i \le 1$$

and boundary conditions

$$u(0,t) = u(1,t) = 0, \; 0 \le t \le T,$$

and the exact solution is given by:

$$U(x_i) = \sin(\pi x)\exp(-\pi^2 t).$$

The numerical results are presented in terms of E^2, E^{∞} and $\mathrm{K}(A)$ are given in table, for h=0.1 and different time-step k =(Δt) and shape parameter c.

Table 4.1 Root Mean Square error, Max. Absolute error and Condition Number for example1,at h=0.1 and Δt =0.01

	Present Method			Dehghan & Tatari(2010)		
c	E^2	E^∞	$\kappa(A)s$	E^2	E^∞	$\kappa(A)s$
0.5	2.0779E-02	2.0883E-01	2.3278E+06	9.0651E+39	7.0000E+73	1.9676E+19
1	3.2486E-04	3.2648E-03	6.5360E+10	3.3136E+17	2.0000E+29	2.0434E+17
2	2.4130E-06	2.4250E-05	1.5298E+16	5.0227E+1	5.0001E+0	9.3751E+17
3	2.1297E-02	2.1403E-01	1.1042E+17	1.0196E-01	7.1266E-03	6.6616E+17
4	1.4966E-06	1.5040E-05	4.2727E+16	1.0384E-01	7.4346E-03	4.0811E+17
5	1.4865E+18	1.4939E+19	1.8801E+18	1.0400E-02	7.6029E+03	1.1529E+16
6	9.8842E-05	9.9335E-04	8.6391E+16	1.0150E-02	7.5571E-03	1.4832E+16
7	1.6051E-04	1.6131E-03	1.1250E+17	9.5715E-03	7.3241E-03	3.0267E+15

Table 4.2. Root Mean Square error, max. Absolute error and Condition number for example1,at h=0.1 , Δt =0.001 and Δt =0.025

Present method						
	Δt =0.001			Δt =0.025		
c	E^2	E^∞	$\mathrm{K}(A)s$	E^2	E^∞	$\mathrm{K}(A)s$
0.5	9.4713E-04	2.9966E-02	2.3278E+06	1.7661E-02	3.0518E-01	2.3278E+06
1	1.4296E-05	4.5230E-04	6.5360E+10	7.4712E-04	4.7839E-03	6.5360E+10
2	2.5550E-07	8.0837E-06	1.5298E+16	5.1281E-06	3.2836E-05	1.5298E+16
3	3.2904E-07	1.0410E-05	1.1042E+17	2.7782E+07	1.7789E+08	1.1042E+17
4	8.5701E-07	2.7115E-05	4.2727E+16	5.2983E-07	3.3926E-06	4.2727E+16
5	2.7049E-04	8.5579E-03	1.8801E+18	5.8119E+53	3.7214E+54	1.8801E+18
6	5.1210E-06	1.6202E-04	8.6391E+16	2.2698E-04	1.4534E-03	8.6391E+16
7	7.0001E-06	2.2147E-04	1.1250E+17	6.3169E-04	4.0448E-03	1.1250E+17

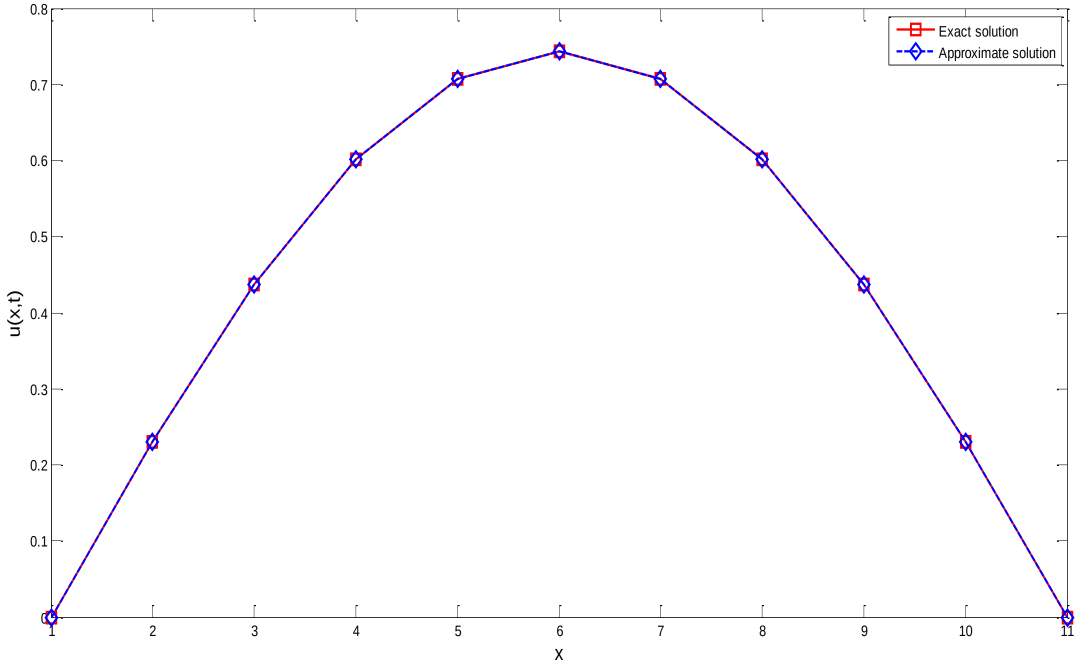

Figure 4.1: Graph of the approximate and Exact solution at c=2, h=0.1, Δt =0.01 and T=1

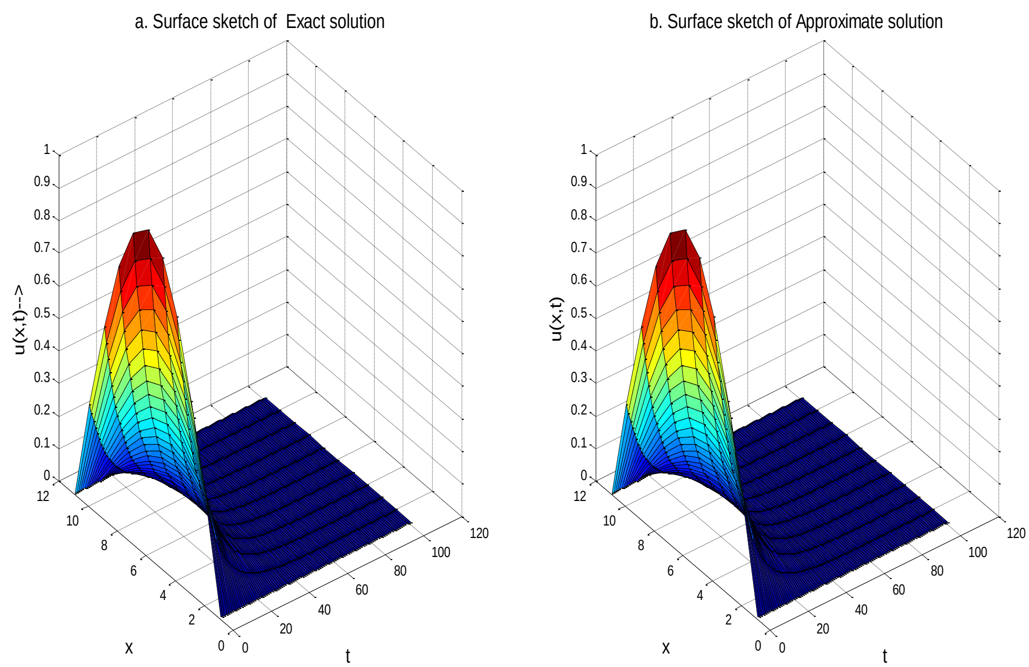

Figure 4.2: Surface graphs of physical behaviour of the given problem for c=2, h=0.1, Δt =0.01 and T=1

4.7 Discussion

In this thesis, radial basis function based on differential quadrature method presented for solving one dimensional heat equation. First, the domain is discretized using the uniform step-length and derivative involving the spatial variable 'x' is replaced by the sum of weighting coefficient times functional values at each grid point via inverse multiquadric radial basis function. Then, the resulting first order linear system of ordinary differential equation is solved by Runge-Kutta 4 solver called ode45.

To validate the applicability of the proposed method, one model example have been considered and the numerical results have been presented in tables 4.1-4.2 for different values of the shape parameter "c" and time-step k, keeping the step-length h fixed. The results obtained by the present method have been compared with numerical results obtained by (Dehghan and Tatari, 2010) and the results are summarized in tables 4.3-4.2.

In table 4.1, numerical values are presented for Δt =0.01, T=1 & h=0.1. As it can easily be seen from table 4.1, the approximate solutions are pretty good irrespective of the ill-conditioned nature of the interpolant matrix (Schaback, 1995).

The result presented in table 4.2 show that the accuracy is further enhanced when Δt =0.001 and declines when Δt =0.025. This confirms that the present method gives more accurate results over a long time interval.

In order to show the physical behavior of the given problem, the surfaces and plots graphs of approximating and exact solution are given in the figure 4.1 and 4.2, for c =2, h=0.01, Δt =0.01, and T=1. As it can be observed from the graphs (fig 4.1-4.2), the present method approximates the exact solution very well for c =2.

In a nutshell, the numerical results presented in tables and graphs confirm that the present method is efficient and accurate for solving one dimensional heat equation.

CHAPTER FIVE

5. CONCLUSION AND SCOPE OF FUTURE WORK

5.1 Conclusion

In this thesis, inverse multiquadric radial basis function has been presented for solving one dimensional heat equation. The proposed method has been applied to one model example for different values of shape parameter and the results are presented in the tables and graphs. The results show that the present method approximates the exact solution very well and it shows that the betterment of the present method over some existing methods reported in the literature.

5.2 Scope of Future Work

In this thesis, inverse multiquadric radial basis function is presented for solving one dimensional heat equation. Here, a variable shape parameter is used for fixed step length to obtain better approximation.

However, if node dependent (optimal) shape parameter is used, the accuracy of the approximation solution can further be enhanced. Besides, the present method can easily be extended to higher-dimensional problems.

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