Spectral Methods to Solve ODEs and PDEs

by

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Dedicated to my late friend Sidra Khalid

Abstract

The aim of this thesis is to gain an in-depth understanding of spectral methods and to investigate and demonstrate the level of accuracy of spectral methods in comparison to other numerical methods. Different aspects of a solution obtained using finite difference method and spectral methods are compared to develop an understanding how latter competes and excels. This thesis explores solutions of different kinds of differential equations, including ordinary and partial differential equations on random domains using `MATLAB`. The collocation method is used extensively here as it produces most accurate results possible. The stability and convergence rate of our numerical method are also investigated here, presenting plots and tables with problems under-consideration for wider understanding. The results in this study show how well this present method works and reduction in error is far more better than other numerical methods.

Preface

Spectral methods especially pseudospectral method have emerged as intriguing option for finding solutions of differential equations in many areas of Science and Mathematics. Spectral methods are one of the superior numerical technique for solution of differential equations on a simple domain and when the data defining the equation is smooth. This thesis describes spectral methods approach for both ordinary differential equations and partial differential equations.

Chapter 1 is the introduction of spectral methods. It presents the basic concept of collocation method and explain its computational aspects. Differentiation matrices and collocation points are discussed in detail for various polynomials.

After a brief introduction of collocation method, in Chapter 2 the main focus is on ordinary differential equations and comparison of different numerical methods. ODEs of second and third order both linear and non-linear on random domains are solved here using spectral methods (using Chebyshev and Laguerre polynomials) and compared with finite difference method and also with their exact solutions. For each problem under consideration the results are displayed in graphical form.

Chapter 3 presents spectral methods for partial differential equations. Homogeneous and non-homogeneous PDEs both linear and nonlinear are solved in this chapter.

In the end, Chapter 4 concludes this thesis.

Acknowledgements

Those scientists who have deep knowledge fear Allah better, Verily; Allah is All-Mighty, Oft-Forgiving. (Quran 35:28)

All praise to Almighty Allah, Who showered His endless blessings on me and for giving me strength to carry out my work successfully. My deepest gratitude to my supervisor Dr. Muhammad Asif Farooq for providing his guidance and constructive comments that has contributed greatly to the success of this research. This thesis would not have been possible without his supervision and persistent help. I would like to thank him for giving me an opportunity to work with him on an interesting topic. Special thanks to my GEC members Prof. Azad A. Siddiqui (SNS), Dr. Yousaf Habib (SNS) and Dr. Adnan Maqsood (RCMS). In the end, I would also like to thank my family especially my parents for their unconditional support and encouragement.

Contents

Chapter 1

Introduction

Differential equations are of basic importance in different fields of Science, Engineering and Mathematics. Differential equations are studied from several prospectives mostly concerning their solutions. There are various numerical techniques available to solve differential equations (ODEs and PDEs). Generally, following numerical techniques are useful in finding the solution of differential equations:

1. Finite Difference Method (FDM).
2. Finite Element Method (FEM).
3. Finite Volume Method (FVM).
4. Spectral Methods.

The numerical method is measured by its accuracy, efficiency and by its convergence rate.

Spectral methods have become popular in the last few decades among all the numerical methods for solving differential equations. It is considered as one of the fastest converging method when compared either with finite difference method or finite element method. Spectral methods can be used to solve ordinary differential equations, partial differential equations and eigenvalue problems efficiently. The main reason for spectral methods being superior is that the unknown solution is expanded as a global interpolant while other methods, like finite difference method uses local interpolant.

The convergence of spectral methods is based on the smoothness of the solution. For smooth functions the convergence rate is $O(N^{-m})$ for every m. The analytic functions converge even faster at the rate of $O(c^N)$ where $0 < c < 1$, see reference [1]. This rate distinguishes spectral methods from finite difference method, where the convergence rate is $O(1/N^p)$ where p is the order of method. Spectral methods often performs extremely well even with the non-smooth functions under certain restrictions, where both solution and variable coefficients are not smooth, see reference [2]. Also computational problem solving spectral methods uses less memory.

However irregular domains, strong shocks and certain boundary conditions can cause inefficiencies while working with spectral methods. So the few restrictions to be kept in mind while using spectral methods includes strict stability restrictions for boundary value problems, use of sparse matrices instead of full matrices and the complicated computer implementations.

Spectral methods is mainly of three different types the Tau method, the Galerkin method and the collocation method. The choice of using any of these methods depend upon the application. The Tau and Galerkin method belong to the weighted residual methods class, while collocation method uses a single global interpolant. The Tau method is best suited for problems with complicated boundary conditions. The boundary conditions can even be non-linear. The Galerikan method has the advantage of more convenient analysis and optimal error estimates while the collocation method works best with nonlinear problems or with complicated coefficients. For the detailed comparison of above three mention methods, refer to [2].

The main idea of spectral methods is to approximate the unknown solution of differential equation by using orthogonal functions. The spatial derivative of the solution is approximated by the derivative of polynomial and if there exist any time derivative in the equation, it is solved through classical finite difference schemes. For periodic problems Fourier series is used. On a periodic domain spectral derivatives are calculated by the Fast Fourier Transform (FFT). For non periodic problems Chebyshev polynomial and Legendre polynomials are used as orthogonal functions. For the approximation on the real line Hermite polynomials and for half line approximations Laguerre polynomials are best suited. In using polynomials for spectral methods, clustering of grid points is of great importance. The grid points should cluster near end points for asymptotic convergence.

In the past few years, the activity on theory as well as application of spectral methods have been concentrated on collocation method. The collocation method, also known as pseudospectral method uses a set of grid points which are called the collocation points or the nodes. The unknown solution is then approximated using the interpolating polynomial at the collocation points.

The complete description of the collocation method is given in [2], [3], [4] and [5].

For scientific computing and matrix based implementations, differentiation matrices are ideal for derivatives involved in any differential equation. Differentiation matrices are basically derived from pseudospectral method for boundary value problems that are based on weighted interpolants of the function $f(x)$ which has the following form

$$f(x) \approx p_{N-1}(x) = \sum_{j=1}^{N} \frac{\alpha(x)}{\alpha(x_j)} \phi_j(x) f_j, \tag{1.1.1}$$

where $\{x_j\}_{j=1}^N$ is the set of distinct interpolation points, $\alpha(x)$ is a weight function, $\{\phi_j(x)\}_{j=1}^N$ is the set of interpolating functions and $f_j = f(x_j)$. Taking l derivatives of Eq.(1.1.1) and evaluating the result at the nodes $\{x_k\}$ gives our required differentiation matrix represented by a matrix $D^{(l)}$, whose entries are

$$D_{k,j}^{(l)} = \frac{d^l}{dx^l}\left[\frac{\alpha(x)}{\alpha(x_j)}\phi_j(x)\right]_{x=x_k}, \tag{1.1.2}$$

and thus we have

$$\mathbf{f}^{(l)} = D^{(l)}\mathbf{f}, \tag{1.1.3}$$

where $\mathbf{f}$ is the vector of function values at the nodes $\{x_k\}$. The weight function depends on the choice of interpolating polynomial. For Hermite polynomial weight function is $e^{-x^2/2}$, for Laguerre polynomial it is $e^{-x/2}$ and weight function is constant for Chebyshev polynomials. The computation of spectral collocation differentiation matrices have been considered by [6] for constant weights. It is the case of Chebyshev polynomial otherwise for Laguerre polynomial, Legendre polynomial or Hermite polynomial arbitrary positive weight functions are taken. For arbitrary weight functions work of [7] can be studied.

The roots of Chebyshev polynomials known as the Chebyshev points are used as the nodes in Eq.(1.1.2) and Eq.(1.1.3). Chebyshev points lie in the interval $[-1, 1]$.

Chebyshev points are defined as

$$x_j = \cos(j\pi/(N-1)). \qquad j = 0, 1, ..., N-1$$

For the differential equation on a random domain $[a, b]$, first the interval should be converted to $[-1, 1]$ by using the following transformation

$$x \longleftrightarrow (1/2)((b-a)x + (b+a)).$$

Another way to construct the differentiation matrix was introduced by [8] using Chebyshev points. The Chebyshev differentiation matrix D_N have $N+1$ rows and columns (for $N \geq 1$) indexing from 0 to N. The entries of this matrix are

$$(D_N)_{00} = \frac{2N^2+1}{6}, \qquad (D_N)_{NN} = -\frac{2N^2+1}{6}$$

$$(D_N)_{jj} = \frac{-x_j}{2(1-x_j^2)}, \qquad j = 1, ..., N-1$$

$$(D_N)_{ij} = \frac{c_i}{c_j}\frac{(-1)^{i+j}}{(x_i - x_j)}, \qquad i \neq j, \quad i, j = 1, ..., N-1$$

where

$$c_i = \begin{cases} 2 & i = 0 \ or \ N \\ 0 & otherwise. \end{cases}$$

However, results obtained using differentiation matrices defined by [8] become less accurate as the derivatives increase in order. The entries of Chebyshev differentiation matrices as defined above are formulated using Lagrange interpolation. For the derivatives, the interpolating polynomial is then differentiated accordingly. The formulas for entries of differentiation matrices were first published by [9]. `MATLAB` codes with the implementations are given in [8] for more understanding.

Hermite polynomials, Laguerre polynomials and Legendre polynomials uses their roots as nodes, in calculating differentiation matrices. The roots of orthogonal polynomials are given by the eigenvalues of the $N \times N$ tridiagonal Jacobian matrix

$$J = \begin{pmatrix} \alpha_o & \beta_1 & & \\ \beta_1 & \alpha_1 & \beta_2 & \\ & & \ddots & \beta_{N-1} \\ & & \beta_{N-1} & \alpha_{N-1} \end{pmatrix}$$

where α_n and β_n are given by the following table

	Legendre	Laguerre	Hermite
α_n	0	$2n+1$	0
β_n	$n/\sqrt{4n^2-1}$	$-n$	$\sqrt{n}$

For the efficient execution of spectral differentiation matrices in `MATLAB`, the barycentric[1] form of interpolants is considered rather than using the form given by Eq.(1.1.1). The barycentric form of interpolant is

$$p_{N-1} = \frac{\alpha(x) \sum\limits_{j=1}^{N} \frac{\omega_j}{x-x_j} \frac{f_j}{\alpha(x_j)}}{\sum\limits_{j=1}^{N} \frac{\omega_j}{x-x_j}}, \qquad (1.1.4)$$

where

$$\omega_j^{-1} = \prod_{m=1}^{N} (x_j - x_m). \qquad (1.1.5)$$

In case of Chebyshev polynomials, where weight function is constant, the above form becomes

[1]Barycentric interpolation is a variant of Lagrange polynomial interpolation which is fast and stable.

$$p_{N-1} = \frac{\sum_{j=1}^{N} \frac{(-1)^j f_j}{c_j(x-x_j)}}{\sum_{j=1}^{N} \frac{(-1)^j}{c_j(x-x_j)}}. \tag{1.1.6}$$

`MATLAB` codes for the computation of spectral differentiation matrices using above mentioned forms of interpolants are given in [10]. The two main algorithms on which the computation of differentiation matrices based on are *poldif.m* and *chebdif.m*. For the computation of differentiation matrices for non-constant weight functions on arbitrary set of points *poldif.m* is used while *chebdif.m* computes differentiation matrices for constant weight function and Chebyshev nodes.

The next step is the implementation of given boundary conditions, after computing the derivatives involved in any differential equation. Implementation of boundary conditions effect the differentiation matrices which will be explained latter. There are two approaches for the implementation of boundary conditions. Either restrict the attention to interpolant that should satisfy the boundary conditions or add an extra equation that would satisfy the boundary conditions completely. For different types of differential equations and boundary conditions, different techniques are to be used to obtain accurate results. This will be more clear in the next chapters where different types of ODEs and PDEs are solved.

This thesis is outlined as follows. In Chapter 2, we present spectral methods for ODEs. The spectral method solution of PDEs is given in Chapter 3. Conclusions and outlook are drawn in Chapter 4.

Chapter 2

Spectral Methods for ODEs

Ordinary differential equations occur in many disciplines like Biology, Chemistry, Physics and Mathematics. Many ODEs occurring in practice are of second order. Higher order ODEs can either be solved directly or by reducing it into a system of first-order ODEs. ODEs are much easier to solve and understand as compared to partial differential equations. The solution of ODEs with constant coefficient and periodic boundary conditions is simple and easy to solve using Fourier spectral method. For non-periodic boundary conditions polynomial spectral method is used. Although spectral methods are much more efficient as compared to other numerical methods but the right selection of N is required for high accuracy.

The solutions of ODEs using different discrete methods like matrices, is an old and most successful way in computational mathematics. Spectral methods for solving ODEs using `MATLAB` is the subject of this section. It includes linear and nonlinear ODEs with random domains and coupled ODEs with mixed boundary conditions.

Laguerre spectral collocation method and Chebyshev spectral collocation method are discussed in detail here for better understanding and comparison. In Laguerre spectral method, the error decays slower than that of Chebyshev spectral method for similar problems, see [11]. Due to poor convergence properties of Laguerre spectral method, Chebyshev spectral method is preferred, even for semi-infinite domains. Both methods are applied to same problems for clarity in accuracy demonstrated by these methods.

This chapter is organized as follows. In section 2.1 linear ODEs are solved by spectral methods. The Darcy-Brinkman-Forchheimer Equation is solved in section 2.2. In section 2.3, Falkner-Skan Equation is solved. In this section we used open-source Software *Chebfun* to find solution. In section 2.4 coupled ODEs are solved using *Chebfun*.

2.1 Spectral Solution of Linear ODEs

We begin with some linear ODEs for understanding of spectral collocation method and its implementations. The exact solutions of ODEs are given so that we can compare our results with other numerical methods. We consider

$$k\frac{d^2T}{dx^2} + s_o x = 0, \qquad (2.1.1)$$

with boundary conditions

$$T(0) = T(L) = 0.$$

Here we will use two different techniques to see the difference in results. The procedure to solve any differential equation using Chebyshev polynomials is same as Laguerre polynomials. Since the domain is $[0, L]$, the natural idea will be to use Laguerre polynomials with rescaling parameter to be chosen according to the selection of differentiation matrix size. Laguerre differentiation matrix is calculated using *lagdif.m* while *lagroots.m* taken from [10] will give us the nodes. `MATLAB` codes for both *lagdif.m* and *lagroots.m* can be found in [10]. Since the boundary conditions are of homogeneous Dirichlet type so we take the interior points as our grid for computation and boundary conditions are enforced latter. Only the deletion of appropriate *(first and last)* rows and columns in differentiation matrix is required along with the deletion of nodes from both ends. This can be understood by considering Eq. (1.1.3) where **f** is a column vector, deletion of its end points required deletion of rows and columns of differentiation matrix, see [8]. `MATLAB` command of *fsolve* then gives the solution of our problem at interior nodes. For end points we have to enforce the boundary condition by adding the values of function at end points. The values of s_o, k and L are all taken to be 1 for convenience. The exact solution of above problem in Eq.(2.1.1) is

$$T(x) = \frac{s_o}{6k}(L^2 - x^2)x.$$

Figure 2.1 shows the solution obtained using Laguerre differentiation matrix compared with exact solution and Table 2.1 display the values of T for different values of x.

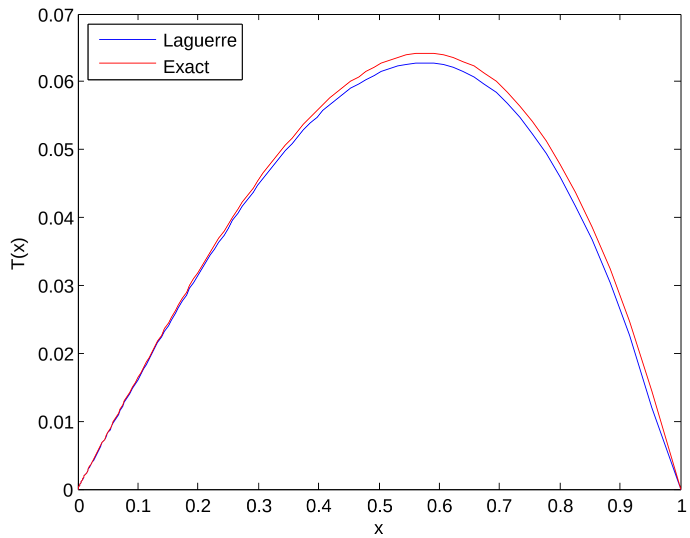

Figure 2.1: *Comparison of Laguerre spectral collocation method and exact solution.*

x	T (Collocation solution)	T (Exact solution)	absolute error
0	0	0	0.00000
0.2062	0.03242159	0.03289889	0.0004773
0.4074	0.05568983	0.05663393	0.0009441
0.5041	0.06149894	0.06266729	0.001168
0.6062	0.06250275	0.06390515	0.001402
0.7133	0.0567439	0.05839188	0.001648
0.8012	0.04596546	0.04780998	0.001845
1	0	0	0.00000

Table 2.1: *Comparison of exact solution and Laguerre spectral collocation method with absolute error.*

Another way to solve Eq.(2.1.1) is by Chebyshev spectral collocation method. The canonical interval of Chebyshev polynomials is $[-1, 1]$, it can be rescaled using the transformation defined in the above section. Eq.(2.1.1) is then transformed to

$$4\frac{d^2T}{dx^2} + \frac{x+1}{2} = 0,$$

and the boundary conditions become

$$T(-1) = T(1) = 0.$$

This equation can now be easily solved by using *chebdif.m* given in [10]. After obtaining the results through Chebyshev spectral method, we transform the solution into the domain $[0, 1]$. Figure 2.2 shows the comparison of Chebyshev spectral collocation method and the exact solution, Figure 2.3 shows the relative percentage error while Table 2.2 also shows relative percentage error for different values of x.

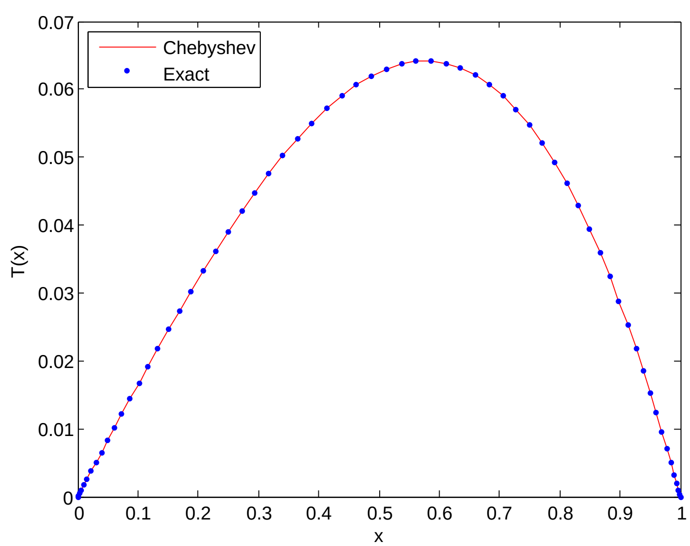

Figure 2.2: *Comparison of Chebyshev spectral collocation method and exact solution.*

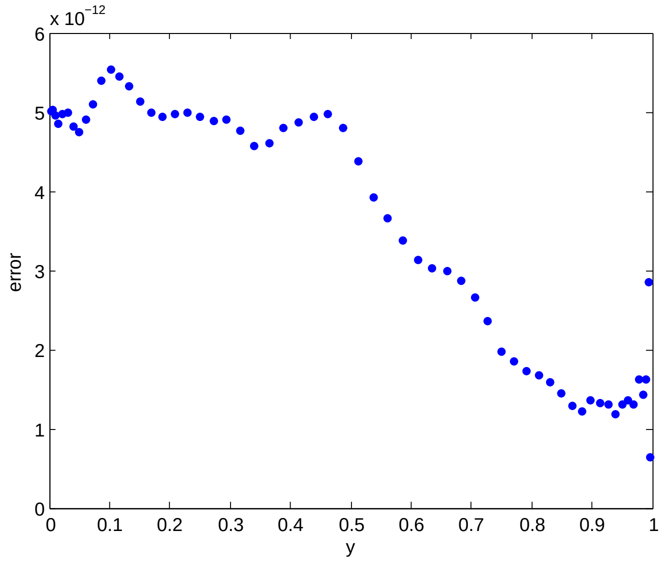

Figure 2.3: *Percentage relative error of exact solution and spectral methods using Chebyshev polynomials.*

x	T (Collocation solution)	T (Exact solution)	Percentage relative error
0.03015	0.005021	0.005021	4.992×10^{-12}
0.08688	0.01437	0.01437	5.396×10^{-12}
0.1509	0.02457	0.02457	5.125×10^{-12}
0.2944	0.04481	0.04481	4.909×10^{-12}
0.4626	0.0606	0.0606	4.981×10^{-12}
0.6354	0.06314	0.06314	3.033×10^{-12}
0.8117	0.046143	0.046143	1.684×10^{-12}
0.9607	0.01233	0.01233	1.365×10^{-12}

Table 2.2: *Comparison of Chebyshev spectral collocation method and exact solution with relative percentage error.*

The huge difference between results of Laguerre spectral method and Chebyshev spectral method can clearly be observed. The reason for high convergence rate of Chebyshev spectral collocation method is clustering at the end points. Evenly spaced points can be used for polynomial interpolation but it does not provide high accuracy. The best option for maximum convergence is the use of unevenly spaced points. As explained in [8], different sets of unevenly points can be taken but all sharing a common property. As $N \longrightarrow \infty$, the density for distribution of points is

$$density \sim \frac{N}{2\sqrt{1-x^2}}.$$

The average spacing between interior points in $O(N^{-1})$ while for end points $x = \pm 1$ the spacing is $O(N^{-2})$. The effect of using these clustered points on accuracy is dramatic. For detailed examination, Chapter 5 of [8] can be studied. Laguerre points lack the clustering property, reducing the convergence rate of Laguerre spectral method. The clustered points at the right end are not considered for Laguerre polynomials which results in poor convergence in our case.

Now we consider another ODE on a domain $[0, 1]$

$$\frac{d^2\phi}{dx^2} + \phi + x^2 = 0, \qquad (2.1.2)$$

with boundary conditions

$$\phi(0) = 0 \ , \ \phi(1) = 0.$$

This is a second-order ODE with homogeneous Dirichlet boundary conditions. Again Laguerre polynomial can be used with appropriate rescaling since the domain is $[0, 1]$.

The exact solution of Eq.(2.1.2) is

$$\phi = 2 - 2\cos x - \frac{1 - 2\cos 1}{\sin 1}\sin x - x^2.$$

The result for solution of Eq.(2.1.2), computed using Laguerre differentiation matrices in spectral collocation method, is given below in Figure 2.4. While Table 2.3 displays different values of $\phi(x)$ along with the absolute error.

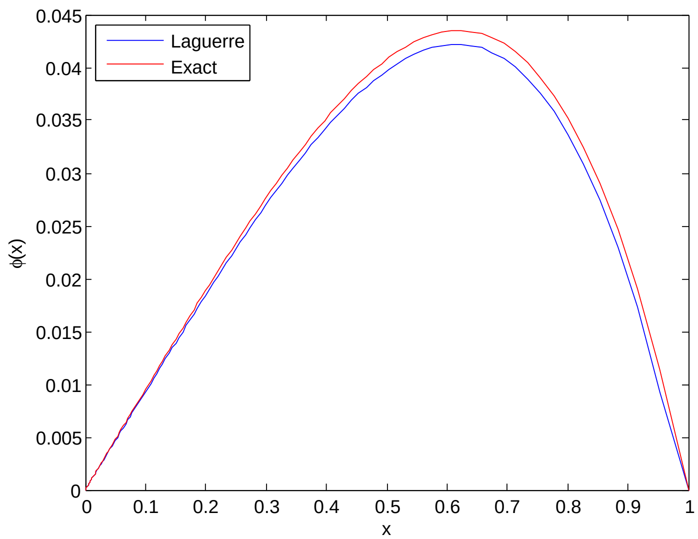

Figure 2.4: *Comparison between Laguerre spectral collocation method and exact solution.*

x	ϕ (Laguerre)	ϕ (Exact solution)	absolute error
0	0	0	0.0000
0.07435	0.006948366	0.007112449	0.0001641
0.2062	0.01900579	0.01945772	0.0004519
0.4074	0.03479872	0.03567416	0.0008754
0.5041	0.03986597	0.04093331	0.001067
0.6062	0.04220312	0.04346008	0.001257
0.7133	0.04002447	0.04146627	0.001442
0.8012	0.03360268	0.03517996	0.001577
1	0	0	0.00000

Table 2.3: *Comparison of exact solution and spectral methods with absolute error.*

Chebyshev polynomials can be used to solve this problem as well, with great accuracy and high convergence rate. Transforming Eq.(2.1.2) on the domain $[-1, 1]$ gives

$$4\frac{d^2\phi}{dx^2} + \phi + \frac{(x+1)^2}{2} = 0,$$

with boundary condition

$$\phi(-1) = \phi(1) = 0.$$

We follow the same steps for the solution of this problem as used in above problem. Figure 2.5 presents the comparison between Chebyshev spectral collocation method and exact solution, Figure 2.6 shows relative percentage error and Table 2.4 below show the results for different values of x.

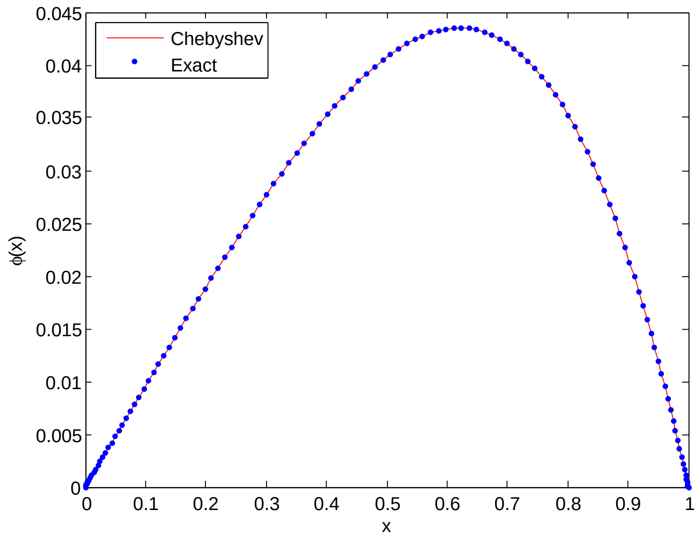

Figure 2.5: Comparison of exact solution and Chebyshev spectral collocation method.

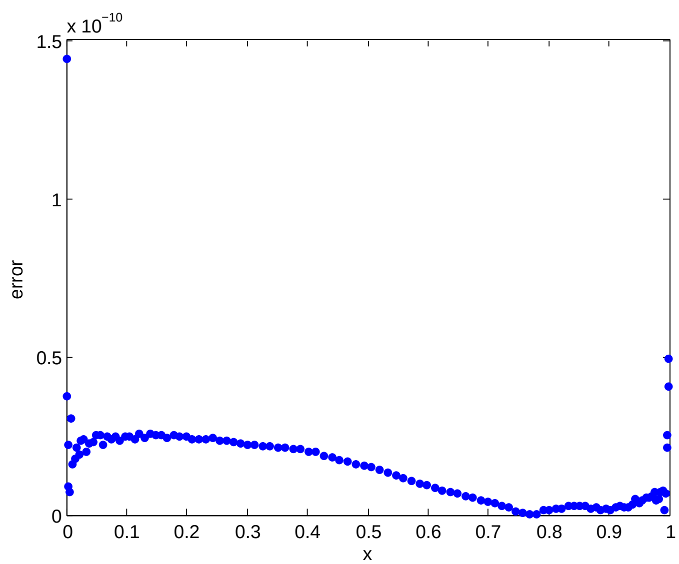

Figure 2.6: *Percentage relative error of exact solution and spectral methods using Chebyshev polynomials.*

x	ϕ (Collocation solution)	ϕ (Exact solution)	Percentage relative error
0.01405	0.001345526	0.001345526	1.779×10^{-11}
0.09705	0.009274349	0.009274349	2.462×10^{-11}
0.1681	0.01595629	0.01595629	2.455×10^{-11}
0.289	0.02672185	0.02672185	2.26×10^{-11}
0.4016	0.03529056	0.03529056	2.013×10^{-11}
0.6241	0.04349706	0.04349706	7.785×10^{-12}
0.8117	0.03409777	0.03409777	1.872×10^{-12}
0.9662	0.008398714	0.008398714	5.68×10^{-12}

Table 2.4: *Comparison of spectral solution and exact solution with relative percentage error.*

2.2 Darcy-Brinkman-Forchheimer Equation

The Darcy-Brinkman-Forchheimer Equation is

$$d^2u/dy^2 - s^2u - Fsu^2 + 1/M = 0, \qquad (2.2)$$

subject to the boundary conditions

$$u(-1) = 0, \;\; u(1) = 0.$$

was considered in [12]. In Eq.(2.2), s is the porous medium shape parameter, F is the Forchheimer number and M is the viscosity ratio. This is a steady state problem of flow through a horizontal channel which is filled with porous medium. This flow inside the channel is governed by the Darcy-Brinkman-Forchheimer momentum equation. Such flows are very important in many physical as well as industrial setting, for example, in the movement of ground water and crude oil through the porous rocky surface. This problem was previously solved analytically in [13] and numerically by asymptotic expansion methods in [14] and also by spectral homotopy analysis method (SHAM).

Since the domain of this problem is [-1,1], Chebyshev spectral collocation method should be the natural choice. First the `MATLAB` function *chebdif.m* in [10] computes the second-derivative matrix along with the chebyshev points and then boundary conditions are implemented. All that remains is to compute the solution of Eq.(2.2). `MATLAB` built-in function *fsolve* is used for this purpose. The values of s, F and M are taken to be same as in [12] for comparison. Passing all the information to the function *fsolve*, yields approximated solution $u(y_k)$, where y_k are the chebyshev nodes corresponding to the differentiation matrix D. The output of *fsolve* gives the result as a column vector, only at the interior nodes. The endpoints and the values at those points are to be enforced for solution on the required domain.

In [12] standard HAM approach is used to solve this model equation along with shooting method which is based on Runge-Kutta method of fourth order. For different values of s and $F = M = 1$, we will see the variation in velocity profiles and comparison between present method and results obtained using *bvp4c*. Figures 2.7-2.9 present the solution for $s = 0.5, 2$ and 5 and it can be observed that as the value of s increases the velocity profile decreases vertically. The efficiency of spectral collocation method for nonlinear boundary value problem can be seen in the graphs below.

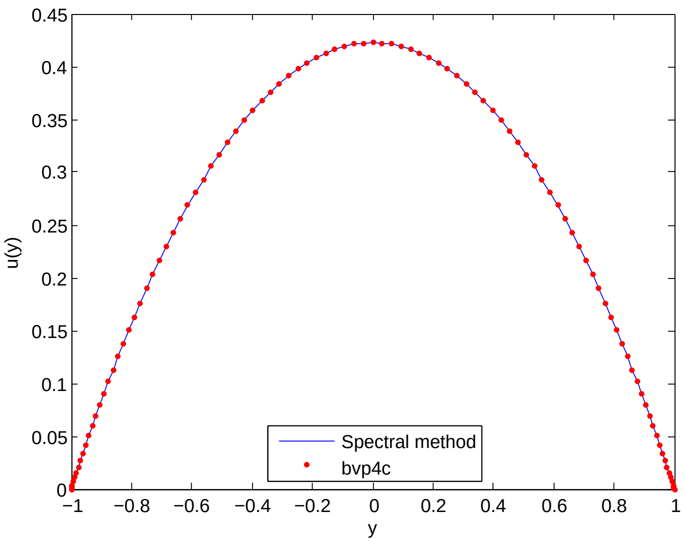

Figure 2.7: *Velocity profile for s=0.5 while F=M=1.*

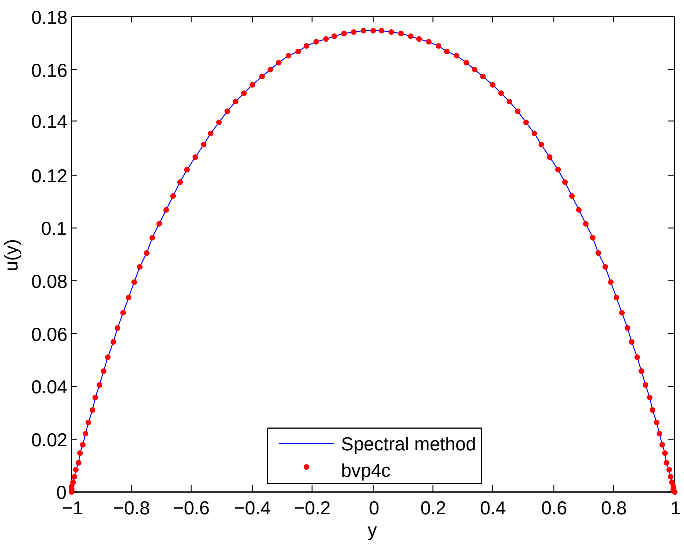

Figure 2.8: *Velocity profile for s=2 and F=M=1.*

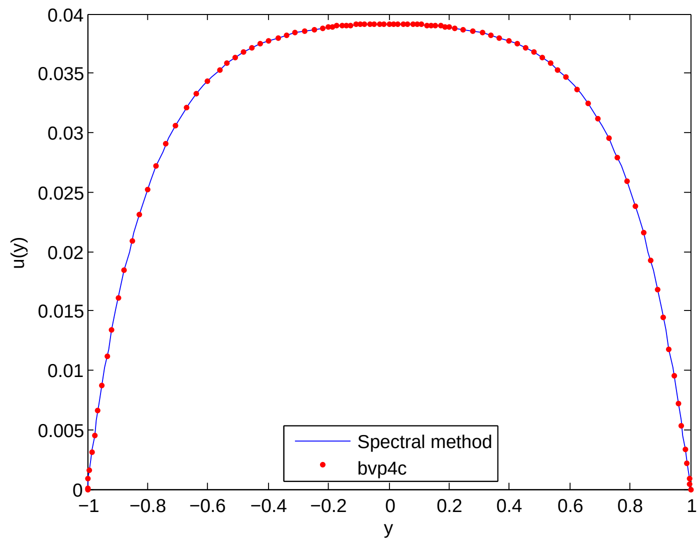

Figure 2.9: *Velocity profile for s=5 and F=M=1.*

For fixed values of s and M with variation in F, the results below in Figures 2.10-2.12 show that velocity profile again decreases with increase in Forchheimer number. However convergence with our numerical method can be observed when compared with *bvp4c*.

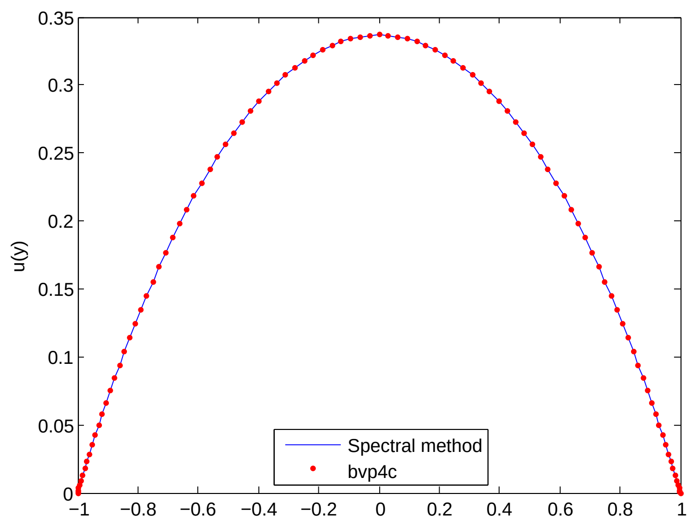

Figure 2.10: *Velocity profile for F=0.5 and s=M=1.*

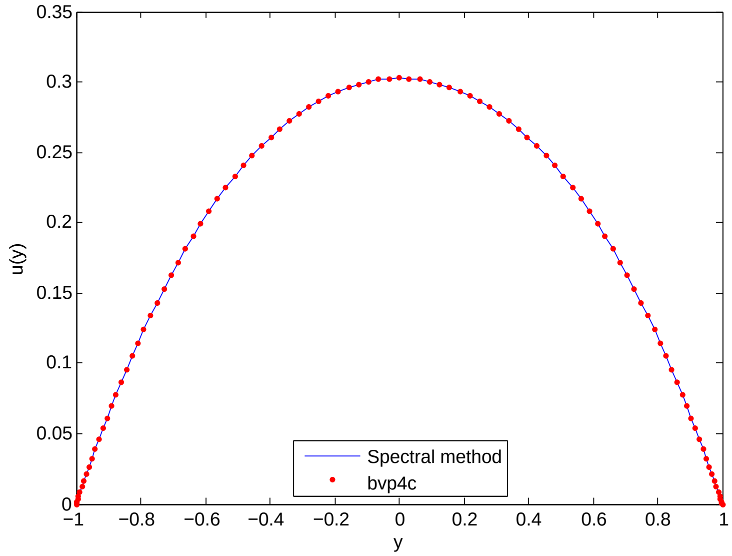

Figure 2.11: *Velocity profile for F=2 and s=M=1.*

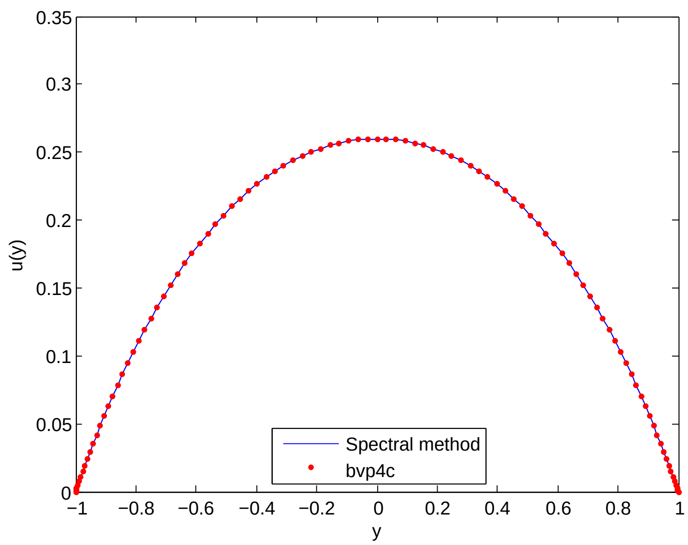

Figure 2.12: *Velocity Profile for F=5 and s=M=1.*

2.3 Falkner-Skan Equation

Considering a boundary layer flow of a steady and incompressible fluid due to a moving plate in viscous fluid. Boundary layer equations are given in Chapter 2 of [15], the simplified form of that gives following equation:

$$ff'' + 2f''' = 0, \qquad (2.3)$$

and the corresponding boundary conditions are

$$f = 0 \ \ on \ \ \eta = 0,$$

$$f' = 1 \ \ on \ \ \eta = 0,$$

$$f' \to 0 \ \ as \ \ \eta \to \infty.$$

This is a third order non-linear ODE with mixed type boundary conditions. Numerical solution of Eq.(2.3) was obtained using Keller-box method in [14]. Here the open-source software *Chebfun*[1] is used for the computation of third order derivative and boundary conditions. *Chebfun* is actually a collection of algorithms and a software system in `MATLAB`. It is an open-source software system which is easily available on internet. It works with Chebyshev polynomials but the choice of domain can be modified. The implementation of *Chebfun* is based on the fact that by using polynomial interpolation in Chebyshev points, smooth functions can be represented quite efficiently. *chebop* is a tool in *Chebfun* for solving differential equations with spectral collocation method. It contains domain, operator and boundary conditions,

[1] *Chebfun* is the name of an open-software system while *chebfun* is a command of that software.

defined according to the problem under consideration. For the solution of Eq.(2.3), *chebfun* and *chebop* are used.

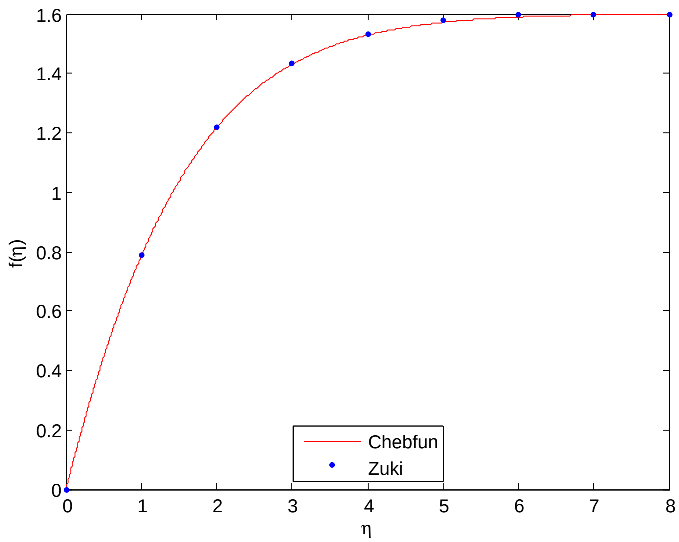

Figure 2.13: *Comparison of Chebfun and Zuki [15].*

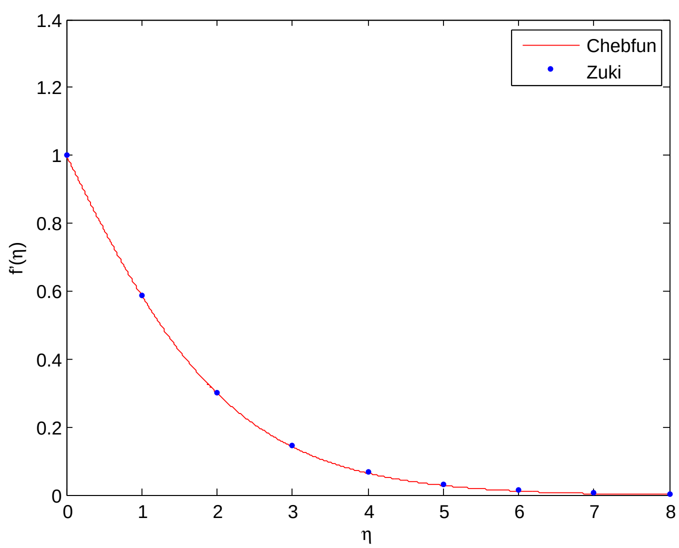

Figure 2.14: *Comparison of velocity profile $f'(\eta)$ of Chebfun and Zuki [15].*

The results obtained using spectral methods (by *chebfun*) is compared with results by [15] to validate the accuracy of spectral collocation method. Graph of $f(\eta)$ is plotted in Figure 2.13 whereas Figure 2.14 shows the velocity profile variation $f'(\eta)$.

Table 2.5 shows the values of $f(\eta)$, $f'(\eta)$ and $f''(\eta)$ for different values of η. The velocity gradient $f''(\eta)$ is plotted in Figure 2.15 and can be compared with the values of $f''(\eta)$ calculated using Keller-box method and Runge-Kutta method in [15].

η	f $(Chebfun)$	f (Zuki)	f' $(Chebfun)$	f' (Zuki)	f'' $(Chebfun)$	f'' (Zuki)
0	0	0	1.0000	1.0000	-0.4446	-0.4439
1.00	0.78581	0.78615	0.5864	0.5870	-0.3590	-0.3584
2.00	1.21711	1.21832	0.3005	0.3015	-0.2150	-0.2146
3.00	1.42973	1.43220	0.1423	0.1436	-0.1102	-0.1099
4.00	1.52814	1.53215	0.0642	0.0658	-0.0524	-0.0522
5.00	1.57169	1.57746	0.0276	0.0294	-0.0241	-0.0239
6.00	1.58988	1.59758	0.0109	0.0129	-0.0109	-0.0108
7.00	1.59655	1.60629	0.0034	0.0054	-0.0049	-0.0048
8.00	1.59802	1.60987	0.0000	0.0021	-0.0022	-0.0021

Table 2.5: *Comparison between Zuki and present method (Chebfun).*

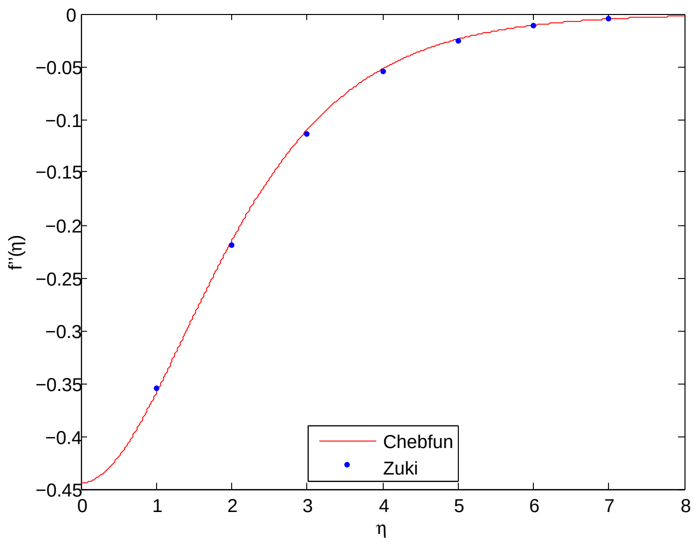

Figure 2.15: *Comparison of velocity gradient* $f''(\eta)$ *of Chebfun and Zuki [15].*

It can be observed that the results obtained using spectral method are quite good when compared with results of Zuki in [15].

2.4 Coupled ODEs

Now moving towards coupled nonlinear equation, concentrating on finding solution with spectral methods. The problem under consideration is a boundary layer flow due to a moving plate in a micropolar fluid. Simplified form of that problem is given in [15] is

$$\left.\begin{aligned} f''' + \tfrac{1}{2}' f f'' = 0, \\ g'' + \tfrac{1}{2}(gf' + fg') = 0, \end{aligned}\right\} \qquad (2.4)$$

and the corresponding boundary conditions are

$$f(0) = 0, \quad f'(0) = 1, \quad f'(\infty) = 0,$$

$$g(0) = -nf''(0), \quad g(\infty) = 0.$$

Keller-box method was used in [15] for solving the above given system of equations numerically. Here *chebfun* will be used for solution of Eq.(2.4). The domain of this problem is $[0, 6]$ so *chebop* is required for domains other than $[-1, 1]$. *chebfun* along with providing the information about differential equations and boundary conditions, solves the problem. It can be seen in figures below that with increase in values of n, $f(\eta)$ remains same. Figure 2.16 and Figure 2.17 displays results of f for $n = 0.2$ and $n = 0.8$.

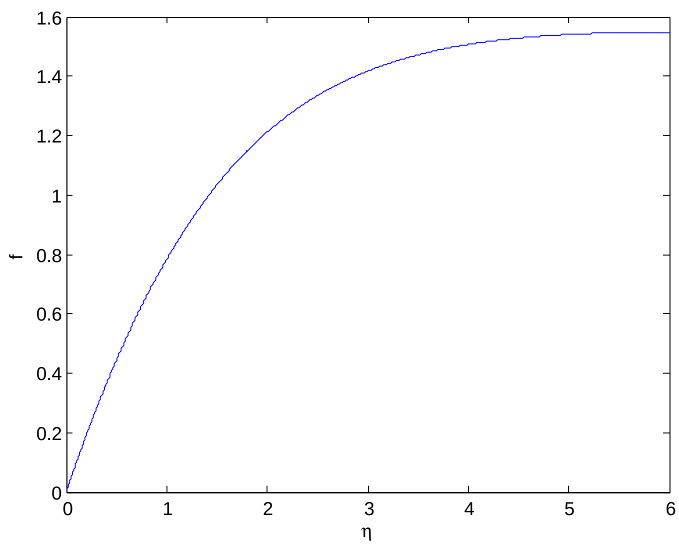

Figure 2.16: *Chebfun* solution of $f(\eta)$ for n=0.2

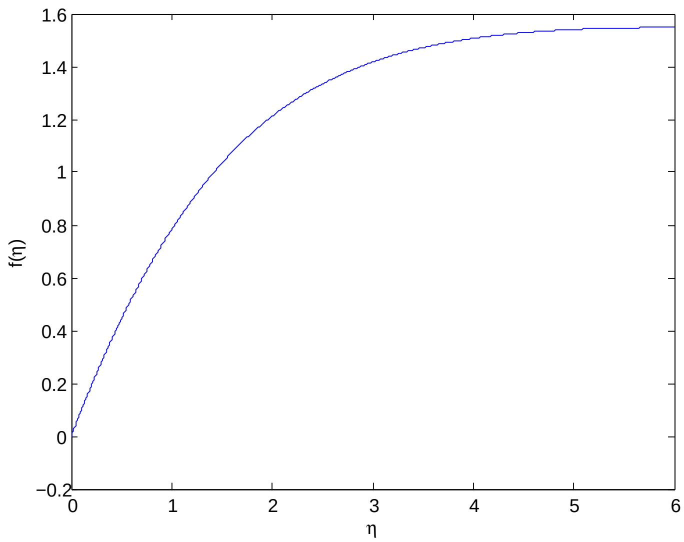

Figure 2.17: *Chebfun* solution of $f(\eta)$ for n=0.8

For $n = 0.8$ and $n = 0.2$ results of $g(\eta)$ are displayed below in Figure 2.18 and Figure 2.19.

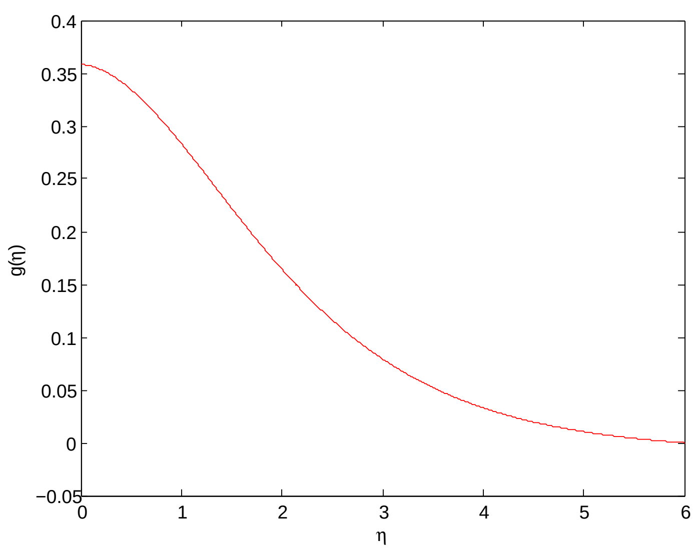

Figure 2.18: *Chebfun* solution of $g(\eta)$ for n=0.8

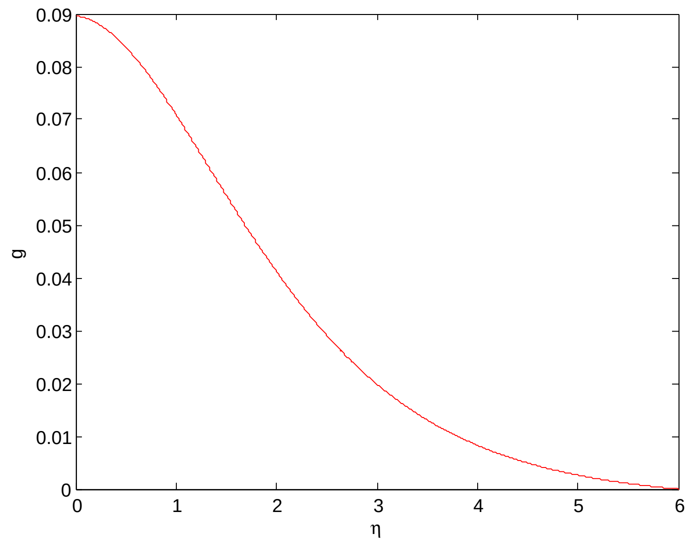

Figure 2.19: *Chebfun* solution of $g(\eta)$ for n=0.2

For any value of n, $g'(\eta)$ lies on the horizontal line. Figure 2.20 shows as n increases graph of $g(\eta)$ reduces getting close to horizontal axis.

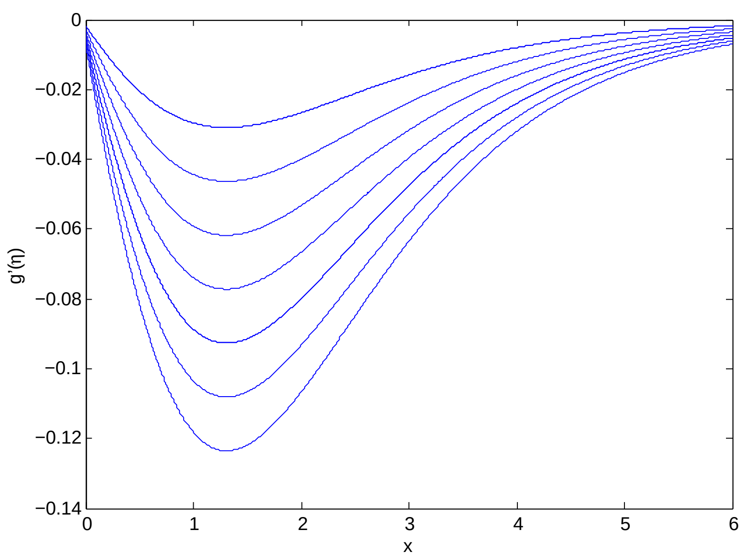

Figure 2.20: *Chebfun* solution of $g'(\eta)$ for x=0.2,0.3,0.4,0.5,0.6,,0.7 and 0.8

Chapter 3

Spectral Methods for PDEs

Partial differential equations describe many different phenomena like sound propagation, heat transfer and fluid flows. As compared to ordinary differential equations, partial differential equations are difficult to solve and require more attention in implementation. Although computationally, spectral methods for partial differential equations are less expensive than finite difference method but less accurate for problems with complex geometries due to Gibbs phenomena and Runge phenomena.

The procedure for solving PDEs is same as discussed for ODEs in previous chapter. Time derivative is also involved in these problems so extra work is needed to find accurate solution. For time stepping Runge-Kutta methods will be considered.

For partial differential equations with periodic boundary conditions spectral methods are very effective but far less potent for problems with non-periodic boundary conditions. Fourier and Chebyshev differencing methods are the most extensively used methods since the base functions used for interpolant expansion gives the most accurate solution.

The main feature here is to solve time-dependent partial differential equations on irregular domains using spectral collocation method and the main focus is on parabolic equations. Chebyshev spectral collocation method is most extensively used here for maximum accuracy due to its clustering property.

This chapter is organized as follows. In section 3.1 the solution of one dimensional heat equation is presented. Non-homogeneous heat equation in one dimensional is solved in section 3.2. Burger's equation is solved in section 3.3.

3.1 Heat Equation in 1D

Consider a uniform rod lying on x-axis from $x = 0$ to $x = \pi$ with insulated sides. The partial differential equation describing flow of heat energy in that rod and the temperature distribution on the domain $[0, \pi]$ is written as

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}, \tag{3.1}$$

with initial temperature distribution is

$$u(x, 0) = \sin(x),$$

and boundary condition given by

$$u(0, t) = u(\pi, t) = 0.$$

Here D is the thermal conductivity also called diffusion coefficient. Since domain is $[0, \pi]$ the natural idea must be Fourier method but here Chebyshev and Laguerre spectral collocation method is our choice, in order to see the accuracy both methods have shown here. To observe the spectral accuracy we take the exact solution for above mentioned heat equation, with $D = 1$, we have

$$u(x,t) = e^{-t}\sin(x).$$

The difference between solutions of this problem using both Laguerre and Chebyshev spectral collocation method can be seen. Laguerre spectral collocation method although enjoys spectral convergence rate but when compared to Chebyshev spectral method for a same problem, the actual error decay is considerably slow. The reason for slow error decay is mentioned in the above chapter but for detailed explanation refer [11] and [17]. Below are the results presenting the solutions of both methods and their comparison with exact solution.

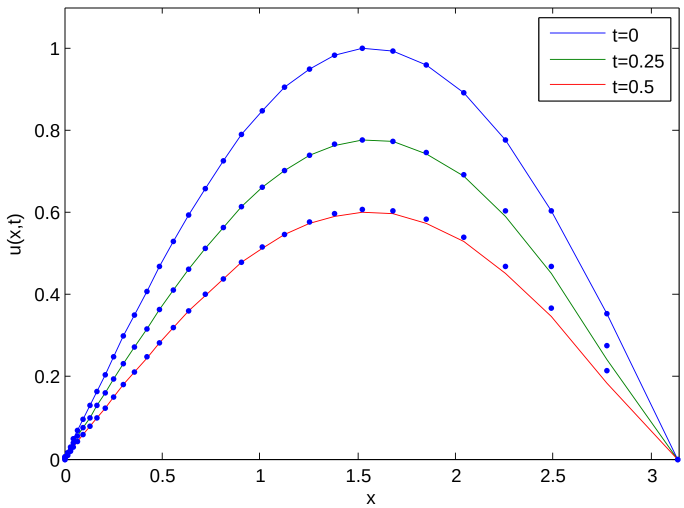

Figure 3.1: *Comparison of exact solution and spectral methods with Laguerre polynomials for t=0,0.25 and 0.5 (where '-' represents spectral solution and '.' represents exact solution).*

Figure 3.1 shows solution using Laguerre spectral method. Due to rescaling in Laguerre nodes from $[0, \infty]$ to $[0, \pi]$, nodes lack the clustering property at right end. This causes loss of accuracy when Laguerre polynomials are used. Table 3.1 displays comparison of exact solution and spectral solution giving different values of T along with absolute error.

η	Spectral solution	Exact solution	t	Absolute error
0.04842	0.04840143	0.04840143	0	0
0.2069	0.2053797	0.2053797	0	0
0.4861	0.4672037	0.4672037	0	0
0.9093	0.7890914	0.7890914	0	0
1.527	0.9990589	0.9990598	0	0
0.04842	0.03768597	0.03769507	0.25	9.109×10^{-6}
0.2069	0.1599629	0.1599499	0.25	1.302×10^{-5}
0.4861	0.3638213	0.3638586	0.25	3.729×10^{-5}
0.9093	0.6144969	0.614545	0.25	4.808×10^{-5}
1.527	0.7765793	0.7780686	0.25	1.489×10^{-3}
0.04842	0.0293189	0.02935695	0.5	3.805×10^{-5}
0.2069	0.1244387	0.1245691	0.5	1.303×10^{-4}
0.4861	0.2829318	0.2833734	0.5	4.416×10^{-4}
0.9093	0.477289	0.4786081	0.5	1.319×10^{-3}
1.527	0.600588	0.6059604	0.5	5.372×10^{-3}

Table 3.1: *Comparison between solution obtained using Laguerre spectral collocation method and exact solution.*

While with Chebyshev spectral method transformation of Eq.(3.1) gives the following PDE

$$\frac{\partial u}{\partial t} = \frac{4}{\pi^2}\frac{\partial^2 u}{\partial x^2},$$

and the initial and boundary conditions on domain $[-1, 1]$ will become

$$u(x, 0) = \sin \pi(\frac{x+1}{2}),$$

$$u(\pm 1, t) = 0.$$

After the whole process of calculation the domain is transformed back to $[0, \pi]$. The solution of Eq.(3.1) is plotted below along with its exact solution in Figure 3.2. Table 3.2 displays comparison of exact solution and spectral solution giving different values of T along with percentage relative error. It is clear that Chebyshev spectral method converges better than Laguerre spectral method even for partial differential equations.

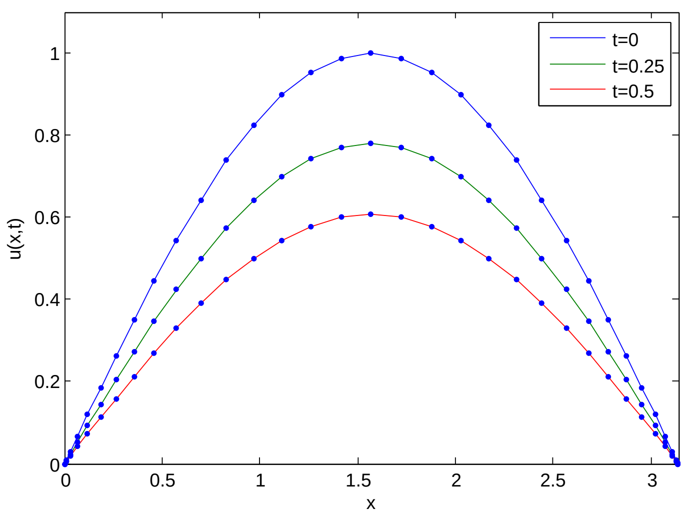

Figure 3.2: *Comparison of exact solution and spectral methods with Chebyshev polynomials for t=0,0.25 and 0.5 (where '-' represents spectral solution and '.' represents exact solution).*

η	Spectral solution	Exact solution	t	percentage relative error
0.1196	0.119285	0.119285	0	0
0.4601	0.4440158	0.4440158	0	0
0.9697	0.824704	0.824704	0	0
1.571	1	1	0	0
2.172	0.824704	0.824704	0	0
2.682	0.4440158	0.4440158	0	0
3.022	0.119285	0.119285	0	0
0.1196	0.09289906	0.09289928	0.25	2.437×10^{-4}
0.4601	0.345799	0.3457999	0.25	2.437×10^{-4}
0.9697	0.6422785	0.6422801	0.25	2.437×10^{-4}
1.571	0.77887989	0.7788008	0.25	2.437×10^{-4}
2.172	0.6422785	0.6422801	0.25	2.437×10^{-4}
2.682	0.345799	0.3457999	0.25	2.437×10^{-4}
3.022	0.09289906	0.9289928	0.25	2.437×10^{-4}
0.1196	0.07234986	0.07235003	0.5	2.388×10^{-4}
0.4601	0.2693086	0.2693092	0.5	2.388×10^{-4}
0.9697	0.5002071	0.5002083	0.5	2.388×10^{-4}
1.571	0.6065292	0.6065307	0.5	2.388×10^{-4}
2.172	0.5002071	0.5002083	0.5	2.388×10^{-4}
2.682	0.2693086	0.2693092	0.5	2.388×10^{-4}
3.022	0.07234986	0.07235003	0.5	2.388×10^{-4}

Table 3.2: *Comparison between exact solution and solution obtained using Chebyshev spectral collocation method.*

For the comparison between spectral methods and finite difference method we will consider the same Eq.(3.1) with different values of conductivity parameter D and the domain will be $[0, 1]$ and time $0 \leq t \leq 1$. For $D = 0.25$ and $D = 1$ the results are shown below. Both results are in good coordination as can be seen in mesh-plots given here using `MATLAB`'s *mesh* function. The mesh-plot proves the efficiency of present method.

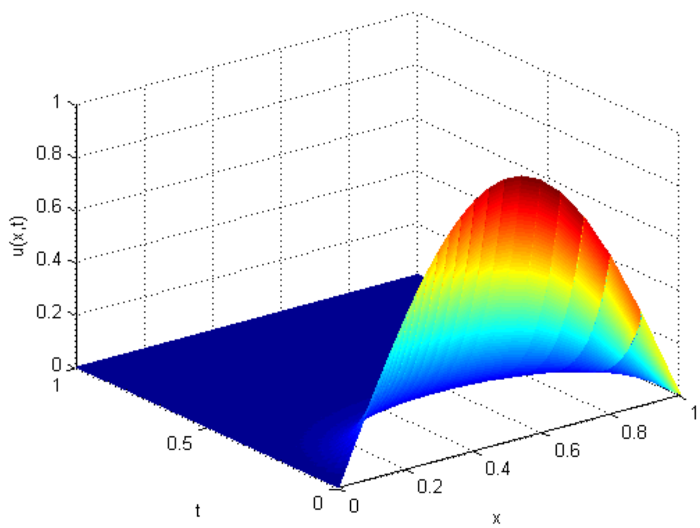

Figure 3.3: *Solution $u(x, t)$ using Laguerre spectral collocation method for $D = 0.25$.*

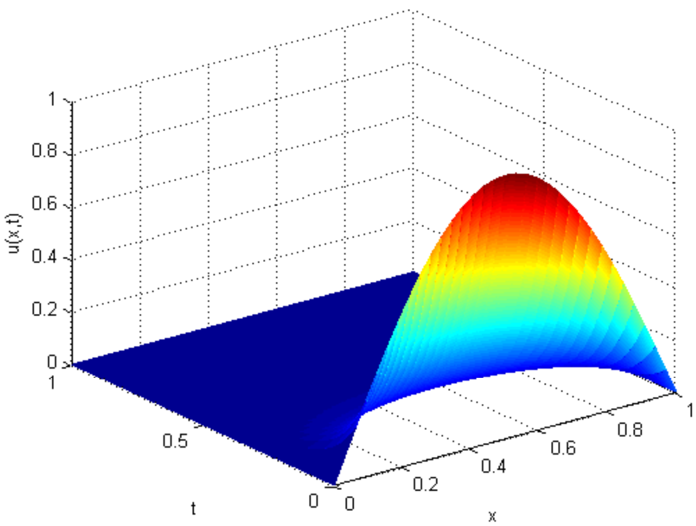

Figure 3.4: *Solution* $u(x,t)$ *using Finite difference method for* $D = 0.25$.

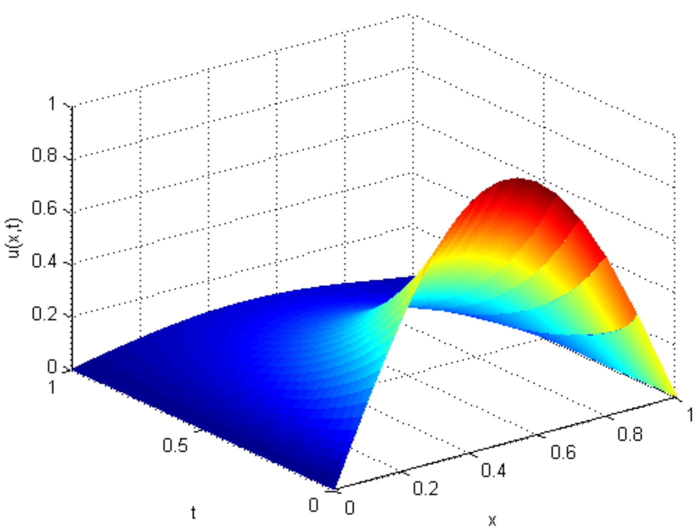

Figure 3.5: *Solution* $u(x,t)$ *using Laguerre spectral collocation method for* $D = 1$.

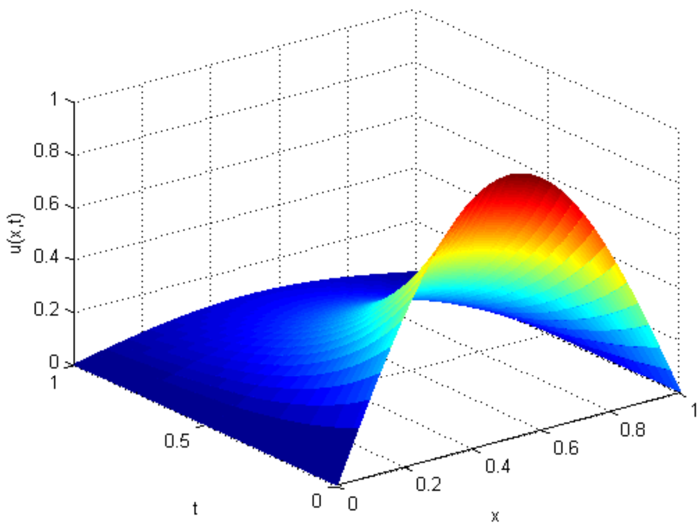

Figure 3.6: *Solution $u(x,t)$ using finite difference method for $D = 1$.*

3.2 Non-Homogeneous Heat Equation in 1D

For the examination of stability of our present numerical method, we will consider a non-homogeneous heat equation from [16], the equation is

$$\frac{\partial T}{\partial t} = 4\alpha \frac{\partial^2 T}{\partial x^2} + (\pi^2 - 1)e^{-t} \sin \pi (\frac{x+1}{2}), \qquad (3.2)$$

with initial and boundary conditions

$$T(-1,t) = T(1,t) = 0,$$

$$T(x,0) = \sin \pi (\frac{x+1}{2}).$$

Finite difference was used in [16] to solve the above problem but the domain for this equation was $[0, 1]$. `MATLAB` code was given in the end of [16] for clear understanding. We can make slight changes to convert the interval in the code to make it work for comparison on our required domain. Results show that the solution obtained using present method is in good agreement with solution computed using finite difference method.

We will use Chebyshev spectral collocation method since the domain is $[-1, 1]$ so no transformation is required. For the incorporation of boundary conditions, rows and columns of D are deleted *(first and last)*. Since we have second order derivative involved in the equation *cheb.m* from [8] can also be used instead of *chebdif.m* with equal efficiency for the computation of chebyshev nodes and differentiation matrix D. It will give first order D, for derivative of our required order we have to take the power of D accordingly.

The accuracy of our method depends highly on the choice of N, the size of differentiation matrix and the number of nodes. If N for current problem given by Eq.(3.2) is taken to be less than 20 the rate of accuracy decreases and difference occurs between results calculated using both spectral methods and finite difference method. On the other hand N could be taken as large as possible to increase the convergence rate. But it is not the case for every problem, sometimes increase in N decrease convergence, that is why selection of proper N is very crucial.

There are various ODE solvers as mentioned above but the right choice matters in time elapsed. Here to see the difference we considered *ode45* and *ode15s*. It was observed that for our problem former takes about 14 *seconds* while latter took only *one second*. Here $\alpha = 1$ and for different values of t results are displayed. Figure 3.7 displays the results obtained using spectral methods compared with finite difference method. It proves that our present method is in good agreement with results in [16].

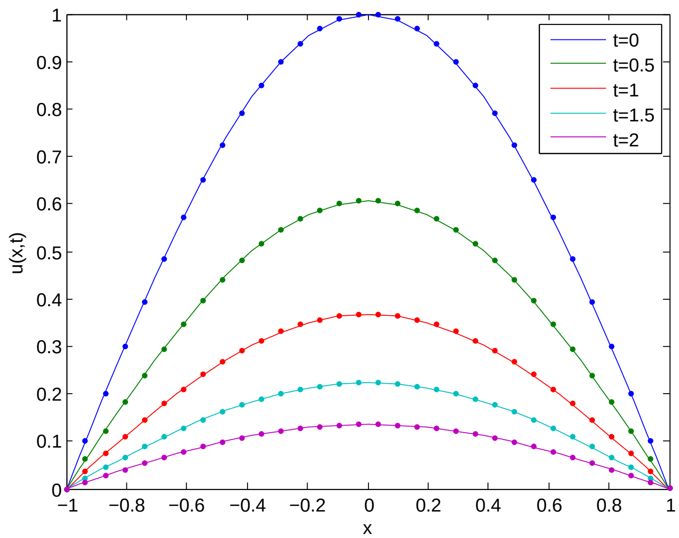

Figure 3.7: *Comparison of spectral method using Chebyshev polynomials and finite difference method for t=0,0.5,1,1.5,2. (where '-' represents the spectral solution and '.' represents the finite difference method.)*

3.3 Burger's Equation

The viscous Burger's equation is a non-linear partial differential equation with interesting application in astrophysics and fluid mechanics. It is an interesting task to solve this equation since common numerical method used for its solution is finite difference method and due to round-off error there is a huge loss of accuracy. Analytical methods for the solution of this problem are also very restricted.

Considering the one-dimensional Burger's equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \varepsilon\frac{\partial^2 u}{\partial x^2}, \qquad (3.3)$$

with boundary conditions

$$u(\pm 1, t) = 0,$$

and initial condition

$$u(x, 0) = -sin\pi x.$$

It is a simplified mathematical model for the motion of a viscous compressible gas. Here u is the speed of gas and ε is the kinematic viscosity and also time derivative is involved in our problem. For high viscosity pseudospectral method can solve the Burger's equation much more efficiently than other numerical methods.

The main idea is to use chebyshev differentiation matrix along with chebyshev collocation points excluding end points, as taken in above examples. Time stepping can be achieved using Runge-Kutta schemes. There are various ODE solvers in `MATLAB` with adaptive time-stepping selection mechanism, *ode45* works effectively for time stepping here. After all the computation, end nodes and deleted rows and columns of solution are included. The solution is displayed in figure below. Many numerical solutions fail for very small value of ε but pseudospectral method works quite efficiently.

The convergence of some problems are limited by Gibbs phenomenon, which are not quite suited for simulation. The most simplified way to understand Gibbs phenomenon is to think of oscillations near discontinuities. There are many factors for such a phenomenon, here in Eq.(3.3) it is because of the presence of shock waves appearing in our solution. The nonlinear factor in our problem creates shock waves. It can be observed below in Figure 3.8 that shock waves appear at $t = 2/\pi$ for $N = 200$. As N is increased the difference in solution curves can be observed in Figure 3.9. For $N = 800$ the results are better than before but still there are shock waves appearing in our solution. The kinematic velocity ε is taken to be $1/(300\pi)$.

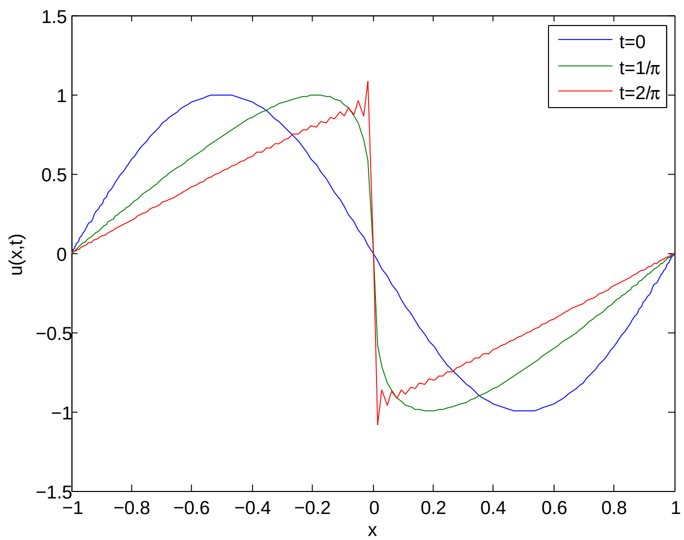

Figure 3.8: *Solution for Burger's equation for* $N = 200$ *with* $t = 0, 1/\pi$ *and* $2/\pi$.

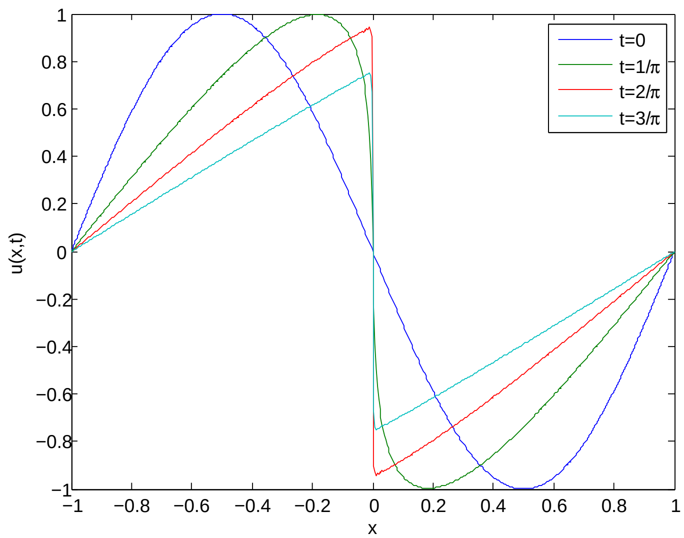

Figure 3.9: *Solution for Burger's equation for* $N = 800$ *with* $t = 0, 1/\pi$, $2/\pi$ *and* $3/\pi$.

Chapter 4

Conclusions and Outlook

This thesis has presented accuracy of solutions for several ODEs and PDEs by applying spectral methods. The problems were solved mostly using Chebyshev polynomials which gave us remarkable results with great efficiency.

In Chapter 2, it can clearly be observed that the results obtained using present method are very accurate. The tables are plotted for ODEs which show error of the order 10^{-12}. Also solutions computed through spectral method are compared with exact solutions to displays how well spectral methods works. In Chapter 3 the PDEs are solved and compared with finite difference method which again is in great agreement with each other.

This thesis has displayed a solid difference in results based on selection of polynomials (Chebyshev and Laguerre). The selection and implementation of different polynomials shows a great difference in accuracy. Throughout this thesis it is clear how Chebyshev spectral method proves to be better than Laguerre spectral method. Solutions using Chebyshev spectral collocation method are far better and close to exact solutions as compared to Laguerre spectral collocation method. Overall spectral collocation method proves to be superior than other numerical methods.

In future we can solve third order differential equations. In this thesis we present solution only in one dimension but this work can be extended for two dimension and comparison can be drawn.

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