

Higher Order Compact Exponential Scheme For Convection-Diffusion Equations

MA 7392 PROJECT REPORT

submitted by

ABHISHEK KUMAR JHA

M190687MA

under the guidance of

Dr. SURESH KUMAR NADUPURI

in partial fulfillment for the award of degree of

MASTER OF SCIENCE (MATHEMATICS)



DEPARTMENT OF MATHEMATICS

NATIONAL INSTITUTE OF TECHNOLOGY CALICUT

KOZHIKODE 673601

MAY, 2021

CERTIFICATE

This is to certify that the project work entitled **Higher Order Compact Exponential Scheme For Convection-Diffusion Equations** submitted by **Abhishek Kumar Jha** to the National Institute of Technology Calicut, in partial fulfillment for the award of degree of Master of Science (Mathematics) is a bonafide record of project work done by him under my supervision.

Dr. Suresh Kumar Nadupuri

Department of Mathematics
National Institute of Technology Calicut
Kozhikode, 673601, Kerala.

Dr. M S Sunitha

Head, Department of Mathematics
National Institute of Technology Calicut
Kozhikode, 673601, Kerala.

Place : NIT Calicut

Date : May 2021

ACKNOWLEDGEMENT

It gives me immense pleasure to express my sincere gratitude to people who helped me through the process of writing the work. I thank my project supervisor Dr. Suresh Kumar Nadupuri for guiding me from the start and always appreciating my work and motivating me throughout, having belief in me and my knowledge and providing invaluable help and support to bring out the best in me. I thank the PhD student Sobin Thomas, department of mathematics for helping me with proper and timely availability of required resources and being an obliging listener and auditor to my work.

I express my sincere thanks to Dr. M S Sunitha, Head of the Department of Mathematics, National Institute of Technology Calicut, for extending her support in the completion of this work.

I express my sincere gratitude to the Director, National Institute of Technology Calicut, for providing me the necessary facilities as and when required.

I thank my family and friends for being a constant support of pillar and encouragement during the whole time.

Abhishek Kumar Jha

ABSTRACT

The report contains the complete background knowledge of solving boundary value problems of non-homogeneous linear differential equations using Green's function and later on using this to develop a fourth-order exponential scheme for spatial variables to find the numerical solution of unsteady 1-D convection-diffusion initial boundary value problems. Green's function is used to solve non-homogeneous differential equations subject to specific boundary conditions. Using Green's functions, it is possible to solve Laplace's equation and Poisson's equation subject to boundary conditions. In this report we first focus on introduction to Green's function followed by stating the fundamental theorem of Green's function. Later we present the construction of Green's function using Heaviside step function whose derivative leads to Dirac delta function helping us to define a special function. Using some properties, finally we develop the Green's function. After this we consider boundary value problems of second order non-homogeneous linear differential equation and solve it using Green's function. Finally we focus on to the development of high order exponential numerical scheme for unsteady 1-D convection diffusion initial boundary value problems. The spatial discretization using the proposed fourth order scheme leads to a system of ODEs. For time integration, third order TVD Runge Kutta method is implemented. Finally we presented the accuracy of the numerical solution and the numerical order of convergence is attained.

Contents

ACKNOWLEDGEMENT	iii
ABSTRACT	iv
1 Introduction	2
2 Green's function	5
3 Construction of Green's function	6
4 Solving boundary value problems using Green's function	9
5 Development of fourth-order exponential scheme	11
6 TVD Runge-Kutta method	16
7 Numerical Solution	17
8 Conclusions	21
9 References	22
10 Appendix	23

1 Introduction

The convection-diffusion equation is a phenomena where particles, energy or other physical quantities are transferred inside a physical system due to two processes: diffusion and convection. Diffusion is the net movement of quantities (for example, atoms, ions, molecules, energy) from a region of higher concentration to a region of lower concentration. Diffusion is driven by a gradient in concentration. The concept of diffusion is widely used in many fields, including physics (particle diffusion), chemistry, biology, sociology, economics and finance. The central idea of diffusion is common to all of these: a substance or collection undergoing diffusion spreads out from a point or location at which there is a higher concentration of that substance or collection. A gradient is the change in the value of a quantity, for example, concentration, pressure, or temperature with the change in another variable, usually distance. A change in concentration over a distance is called a concentration gradient, a change in pressure over a distance is called a pressure gradient, and a change in temperature over a distance is called a temperature gradient. Convection is the transfer of heat due to the bulk movement of molecules within fluids (gases and liquids), including molten rock. In this project we consider the following unsteady 1D convection-diffusion equation which is represented as:

$$\frac{\partial v}{\partial t} + p \frac{dv}{dx} = a \frac{\partial^2 v}{\partial x^2}, \quad (x, t) \in (0, l) \times (0, T] \quad (1)$$

with initial condition

$$v(x, 0) = \xi(x), \quad x \in [0, l] \quad (2)$$

and Dirichlet boundary condition

$$v(0, t) = g_1, \quad v(l, t) = g_2, \quad t \in (0, T] \quad (3)$$

where $(0, T]$ is the time interval, ξ is given sufficient smooth function and $v(x, t)$ represents a scalar variable which is convected in the x -direction with constant velocity and is spread with constant diffusivity $a > 0$, and g_1 and g_2 are constants. The equation has various application in the real world such as thermal pollution in river system, water transfer in soil, mathematical physics, flow of porous media, heat transfer in draining films, particle deposition in the respiratory tract etc.

The principle of finite difference methods is well known numerical schemes used to solve ordinary as well as partial differential equations. It consists in approximating the differential operator by replacing the derivatives in the equation using differential quotients. The domain is partitioned in space and in time and approximations of the solution are computed at the space or time points. The finite difference approximations for derivatives are one of the simplest and of the oldest methods to solve differential equations. It was already known by L. Euler (1707-1783) in one dimension of space and was probably extended to dimension two by C. Runge (1856-1927). The advent of finite difference techniques in numerical applications began in the early 1950s and their development was stimulated by the emergence of computers that offered a convenient framework for dealing with complex problems of science and technology. Theoretical results have been obtained during the last five decades regarding the accuracy, stability and convergence of the finite difference method for partial differential equations. High-order compact finite difference schemes in which the value of the function and its first or higher derivatives are considered as unknowns at each discretization point are discussed in this article. High-order compact finite difference schemes have been extensively studied and widely used to compute the numerical solution of problems involving incompressible, compressible, and hypersonic flows. High-order compact finite difference schemes give high-order accuracy and better resolution characteristics as compared to classical finite difference schemes for the same number of grid points. There exist various approaches in the literature to derive compact finite difference schemes for derivative approximations[5]. Adam (1975) presented highly accurate difference schemes for the solution

of evolution equations of parabolic type. In that same year, Hirsh (1975) discussed higher order accurate solutions of fluid mechanics problems by a compact finite difference schemes. Two methods based on compact scheme are presented by Adam (1977) to eliminate the second-order derivatives in parabolic equations while keeping the fourth-order accuracy and the tridiagonal nature of the schemes. In Adam (1977), a high-order accurate additional boundary condition is also proposed, which is consistent with the high accuracy of the inner scheme. A fourth-order nonuniform combined compact finite difference scheme using truncated Taylor series is discussed by Geodheer and Potters (1985) and is used by them to solve a model transport problem in one dimension. Lele (1992) discussed various-order compact finite difference approximations for first and second derivatives. The main aim is to introduce a high-order exponential method for solving numerically the above equation.

The thesis is organised as follows. We start with introduction and in the next section we describe Green's function. In section 3, the construction of Green's function is presented in detail. In section 4, boundary value problems are solved using the Green's function. A fourth order exponential scheme for the unsteady 1-D convection-diffusion equation with boundary conditions is presented in section 5. A third order TVD Runge-Kutta method is briefly illustrated in section 6. The numerical results are presented in section 7 and conclusions are given in section 8.

2 Green's function

A second order non-homogeneous linear differential equation is written in the following form: $Ly(x) = f(x)$ defined on $x \in [a, b]$ with given boundary conditions. Here L is a second order linear operator. We will define Green's function eventually helping us in finding the solution for the given boundary value problems. Green's functions come in many disguises and are used in various field, so it can be difficult to see the unification of the Green's function concept. The original sense of the Green's function is a function of two variables that when acted up by a particular linear differential operator that acts on the first variable, produces the appropriate delta function which is zero when the variables are not equal. The main advantage is that Green's function is only dependent on the linear operator and is independent of the changing $f(x)$ function in different problems. The fundamental theorem of Green's function states that if a function $f(x)$ is continuous in the interval $[a, b]$, then the function given by

$$y(x) = \int_a^b G(x, \xi) f(\xi) d\xi,$$

is a solution of non-homogeneous linear differential equation of the form $Ly(x) = f(x)$ with given boundary conditions, where $a < \xi < b$ and $G(x, \xi)$ is Green's function defined as,

$$G(x, \xi) = \begin{cases} c_1 y_1(x) + c_2 y_2(x), & a < x < \xi \\ d_1 y_1(x) + d_2 y_2(x), & \xi < x < b. \end{cases}$$

The Green's function has the following properties:

Property 1: $G(x, \xi)$ is continuous at $x = \xi$.

Property 2: $\frac{\partial G}{\partial x}$ has a jump discontinuity of magnitude 1 at $x = \xi$.

3 Construction of Green's function

In this section we present the construction of the Green's function. Initially we state the Heaviside step function which will be differentiated which gives the Dirac delta function.

The Heaviside step function is defined as $H(x - a) = \begin{cases} 0, & x < a \\ 1, & x \geq a. \end{cases}$

At $x = a$ there is a jump discontinuity of magnitude 1.

Taking the derivative of the Heaviside function we get, $\frac{dH(x - a)}{dx} = \begin{cases} 0, & x \neq a \\ \infty, & x = a. \end{cases}$

The Dirac delta function is defined as $\delta(x - a) = \begin{cases} 0, & x \neq a \\ \infty, & x = a. \end{cases}$

$\Rightarrow \delta(x - a) = \frac{dH(x - a)}{dx}$ with a property $\int_{-\infty}^{\infty} \delta(x - a) dx = 1$.

In order to prove the above property consider a special function defined as

$$f(x, \epsilon) = \begin{cases} \frac{1}{2\epsilon}, & -\epsilon < x < \epsilon \\ 0, & \text{otherwise.} \end{cases}$$

Without loss of generality, take ϵ about $x = 0$.

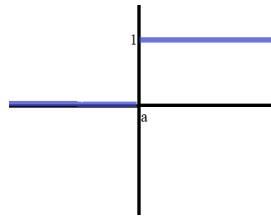


Figure 1.1 Graph of Heaviside step function.

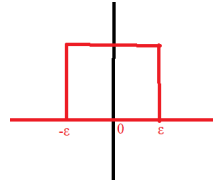


Figure 1.2 Graph of $f(x, \epsilon)$

The area under the graph of $f(x, \epsilon)$ from $-\epsilon$ to $\epsilon = \int_{-\epsilon}^{\epsilon} f(x, \epsilon) dx = \frac{1}{2\epsilon} [x]_{-\epsilon}^{\epsilon} = 1$.

$$\implies \int_{-\infty}^{\infty} f(x, \epsilon) dx = \int_{-\infty}^{-\epsilon} f(x, \epsilon) dx + \int_{-\epsilon}^{\epsilon} f(x, \epsilon) dx + \int_{\epsilon}^{\infty} f(x, \epsilon) dx = 1.$$

$$\implies \int_{-\infty}^{\infty} f(x, \epsilon) dx = 1.$$

As ϵ tends to 0 the function becomes unbounded. The value of ϵ is taken around $x = 0$.

$$\implies \lim_{\epsilon \rightarrow 0} f(x, \epsilon) = \begin{cases} 0, & x \neq 0 \\ \infty, & x = 0 \end{cases} = \delta(x - 0) = \delta(x). \quad 1.1$$

Taking limit on both sides of $\int_{-\infty}^{\infty} f(x, \epsilon) dx = 1$ we get,

$$\lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} f(x, \epsilon) dx = 1.$$

.

By Leibniz's Rule we get, $\int_{-\infty}^{\infty} \lim_{\epsilon \rightarrow 0} f(x, \epsilon) dx = 1$.

Using 1.1, we get $\int_{-\infty}^{\infty} \delta(x) dx = 1$ which leads to the required proof that is,

$$\int_{-\infty}^{\infty} \delta(x - a) dx = 1.$$

Now we define a function f as $f(x, \epsilon) = \begin{cases} \frac{g(x)}{2\epsilon}, & -\epsilon < x < \epsilon \\ 0, & \text{otherwise.} \end{cases}$

Integrating both sides from $-\epsilon$ to ϵ we get $\int_{-\epsilon}^{\epsilon} f(x, \epsilon) g(x) dx = \int_{-\epsilon}^{\epsilon} \frac{g(x)}{2\epsilon} dx$.

Since the interval is about $x = 0$, approximating $g(x)$ as $g(x = 0)$ we get,

$$\int_{-\epsilon}^{\epsilon} \frac{g(x)}{2\epsilon} dx = \int_{-\epsilon}^{\epsilon} \frac{g(x=0)}{2\epsilon} dx = g(0) \int_{-\epsilon}^{\epsilon} \frac{1}{2\epsilon} dx = g(0) \cdot 1 = g(0).$$

$$\implies \int_{-\epsilon}^{\epsilon} f(x, \epsilon) g(x) dx = g(0).$$

$$\implies \int_{-\infty}^{\infty} f(x, \epsilon) g(x) dx = g(0).$$

$$\implies \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} f(x, \epsilon) g(x) dx = \int_{-\infty}^{\infty} \lim_{\epsilon \rightarrow 0} f(x, \epsilon) g(x) dx,$$

$$= \int_{-\infty}^{\infty} \delta(x)g(x)dx = g(0). \quad [\text{Using 1.1}]$$

$$\implies \int_{-\infty}^{\infty} \delta(x-a)g(x)dx = g(a).$$

Over an interval $[a, b]$ we obtain,

$$\int_a^b \delta(x-a)g(x)dx = g(a).$$

Next we develop the Green's function $G(x, \xi)$ using the above derived results. We define a linear operator on Green's function given by,

$$LG(x, \xi) = \delta(x - \xi) = \begin{cases} 0, & x \neq \xi \\ \infty, & x = \xi. \end{cases} \quad 1.3$$

Where, $LG(x, \xi)$ is a linear operator on Green's function.

From fundamental theorem of Green's function we have, $y(x) = \int_a^b G(x, \xi) f(\xi) d\xi$ is a solution of the Linear differential equation $Ly(x) = f(x)$.

$$\text{We have } Ly(x) = L \int_a^b G(x, \xi) f(\xi) d\xi = \int_a^b LG(x, \xi) f(\xi) d\xi,$$

$$= \int_a^b \delta(x - \xi) f(\xi) d\xi = f(x). \quad [\text{Using 1.2}]$$

We get $Ly(x) = f(x)$, therefore it is evident that the above function $LG(x, \xi)$ is a leading path to the solution of the given differential equation $Ly(x) = f(x)$.

The case of $x \neq \xi$, $LG(x, \xi) = 0$ is equivalent to solving homogeneous differential equation of order 2. Let $y_1(x)$ and $y_2(x)$ be the two linearly independent solution of the given differential equation $Ly(x) = 0$. Then, $y_c(x) = c_1y_1(x) + c_2y_2(x)$ is the complementary function.

$$\implies G(x, \xi) = \begin{cases} c_1y_1(x) + c_2y_2(x), & a < x < \xi \\ d_1y_1(x) + d_2y_2(x), & \xi < x < b. \end{cases}$$

The constants c_1, d_1, c_2, d_2 are to be determined with help of the properties of Green's function mentioned below.

Property 1: $G(x, \xi)$ is continuous at $x = \xi$.

$$\implies c_1y_1(\xi) + c_2y_2(\xi) = d_1y_1(\xi) + d_2y_2(\xi),$$

$$\implies (c_1 - d_1)y_1(\xi) + (c_2 - d_2)y_2(\xi) = 0. \quad (4)$$

Property 2: $\frac{\partial G}{\partial x}$ has a jump discontinuity of magnitude 1 at $x = \xi$.

$$\begin{aligned} \implies \left[\frac{\partial G}{\partial x} \right]_{x < \xi}^{x > \xi} &= 1, \\ \implies (d_1 - c_1)y_1'(\xi) + (d_2 - c_2)y_2'(\xi) &= 1. \end{aligned} \quad (5)$$

(4) and (5) are two equations with four variables. In order to solve the given boundary value problem, two more equations are required. This will be provided by the boundary conditions. In the next section we deal with solving boundary value problems using Green's function.

4 Solving boundary value problems using Green's function

In this section, the solution of boundary value problems of second order non-homogeneous equation using Green's function are presented. We consider a second order non-homogeneous linear differential function defined as $y''(x) = f(x)$ with boundary conditions given by $y(0) = 0$, $y'(1) = 0$, $0 \leq x \leq 1$.

Using the equation 1.3 we get, $\frac{d^2 G(x, \xi)}{dx^2} = \delta(x - \xi) = 0$, $x \neq \xi$.

$$\implies G(0, \xi) = 0, G_x(1, \xi) = 0.$$

Solving the homogeneous equation $y''(x) = 0$, we get the complementary solution as $y(x) = c_1x + d_1$.

$$\implies G(x, \xi) = \begin{cases} c_1x + d_1, & x < \xi \\ c_2x + d_2, & x > \xi. \end{cases}$$

Using the Property 1 we get, $c_1\xi + d_1 = c_2\xi + d_2$,

$$\implies (c_1 - c_2)\xi + (d_1 - d_2) = 0.$$

Apply the boundary condition we get,

$$G(0, \xi) = c_1 \cdot 0 + d_1 = 0,$$

$$G_x(1, \xi) = c_2 = 0.$$

$$\implies G(x, \xi) = \begin{cases} c_1 x, & x < \xi \\ d_2, & x > \xi. \end{cases}$$

Also, $c_1 \xi = d_2$.

Using the property 2 we get, $\left[\frac{\partial G}{\partial x} \right]_{x < \xi}^{x > \xi} = 1$.

$\implies 0 - c_1 = 1$, i.e. $c_1 = -1$ and $d_1 = -\xi$.

$$\implies G(x, \xi) = \begin{cases} -x, & x < \xi \\ -\xi, & x > \xi. \end{cases}$$

From the fundamental theorem of Green's function we have, $y(x) = \int_a^b G(x, \xi) f(\xi) d\xi$

which is the solution of the given boundary value problem.

Case 1 Consider $f(x) = x^2$

$$\implies y(x) = \int_0^x G(x, \xi) \xi^2 d\xi + \int_x^1 G(x, \xi) \xi^2 d\xi$$

$$\implies y(x) = \int_0^x -\xi \xi^2 d\xi + \int_x^1 -x \xi^2 d\xi$$

$$\implies y(x) = - \left[\frac{\xi^4}{4} \right]_0^x - x \left[\frac{\xi^3}{3} \right]_x^1 = \frac{x^4}{12} - \frac{x}{3}.$$

Case 2 Consider $f(x) = e^x$

$$\implies y(x) = \int_0^x G(x, \xi) \xi^2 d\xi + \int_x^1 G(x, \xi) \xi^2 d\xi$$

$$\implies y(x) = \int_0^x -\xi e^\xi d\xi + \int_x^1 -x e^\xi d\xi$$

$$\implies y(x) = - [e^\xi \xi - e^\xi]_0^x - x [e^\xi]_x^1 = e^x - ex - 1.$$

In the next section, development of fourth-order exponential scheme will be obtained where Green's function plays a major role in obtaining the solution of differential equation associated with convection diffusion equation.

5 Development of fourth-order exponential scheme

In this section we focus on the development of a higher-order exponential compact scheme for solving one dimensional convection diffusion equation with initial and boundary conditions. Consider the following unsteady 1D convection-diffusion equation which is represented as:

$$\frac{\partial v}{\partial t} + p \frac{dv}{dx} = a \frac{\partial^2 v}{\partial x^2}, \quad (x, t) \in (0, l) \times (0, T]$$

with initial condition

$$v(x, 0) = \xi(x), \quad x \in [0, l]$$

and Dirichlet boundary condition

$$v(0, t) = g_1, \quad v(l, t) = g_2, \quad t \in (0, T]$$

where $(0, T]$ is the time interval, ξ is given sufficient smooth function and $v(x, t)$ represents a scalar variable which is convected in the x -direction with constant velocity and is spread with constant diffusivity $a > 0$, and g_1 and g_2 are constants. we start with considering a steady 1D convection-diffusion equation

$$-av_{xx} + pv_x = f, \quad (6)$$

where a is the positive constant conductivity, p is the constant convective velocity and f is a sufficiently smooth function of x . To formulate high-order compact schemes, we first consider the following two-point boundary value problem in the subdomain $[x_{i-1}, x_{i+1}]$, $(i = 1, 2, 3, \dots, n-1)$

$$\begin{cases} -av_{xx} + pv_x = f, & x_{i-1} < x < x_{i+1} \\ v(x_{i-1}) = v_{i-1}, & v(x_{i+1}) = v_{i+1}. \end{cases} \quad (7)$$

Using Green's function method described in previous section, we obtain the solution of problem (7) as

$$v(x) = \xi_1(x) v_{i-1} + \xi_2(x) v_{i+1} + \int_{x_{i-1}}^{x_{i+1}} G(x, \eta) f(\eta) d\eta,$$

where the functions $\xi_1(x)$ and $\xi_2(x)$ are the solutions of the following problems respectively,

$$\begin{cases} -a\xi_{xx} + p\xi_x = 0, & x_{i-1} < x < x_{i+1} \\ \xi(x_{i-1}) = 1, \quad \xi(x_{i+1}) = 0. \end{cases} \quad (8)$$

and

$$\begin{cases} -a\xi_{xx} + p\xi_x = 0, & x_{i-1} < x < x_{i+1} \\ \xi(x_{i-1}) = 0, \quad \xi(x_{i+1}) = 1. \end{cases} \quad (9)$$

$\xi_1(x)$, $\xi_2(x)$ and $G(x, \eta)$ are to be determined. Characteristic equation of equation (9) is $-am^2 + pm = 0$. The roots of the equation are $m = 0$, $m = -\frac{p}{a}$. The general solution of (4) is given as:

$$\xi_1(x) = c_1 + c_2 e^{\frac{px}{a}}$$

Applying the boundary conditions of equation (8), we get

$$1 = c_1 + c_2 e^{\frac{p(x_{i-1})}{a}},$$

$$0 = c_1 + c_2 e^{\frac{p(x_{i+1})}{a}}.$$

Solving the above two equations, we obtain

$$\begin{aligned} c_1 &= \frac{e^{\frac{p(x_{i+1})}{a}}}{e^{\frac{p(x_{i+1})}{a}} - e^{\frac{p(x_{i-1})}{a}}} \text{ and } c_2 = \frac{-1}{e^{\frac{p(x_{i+1})}{a}} - e^{\frac{p(x_{i-1})}{a}}} \\ \implies \xi_1(x) &= c_1 + c_2 e^{\frac{px}{a}} = \frac{e^{\frac{p(x_{i+1})}{a}}}{e^{\frac{p(x_{i+1})}{a}} - e^{\frac{p(x_{i-1})}{a}}} - \frac{e^{\frac{px}{a}}}{e^{\frac{p(x_{i+1})}{a}} - e^{\frac{p(x_{i-1})}{a}}}. \\ \implies \xi_1(x) &= \frac{e^{\frac{p(x_{i+1})}{a}} - e^{\frac{px}{a}}}{e^{\frac{p(x_{i+1})}{a}} - e^{\frac{p(x_{i-1})}{a}}} = \frac{1 - e^{\frac{p}{a}(x-x_{i+1})}}{1 - e^{\frac{p}{a}(x_{i-1}-x_{i+1})}} = \frac{1 - e^{\frac{p}{a}(x-x_{i+1})}}{1 - e^{-\frac{2p}{a}h_x}}. \end{aligned}$$

Similarly the solution of the BVP (9) is obtained as

$$\xi_2(x) = \frac{e^{\frac{p}{a}(x-x_{i-1})} - 1}{e^{\frac{2p}{a}h_x} - 1}.$$

The Green's function $G(x, \eta)$ of the following BVP

$$\begin{cases} -av_{xx} + pv_x = 0, & x_{i-1} < x < x_{i+1} \\ u(x_{i-1}) = 0, & u(x_{i+1}) = 0 \end{cases}$$

can be expressed as

$$G(x, \eta) = \frac{1}{W(\eta)} \begin{cases} \xi_1(x) \xi_2(\eta), & x_{i-1} \leq \eta < x \\ \xi_1(\eta) \xi_2(x), & x \leq \eta \leq x_{i+1}, \end{cases}$$

where $W(\eta)$ is obtained as $W(\eta) = \frac{p}{a} \frac{e^{\frac{p}{a}(\eta-x_i)}}{e^{\frac{p}{a}h_x} - e^{-\frac{p}{a}h_x}}$ using Abel's formula in given differential equation. Therefore, the solution is given as:

$$v_i(x) = \xi_1(x) v_{i-1} + \xi_2(x) v_{i+1} + \int_{x_{i-1}}^{x_{i+1}} G(x_i, \eta) f(\eta) d\eta.$$

Consider the case of homogeneous 1D convection-diffusion equation.

The solution of the equation is:

$$v_i(x) = \xi_1(x) v_{i-1} + \xi_2(x) v_{i+1}.$$

$$\text{Using } \xi_1(x) = \frac{1 - e^{-\frac{ph_x}{a}}}{1 - e^{-\frac{2ph_x}{a}}}, \quad \xi_2(x) = \frac{e^{\frac{ph_x}{a}} - 1}{e^{\frac{2ph_x}{a}} - 1}.$$

$$\implies v_i = \frac{1 - e^{-\frac{ph_x}{a}}}{1 - e^{-\frac{2ph_x}{a}}} v_{i-1} + \frac{e^{\frac{ph_x}{a}} - 1}{e^{\frac{2ph_x}{a}} - 1} v_{i+1}.$$

$$\implies v_i = \frac{e^{\frac{ph_x}{a}} - 1}{e^{\frac{ph_x}{a}} - e^{-\frac{ph_x}{a}}} v_{i-1} + \frac{1 - e^{-\frac{ph_x}{a}}}{e^{\frac{ph_x}{a}} - e^{-\frac{ph_x}{a}}} v_{i+1}.$$

Let us take $\frac{ph_x}{a} = 2\beta$, then

$$v_i = \frac{e^{2\beta} - 1}{e^{2\beta} - e^{-2\beta}} v_{i-1} + \frac{1 - e^{-2\beta}}{e^{2\beta} - e^{-2\beta}} v_{i+1}.$$

$$\implies v_i = \frac{e^\beta (e^\beta - e^{-\beta})}{(e^\beta - e^{-\beta})(e^\beta + e^{-\beta})} v_{i-1} + \frac{e^{-\beta} (e^\beta - e^{-\beta})}{(e^\beta - e^{-\beta})(e^\beta + e^{-\beta})} v_{i+1}.$$

$$\implies \frac{(e^\beta + e^{-\beta})}{(e^\beta - e^{-\beta})} v_i = \frac{e^\beta}{(e^\beta - e^{-\beta})} v_{i-1} + \frac{e^{-\beta}}{(e^\beta - e^{-\beta})} v_{i+1}.$$

$$\implies \frac{2(e^\beta + e^{-\beta})}{(e^\beta - e^{-\beta})} v_i = \frac{2e^\beta}{(e^\beta - e^{-\beta})} v_{i-1} + \frac{2e^{-\beta}}{(e^\beta - e^{-\beta})} v_{i+1}.$$

Using $\coth(\beta) = \frac{(e^\beta + e^{-\beta})}{(e^\beta - e^{-\beta})}$, $1 + \coth(\beta) = \frac{2e^\beta}{(e^\beta - e^{-\beta})}$, $\coth(\beta) - 1 = \frac{2e^{-\beta}}{(e^\beta - e^{-\beta})}$, we get the following,

$$2 \coth(\beta) v_i = (1 + \coth(\beta)) v_{i-1} + (\coth(\beta) - 1) v_{i+1}.$$

$$\implies -\coth(\beta) (v_{i+1} - 2v_i + v_{i-1}) + v_{i+1} - v_{i-1} = 0.$$

$$\implies -h_x^2 \coth(\beta) \left(\frac{v_{i+1} - 2v_i + v_{i-1}}{h_x^2} \right) + 2h_x \frac{v_{i+1} - v_{i-1}}{2h_x} = 0.$$

The above equation can be expressed as:

$$-h_x^2 \coth(\beta) \delta_x^2 v_i + 2h_x \delta_x v_i = 0,$$

where $\frac{v_{i+1} - 2v_i + v_{i-1}}{h_x^2} = \delta_x^2 v_i$, $\frac{v_{i+1} - v_{i-1}}{2h_x} = \delta_x v_i$ are the standard central difference operators. Multiplying by $\frac{p}{2h_x}$, we get

$$-\frac{ph_x}{2} \coth(\beta) \delta_x^2 v_i + p \delta_x v_i = 0.$$

Substitute back $\beta = \frac{ph_x}{2a}$ and taking $\alpha = \frac{ph_x}{2} \coth\left(\frac{ph_x}{2a}\right)$, we get

$$-\alpha \delta_x^2 v_i + p \delta_x v_i = 0.$$

We now consider the non-homogeneous equation:

$$-\alpha \delta_x^2 v_i + p \delta_x v_i = f(x).$$

The function $f(x)$ is approximated using the expansion, $f(x) = f_i + \alpha_1 f_{xi} + \alpha_2 f_{xxi} + O(h_x^3)$.

It can also be approximated using parabolic interpolation method. Therefore we get,

$$-\alpha \delta_x^2 v_i + p \delta_x v_i = f_i + \alpha_1 f_{xi} + \alpha_2 f_{xxi} + O(h_x^3) \quad (10)$$

Using the equation (6) in (10) gives,

$$\begin{aligned} -\alpha \delta_x^2 v_i + p \delta_x v_i &= (-av_{xx} + pv_x)_i + \alpha_1 (-av_{xx} + pv_x)_{xi} + \alpha_2 (-av_{xx} + pv_x)_{xxi}. \\ -\alpha \delta_x^2 v_i + p \delta_x v_i &= -av_{xxi} + pv_{xi} - \alpha_1 av_{xxxi} + \alpha_1 pv_{xxi} - \alpha_2 av_{xxxixi} + \alpha_2 pv_{xxxixi}. \end{aligned}$$

Hence we get,

$$-\alpha \delta_x^2 v_i + p \delta_x v_i + av_{xxi} - pv_{xi} + \alpha_1 av_{xxxi} - \alpha_1 pv_{xxi} + \alpha_2 av_{xxxixi} - \alpha_2 pv_{xxxixi} = 0. \quad (11)$$

Consider the Taylor series expansion about the point v_i ,

$$\begin{aligned} v_{i-1} &= v_i - h_x v_{xi} + \frac{1}{2} h_x^2 v_{xxi} - \frac{1}{6} h_x^3 v_{xxxixi} + O(h_x^4). \\ v_{i+1} &= v_i + h_x v_{xi} + \frac{1}{2} h_x^2 v_{xxi} + \frac{1}{6} h_x^3 v_{xxxixi} + O(h_x^4). \end{aligned}$$

We write the following operators as:

$$\begin{cases} \delta_x v_i = \frac{v_{i+1} - v_{i-1}}{2h_x} = v_{xi} + \frac{h_x^2}{6} v_{xxxixi}, \\ \delta_x^2 v_i = \frac{v_{i+1} - 2v_i + v_{i-1}}{h_x^2} = v_{xxi} + \frac{O(h_x^4)}{h_x^2}. \end{cases} \quad (12)$$

Using the equations (11) and (12),

$$-\alpha v_{xxi} + p v_{xi} + \frac{p h_x^2}{6} v_{xxxi} + a v_{xxi} - p v_{xi} + \alpha_1 a v_{xxxi} - \alpha_1 p v_{xxi} + \alpha_2 a v_{xxxxi} - \alpha_2 p v_{xxxi} = 0.$$

We get $-\alpha + a - p\alpha_1 = 0$ and $\frac{p h_x^2}{6} - \alpha_2 p + \alpha_1 a = 0$.

Simplifying we obtain $\alpha_1 = \frac{a - \alpha}{p}$ and $\alpha_2 = \frac{a(a - \alpha)}{p^2} + \frac{h_x^2}{6}$.

Omitting the truncation error $O(h_x^4)$, we obtain the following three-point fourth order compact finite difference formulation for equation (6).

$$-\alpha \delta_x^2 v_i + p \delta_x v_i = f_i + \alpha_1 f_{xi} + \alpha_2 f_{xxi},$$

which can be given by

$$(-\alpha \delta_x^2 + p \delta_x) v_i = (1 + \alpha_1 \delta_x + \alpha_2 \delta_x^2) f_i. \quad (13)$$

Replacing f in (13) by $-\frac{\partial v}{\partial t}$ we get

$$(-\alpha \delta_x^2 + p \delta_x) v_i^n = (1 + \alpha_1 \delta_x + \alpha_2 \delta_x^2) \left(-\frac{\partial v}{\partial t} \right)_i^n. \quad (14)$$

Using (12) and (14), equation (13) can be written as

$$\begin{aligned} & \left(\frac{\alpha_2}{h_x^2} - \frac{\alpha_1}{2h_x} \right) \left(\frac{\partial v}{\partial t} \right)_{i-1}^n + \left(1 - \frac{2\alpha_2}{h_x^2} \right) \left(\frac{\partial v}{\partial t} \right)_i^n + \left(\frac{\alpha_2}{h_x^2} + \frac{\alpha_1}{2h_x} \right) \left(\frac{\partial v}{\partial t} \right)_{i+1}^n \\ & = \left(\frac{\alpha}{h_x^2} + \frac{p}{2h_x} \right) v_{i-1}^n - \frac{2\alpha}{h_x^2} v_i^n + \left(\frac{\alpha}{h_x^2} - \frac{p}{2h_x} \right) v_{i+1}^n, \end{aligned} \quad (15)$$

for $i = 1, 2, \dots, N-1$. Here $i = 0$ and $i = N$ are boundary nodes. Taking the time level $t = n\Delta t$ and applying (15) with (2) and (3) leads to a system of first order differential equations given by

$$\begin{cases} P \frac{dV(t)}{dt} = QV(t) + g, \\ V(0) = \xi_0 \end{cases} \quad (16)$$

where $V(t) = [v_1(t), v_2(t), \dots, v_{N-2}(t), v_{N-1}(t)]^T$, $\xi_0 = [\xi_1, \xi_2, \dots, \xi_{N-2}, \xi_{N-1}]^T$ and $g = \left[\left(\frac{\alpha}{h_x^2} + \frac{p}{2h_x} \right) g_1, 0, \dots, 0, \left(\frac{\alpha}{h_x^2} - \frac{p}{2h_x} \right) g_2 \right]^T$.

In (16) the matrix P and Q of order $N - 1$ are given by

$$P = \begin{pmatrix} 1 - \frac{2\alpha_2}{h_x^2} & \frac{\alpha_2}{h_x^2} + \frac{\alpha_1}{2h_x} & 0 & \dots & 0 & 0 \\ \frac{\alpha_2}{h_x^2} - \frac{\alpha_1}{2h_x} & 1 - \frac{2\alpha_2}{h_x^2} & \frac{\alpha_2}{h_x^2} + \frac{\alpha_1}{2h_x} & 0 & \dots & 0 \\ 0 & \frac{\alpha_2}{h_x^2} - \frac{\alpha_1}{2h_x} & 1 - \frac{2\alpha_2}{h_x^2} & \frac{\alpha_2}{h_x^2} + \frac{\alpha_1}{2h_x} & 0 & \dots \\ \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ \dots & 0 & \frac{\alpha_2}{h_x^2} - \frac{\alpha_1}{2h_x} & 1 - \frac{2\alpha_2}{h_x^2} & \frac{\alpha_2}{h_x^2} + \frac{\alpha_1}{2h_x} & 0 \\ 0 & \dots & 0 & \frac{\alpha_2}{h_x^2} - \frac{\alpha_1}{2h_x} & 1 - \frac{2\alpha_2}{h_x^2} & \frac{\alpha_2}{h_x^2} + \frac{\alpha_1}{2h_x} \\ 0 & 0 & \dots & 0 & \frac{\alpha_2}{h_x^2} - \frac{\alpha_1}{2h_x} & 1 - \frac{2\alpha_2}{h_x^2} \end{pmatrix}$$

$$Q = \begin{pmatrix} -\frac{2\alpha}{h_x^2} & \frac{\alpha}{h_x^2} - \frac{p}{2h_x} & 0 & \dots & 0 & 0 \\ \frac{\alpha}{h_x^2} + \frac{p}{2h_x} & -\frac{2\alpha}{h_x^2} & \frac{\alpha}{h_x^2} - \frac{p}{2h_x} & 0 & \dots & 0 \\ 0 & \frac{\alpha}{h_x^2} + \frac{p}{2h_x} & -\frac{2\alpha}{h_x^2} & \frac{\alpha}{h_x^2} - \frac{p}{2h_x} & 0 & \dots \\ \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ \dots & 0 & \frac{\alpha}{h_x^2} + \frac{p}{2h_x} & -\frac{2\alpha}{h_x^2} & \frac{\alpha}{h_x^2} - \frac{p}{2h_x} & 0 \\ 0 & \dots & 0 & \frac{\alpha}{h_x^2} + \frac{p}{2h_x} & -\frac{2\alpha}{h_x^2} & \frac{\alpha}{h_x^2} - \frac{p}{2h_x} \\ 0 & 0 & \dots & 0 & \frac{\alpha}{h_x^2} + \frac{p}{2h_x} & -\frac{2\alpha}{h_x^2} \end{pmatrix}$$

A suitable time integration is to be used to solve the system of ODEs (16).

6 TVD Runge-Kutta method

To achieve higher order accuracy in the temporal discretization, one can use total variation diminishing (TVD) Runge-Kutta (RK) methods. These methods guarantee that the total variation of the solution does not increase, so that no new extrema are generated. For example, if the solution represents a temperature profile, spurious oscillations caused by the numerical method may trigger a chemical reaction in the simulation. Using a TVD method would ensure that this situation does not occur. Higher order TVD (total variation diminishing) Runge-Kutta time discretization method is used to solve the system of ODEs with suitable initial conditions.

The optimal third order TVD Runge-Kutta method [7] to solve (16) is given by:

$$\begin{cases} v^{(1)} = v^{(n)} + \Delta t V(v^{(n)}), \\ v^{(2)} = \frac{3}{4}v^{(n)} + \frac{1}{4}v^{(1)} + \frac{1}{4}\Delta t V(v^{(1)}), \\ v^{(n+1)} = \frac{1}{3}v^{(n)} + \frac{2}{3}v^{(2)} + \frac{2}{3}\Delta t V(v^{(2)}) \end{cases} \quad (17)$$

7 Numerical Solution

Problem 1

Consider the following convection-diffusion equation in the unit interval $0 \leq x \leq 1$:

$$\frac{\partial u}{\partial t} + 0.1 \frac{\partial u}{\partial x} = 0.01 \frac{\partial^2 u}{\partial x^2}, \quad t > 0.$$

with initial and boundary conditions

$$u(0, t) = u(1, t) = 0, \quad u(x, 0) = e^{5x} \sin \pi x.$$

Here we follow the method of lines approach to obtain the numerical solution, let

$$\frac{\partial u}{\partial t} = -0.1 \frac{\partial u}{\partial x} + 0.01 \frac{\partial^2 u}{\partial x^2}.$$

First we discretize the right hand side of the above equation using the proposed spatial discretization (15). This leads to a system of ordinary differential equations

which are solved using third order TVD Runge kutta method described in Section 6.

The analytical solution to the considered IBVP is $u(x, t) = e^{5x-t(0.01\pi^2+0.25)} \sin \pi x$.

The spatial 2-norm for different values of space step size h using the proposed fourth order scheme in space and third order scheme in time is presented in Table 1. The MATLAB code is given in the appendix.

h	2-norm error	order of convergence
0.20	9.9569e-04	3.6960
0.10	7.6825e-05	3.6013
0.05	6.3298e-06	—

Table 1. Spatial 2-norm error for problem 1 with time T=20.

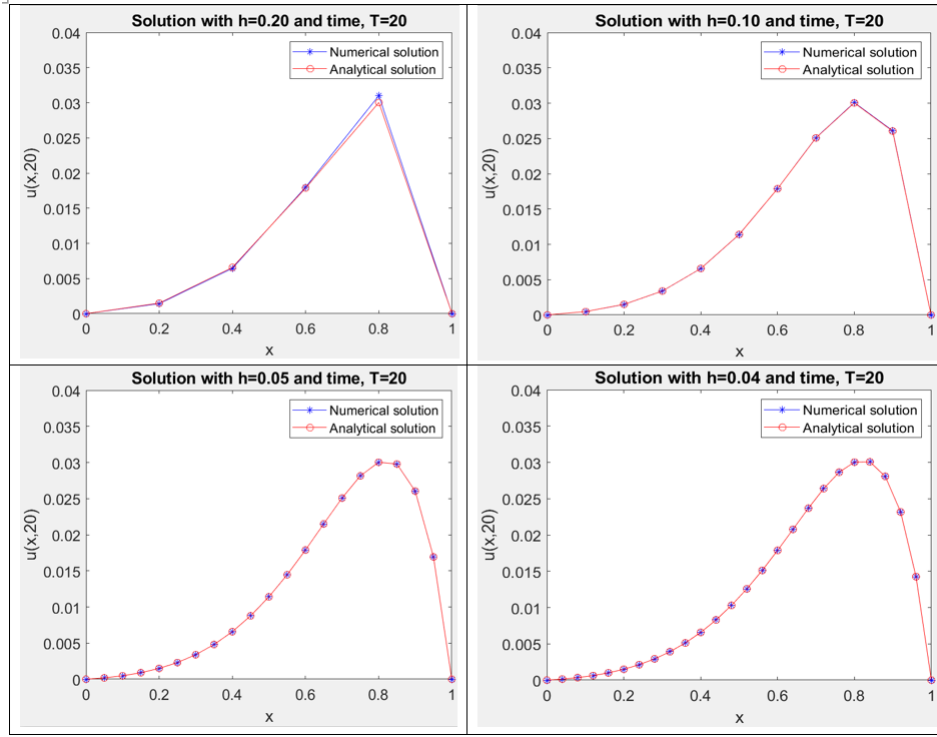


Figure 1: Numerical and analytical solution corresponding to different values of h .

As the space step size h decreases, the error in the numerical solution decreases. This can be noticed from Figure 1 and Table 1. The numerical and analytical solutions with different h values at $T = 20$ are shown in Figure 1. For the derived scheme, the order of convergence [1] will be approximated using the formula $\log_2 \left(\frac{e_1}{e_2} \right)$ where e_1 and e_2 are the 2-norm error at h and $0.5h$ respectively. From the Table 1, it is clearly evident the proposed scheme is highly accurate and also the fourth order convergence is achieved.

Problem 2

Consider the following convection-diffusion equation in the unit interval $0 \leq x \leq 1$:

$$\frac{\partial u}{\partial t} + 0.1 \frac{\partial u}{\partial x} = 0.2 \frac{\partial^2 u}{\partial x^2}, \quad t > 0.$$

with initial and boundary conditions

$$u(0, t) = u(1, t) = 0, \quad u(x, 0) = e^{0.25x} \sin \pi x.$$

Working with the similar approach as in problem 1 we follow the method of lines approach to obtain the numerical solution, let $\frac{\partial u}{\partial t} = -0.1 \frac{\partial u}{\partial x} + 0.21 \frac{\partial^2 u}{\partial x^2}$.

First we discretize the right hand side of the above equation using the proposed spatial discretization (15). This leads to a system of ordinary differential equations which are solved using third order TVD Runge kutta method described in Section 6.

The analytical solution to the considered IBVP is $u(x, t) = e^{0.25x - t(0.2\pi^2 + 0.0125)} \sin \pi x$.

The spatial 2-norm for different values of space step size h using the proposed fourth order scheme in space and third order scheme in time is presented in Table 2.

h	2-norm error	order of convergence
0.20	5.7964e-11	3.5246
0.10	5.0367e-12	3.5046
0.05	4.4377e-13	—

Table 2. Spatial 2-norm error for problem 2 with time T=10.

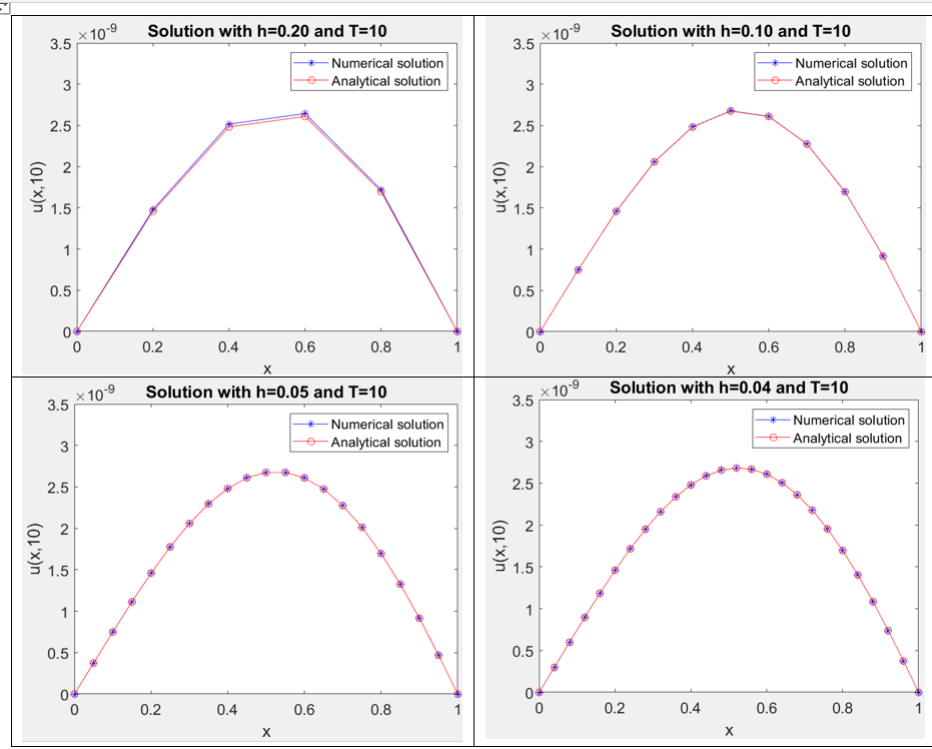


Figure 2: Numerical and analytical solution corresponding to different values of h

In this case too, as the space step size h decreases, the error in the numerical solution decreases. This can be noticed from Figure 2 and Table 2. The numerical and analytical solution with different h values at $T = 10$ are shown in Figure 2. For the derived scheme, the order of convergence [1] is approximated using the formula $\log_2 \left(\frac{e_1}{e_2} \right)$ where e_1 and e_2 are the 2-norm error at h and $0.5h$ respectively. From the Table 2, it is clearly evident that the proposed scheme gives high accuracy. Also the fourth order convergence is achieved.

8 Conclusions

In this report we initially presented Green's function to solve non-homogeneous second order linear differential function with given boundary conditions. In the beginning we started with the introduction to Green's function followed by stating the fundamental theorem of Green's function. Then we presented the construction of Green's function. Heaviside step function is used whose derivative leads to Dirac delta function helping to define special function and using some properties to finally develop the Green's function. Next boundary value problems of second order non-homogeneous linear differential equations are solved using Green's function. In this report Green's function is derived in a detailed and well explained step by step manner. Later we focused on the development of fourth-order exponential equation. The derivation of a fourth order exponential scheme for spatial discretization of unsteady 1D convection-diffusion equations is presented with the help of standard central difference operators, Taylor series expansion and Green's function. With the formulated spatial discretization, the unsteady 1D convection diffusion initial boundary value problem was converted to a system of first-order differential equations with initial conditions. We used third order TVD RK method for the time integration. We implemented the proposed scheme on some test problems and the accuracy of the numerical scheme is presented. The proposed scheme achieves high accuracy and also the numerical order of convergence is achieved.

9 References

- [1] G.D. Smith, *Numerical Solution of Partial Differential Equations (Finite Difference Method)*, Volume 38, Oxford University Press, Oxford, 527–543, 1998.
- [2] Hengfei Ding, Yuxin Zhang, *A new difference scheme with high accuracy and absolute stability for solving convection–diffusion equations*, Journal of Computational and Applied Mathematics 230 (2009) 600–606, 2008.
- [3] I. Stakglod, *Green’s Function and Boundary Value Problems*, John Wiley and Sons, New York, 1979.
- [4] J.H. Williamson, *Low-storage Runge-Kutta schemes*, J. Comput. Physics, Volume 35, 1980.
- [5] M.K. Jain, *Numerical Solution of Differential Equations*, Wiley Eastern Limited, 1991.
- [6] Shepley L. Ross, *Differential Equations*, 3rd Edition, Wiley India Edition, 2010.
- [7] Sigal Gottlieb and Chi-Wang Shu, *Total variation diminishing Runge-Kutta schemes*, American Mathematical Society, Math. Comp. 67, 1998.
- [8] S. N. Ha and C. R. Lee, *Numerical Study for two- point boundary value problems using Green’s function*, Pergamon, Computers and Mathematics with Applications 44 (2002) 1599-1608.
- [9] Tyn Myint-U, *Ordinary Differential Equations*, North-Holland Publishing Company, 1978.
- [10] Zhen F. Tian and P.X. Yu, *A high-order exponential scheme for solving 1D unsteady convection-diffusion equations*, Journal of Computational and Applied Mathematics 235 (2011) 2477-2991.

10 Appendix

MATLAB code for problem 1.

```
1 %Fourth order exponential scheme with TVD RK-3
2 %for solving 1-D convection diffusion IBVP
3 clc;
4 close all;
5 clear all;
6 %Space and time step sizes
7 h=0.04;
8 k=.05;
9 %Final time
10 time=20;
11 % Coefficients in the PDE
12 a=.01;
13 p=0.1;
14 l1=0;
15 l2=1;
16 n=( (l2-l1)/h)+1;
17 x=linspace(l1,l2,n);
18 alpha=p*h/2*coth(p*h/(2*a));
19 alpha1=(a-alpha)/p;
20 alpha2=(a*(a-alpha))/p^2+h^2/6;
21 %Initial Condition
22 u0=zeros(1,n);
23 for i=1:n
24     u0(1,i)=exp(5*x(i))*sin(pi*x(i));
25 end
26 %Boundary Conditions
27 g1=0;
28 g2=0;
```

```

29 % Numerical Scheme
30 A=zeros(n-2,n-2);
31 A(1,1)=1-(2*alpha2/h^2);
32 A(n-2,n-2)=1-(2*alpha2/h^2);
33 A(1,2)=alpha2/h^2+alpha1/(2*h);
34 A(n-2,n-3)=alpha2/h^2-alpha1/(2*h);
35 for i=2:n-3
36     A(i,i)=1-(2*alpha2/h^2);
37     A(i,i+1)=alpha2/h^2+alpha1/(2*h);
38     A(i,i-1)=alpha2/h^2-alpha1/(2*h);
39 end
40 B=zeros(n-2,n-2);
41 B(1,1)=-2*alpha/h^2;
42 B(1,2)=alpha/h^2-p/(2*h);
43 B(n-2,n-3)=alpha/h^2+p/(2*h);
44 B(n-2,n-2)=-2*alpha/h^2;
45 for i=2:n-3
46     B(i,i)=-2*alpha/h^2;
47     B(i,i+1)=alpha/h^2-p/(2*h);
48     B(i,i-1)=alpha/h^2+p/(2*h);
49 end
50 g=zeros(n-2,1);
51 g(1,1)=(alpha/h^2+p/(2*h))*g1;
52 g(n-2,1)=(alpha/h^2-p/(2*h))*g2;
53 un=zeros(n-2,1);
54 u0=zeros(n-2,1);
55 u0=u00(2:n-1)';
56 t=0;
57 while t<=time
58     L1=(A\B)*(u0)+(A\g);
59     C1=u0+k*L1;
60     L2=(A\B)*(C1)+(A\g);
61     C2=(3/4)*u0+(1/4)*C1+(1/4)*k*L2;
62     L3=(A\B)*(C2)+(A\g);
63     un=(1/3)*u0+(2/3)*C2+(2/3)*k*L3;

```

```

64  u0=un;
65  t=t+k;
66  end
67  una=zeros(n,1);
68  una(1)=g1;
69  una(n)=g2;
70  una(2:n-1)=un(1:n-2);
71  %Analytical Solution
72  ua=zeros(n,1);
73  for i=1:n
74      ua(i,1)=exp(5*x(i)-time*(0.01*pi^2+0.25))*sin(pi*x(i));
75  end
76  %Error
77  err=norm((ua-una),2)
78  %Order of convergence
79  order=log2(7.6825e-05/6.3298e-06)
80  plot(x,una,'*b-');
81  hold on
82  plot(x,ua,'*r');
83  axis([0 1 0 0.035])
84  xlabel('x');
85  ylabel('u(x,20)');
86  legend('una', 'ua');
87  title('Solution with h=0.04 and time, T=20')
88  %-----

```