HIGHER ORDER COMPACT SCHEME FOR CONVECTION-DIFFUSION EQUATIONS

Thesis submitted in partial fulfillment of the requirements for
The award of degree of
Masters of Science
In
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Submitted by
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Under
the guidance of
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CERTIFICATE

I hereby certify that the work which is being presented in the thesis entitled **"Higher order compact scheme for convection-diffusion equations"** in partial fulfillment of the requirements for the award of degree of Master of Science, School of Mathematics, Thapar University, Patiala is an authentic record of my own work studied under the supervision of Dr. Vivek Sangwan. *The matter presented in this thesis has not been submitted for the award of any other degree of this or any other university.*

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This is to certify that the above statement made by the candidate is correct and true to the best of my knowledge.

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(MANDEEP KAUR)

ABSTRACT

Differential equations arise in almost all areas of science and engineering including fluid dynamics, fluid mechanics, aerodynamics, medicines, whether predictions etc. Most of the realistic model problems are defined in terms of differential equations or system of differential equations. But most of these model problems or differential equations are not solvable by analytical methods because of the complexity of the coefficients or nonlinearity or due to complex domains etc. Therefore, we need to depend on numerical technics to find the approximate solutions of the differential equations. In the present study, higher order compact finite difference schemes has been presented for solving the differential equations. A brief outline of the thesis is as follows:

Chapter 1 includes the basic definitions and concepts related to the differential equations. Types of differential equations and solution methodology has been discussed. Analytical and numerical schemes has been explained with the help of examples.

In Chapter 2, a fourth order compact scheme has been proposed for a convection-diffusion differential equation with variable coefficients. In the derivation of the difference scheme, the solution $u(x, y)$ is first expressed locally on a mesh element in terms of a linear combination of polynomial functions. The coefficients $p(x, y)$, $q(x, y)$, and $f(x, y)$ are expended in a similar manner. A set of linear equations for the unknown coefficients in the expansion of $u(x, y)$ are obtained by demanding that the governing differential equation be satisfied locally at each mesh point. Additional equations are obtained by interpolating the solution over a set of mesh points which lie on the cell. The difference scheme is defined on a single square cell of size $2h$ over a 9-point stencil. Only those mesh points which lie on a single square cell of side $2h$ are involved, thereby keeping the bandwidth as small as possible for the order of the truncation error achieved. The proposed compact scheme has a truncation error of order h^4. The resulting scheme has been applied to a flow problem in porous media.

In Chapter 3, a fourth order compact finite difference scheme for a second order ordinary differential equation has been presented. To formulate the proposed scheme, the second-order differential equation has been supplemented with fourth order relations between the function value y and the spatial first and second derivatives, $F(=y')$ and $S(=y'')$, on three adjacent mesh points and the derivatives F and S has been eliminated from the system. In this way, a scheme of fourth order, yet based on only three points, is constructed. A proper combination of fourth order relations with boundary conditions and the differential equation ensures a fourth order truncation error also at the boundaries. The scheme is based on a non-equidistant mesh, which makes it particularly useful in problems involving shard boundary layers.

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Contents

Chapter 1

Differential equations - An overview

1.1 Introduction

Differential equations have a remarkable ability to predict the world around us. They are used in a wide variety of disciplines, from biology, economics, physics, chemistry and engineering. Differential equation is a mathematical equation that relates some function with its derivatives. In applications, the functions usually represent physical quantities, the derivative represent their rate of change, and the equation defines a relationship between the two. They can describe exponential growth and decay, the population growth of species or change in investment return over time.

A differential equation is one which can be written in the form $f(x, y, y', y'') = 0$, where prime denote the derivative of the dependent variable w.r.t the independent variable x. Some of the differential equations can be solved simply by integrating, others require much more complex mathematics.

Differential equations are widely used in science and engineering in different forms, such as:

1. In medicine, for modeling cancer growth or the spread of diseases etc.
2. In physics, to describe the motion of waves, pendulums or chaotic systems etc.
3. In chemistry, for modeling chemical reactions etc.
4. In economics, to find optimum investment strategies etc.
5. In engineering, for describing the movement of electricity etc.

Differential equations are studied from several different perspectives, mostly concerned with their solutions – the set of functions that satisfy the equations, but not all the differential equations are solvable by explicit or predefined methods, however, some properties of the solutions of given differential equations may be determined without finding the exact form.

In the present study, we are interested in finding the approximate solution of some differential equations using higher order compact finite difference scheme. Before proceeding to higher order compact scheme, we present below the definitions of some basic concepts and some finite difference schemes which are widely used in differential equations.

1.2 Differential equation

A differential equation is a relation which contains one or more terms involving derivatives the dependent variables with respect to the independent variables.

For example:

$$\frac{dy}{dt} = 3y + 6.$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0.$$

Order of a differential equation: The order of a differential equation is the order of highest differential coefficients occurring in it.

For example:

$$\frac{dy}{dt} + 7x + 5 = 0, \qquad order = 1.$$

$$\frac{d^2y}{dx^2} + x\frac{dy}{dx} + 2 = 0, \qquad order = 2.$$

Degree of a differential equation: The degree of a differential equation is the degree of the highest differential coefficients, when the equation has been made free from fractions and radicals.

For example:

$$\frac{d^2y}{dx^2} + 7\frac{dy}{dx} + 2 = 0, \qquad degree = 1.$$

$$\left(\frac{d^2y}{dx^2}\right)^2 + \frac{dy}{dx} + y^2 = 0, \qquad degree = 2.$$

Homogeneous linear differential equation: A linear differential equation is said to be homogeneous provided if $y(x)$ is a solution of the differential equation, then so is $cy(x)$, where c is any arbitrary constant.

For example:

$$\frac{d^4y}{dx^4} + x\frac{d^2y}{dx^2} + y = 0.$$

$$x^2\frac{d^2y}{dx^2} - 3x\frac{dy}{dx} + 4y = 0.$$

Non-Homogeneous linear differential equation: A linear differential equation is said to be non-homogeneous if it is not homogeneous.

For example:

$$\frac{d^4y}{dx^4} + x\frac{d^2y}{dx^2} + y = 6x + 3.$$

$$3\frac{\partial^2 z}{\partial x \partial y} + \frac{\partial^2 z}{\partial y^2} - 5\frac{\partial z}{\partial y} = e^{x+4y}.$$

1.3 Classification of differential equations

Differential equations are classified into two categories:
1. Ordinary differential equations
2. Partial differential equations

1.4 Ordinary differential equation

An ordinary differential equation is an equation containing a function of one independent variable and its derivatives.

For example:

$$\frac{dy}{dx} + x + 1 = 0.$$

$$\frac{d^2y}{dx^2} + \frac{dy}{dx} = x^2.$$

Types of ordinary differential equation can be classified into two types:
(a) Linear ordinary differential equation.
(b) Non–linear ordinary differential equation.

1.4.1 Linear differential equation

A differential equation is said to be linear if the unknown function and all of its derivatives occurring in the equation occur only in the first degree and are not multiplied together.

For example:

$$\frac{dy}{dx} = sinx.$$

$$\frac{d^2y}{dx^2} + y = 0.$$

1.4.2 Non-linear differential equation

A differential equation which is not linear is called non-linear differential equation.

For example:

$$\frac{d^2y}{dx^2} + \left(\frac{dy}{dx}\right)^2 + y^2 = 0.$$

$$y = \sqrt{x}\left(\frac{dy}{dx}\right) + \frac{k}{\left(\frac{dy}{dx}\right)}.$$

1.5 Partial differential equation

A differential equation which contains one or more partial derivatives of an unknown function of two or more independent variables is said to be partial differential equation.

For example:

$$\frac{\partial z}{\partial x} - 5\frac{\partial z}{\partial y} = 2z + sin(x - 2y).$$

$$\frac{\partial^2 z}{\partial x^2} - \frac{\partial^2 z}{\partial x \partial y} + 3\left(\frac{\partial^2 z}{\partial y^2}\right) = 0.$$

Partial differential equations can be classified into the following types:
(a) Linear partial differential equation
(b) Semi–linear partial differential equation
(c) Quasi–linear partial differential equation
(d) Non–linear partial differential equation.

1.5.1 Linear partial differential equation

A differential equation which can be written in the form

$$P(x,y)p + Q(x,y)q = R(x,y)z + S(x,y)$$

is said to be a linear partial differential equation.
For example:

$$p + 3q = 5z - tan(3x - y)$$

$$(x - \alpha)p + (y - \beta)q = z - \gamma.$$

1.5.2 Semi-linear partial differential equation

A differential equation which can be written in the form

$$P(x,y)p + Q(x,y)q = R(x,y,z)$$

is said to be a semi-linear partial differential equation.
For example:

$$x^2p + y^2q = x^2y^2z^2.$$

$$xy^2p - y^3q = \alpha xz^4.$$

1.5.3 Quasi-linear partial differential equation

A differential equation which can be written in the form

$$P(x,y,z)p + Q(x,y,z)q = R(x,y,z)$$

is said to be a quasi-linear partial differential equation.
For example:

$$x^2(y-z)p + y^2(z-x)q = z^2(x-y)$$

$$\left(\frac{1}{z} - \frac{1}{y}\right)p + \left(\frac{1}{x} - \frac{1}{z}\right)q = \frac{1}{y} - \frac{1}{x}.$$

1.5.4 Non-linear partial differential equation

A differential equation which does not come under the above three types is said to be a non-linear partial differential equation.
For example:

$$p^2e^{2y} = qe^{2x}.$$
$$x(1+y)p = y(1+x)q^2.$$

1.6 Solutions of differential equations

1.6.1 General solution

The solution of a differential equation which involves as many arbitrary constants as the order of the differential equation is called the general solution.

1.6.2 Particular solution

A particular solution of a differential equation is that which contains no arbitrary constant and is obtained from the general solution by giving particular values to the arbitrary constants.

1.6.3 Singular solution

A singular solution of a differential equation is that which contains no arbitrary constant and cannot be obtained from the general solution by giving any particular values to the arbitrary constants.

1.7 Solution methodology

Broadly, we can categorize the solution approaches for differential equations into two categories:

1. Analytical approach
2. Numerical approach.

1.8 Analytical techniques

Using these techniques, we get exact solution. Some of the analytical techniques include:

1. Variable separable method
2. Method for linear differential equation
3. Method of undetermined coefficients
4. Method of variation of parameters, etc

Now, I will present one of the analytical techniques to find the general solution of a differential equation.

1.8.1 Variable separable method

Consider a differential equation

$$x(1+y^2)dx + y(1+x^2)dy = 0.$$

The equation can be written as

$$y(1+x^2)dy = -x(1+x^2)dx$$

$$\Rightarrow \frac{y}{1+y^2}dy = -\frac{x}{1+x^2}dx$$

Integrating, we get

$$\int \frac{2y}{1+y^2}dy = -\int \frac{2x}{1+x^2}dx$$

$$\Rightarrow \log(1+y^2) = -\log(1+x^2) + \log c$$
$$\Rightarrow \log(1+x^2) + \log(1+y^2) = \log c$$
$$\Rightarrow \log[(1+x^2)(1+y^2)] = \log c$$
$$\Rightarrow (1+x^2)(1+y^2) = c$$

which is the required general solution.

1.9 Numerical techniques

Since most of differential equations cannot be solved using analytical techniques. Therefore, we need to take help of numerical techniques for finding the approximate solution of differential equations. Using these techniques, we get approximate solution. Some of the widely used numerical techniques include:

1. Finite difference methods
2. Finite element methods
3. Finite volume methods etc.

For the present study, I will focus on numerical techniques, in particular, finite difference method for finding the approximate solutions of differential equations.

1.9.1 Finite difference methods

In finite difference methods, we first discretize the domain and construct the mesh. Then at each nodal point of the mesh, we approximate the differential coefficients appearing in the differential equation using Taylor's series expansion. Thus, we get a system of equations in the unknown function values at the nodal points. Simplifying the system of equations, we get the solution values at the nodal points of the mesh. Depending on the Taylor's series approximations, we get different finite difference schemes.

Finite difference formulae for first order derivative terms:

Forward Difference:

$$y^{'}(x_i) = \frac{y_{i+1} - y_i}{h} + O(h)$$

Backward Difference:

$$y^{'}(x_i) = \frac{y_i - y_{i-1}}{h} + O(h)$$

Central Difference:

$$y^{'}(x_i) = \frac{y_{i+1} - y_{i-1}}{2h} + O(h^2)$$

Finite difference formulae for second order derivative terms:

Forward Difference:

$$y^{''}(x_i) = \frac{y_{i+2} - 2y_{i+1} + y_i}{h^2} + O(h)$$

Backward Difference:

$$y^{''}(x_i) = \frac{y_i - 2y_{i-1} + y_{i-2}}{h^2} + O(h)$$

Central Difference:

$$y^{''}(x_i) = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + O(h^2).$$

Next, we solve heat equation using finite difference method.

Example:
Consider the heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad 0 \leq x \leq 1, t > 0 \tag{1.9.1}$$

with boundary conditions $u(0,t) = u(1,t) = 1$ and initial condition

$$u(x,0) = \begin{cases} 1 + 2x & 0 \leq x \leq \frac{1}{2} \\ 3 - 2x & \dfrac{1}{2} \leq x \leq 1. \end{cases}$$

We will use explicit finite difference method for finding the approximate solution of the differential equation. We will take $\Delta x = 0.2$ and $\Delta t = 0.02$ and compute the solution upto time interval $t = 0.24$ correct to six decimal places.

We note that the problem is symmetric about $x = 0.5$, since the initial temperature at $u(x,0)$ is symmetric about $x = 0.5$ and the boundary conditions at $x = 0$ and $x = 1.0$ are also same. Therefore, the temperature at the subsequent times will remain also symmetric about $x = 0.5$.

The domain $0 \leq x \leq 1.0$ is subdivided into five equal sub-intervals each of width $\Delta x = 0.2$.

Therefore, the nodal points x_i are given by
$x_i = 0.2 \times i, i = 0(1)5$.
Also, $t_i = \triangle t \times i$; i=0(1)12.

Now, in equation (1.9.1) the time derivative $\dfrac{\partial u}{\partial t}$ is replaced by forward difference approximation and the space derivative $\dfrac{\partial^2 u}{\partial x^2}$ by central difference approximation. In operator form we can write,

$$\frac{1}{\triangle t} \triangle t u(x_i, t_j) + O(\triangle t) = \frac{1}{(\triangle x)^2} (\delta_x^2) u(x_i, t_j) + O(\triangle x^2), \tag{1.9.2}$$

where $\triangle_t$ and (δ_x^2) denote forward difference and central difference in the direction of t and x respectively. The formulation (1.9.2) can be written in the terms of the unknown function values at the nodal points as,

$$\frac{u(x_i, t_j + \triangle t) - u(x_i, t_j)}{\triangle t} = \frac{u(x_i - \triangle x, t_j) - 2u(x_i, t_j) + u(x_i + \triangle x, t_j)}{(\triangle x)^2} + O(\triangle t) + O(\triangle x^2)$$

$$\frac{u(x_i, t_{j+1}) - u(x_i, t_j)}{\triangle t} = \frac{u(x_{i-1}, t_j) - 2u(x_i, t_j) + u(x_{i+1}, t_j)}{(\triangle x)^2} + O(\triangle t) + O(\triangle x^2) \tag{1.9.3}$$

Here, the term $O(\triangle t) + O(\triangle x^2)$ is called truncation error. Denoting the computed values at the mesh points (i, j) by $u_{i,j}$ etc and neglecting the truncation error, the finite difference approximation scheme can be written as

$$u_{i,j+1} = r \times u_{i-1,j} + (1 - 2 \times r) \times u_{i,j} + r \times u_{i+1,j}, \tag{1.9.4}$$

where $r = \dfrac{\triangle t}{\triangle x^2}$.
Due to symmetry at $x = 0.5$, for all j, we have

$$u_{0,j} = u_{5,j}, \quad u_{1,j} = u_{4,j}, \quad u_{2,j} = u_{3,j}.$$

Also,

$$r = \frac{\Delta t}{\Delta x^2} = \frac{0.02}{0.04} = 0.5.$$

Putting $r = 0.5$ in (1.9.4), we get

$$u_{i,j+1} = \frac{1}{2}(u_{i-1,j} + u_{i+1,j}), \quad i = 1, 2.$$

The values for i=3 and i=4 can be obtained using symmetry.

Computed values are:

x	0	0.2	0.4	0.6	0.8	1.0
t=0.00	1.0	1.4	1.8	1.8	1.4	1.0
0.02	1.0	1.4	1.6	1.6	1.4	1.0
0.04	1.0	1.3	1.5	1.5	1.3	1.0
0.06	1.0	1.25	1.4	1.4	1.25	1.0
0.08	1.0	1.20	1.325	1.325	1.20	1.0
0.10	1.0	1.1625	1.2625	1.2625	1.1625	1.0
0.12	1.0	1.13125	1.21250	1.21250	1.13125	1.0
0.14	1.0	1.10625	1.171875	1.171875	1.10625	1.0
0.16	1.0	1.085938	1.139062	1.139062	1.085938	1.0
0.18	1.0	1.069531	1.12500	1.12500	1.069531	1.0
0.20	1.0	1.056250	1.091016	1.091016	1.056250	1.0
0.22	1.0	1.045508	1.073633	1.073633	1.045508	1.0
0.24	1.0	1.036816	1.059570	1.059570	1.036816	1.0

Chapter 2

A single cell high order scheme for convection-diffusion equation with variable coefficients (Review)

2.1 Introduction

In this paper [6], a new finite difference scheme for the convection-diffusion equation with variable coefficients is proposed. The difference scheme is defined on a single square cell of size $2h$ over a 9-point stencil and has a truncation error of order h^4. The resulting system of equations has been solved by iterative methods.

Consider the convection-diffusion equation

$$Lu \equiv u_{xx} + u_{yy} + p(x,y)u_x + q(x,y)u_y = f(x,y) \tag{2.1.1}$$

This equation often appear in the description of transport phenomena. The magnitudes of $p(x,y)$ and $q(x,y)$ determine the ratio of the convection to diffusion. In many problems of practical interest, the convective terms dominate the diffusion terms. Numerical simulation of such equations becomes increasingly difficult as the ratio of the convection to diffusion increases.

When the equation is discretized using central difference, the resulting scheme, called CDS, has a truncation error of order h^2. In the case of CDS, iterative method for solving the resulting system of linear equations do not converge when the convective terms dominate and the cell Reynolds number is greater than a certain constant. In addition, direct method for solving the system of linear equations may give erroneous results. If the convective terms are approximated by suitable forward or backward differences and the diffusion terms by central differences, the resulting scheme is called the upwind or the upstream scheme or the upwind differencing scheme (UDS). There are several variations of UDS and also combinations of the CDS and the UDS schemes. The UDS introduces artificial viscosity and hence the results contain more error when the convection dominates. Both the truncation and the discretization errors of UDS are of order h and hence a very fine mesh is needed if accurate results are required. Such a refinement of the mesh is often uneconomical.

Recently, a new finite difference scheme has been proposed by the Gupta et al. [5] for the special case of equation (2.1.1) where p and q are constants. In the present study a generalization of the scheme has been presented to the case of variable coefficients $p(x, y)$ and $q(x, y)$. The new scheme has a truncation error of order h^4 and the resulting system of linear equation can be solved by iterative methods even for large absolute values of $p(x, y)$ and $q(x, y)$.

The truncation error of this scheme is of order h^4. The coefficients of the non-diagonal terms in the difference equation do not have the same sign for all values of $p(x, y)$ and $q(x, y)$, therefore, it is not possible to predict the order of the discretization error from that of the truncation error using the theoretical results. The order of discretization error is defined for the asymptotic case when the mesh size $h \to 0$. The numerical estimates of the order determined from the errors calculated by using two different mesh sizes may not reach its asymptotic value as long as the derivatives appearing in the expression for the truncation error vary with the change in the mesh. This is indeed the case when the transport number is large. A better estimate of the order of the discretization error is obtained in such cases by refining the mesh.

Gupta et al. [5] have solved several test problems using the present scheme and also the upwind differencing scheme and the CDS. Such schemes are more complicated and difficult to implement. The rate at which the error decreases as the mesh is refined is not as fast as that of the presented scheme, and hence this scheme gives better results as the mesh is refined.

In the present scheme [6], the coefficients can be computed easily when the grid is uniform. The difference scheme is not obtained explicitly for each mesh point but is computed as the difference equations are assembled. The procedure has been generalized to the case of the convection diffusion equation when the diffusion coefficients are variable, and the resulting scheme has been applied to some flow problems in porous media.

In the derivation of the difference scheme, the solution $u(x, y)$ is first expressed locally on a mesh element in terms of a linear combination of functions which are use to be polynomials. The functions $p(x, y)$, $q(x, y)$, and $f(x, y)$ are expended in a similar manner. A set of linear equations for the unknown coefficients in the expansion of $u(x, y)$ are obtained by demanding that the differential equation (2.1.1) be satisfied locally. Additional equations are obtained by interpolating the solution over a set of mesh points which lie on the cell. This technique has been used to obtain single cell high order schemes for the Poisson, the Helmholtz, the biharmonic and other linear equations [10, 11].

The difference scheme derived here is a 9-point scheme [6]. Only those mesh points which lie on a single square cell of side $2h$ are involved, thereby keeping the bandwidth as small as possible for the order of the truncation error achieved. No special formulae are needed for points near the boundary. The new finite difference compact scheme for equation(2.1.1) is presented in the next section.

2.2 Compact finite difference scheme

The finite difference approximation for diffusion and convection terms at a mesh point (x, y) which is denoted by '0' in Figure 1 involves the other eight mesh points at$(x \pm h, y)$, $(x, y \pm h)$, $(x \pm h, y \pm h)$. These points are denoted either by numbers 1– 8 or by the letters showing their directions with respect to the point '0' as in Figure 1. The difference formula involves the coefficients $\lambda_{i,j}$, $\mu_{i,j}$, and $c_{i,j}$ which appear in the expansion of $p(x, y)$, $q(x, y)$ and $f(x, y)$ along with the nodal values $u_k = u(x_k, y_k)$ for $k = 0, 1, 2....$ Alternatively, the coefficients in the expansion of the known functions can be expressed in terms of their partial derivatives. In practice it is more convenient to use the nodal values of the known functions rather than their derivatives. Therefore, an alternative formulation of the difference formula involving the nodal values of $p(x, y)$, $q(x, y)$ and $f(x, y)$ is also given.

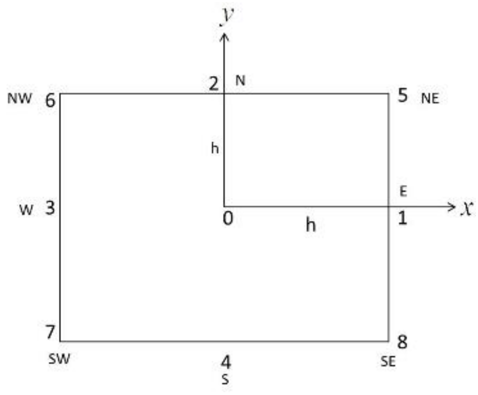

Figure 1: Labelling of grid points

The differential equation considered is

$$u_{xx} + u_{yy} + p(x,y)u_x + q(x,y)u_y = f(x,y). \tag{2.2.1}$$

We assume that locally, the solution $u(x,y)$ and the function p, q, f can be expressed by two-dimensional power series:

$$\begin{aligned} u(x,y) &= \sum a_{i,j}x^i y^j, \\ f(x,y) &= \sum c_{i,j}x^i y^j, \\ p(x,y) &= \sum \lambda_{i,j}x^i y^j, \\ q(x,y) &= \sum \mu_{i,j}x^i y^j. \end{aligned} \tag{2.2.2}$$

Substituting (2.3) into (2.2), we get

$$\begin{aligned} \sum c_{i,j}x^i y^j &= i(i-1)\sum a_{i,j}x^{i-2}y^j + j(j-1)\sum a_{i,j}x^i y^{j-2} \\ &\quad + i\sum\sum a_{i,j}\lambda_{i,j}x^{i-1}y^j + j\sum\sum a_{i,j}\mu_{i,j}x^i y^{j-1} \end{aligned}$$

Comparing the coefficients of $x^i y^j$ on both sides, we get

$$\begin{aligned} c_{i,j} &= (i+1)(i+2)a_{i+2,j} + (j+1)(j+2)a_{i,j+2} + \\ &\quad + \sum_{i\le r,s\le j} [(i-r+1)\lambda_{r,s}a_{i+1-r,j-s} + (j-s+1)\mu_{r,s}a_{i-r,j+1-s}] \end{aligned} \tag{2.2.3}$$

The equation (2.2.3) constitute the constraints, imposed by the differential equation (2.2.1), on the coefficients $a_{i,j}$, $c_{i,j}$, $\lambda_{i,j}$ and $\mu_{i,j}$ of the expansion (2.2.2). In particular,

$$\begin{aligned}
c_{0,0} &= 2(a_{2,0} + a_{0,2}) + \lambda_{0,0}a_{1,0} + \mu_{0,0}a_{0,1} \\
c_{1,0} &= 6a_{3,0} + 2a_{1,2} + 2\lambda_{0,0}a_{2,0} + \lambda_{1,0}a_{1,0} + \mu_{0,0}a_{1,1} + \mu_{1,0}a_{0,1} \\
c_{0,1} &= 2a_{2,1} + 6a_{0,3} + \lambda_{0,0}a_{1,1} + \lambda_{0,1}a_{1,0} + 2\mu_{0,0}a_{0,2} + \mu_{0,1}a_{0,1} \\
c_{2,0} &= 12a_{4,0} + 2a_{2,2} + 3\lambda_{0,0}a_{3,0} + 2\lambda_{1,0}a_{2,0} + \lambda_{2,0}a_{1,0} + \mu_{0,0}a_{2,1} + \mu_{1,0}a_{1,1} + \mu_{2,0}a_{0,1} \\
c_{0,2} &= 2a_{2,2} + 12a_{0,4} + \lambda_{0,0}a_{1,2} + \lambda_{0,1}a_{1,1} + \lambda_{0,2}a_{1,0} + 3\mu_{0,0}a_{0,3} + 2\mu_{0,1}a_{0,2} + \mu_{0,2}a_{0,1} \\
c_{1,1} &= 6a_{3,1} + 6a_{1,3} + 2\lambda_{0,0}a_{2,1} + \lambda_{1,0}a_{1,1} + \lambda_{1,1}a_{1,0} + 2\mu_{0,0}a_{1,2} + \mu_{0,1}a_{1,1} + \mu_{1,1}a_{0,1}
\end{aligned} \tag{2.2.4}$$

The above six constraints ensure the satisfaction of the differential equation (2.2.1) for $u = x^i y^j$ for $i + j \leq 4$. These constraints involve 15 unknown values of $a_{i,j}$, $0 \leq i + j \leq 4$. The remaining nine equations, relating the values of $a_{i,j}$ are obtained by collocation on the nine points $0-8$ of the single cell of side $2h$ (see figure 1). In particular,

$$\begin{aligned}
u_0 &= a_{0,0} \\
u_E \equiv u_1 &= a_{0,0} + a_{1,0}h + a_{2,0}h^2 + a_{3,0}h^3 + ... \\
u_N \equiv u_2 &= a_{0,0} + a_{0,1}h + a_{0,2}h^2 + a_{0,3}h^3 + a_{0,4}h^4 + ... \\
u_W \equiv u_3 &= a_{0,0} + a_{1,0}h + a_{2,0}h^2 + a_{3,0}h^3 + ... \\
u_S \equiv u_4 &= a_{0,0} - a_{0,1}h + a_{0,2}h^2 - a_{0,3}h^3 + ... \\
u_{NE} \equiv u_5 &= a_{0,0} + (a_{0,1} + a_{1,0})h + (a_{0,2} + a_{1,1} + a_{2,0})h^2 + ... \\
u_{NW} \equiv u_6 &= a_{0,0} + (a_{0,1} - a_{1,0})h + (a_{0,2} - a_{1,1} - a_{2,0})h^2 + ... \\
u_{SW} \equiv u_7 &= a_{0,0} + (-a_{0,1} - a_{1,0})h + (-a_{0,2} + a_{1,1} - a_{2,0})h^2 + ... \\
u_{SE} \equiv u_8 &= a_{0,0} + (a_{1,0} - a_{0,1})h + (a_{2,0} - a_{0,2} - a_{1,1})h^2 + ...
\end{aligned} \tag{2.2.5}$$

We use the notation

$$\begin{aligned}
\diamond u_0 &= u_1 + u_2 + u_3 + u_4 \\
\Box u_0 &= u_5 + u_6 + u_7 + u_8
\end{aligned} \tag{2.2.6}$$

From (2.2.5), we obtain relation of the form

$$
\begin{aligned}
u_1 - u_0 &= (a_{0,0} + a_{1,0}h + a_{2,0}h^2 + a_{3,0}h^3 + ...) - (a_{0,0}) \\
&= a_{1,0}h + a_{2,0}h^2 + a_{3,0}h^3 + ... \\
u_2 + u_4 - 2u_0 &= (a_{0,0} + a_{0,1}h + a_{0,2}h^2 + a_{0,3}h^3 + a_{0,4}h^4 + ...) \\
&\quad + (a_{0,0} - a_{0,1}h + a_{0,2}h^2 - a_{0,3}h^3 + ...) - (a_{0,0}) \\
&= 2a_{0,2}h^2 + 2a_{0,4}h^4 + ... \\
/ \; u_5 + u_7 - u_6 - u_8 &= (a_{0,0} + (a_{0,1} + a_{1,0})h + (a_{0,2} + a_{1,1} + a_{2,0})h^2 + ...) \\
&\quad + (a_{0,0} + (-a_{0,1} - a_{1,0})h + (-a_{0,2} + a_{1,1} - a_{2,0})h^2 + ...) \\
&\quad - (a_{0,0} + (a_{0,1} - a_{1,0})h + (a_{0,2} - a_{1,1} - a_{2,0})h^2 + ...) \\
&\quad - (a_{0,0} + (a_{1,0} - a_{0,1})h + (a_{2,0} - a_{0,2} - a_{1,1})h^2 + ...) \\
&= 4a_{1,1}h^2 + O(h^4)
\end{aligned}
\tag{2.2.7}
$$

Now, from(2.2.4), we get

$$
\begin{aligned}
h^2(c_{0,0}) &= h^2(2(a_{2,0} + a_{0,2}) + \lambda_{0,0}a_{1,0} + \mu_{0,0}a_{0,1}) \\
&= 2h^2(a_{2,0} + a_{0,2}) + \lambda_{0,0}h(a_{1,0}h) + \mu_{0,0}h(a_{0,1}h) \\
&= 2h^2(a_{2,0} + a_{0,2}) + \lambda_{0,0}h(u_1 - u_0 - a_{2,0}h^2 - a_{3,0}h^3...) + \\
&\quad \mu_{0,0}h(u_2 - u_0 - a_{0,2}h^2 - a_{0,3}h^3...) \\
&= (u_1 + u_2 + u_3 + u_4 - 4u_0 - 2a_{4,0}h^4 - 2a_{0,4}h^4) + \lambda_{0,0}h(u_1 - u_0 \\
&\quad - a_{2,0}h^2) + \mu_{0,0}h(u_2 - u_0 - a_{0,2}h^2) + O(h^4) \\
&= (\diamond u_0 - 4u_0 - 2a_{4,0}h^4 - 2a_{0,4}h^4) + \lambda_{0,0}h(u_1 - u_0 - a_{2,0}h^2) + \\
&\quad \mu_{0,0}h(u_2 - u_0 - a_{0,2}h^2) + O(h^4)
\end{aligned}
\tag{2.2.8}
$$

Neglecting terms of order h^3 and of higher orders, we obtain the well known upwind difference scheme of order h^2 as

$$
h^2(c_{0,0}) = \diamond u_0 - 4u_0 + \lambda_{0,0}h(u_1 - u_0) + \mu_{0,0}h(u_2 - u_0) \tag{2.2.9}
$$

If the terms containing h^3 are eliminated in (2.2.7), we obtain

$$
\begin{aligned}
h^2(c_{0,0}) &= (u_1 + u_2 + u_3 + u_4 - 4u_0 - 2a_{4,0}h^4 - 2a_{0,4}h^4) + \lambda_{0,0}h(u_1 - u_0 \\
&\quad - a_{2,0}h^2) + \mu_{0,0}h(u_2 - u_0 - a_{0,2}h^2) + O(h^4) - \frac{\lambda_{0,0}h}{2}(u_1 + u_3 - 2u_0) \\
&\quad + O(h^4) - \frac{\mu_{0,0}h}{2}(u_2 + u_4 - 2u_0) + O(h^4) \\
&= \diamond u_0 - 4u_0 + \frac{\lambda_{0,0}h}{2}(u_1 - u_3) + \frac{\mu_{0,0}h}{2}(u_2 - u_4) + O(h^4)
\end{aligned} \tag{2.2.10}
$$

The central difference scheme results when $O(h^4)$ terms are neglected in (2.2.10). This result cannot be improved any further without using more constraints from (2.2.4), (2.2.5). The two constraints involving $c_{1,0}$, $c_{0,1}$ contain $a_{3,0}$, $a_{0,3}$ which also appear in the next set of constraints for $c_{2,0}$, $c_{0,2}$. Using these constraints and the relations (2.2.7), (2.2.8), (2.2.9), we obtain

$$
\begin{aligned}
6h^2c_{0,0} + \frac{h^4}{2}(c_{1,0}\lambda_{0,0} + c_{0,1}\mu_{0,0}) + h^4(c_{2,0} + c_{0,2}) &= 6 \diamond u_0 - 24u_0 \\
+3h\lambda_{0,0}(u_2 - u_4) + 2h^4(\lambda_{0,0}a_{1,2} + \mu_{0,0}a_{2,1})a_{2,0}h^4(\lambda_{0,0}^2 + 2\lambda_{1,0}) \\
+a_{0,2}h^4(\mu_{0,0}^2 + 2\mu_{0,1}) + a_{1,1}h^4(\lambda_{0,0}\mu_{0,0} + \lambda_{0,1} + \mu_{1,0}) \\
+a_{1,0}h^4(\lambda_{2,0} + \lambda_{0,2} + \frac{1}{2}\lambda_{0,0}\lambda_{1,0} + \frac{1}{2}\mu_{0,0}\lambda_{0,1}) \\
+a_{0,1}h^4(\mu_{2,0} + \mu_{0,2} + \frac{1}{2}\lambda_{0,0}\mu_{1,0} + \frac{1}{2}\mu_{0,0}\mu_{0,1}) + 4h^4a_{2,2} + O(h^4).
\end{aligned}
$$

$$
\begin{aligned}
&= 4 \diamond u_0 + \Box u_0 - 20u_0 + 2h\lambda_{0,0}(u_1 - u_3) + 2h\mu_{0,0}(u_2 - u_4) \\
&+\lambda_{0,0}\frac{h}{2}(u_5 - u_6 \quad - u_7 + u_8) + \mu_{0,0}\frac{h}{2}(u_5 + u_6 - u_7 - u_8) \\
&+\frac{1}{2}h^2(\lambda_{0,0}^2 + 2\lambda_{1,0})(u_1 + u_3) + \frac{1}{2}h^2(\mu_{0,0}h^2 + 2\mu_{0,1})(u_2 + u_4) \\
&-h^2(\lambda_{0,0}^2 + \mu_{0,0}^2 + 2\lambda_{1,0} + 2\mu_{0,1})u_0 \\
&+\frac{1}{4}h^2(\lambda_{0,0}\mu_{0,0} + \lambda_{0,1} + \mu_{1,0})(u_5 - u_6 + u_7 - u_8) \\
&+\frac{h^3}{2}(\lambda_{2,0} + \lambda_{0,2} + \frac{1}{2}\lambda_{0,0}\lambda_{1,0} + \frac{1}{2}\mu_{0,0}\lambda_{0,1})(u_1 - u_3) \\
&+\frac{h^3}{2}(\mu_{2,0} + \mu_{0,2} + \frac{1}{2}\lambda_{0,0}\mu_{1,0} + \frac{1}{2}\mu_{0,0}\mu_{0,1})(u_2 - u_4) + O(h^6)
\end{aligned} \tag{2.2.11}
$$

Neglecting the term of order h^6, we get the forth order difference scheme given by equation. The scheme can be written as

$$\sum a_k u_k = 6h^2 c_{0,0} + \frac{h^4}{2}(c_{1,0}\lambda_{0,0} + c_{0,1}\mu_{0,0}) + h^4(c_{2,0} + c_{0,2}) \tag{2.2.12}$$

The truncation error of this scheme is given by $\frac{1}{6}h^4\psi(x, y)$ where $\psi(x, y)$ represents the coefficients of $O(h^6)$ on the right hand side of (2.2.11). The function $\psi(x, y)$ is given by

$$\begin{aligned}
\psi(x, y) = {} & 12(a_{6,0} + a_{0,6}) + 6(\lambda_{0,0}a_{5,0} + \mu_{0,0}a_{0,5}) + 4(a_{4,2} + a_{2,4}) \\
& + 2\lambda_{0,0}(a_{3,2} + a_{1,4}) + 2\mu_{0,0}(a_{4,1} + a_{3,2}) + a_{4,0}(\lambda_{0,0}^2 + 2\lambda_{1,0}) \\
& + a_{0,4}(\mu_{0,0}^2 + 2\mu_{0,1}) + (a_{3,1} + a_{1,3})(\lambda_{0,0}\mu_{0,0} + \lambda_{0,1} + \mu_{1,0}) \\
& + (\lambda_{2,0} + \lambda_{0,2} + \frac{1}{2}\lambda_{0,0}\mu_{1,0} + \frac{1}{2}\mu_{0,0}\lambda_{0,1})a_{3,0} \\
& + (\mu_{2,0} + \mu_{0,2} + \frac{1}{2}\lambda_{0,0}\mu_{1,0} + \frac{1}{2}\mu_{0,0}\mu_{0,1})a_{0,3}
\end{aligned} \tag{2.2.13}$$

In above expressions, $a_{i,j}, \lambda_{i,j}$, and $\mu_{i,j}$ are defined as follows:

$$a_{i,j} = \frac{1}{i!j!}\frac{\partial^{i+1}u}{\partial x^i \partial y^j}$$

$$\lambda_{i,j} = \frac{1}{i!j!}\frac{\partial^{i+1}p}{\partial x^i \partial y^j} \tag{2.2.14}$$

$$\mu_{i,j} = \frac{1}{i!j!}\frac{\partial^{i+1}q}{\partial x^i \partial y^j}$$

Now, from equation (2.2.12), we get

$$
\begin{aligned}
a_1 \equiv a_E &= 4 + 2h\lambda_{0,0} + h^2 R_3 + \frac{h^3}{2} R_6 \\
a_2 \equiv a_N &= 4 + 2h\mu_{0,0} + h^2 R_4 + \frac{h^3}{2} R_5 \\
a_3 \equiv a_W &= 4 - 2h\lambda_{0,0} + h^2 R_3 - \frac{h^3}{2} R_6 \\
a_4 \equiv a_S &= 4 - 2H\mu_{0,0} + h^2 R_4 - \frac{h^3}{2} R_5 \\
a_5 \equiv a_{NE} &= 1 + \frac{h}{2}(\lambda_{0,0} + \mu_{0,0}) + \frac{h^2}{4} R_2 \\
a_6 \equiv a_{NW} &= 1 - \frac{h}{2}(\lambda_{0,0} - \mu_{0,0}) - \frac{h^2}{4} R_2 \\
a_7 \equiv a_{SW} &= 1 - \frac{h}{2}(\lambda_{0,0} + \mu_{0,0}) + \frac{h^2}{2} R_2 \\
a_8 \equiv a_{SE} &= 1 + \frac{h}{2}(\lambda_{0,0} - \mu_{0,0}) - \frac{h^2}{4} R_2 \\
a_0 \equiv &- 20 - h^2 R_1,
\end{aligned}
\tag{2.2.15}
$$

where

$$
\begin{aligned}
R_1 &= \lambda_{0,0}^2 + \mu_{0,0}^2 + 2\lambda_{1,0} + 2\mu_{0,1} \\
R_2 &= \mu_{1,0} + \lambda_{0,1} + \lambda_{0,0}\mu_{0,0} \\
R_3 &= \frac{1}{2}\lambda_{0,0}^2 + \lambda_{1,0} \\
R_4 &= \frac{1}{2}\mu_{0,0}^2 + \mu_{0,1} \\
R_5 &= \mu_{2,0} + \mu_{0,2} + \frac{1}{2}\lambda_{0,0}\mu_{1,0} + \frac{1}{2}\mu_{0,0}\mu_{0,1} \\
R_6 &= \lambda_{2,0} + \lambda_{0,2} + \frac{1}{2}\lambda_{0,0}\lambda_{1,0} + \frac{1}{2}\mu_{0,0}\lambda_{0,1}.
\end{aligned}
\tag{2.2.16}
$$

Replacing $\lambda_{i,j}$, $\mu_{i,j}$ and $c_{i,j}$ in terms of the nodal values of the functions $p(x, y)$, $q(x, y)$ and $f(x, y)$, we get the compact finite difference scheme given by:

$$\sum_{i=0}^{8} a_j u_j = \frac{h^2}{2}[f_N + f_S + f_E + f_W + 8f_0] + \frac{h^3}{4}[p_0(f_E - f_W)] + q_0(f_N - f_S)]$$

(2.2.17)

where

$$a_1 \equiv a_E = 4 + \frac{h}{4}[4p_0 + 3p_E - p_W + p_N + p_S] + \frac{h^2}{8}[4p_0^2 + p_0(p_E - p_W) + q_0(p_N - p_S)]$$
$$a_2 \equiv a_N = 4 + \frac{h}{4}[4q_0 + 3q_N - q_S + q_E + q_W] + \frac{h^2}{8}[4q_0^2 + p_0(q_E - q_W) + q_0(q_N - q_S)]$$
$$a_3 \equiv a_W = 4 - \frac{h}{4}[4p_0 - p_E - 3p_W + p_N + p_S] + \frac{h^2}{8}[4p_0^2 + p_0(p_E - p_W) + q_0(q_N - p_S)]$$
$$a_4 \equiv a_S = 4 - \frac{h}{4}[4q_0 - q_N - 3q_S + q_E + q_W] + \frac{h^2}{8}[4q_0^2 + p_0(q_E - q_W) + q_0(q_N - q_S)]$$
$$a_5 \equiv a_{NE} = 1 + \frac{h}{2}(p_0 + q_0) + R_7$$
$$a_6 \equiv a_{NW} = 1 - \frac{h}{2}(p_0 - q_0) - R_7$$
$$a_7 \equiv a_{SW} = 1 - \frac{h}{2}(p_0 + q_0) + R_7$$
$$a_8 \equiv a_{SE} = 1 + \frac{h}{2}(p_0 - q_0) - R_7$$
$$a_0 = -[20 + h^2(p_0^2 + q_0^2) + h(p_E - p_W + h(q_N - q_S)$$

and where

$$R_7 = \frac{h}{8}(q_E - q_W + p_N - p_S) + \frac{h^2}{4}p_0 q_0.$$

2.3 Numerical results

As an example, consider the following boundary value problem [6]

$$\begin{cases} -\varepsilon\left(u_{xx}+u_{yy}\right)+u_x=0, & & 0\le x,y\le 1 \\ u_{x,0}=0, & u_{x,1}=0, & 0\le x\le 1 \\ u_{0,y}=sin\pi y, & u_{1,y}=2sin\pi y, & 0\le y\le 1 \end{cases} \tag{2.3.1}$$

Comparison of (2.3.1) and (2.2.1) shows that $-p(x,y) = \dfrac{1}{\varepsilon} = P(say)$, $q(x,y) \equiv 0$ and $f(x,y) \equiv 0$. The exact solution

$$u = e^{px/2} sin\pi y[2e^{-p/2}\sinh\sigma + \sinh\sigma(1-x)]/\sinh\sigma$$

where $\sigma^2 = \pi^2 + P^2/4$, shows the presence of a boundary layer near $x = 1$ whose thickness is of order $1/P$ for P large. The boundary layer is expected to affect the numerical results adversely as P increases.
This problem has been studied by Gartland et al. [2], who proposed a special five point stencil involving modified bessel functions. In *table* $2.1-2.3$ we give some results for this problem.

Table 2.1: Maximum relative error, h=1/32

P	UDS	CDS	SCHOS
10	0.91666(-1)	0.4537(-2)	0.6011(-4)
20	0.1262	0.1576(-1)	0.1399(-3)
40	0.1686	0.5925(-1)	0.1511(-2)
100	0.2264	0.3002	0.3517(-1)

In $Table$ 2.1 the maximum relative errors for $P = 10, 20, 40,$ and 100 for $h = 1/32$ show that the error due to UDS range between 9 and 23 per cent, whereas the CDS gives acceptable results for $P \le 40$ but not for $P = 100$. The errors for SCHOS remain $\le$ 4 per cent. As expected, the maximum relative occur near the corners at $x = 1$ in all cases.

In $Table$ 2.2 the maximum absolute errors for different values of h are given. Numerical estimates for the order of the discretization errors which are obtained by considering the errors due to mesh sizes h and $2h$ are also given. It is clear from the table that the order of SCHOS is about twice that of CDS.

Table 2.2: Maximum absolute error and the estimated orders

P	h^{-1}	CDS	Order	SCHOS	Order
40	8	0.5122		0.1256	
	16	0.2310	1.15	0.2009(-1)	2.65
	32	0.6723(-1)	1.78	0.1712(-2)	3.55
100	8	0.9060		0.4249	
	16	0.5618	0.68	0.1670	1.35
	32	0.2872	0.97	0.3365	2.31
	64	0.9493(-1)	1.60	0.3151(-2)	3.41

Table 2.3: Average relative errors

h^{-1}	CDS	SCHOS	Gartland
8	1.18(-1)	8.13(-2)	6.81(-3)
16	1.46(-1)	1.25(-2)	4.94(-3)
24	1.61(-2)	1.26(-3)	1.90(-3)
32	2.23(-3)	1.79(-4)	5.71(-4)

In order to compare our results with those given by Gartland, we give the average relative error for $P = 100$ in $Table$ 2.3. Clearly, the special method proposed by Gartland gives better results when the mesh is crude. However, as the mesh is refined, the error due to SCHOS are consistently smaller. The order of the Gartland method is not even as high as that of the CDS.

Gartland proposed a boundary correction stencil to be used at mesh points on $x = 1 - h$. Once this correction is done, the results obtained by CDS, SCHOS, and the Gartland scheme are comparable for $h = 1/8$. However, as the mesh is refined, the results given by SCHOS are better than those given by the other two methods.

Chapter 3

A compact finite difference scheme on a non-equidistant mesh (Review)

3.1 Introduction

In this chapter a fourth order compact finite difference scheme for a set of second order ordinary differential equations has been presented [3]. The scheme is based on a non-equidistant mesh, which makes it particularly useful in problems involving shard boundary layers. The derivation of the purely tridiagonal scheme, including boundary conditions, is presented on a one-dimensional non-equidistant mesh.

Generalization of the scheme in more dimensions, using ADI- type schemes, is straightforward. For one-dimensional problems such as

$$c_1y^{''} + c_2y^{'} + c_3y = d$$

with coefficients and right-hand sides that are computed with few arithmetic operations, the fourth-order scheme requires approximately the same computational effort of a second-order scheme for the same accuracy. The coefficients and right hand side are obtained from lengthy calculation and here the use of fourth-order scheme pays because of the reduction of the required number of mesh points.

The basic idea behind compact schemes is that one supplements the second-order differential equation with fourth order relations between the function value y and the spatial first and second derivatives, $F(= y^{'})$ and $S(= y^{''})$, on three adjacent mesh points. In this way, a scheme of fourth order, yet based on only three points, is constructed by Ciment et al. [1]. The required fourth-order relations can be obtained in various ways, e.g., from Taylor's expansion which has been shown later in this chapter. A review on compact methods has been carried out by Hirish [7].

The most straightforward method in which one adds two relations to the differential equation at each inner mesh point and solves the resulting block tridiagonal system for y, F and S has the disadvantage that it requires a boundary condition on the second derivative Ciment et al. [1, 7]. In order to avoid the use of points outside the computational domain, this boundary condition must be based on only two points, which at best is of third order as shown by Hirish [7].

A different approach, attributes to Krause and Hirish [7, 9], does not have this advantage. Here, a system of fourth order relations together with the differential equation on three adjacent mesh points is formulated such that the derivatives F and S can be eliminated [3]. Just one equation for the three function values remains, and one ends up with a purely tridiagonal system. A proper combination of fourth order relations with boundary conditions and the differential equation ensures a fourth order truncation error also at the boundaries. In the present study, the fourth order relations have been derived which has been used as a supplement to the differential equation. Also, the reduction of the system to a tridiagonal one has been discussed and the inclusion of general boundary conditions on the function and its first derivative has been shown.

3.2 Higher order compact finite difference scheme

Consider the one-dimensional convection-diffusion equation

$$c_1 y^{''} + c_2 y^{'} + c_3 y = d. \qquad (3.2.1)$$

We will use the following notations:
$F \equiv y^{'}$, $S \equiv y^{''}$, superscripts +,0,− indicate points $j+1, j$ and $j-1$; $\triangle_+ \equiv x^+ - x^0, \triangle_- \equiv x^0 - x^-$, and $\triangle_t \equiv \triangle_+ + \triangle_-$.

The Taylor's series expansion for the function values of y at points x_{j+1} and x_{j-1} gives

$$y^+ - y^0 \approx \triangle_+ F^0 + \frac{1}{2}\triangle_+^2 S^0 + \frac{1}{6}\triangle_+^3 y^{iii} + \frac{1}{24}\triangle_+^4 y^{iv} + \frac{1}{120}\triangle_+^5 y^v + \frac{1}{720}\triangle_+^6 y^{vi}, \tag{3.2.2}$$

$$y^0 - y^- \approx \triangle_- F^0 - \frac{1}{2}\triangle_-^2 S^0 + \frac{1}{6}\triangle_-^3 y^{iii} + \frac{1}{24}\triangle_-^4 y^{iv} + \frac{1}{120}\triangle_-^5 y^v + \frac{1}{720}\triangle_-^6 y^{vi}, \tag{3.2.3}$$

$$\begin{aligned}\Rightarrow \triangle_- y^+ - \triangle_t y^0 + \triangle_+ y^- \approx & \frac{1}{2}\triangle_+\triangle_-\triangle_t S^0 + \frac{1}{6}\triangle_+\triangle_-(\triangle_+^2 - \triangle_-^2) y^{iii} \\ & + \frac{1}{24}\triangle_+\triangle_-(\triangle_+^3 + \triangle_-^3) y^{iv} \\ & + \frac{1}{120}\triangle_+\triangle_-(\triangle_+^4 - \triangle_-^4) y^{v} \\ & + \frac{1}{720}\triangle_+\triangle_-(\triangle_+^5 + \triangle_-^5) y^{vi}\end{aligned} \tag{3.2.4}$$

$$\begin{aligned}\Rightarrow \triangle_-^2 y^+ + (\triangle_+^2 - \triangle_-^2) y^0 - \triangle_+^2 y^- \approx & \triangle_+\triangle_-\triangle_t + F^0 \frac{1}{6}\triangle_+^2\triangle_-^2\triangle_t y^{iii} \\ & + \frac{1}{24}\triangle_+^2\triangle_-^2(\triangle_+^2 - \triangle_-^2) y^{iv} \\ & + \frac{1}{120}\triangle_+^2\triangle_-^2(\triangle_+^3 + \triangle_-^3) y^{v} \\ & + \frac{1}{720}\triangle_+^2\triangle_-^2(\triangle_+^4 - \triangle_-^4) y^{vi}\end{aligned} \tag{3.2.5}$$

Equation(3.2.4) and (3.2.5) form the basis for the derivation of fourth order relations between $y^{+,0,-}$, $F^{+,0,-}$ and $S^{+,0,-}$.

Differentiating equation (3.2.4) gives

$$\begin{aligned}\triangle_- F^+ - \triangle_t F^0 + \triangle_+ F^- \approx & \frac{1}{2}\triangle_+\triangle_-\triangle_t y^{iii} \\ & + \frac{1}{6}\triangle_+\triangle_-(\triangle_+^2 - \triangle_-^2) y^{iv} \\ & + \frac{1}{24}\triangle_+\triangle_-(\triangle_+^3 + \triangle_-^3) y^{v} \\ & + \frac{1}{120}\triangle_+\triangle_-(\triangle_+^4 - \triangle_-^4) y^{vi}.\end{aligned} \tag{3.2.6}$$

Similarly, differentiating equation (3.2.5) gives

$$\begin{aligned}\triangle_- S^+ - \triangle_t S^0 + \triangle_+ S^- \approx \frac{1}{2}\triangle_+\triangle_-\triangle_t y^{iv} + \frac{1}{6}\triangle_+\triangle_-(\triangle_+^2 - \triangle_-^2)y^v \\ + \frac{1}{24}\triangle_+\triangle_-(\triangle_+^3 + \triangle_-^3)y^{vi},\end{aligned} \tag{3.2.7}$$

Differentiating both these equations once again, we get

$$\begin{aligned}\triangle_-^2 F^+ + (\triangle_+^2 - \triangle_-^2)F^0 - \triangle_+^2 F^- \approx \triangle_+\triangle_-\triangle_t S^0 + \frac{1}{6}\triangle_+^2\triangle_-^2\triangle_t y^{iv} \\ + \frac{1}{24}\triangle_+^2\triangle_-^2(\triangle_+^2 - \triangle_-^2)y^v \\ + \frac{1}{120}\triangle_+^2\triangle_-^2(\triangle_+^3 + \triangle_-^3)y^{vi}\end{aligned} \tag{3.2.8}$$

$$\begin{aligned}\triangle_-^2 S^+ + (\triangle_+^2 - \triangle_-^2)S^0 - \triangle_+^2 S^- \approx \triangle_+\triangle_-\triangle_t y^{iii} + \frac{1}{6}\triangle_+^2\triangle_-^2\triangle_t y^v \\ + \frac{1}{24}\triangle_+^2\triangle_-^2(\triangle_+^2 - \triangle_-^2)y^{vi}\end{aligned} \tag{3.2.9}$$

Substitution of y^{iii} from (3.2.9) and of y^{iv} from (3.2.7) into Eqs. (3.2.4), (3.2.5), (3.2.6) and (3.2.8) yeilds

$$\begin{aligned}\triangle_+\triangle_-\triangle_t y^{iii} \approx \triangle_-^2 S^+ + (\triangle_+^2 - \triangle_-^2)S^0 - \triangle_+^2 S^- - \frac{1}{6}\triangle_+^2\triangle_-^2\triangle_t y^v \\ - \frac{1}{24}\triangle_+^2\triangle_-^2(\triangle_+^2 - \triangle_-^2)y^{vi}\end{aligned}$$

$$\begin{aligned}\frac{1}{2}\triangle_+\triangle_-\triangle_t y^{iv} \approx \triangle_- S^+ - \triangle_t S^0 + \triangle_+ S^- - \frac{1}{6}\triangle_+\triangle_-(\triangle_+^2 - \triangle_-^2)y^v \\ - \frac{1}{24}\triangle_+\triangle_-(\triangle_+^3 + \triangle_-^3)y^{vi}\end{aligned}$$

$$\begin{aligned}&\triangle_- y^+ - \triangle_t y^0 + \triangle_+ y^- - \frac{\triangle_-}{12}(\triangle_+^2 + \triangle_+\triangle_- - \triangle_-^2)S^+ \\ &- \frac{\triangle_t}{12}(\triangle_+^2 + 3\triangle_+\triangle_- + \triangle_-^2)S^0 + \frac{\triangle_+}{12}(\triangle_+^2 - \triangle_+\triangle_- - \triangle_-^2)S^- \\ &\approx \frac{-\triangle_+\triangle_-\triangle_t}{1440}\big(4(\triangle_+ - \triangle_-)(2\triangle_+^2 + 5\triangle_+\triangle_- + 2\triangle_-^2)y^v \\ &+ (3\triangle_+^4 + 2\triangle_+^3\triangle_- - 7\triangle_+^2\triangle_-^2 + 2\triangle_+\triangle_-^3 + 3\triangle_-^4)y^{vi}\big),\end{aligned} \tag{3.2.10}$$

$$
\begin{aligned}
\triangle_- F^+ - \triangle_t F^0 + \triangle_+ F^- - \frac{\triangle_-}{6}(\triangle_- + 2\triangle_+)S^+ \\
-\frac{\triangle_t}{6}(\triangle_+ - \triangle_-)S^0 + \frac{\triangle_+}{6}(\triangle_+ + 2\triangle_-)S^- \\
\approx \frac{-\triangle_+\triangle_-\triangle_t}{720}\big(10(\triangle_+^2 + \triangle_+\triangle_- + \triangle_-^2)y^v \\
+(\triangle_+ - \triangle_-)(4\triangle_+^2 + 5\triangle_+\triangle_- + 4\triangle_-^2)y^{vi}\big)\,,
\end{aligned}
\tag{3.2.11}
$$

$$
\begin{aligned}
\triangle_-^2 y^+ + (\triangle_+^2 - \triangle_-^2)y^0 - \triangle_+^2 y^- - \triangle_+\triangle_-\triangle_t F^0 \\
-\frac{1}{12}\triangle_+\triangle_-^2\triangle_t S^+ - \frac{1}{12}\triangle_+\triangle_-\triangle_t(\triangle_+ - \triangle_-)S^0 \\
+\frac{1}{12}\triangle_+^2\triangle_-\triangle_t S^- \\
\approx \frac{-\triangle_+\triangle_-\triangle_t}{1440}\big(4(2\triangle_+^2 + 3\triangle_+\triangle_- + 2\triangle_-^2)y^v \\
+(\triangle_+ - \triangle_-)(3\triangle_+^2 + 5\triangle_+\triangle_- + 3\triangle_-^2)y^{vi}\big)
\end{aligned}
\tag{3.2.12}
$$

$$
\begin{aligned}
\triangle_-^2 F^+ + (\triangle_+^2 - \triangle_-^2)F^0 - \triangle_+^2 F^- - \frac{1}{3}\triangle_+\triangle_-^2 S^+ \\
-\frac{2}{3}\triangle_+\triangle_-\triangle_t S^0 - \frac{1}{3}\triangle_+^2\triangle_- S^- \\
\approx \frac{-\triangle_+\triangle_-\triangle_t}{360}\big(5(\triangle_+ - \triangle_-)y^v \\
+2(\triangle_+^2 - \triangle{+}\triangle_- + \triangle_-^2)y^{vi}\big)
\end{aligned}
\tag{3.2.13}
$$

Neglecting the fourth order truncation errors, equations (3.2.10)–(3.2.13) supplement the differential equation at the three points considered, i.e, the linear equations

$$c_3^+ y^+ + c_2^+ F^+ + c_1^+ S^+ = d^+ \tag{3.2.14}$$

$$c_3^0 y^0 + c_2^0 F^0 + c_1^0 S^0 = d^0 \tag{3.2.15}$$

$$c_3^- y^- + c_2^- F^- + c_1^- S^- = d^- \tag{3.2.16}$$

form a system of seven equations in nine unknowns. This system is the required compact relation, the tridiagonal scheme. The algebraic manipulation has been used to perform the major part of the elimination process.

Finally, the following compact relation is obtained

$$F_1 y^+ + F_2 y^0 + F_3 y^- = R, \tag{3.2.17}$$

where

$$F_K = E_{1K}E_{24} - E_{2K}E_{14} \qquad (K = 1,2,3), \tag{3.2.18}$$
$$E_K = D_{1K}D_{35} - D_{3K}D_{15} \qquad (K = 1,2,3,4), \tag{3.2.19}$$
$$E_{2K} = D_{2K}D_{35} - D_{3K}D_{25} \qquad (K = 1,2,3,4), \tag{3.2.20}$$
$$R = S_1E_{24} - S_2E_{14} \tag{3.2.21}$$
$$S_1 = T_1D_{35} - T_3D_{15} \tag{3.2.22}$$
$$S_2 = T_2D_{35} - T_3D_{25} \tag{3.2.23}$$

and

$$\begin{aligned}
D_{11} &= -\triangle_-^3 \left(2(6\triangle_+^2 + 6\triangle_+\triangle_- + \triangle_-^2)c_1^+ + \triangle_t^2\triangle_+^2 c_3^+ + 2\triangle_t(2\triangle_+ + \triangle_-)\triangle_+ c_2^+\right), \\
D_{12} &= -2\triangle_t^3 \left((6\triangle_+^2 - 3\triangle_+\triangle_- - \triangle_-^2)c_1^+ + \triangle_t(\triangle_+ - \triangle_-)\triangle_+ c_2^+\right), \\
D_{13} &= 2\triangle_t^3 \left((6\triangle_+^2 + 15\triangle_+\triangle_- + 8\triangle_-^2)c_1^+ + \triangle_t(\triangle_+ + 2\triangle_-)\triangle_+ c_2^+\right), \\
D_{14} &= \triangle_t^3\triangle_+\triangle_- \left(2(3\triangle_+ + \triangle_-)c_1^+ + \triangle_t\triangle_+ c_2^+\right), \\
D_{15} &= \triangle_t\triangle_+^3\triangle_{-0} \left(2(3\triangle_+ + 2\triangle_-)c_1^+ + \triangle_t\triangle_+ c_2^+\right), \\
T_1 &= -\triangle_t^3\triangle_+^2\triangle_-^3 d^+, \\
D_{21} &= 2\triangle_t^4 - c_1^0, \\
D_2 &= \triangle_t^2 \left(-2(3\triangle_+^2 - 2\triangle_+\triangle_- + \triangle_-^2)c_1^0 + \triangle_+^2\triangle_-^2 c_3^0\right), \\
D_{23} &= 2(3\triangle_+ + 4\triangle_-)\triangle_+^3 c_1^0, \\
D_{24} &= \triangle_t\triangle_+\triangle_- \left(2(2\triangle_+^2 + \triangle_+\triangle_- - \triangle_-^2)c_1^0 + \triangle_t\triangle_+\triangle_- c_2^0\right), \\
D_{25} &= 2\triangle_t\triangle_+^3\triangle_- c_1^0, \\
T_2 &= \triangle_t^2\triangle_+^2\triangle_-^2 d^0, \\
D_{31} &= -2\triangle_-^4 c_1^-, \\
D_{32} &= -2\triangle_t^3(3\triangle_+ - \triangle_-)c_1^-, \\
D_{33} &= \triangle_+^2 \left(2(3\triangle_+^2 + 6\triangle_-^2 + 8\triangle_+\triangle_-)c_1^- - \triangle_1^2\triangle_-^2 c_3^-\right), \\
D_{34} &= 2\triangle_t^3\triangle_+\triangle_- c_1^-, \\
D_{35} &= \triangle_t\triangle_+^2\triangle_- \left(2(2\triangle_+ + 3\triangle_-)c_1^- - \triangle_-\triangle_t c_2^-\right), \\
T_3 &= -\triangle_t^2\triangle_+^2\triangle_-^2 d^-.
\end{aligned} \tag{3.2.24}$$

General boundary conditions

$$\beta y + \gamma F = \delta \tag{3.2.25}$$

are easily inserted. We add the linear equation in y and F representing the boundary condition to the system of seven equations (3.2.10)–(3.2.16) for the first interior point from the boundary. Thus, we have eight equations in nine unknowns. Now, processing the elimination procedure not only for $F^{+,0,-}$ and $S^{+,0,-}$, but also for y^{-}(right boundary) or y^{+} (left boundary) yields one equation in two unknown function values, y_{N-1} and y_N respectively. This completes the tridiagonal system with fourth-order boundary conditions on both sides. The coefficients resulting from the elimination procedure at the boundaries are as follows.
At the left boundary

$$H_3 y_1 + H_2 y_2 = P, \tag{3.2.26}$$

with

$$\begin{aligned} H_k &= F_1 G_k - F_k G_1, \qquad && (k = 1, 2, 3), \\ P &= F_1 Q - G_1 R \\ G_k &= \gamma(D_{34} E_{2k} - E_{24} D_{3K}) \qquad && (K = 1, 2), \\ G_3 &= \beta E_{24} D_{35} + \gamma(D_{34} E_{23} - D_{33} E_{24}), \\ Q &= \delta E_{24} D_{35} + \gamma(D_{34} S_2 - E_{24} T_3), \end{aligned} \tag{3.2.27}$$

where F_1, F_2, F_3, D_{ij}, E_{ij}, R, S_2, and T_3 are to be taken from the compact scheme (eqs(3.2.17) $-$ (3.2.24)) at point $j = 2$.
At the right boundary

$$L_1 y_N + L_2 y_{N-1} = M \tag{3.2.28}$$

with

$$L_k = K_k F_3 - K_3 F_k \qquad (k = 1, 2), \tag{3.2.29}$$

$$
\begin{aligned}
M &= F_3 O - K_3 R, \\
K_k &= E_{24} H_k - E_{2k} H_4 \qquad\qquad (k = 1, 2, 3), \\
O &= E_{24} P - H_4 S_2, \\
H_k &= G_k D_{35} - G_5 D_{3k} \qquad\qquad (k = 1, 2, 3, 4), \\
P &= D_{35} Q - G_5 T_3, \\
G_1 &= -\triangle_-^3 \triangle_+ \triangle_t \beta - 2\triangle_-^3 (2\triangle_+ + \triangle_-)\gamma, \\
G_2 &= -2\triangle_t^3 (\triangle_+ - \triangle_-)\gamma, \\
G_3 &= 2\triangle_+^3 (\triangle_+ - 2\triangle_-)\gamma, \\
G_4 &= \triangle_t^3 \triangle_+ \triangle_- \gamma, \\
G_5 &= \triangle_t^3 \triangle_- \triangle_t \gamma, \\
Q &= -\triangle_t \triangle_+ \triangle_-^3 \delta,
\end{aligned}
\tag{3.2.30}
$$

where F_1, F_2, F_3, D_{ij}, E_{ij}, R, S_2, T_3, $\triangle_+$, $\triangle_-$, and $\triangle_t$ are to be taken from the compact scheme at point $j = N - 1$.

3.3 Numerical results

As an example, a simple problem in which a particle source is prescribed as $\alpha x^k y$ has been chosen where α is a constant and x is the spatial coordinate, the particle flux Γ is coupled to the gradient of the density y by a constant diffusion coefficient D [3]. Thus, in a plane geometry, we have

$$\frac{d\Gamma}{dx} = \alpha x^k y \tag{3.3.1}$$

$$\Gamma = -D \frac{dy}{dx}. \tag{3.3.2}$$

These equations combine to the second–order ODE

$$y'' + a x^k y = 0, \tag{3.3.3}$$

with a= $\frac{\alpha}{D}$. The analytical solution is given by

$$y(x) = C_1 \sqrt{x} J_{1/p}\left(\frac{2\sqrt{a}}{p} x^{p/2}\right) + C_2 \sqrt{x} J_{-1/p}\left(\frac{2\sqrt{a}}{p} x^{p/2}\right) \tag{3.3.4}$$

where $J_{1/p}$ is the Bessel function of fractional order $1/p$, p=k+2, and $C_{1,2}$ are the integration constants. Insertion of boundary conditions $y(1) = y_w$ and $y^{'}(0) = 0$, the solution can be written in the form of a power series as

$$y(x) = \frac{y_w}{\sum_{j=0}^{\infty} g_j} \sum_{j=0}^{\infty} g_j x^{(k+2)j} \tag{3.3.5}$$

with

$$g_j = \frac{(-1)^j}{j!\Gamma(1 + j - 1/(k+2))} \left(\frac{\sqrt{a}}{k+2} \right)^{2j-1/(k+2)} \tag{3.3.6}$$

Figure 2 shows the solution of this model equation for $a = 150$ and $k = 10$.

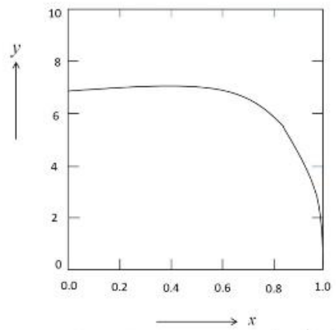

Fig. 2. The solution of the differential equation : $y'' + ax^k y = 0$ for $a = 150$ and $k = 10$.

The coefficients a and k allow for tuning of the width of the boundary layer and of the value of the function at $x = 0$.
The meshes used for numerically solving the equation (3.3.3) are given by

$$x_j = 1 - \left(1 - \frac{j-1}{N-1}\right)^m; \qquad m = 1, 2, 3, 4, \quad j = 1, 2, ..., N. \tag{3.3.7}$$

which enables us to take meshes from equidistant (m=1) to meshes with a high density of points in the boundary layer.

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