COMPUTATIONAL FLUID DYNAMICS [1]

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Contents

Module Information

0.1 Syllabus

Introduction to computational fluid dynamics (CFD), mathematical and numerical models, Navier-Stokes equations, Spatial and temporal discretizations and examples, Finite difference and finite volume schemes and examples, Finite element schemes and examples, Stabilized solution algorithms and examples, Advanced topics including turbulence, examples.

0.2 Assignments and marking scheme

Assignment 1: Allocated 1D finite difference schemes - Programming and writing a report on the performance of the schemes (see Chapter 7 for more details) **Deadline: 5PM, 01.03.2024** [**15% Points**]

Assignment 2: Programming a 1D finite element code and demonstrating the performance of standard and Petrov-Galerkin methods and writing a report (see Chapter 7 for more details)**Deadline: 5PM, 22.03.2024** [**15% Points**]

Optional project: Programming 2D incompressible Navier-Stokes equations using an explicit artificial compressibility method to solve isothermal flow past a square cylinder. [**No points awarded. For your own experience. Deadline: End of Semester**]

0.3 Examination and marking scheme

You will be expected to answer all three questions. All three questions carry equal marks.

There is no guarantee that the examination questions will be uniformly shared between syllabus topics. Thus, you are encouraged to study the entire syllabus. You are also encouraged to prepare from the past examination papers but similar or identical questions from the past papers are not guaranteed. [**70% points**]

Chapter 1

Introduction

1.1 Definition

Computational Fluid Dynamics (CFD) is a subject in which continuous movement of a fluid is modelled using numerical methods. CFD combines several aspects of fluid dynamics including setting up a physical problem, boundary conditions, discretization methods, convergence and accuracy checks and interpretation of results.

1.2 Importance of the Subject

Fluid motion is very common in both natural and man made engineering problems. Following points explain the importance of the topic[1, 2, 3, 4].

(i) Carrying out experiments on certain fluid dynamic problems such as weather forecasting, nuclear explosion and ocean currents is impossible. Computational fluid dynamics plays an important role in obtaining a modelled solution to these problems.

(ii) Cost of carrying out experiments in aerospace and some other applications is very high. A new model aircraft can be analysed and changed using CFD tools before a final wind tunnel test. Thus, CFD saves money and time during the design process.

(iii) Directly measuring certain quantities (Example: drag, Nusselt number) using experimental methods is very difficult. However, using CFD tools these quantities can easily be calculated. Nowadays, it is very common to employ millions of points in a flow calculation. It is, therefore, equivalent to using millions of experimental probes in the flow field. In real experiments, using millions of probes to measure velocity, temperature and pressure is not trivial and is very very expensive.

(iv) In the present age of high performance computing, solution to several complicated turbulent flow problems is possible.

1.3 Numerical Approximations

Figure 1.1 shows some variations of a typical function used in fluid dynamics. If this variation is linear (Figure 1.1, top left), it is a matter of determining two constants from appropriate conditions to represent this variable. The situation is similar if the variation is quadratic

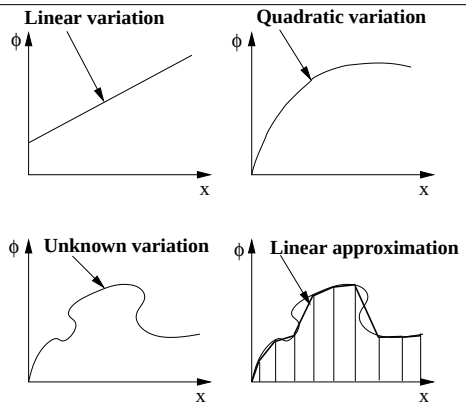


Figure 1.1: Numerical approximation in space

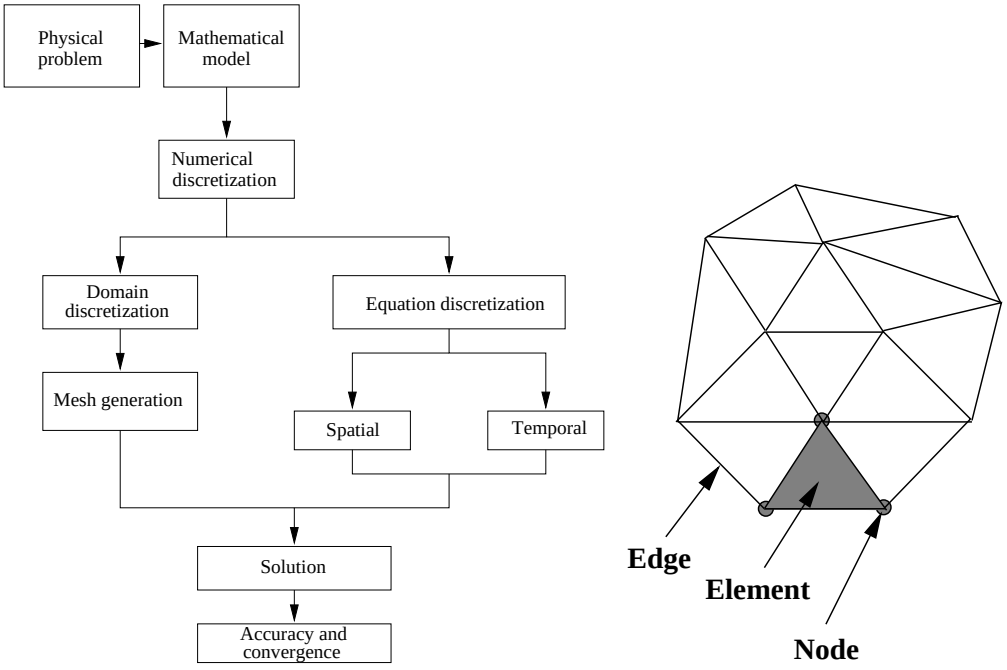
(Figure 1.1, top right) but now we need at least three known conditions to determine this variation. However, if the representation of a variable using analytical relations is either difficult or not possible (Figure 1.1, bottom left), then we may employ an approximation similar to the one shown in Figure 1.1, bottom right. In this figure, a linear variation is applied in small spatial intervals in order to closely represent the true variation. It is obvious from the figure that if the size of the small *spatial* interval introduced approaches zero, the approximate numerical solution approaches the exact solution.

The principles of all numerical approximations are similar to the one explained in Figure 1.1. In a similar fashion, a fluid flow variable can also be *discretized* in time (so called *temporal discretization*).

1.4 Computational Fluid Dynamics (CFD) Model

Figure 1.2 (a)shows a typical CFD model[1, 5]. A CFD model starts with a physical problem and physical approximations to the problem (problem driven approach). The second step is to select an appropriate mathematical model, initial and boundary conditions and then comes the numerical discretization. If a commercial software is employed, the remaining steps to obtain a solution needs little input from a scientist. On the other hand, if the problem is new or a scientist is interested in making progress in the area of algorithms or if he or she is interested to work only with their own numerical codes, then the remaining parts of a CFD model will be essential.

A numerical discretization now has two well coupled divisions as shown in Figure 1.2(a). The first one on the left is domain discretization to physically divide the domain into discrete sub-domains (or points) and the one on the right discretizes the equations for suitably approximating the field variables over the sub-domains. The equation discretization can be further divided into time dependent (temporal) and space dependent (spatial) discretizations. Both the domain and equation discretizations are then combined to get a solution to the physical problem posed at the beginning. Once the solution is obtained and verified, a post processing step will be used to display the results that can be easily understood by an user with fluid dynamics background. A typical domain discretization is shown in Figure 1.2(b).



(a) A typical CFD model

(b) Typical grid or mesh. Elements, nodes and edges

Figure 1.2: CFD model and domain discretization.

1.4.1 Equations and Boundary Conditions

We assume that the Navier-Stokes (NS) equations are the basis for the problems treated in this book. The NS equations can be simplified if necessary. Some of the simplifications include Euler equations, incompressible flow form and Stokes problem. Depending upon the situation, a problem can be approximated in one- or multi-dimensions. Some problems need fluid property variations. Some are initial value problems and others are boundary value problems. Many are initial-boundary value problems. To correctly solve a problem, boundary and initial conditions need to be appropriately established. More details on the NS equations are discussed in Chapter 2. In addition to the NS equations, some additional scalar equations are often necessary to solve some complex problems, such as reactive and turbulent flows.

1.4.2 Numerical Algorithm, Spatial and Temporal Approximations

As mentioned before, an appropriate numerical algorithm needs to be devised. There are several numerical algorithms to solve the Navier-Stokes equations. However, need for fast and accurate solution procedures is, even today, an active research topic. Details of several numerical algorithms are discussed in the latter chapters.

1.4.3 Programming

Once the algorithm to be used is decided, appropriate mathematical expressions and equations need to be programmed using any standard programming tool. The program needs appropriate inputs of the geometry, boundary and initial conditions and it outputs the field variable distributions (velocity components and pressure). Note that in some discretization procedures, the field variables are given at the centre of the elements (Example: cell centered finite volume method).

1.4.4 Pre- and Post- Processing

The mesh generation (domain discretization) and mesh related calculations such as area/volume of the elements or edge coefficients are generally computed at the pre-processing stages. The mesh generation routine may either be part of a main solution routine or a separate program. However, it is very common to do the rest of the pre-processing within the main solution module.

Any calculations or graphical representation of the solution after obtaining the field variable distributions on the nodes is part of a post-processing module. For instance, calculation of stream function, skin-friction or plotting the velocity distribution are part of a post-processing module.

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Chapter 2

Navier-Stokes Equations

2.1 Navier-Stokes Equation in Conservation Form

The Navier-Stokes equations for calculating compressible fluid flow may be written in general conservation form as [1, 2, 3]:

$$\frac{\partial \mathbf{W}}{\partial t} + \frac{\partial \mathbf{F}_j}{\partial x_j} + \frac{\partial \mathbf{G}_j}{\partial x_j} + \mathbf{Q} = \mathbf{0} \tag{2.1}$$

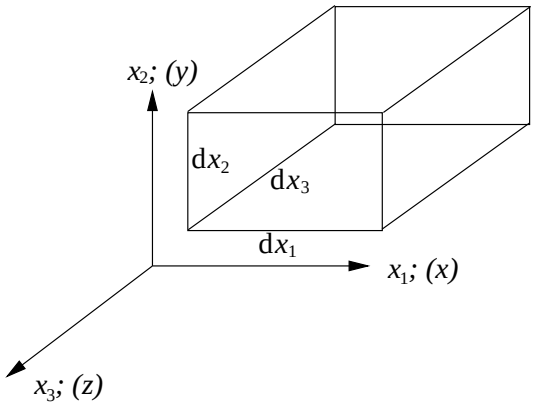

Figure 2.1: Coordinate direction and control volume

where $\mathbf{W}$ is the vector of conservation variables, $\mathbf{F}$ is the Euler flux vector, $\mathbf{G}$ represents the viscous flux vector and $\mathbf{Q}$ the source vector. These terms may be expressed in indicial notation as (see Figure 2.1)

$$\mathbf{W} = \begin{pmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho E \end{pmatrix} \quad \mathbf{F_j} = \begin{pmatrix} \rho u_j \\ \rho u_1 u_j + p\delta_{1j} \\ \rho u_2 u_j + p\delta_{2j} \\ \rho u_3 u_j + p\delta_{3j} \\ \rho E u_j + p u_j \end{pmatrix}$$

$$\mathbf{G_j} = \begin{pmatrix} 0 \\ -\tau_{1j} \\ -\tau_{2j} \\ -\tau_{3j} \\ -u_k\tau_{jk} + q \end{pmatrix} \quad \mathbf{Q} = \begin{pmatrix} 0 \\ -\rho g_1 \\ -\rho g_2 \\ -\rho g_3 \\ -q_h \end{pmatrix}$$

where q is the heat flux ($-k\partial T/\partial x_j$), $\mathbf{g}$ is the acceleration due to gravity, q_h is the heat source. The viscous stress is defined as

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right)$$

where μ is the dynamic viscosity and δ_{ij} is the Kroneker delta ($= 1$ if $i = j$ and $= 0$ if $i \neq j$).

2.2 Navier-Stokes Equation in Non-Conservation Form

To derive the Navier-Stokes Equations in the non-conservation form, we start with the conservation form. The conservation of mass equation is

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0. \tag{2.2}$$

The conservation of momentum equation is

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (u_j \rho u_i)}{\partial x_j} + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} = 0 \tag{2.3}$$

and the conservation of energy equation is

$$\frac{\partial (\rho E)}{\partial t} + \frac{\partial (u_j \rho E)}{\partial x_j} - \frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right) + \frac{\partial (u_j p)}{\partial x_j} - \frac{\partial (\tau_{ij} u_i)}{\partial x_i} = 0. \tag{2.4}$$

Rewriting the momentum equation with terms differentiated as

$$\rho\frac{\partial u_i}{\partial t} + u_i\left(\frac{\partial \rho}{\partial t} + \rho\frac{\partial u_j}{\partial x_j} + u_j\frac{\partial \rho}{\partial x_j}\right) + \rho u_j\frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} = 0. \tag{2.5}$$

The reduced momentum equation is obtained by substituting equation 2.2 into the above equation as

$$\frac{\partial u_i}{\partial t} + u_j\frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} - \frac{1}{\rho}\frac{\partial \tau_{ij}}{\partial x_j} = 0 \tag{2.6}$$

Similarly equation 2.4 can be written with differentiated terms as

$$\begin{aligned} E\left(\frac{\partial \rho}{\partial t} + \rho\frac{\partial u_j}{\partial x_j} + u_j\frac{\partial \rho}{\partial x_j}\right) \quad &+ \quad \rho\frac{\partial E}{\partial t} + \rho u_j\frac{\partial E}{\partial x_j} \\ &- \quad \frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right) + \frac{\partial (u_j p)}{\partial x_j} - \frac{\partial (\tau_{ij} u_j)}{\partial x_i} = 0. \end{aligned} \tag{2.7}$$

Again by substituting equation 2.2 into the above equation, the reduced energy equation is obtained as

$$\frac{\partial E}{\partial t} + u_j \frac{\partial E}{\partial x_j} - \frac{1}{\rho}\frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right) + \frac{1}{\rho}\frac{\partial\left(u_j p\right)}{\partial x_j} - \frac{1}{\rho}\frac{\partial\left(\tau_{ij}u_j\right)}{\partial x_i} = 0. \tag{2.8}$$

The non-conservation form is not suitable for the numerical modelling of compressible flows with strong discontinuities.

2.3 Perfect Gas Model

The compressible flow equations include the variables ρ, u_1, u_2, u_3, p and E. Thus, we need to compute the values of these six variables. However, we only have five equations (Equation 2.1) and an additional equation or constitutive relation is required to close the problem. Here we use the ideal gas law to close the problem. The ideal gas law is given as

$$p = \rho RT; \quad R = c_p - c_v; \quad \gamma = \frac{c_p}{c_v}; \quad c_p = \frac{\gamma}{\gamma - 1}R \tag{2.9}$$

where p is the pressure, ρ is the density, R is the gas constant per unit mass T is the temperature, c_p is the specific heat at constant temperature and c_v is the specific heat at constant volume.

Specific energy, total energy per unit mass and enthalpy

$$e = c_v T = \frac{1}{\gamma - 1}\frac{p}{\rho}; \quad E = e + \frac{1}{2}u_i u_i; \quad h = c_p T = \frac{\gamma}{\gamma - 1}\frac{p}{\rho} \tag{2.10}$$

Mach number and speed of sound

$$M = \frac{|V|}{c}; \quad c^2 = \left(\frac{\partial p}{\partial \rho}\right)_s = \gamma RT = \frac{\gamma p}{\rho} \tag{2.11}$$

Stagnation pressure and temperature

$$\frac{p_o}{p} = \left(\frac{T_o}{T}\right)^{\frac{\gamma}{\gamma-1}} = \left(1 + \frac{\gamma - 1}{2}M^2\right)^{\frac{\gamma}{\gamma-1}}; \quad \frac{T_o}{T} = 1 + \frac{\gamma - 1}{2}M^2 \tag{2.12}$$

2.4 Various Flow Models

Some of the flow models derived from the NS equations are:

(i) Reynolds-averaged Navier-Stokes Equation; (ii) Boundary layer approximation; (iii) Inviscid flow - Euler model; (iv) Inviscid flow - Potential flow model (v) Incompressible flow model

2.4.1 Reynolds-averaged Navier-Stokes Equation

Reynolds averaging is introduced to remove the fluctuations caused by turbulence, without disrupting the other time dependent phenomena.

For any variable A

$$A = \bar{A} + A'$$

where

$$\bar{A}(\vec{x}, t) = \frac{1}{T} \int_{-\frac{-T}{2}}^{\frac{T}{2}} A(\vec{x}, t + \tau)\, d\tau$$

where T is sufficiently large time interval compared to the time scale of the turbulence, yet small enough for the other unsteady phenomena.

For compressible flows, a density weighted average is necessary

$$\tilde{A} = \frac{\overline{\rho A}}{\bar{\rho}}$$

with

$$A = \tilde{A} + A''$$

and

$$\overline{\rho A''} = 0$$

2.4.2 Inviscid flow. Euler flow

The viscous and heat flux terms are removed from the Navier-Stokes equation 2.1, i.e.

$$\frac{\partial \mathbf{W}}{\partial t} + \frac{\partial \mathbf{F}_j}{\partial x_j} + \mathbf{Q} = \mathbf{0} \tag{2.13}$$

2.4.3 Inviscid flow. Potential flow model

- The potential flow model is for non-viscous irrotational flows
- The potential model assumes that the velocity flow field can be modelled by a single scalar function ϕ

The velocity potential ϕ is defined as

$$u = -\frac{\partial \phi}{\partial x}; v = -\frac{\partial \phi}{\partial y}; w = -\frac{\partial \phi}{\partial z} \tag{2.14}$$

Substitution of the above into the Euler equation at steady state leads to

$$\frac{\partial}{\partial x_i}\left(\rho \frac{\partial \phi}{\partial x_i}\right) = 0 \tag{2.15}$$

2.4.4 Isothermal Incompressible Flow

The conservation of mass and momentum equations for an isothermal incompressible flow (no density or temperature variation) may be written as
Continuity

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{2.16}$$

and *Momentum*

$$\rho\frac{\partial u_i}{\partial t} + \rho u_j\frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{2.17}$$

The deviatoric stress components τ_{ij} are related to velocity as

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{2.18}$$

2.5 Non-Dimensional form

The non-dimensional form of the governing equations (example: isothermal incompressible flows) can be obtained by employing a set of approximate non-dimensional scales, such as the ones below.

$$\begin{aligned} u_i^* = \frac{u_i}{u_\infty};\quad \rho^* = \frac{\rho}{\rho_\infty};\quad x_i^* = \frac{x_i}{L};\\ t^* = \frac{tu_\infty}{L};\quad p^* = \frac{p}{\rho_\infty u_\infty^2} \end{aligned} \tag{2.19}$$

where u_∞ is the free stream velocity, ρ_∞ is the free stream density and L is any characteristic length. The non-dimensional form of the equations are (assuming $\rho^* = 1$ for incompressible flows):

The continuity equation:

$$\frac{\partial u_i^*}{\partial x_i^*} = 0 \tag{2.20}$$

and the momentum equation:

$$\frac{\partial u_i^*}{\partial t^*} + u_j^*\frac{\partial u_i^*}{\partial x_j^*} = -\frac{\partial p^*}{\partial x_i^*} + \frac{1}{Re}\frac{\partial \tau_{ij}^*}{\partial x_j^*} \tag{2.21}$$

In the above non-dimensional equations

$$\tau_{ij}^* = \left(\frac{\partial u_i^*}{\partial x_j^*} + \frac{\partial u_j^*}{\partial x_i^*}\right) \tag{2.22}$$

and Re is the Reynolds number given by

$$Re = \frac{u_\infty L}{\nu} \tag{2.23}$$

here $\nu = \mu/\rho_\infty$ is the kinematic viscosity.

2.6 Exercises

E2.1. Derive the non-conservation form of the Euler equations. (substitute continuity equation into other equations). Also reduce the compressible flow equations to non-conservation form of incompressible flow equations.
E2.2. Non-dimensionalise the compressible N-S equations using following scales. Identify the non-dimensional numbers.

$$\begin{aligned} u_i' = \frac{u_i}{u_\infty}; p' = \frac{p}{\rho u_\infty^2}; e' = \frac{e}{u_\infty^2}; t' = \frac{t u_\infty}{L} \\ T' = \frac{T c_p}{u_\infty^2}; x_i' = \frac{x_i}{L}; \mu' = \frac{\mu}{\mu_\infty}; \rho' = \frac{\rho}{\rho_\infty} \end{aligned} \tag{2.24}$$

E2.3. Non-dimensionalise the incompressible N-S equations using following scales and identify the non-dimensional numbers.

$$u_i' = \frac{u_i}{u_\infty}; p' = \frac{p}{\rho u_\infty^2}; t' = \frac{t u_\infty}{L}; x_i' = \frac{x_i}{L}; \mu' = \frac{\mu}{\mu_\infty} \tag{2.25}$$

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Chapter 3

Spatial and temporal discretizations

3.1 Introduction

The discretization method involves two components: spatial and temporal discretizations. The spatial discretization consists of setting up a mesh or a grid by which the continuum of space is replaced by a finite number of points where the numerical values of the variables will have to be determined. It is intuitively obvious that the accuracy of a numerical approximation will be directly dependent on the size of the mesh, that is, the better the discretized space approaches the continuum, the better the approximation of the numerical scheme. In other words, the error of a numerical simulation tends to zero when the mesh size tends to zero, and the rapidity of this variation will be characterized by the order of the numerical discretization of the equations. On the other hand, for complex geometries the solution will also be dependent on the form of the mesh.

Once a mesh has been defined, the equations can be discretized, leading to the transformation of the differential or integral equations to discrete algebraic operations involving the values of the unknowns at the mesh points. For time-dependent problems an intermediate step is obtained, namely a system of ordinary differential equations (ODE's) in time which,through an integration scheme in time, will ultimately lead to an algebraic system for the unknowns at a given time level. For physical time-dependent problems, such as those associated with transient flow behaviour or those connected to time-varying boundary conditions, there is obviously no alternative to the use of a time-dependent mathematical model whereby, in addition, time accuracy of the numerical solution is required. However, with stationary problems an alternative exists, and the user can decide to work with a time-independent formulation, or apply a time-dependent model, and follow the numerical solution in time until the steady state is reached.

3.2 Spatial Discretization

The major spatial discretization methods are the finite difference method, finite volume method and finite element method. The finite difference method (FDM) is a popular technique, whilst the finite element method (FEM) is increasingly used in a variety of problems of fluid dynamics. The finite volume method (FVM) by which the integral form of the conservation laws are discretized can be treated as an independent method due to its flexibility

on unstructured meshes.

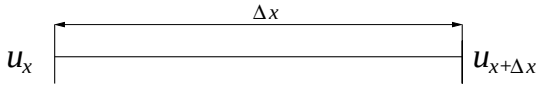

Figure 3.1: One dimensional FDM discretization

3.2.1 Finite Difference Method

The finite difference method is based on the properties of Taylor expansions. It is the oldest of the methods applied to obtain numerical solutions of differential equations, and the first application is considered to have been developed by Euler in 1768. However, it may be the simplest method to apply, especially on uniform meshes, but it requires a high degree of regularity of the mesh. In particular, the mesh have to be set up in a structured way, by which means the mesh points, in an n-dimensional space, are located at the intersections of n family of rectilinear or curved lines. These curves appear as a form of numerical coordinate lines and each point must lie on one, and only one, line of each family.

The forward Taylor expansion of a variable u in space may be written as(Figure 3.1)

$$u_{(x+\Delta x)} = u_{(x)} + \frac{\Delta x}{1!}\frac{\partial u_{(x)}}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 u_{(x)}}{\partial x^2} + \frac{(\Delta x)^3}{3!}\frac{\partial^3 u_{(x)}}{\partial x^3} + \cdots \tag{3.1}$$

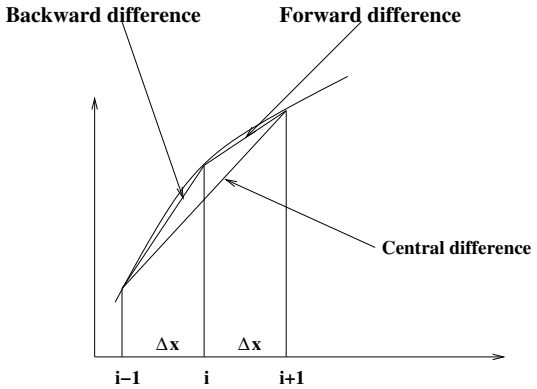

Figure 3.2: Spatial gradient approximations

Similarly a backward Taylor series may be written as

$$u_{(x-\Delta x)} = u_{(x)} - \frac{\Delta x}{1!}\frac{\partial u_{(x)}}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 u_{(x)}}{\partial x^2} - \frac{(\Delta x)^3}{3!}\frac{\partial^3 u_{(x)}}{\partial x^3} + \cdots \tag{3.2}$$

The idea of finite difference methods is actually quite simple, since it corresponds to an estimation of a derivative by the ratio of two differences according to the definition of the derivative. Now we consider three different formula (Figure 3.2). We can write a forward difference formula for a first order derivative by either taking the difference between $i + 1^{th}$

(or $x + \Delta x^{th}$) and i^{th}(or $x^t h$) values of the variable and dividing by the distance between the two points or by using the forward Taylor expansion as

$$\frac{u_{i+1} - u_i}{\Delta x} = \frac{\partial u_i}{\partial x} + O(\Delta x) \tag{3.3}$$

Similarly the backward difference (Figure 3.2 or Equation 3.2) may be written as

$$\frac{u_i - u_{i-1}}{\Delta x} = \frac{\partial u_i}{\partial x} + O(\Delta x) \tag{3.4}$$

The central difference is obtained by taking the difference between the points on both sides of the i^{th} point and dividing the difference by the distance between $i + 1^{th}$ and $i - 1^{th}$ points. Alternatively the central difference formula can be obtained by adding Equations 3.1 and 3.2.

$$\frac{u_{i+1} - u_{i-1}}{2\Delta x} = \frac{\partial u_i}{\partial x} + O(\Delta x)^2 \tag{3.5}$$

The forward difference formula for $\partial u_i / \partial x$ can be considered as a central difference with respect to the point (Figure 3.3)

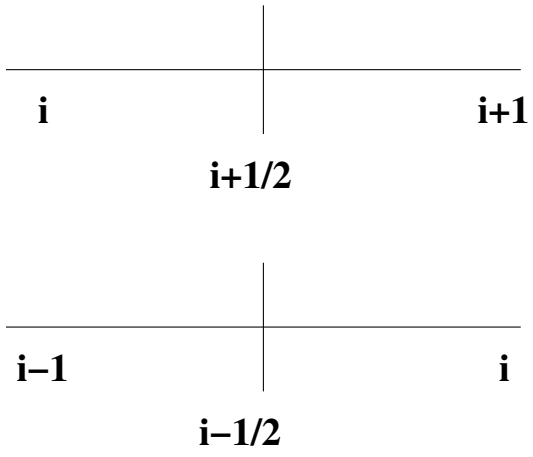

Figure 3.3: Central difference between adjacent points.

$$x_{i+1/2} = \frac{x_i + x_{i+1}}{2} \tag{3.6}$$

$$\left[\frac{\partial u}{\partial x}\right]_{i+1/2} = \frac{u_{i+1} - u_i}{\Delta x} + O(\Delta x)^2 \tag{3.7}$$

$$\left[\frac{\partial u}{\partial x}\right]_{i-1/2} = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x)^2 \tag{3.8}$$

For difference formulas using an arbitrary number of points, a one-side, second-order difference formula for $\partial u_i/\partial x$, containing only the upstream points $i-2$, $i-1$, i, can be obtained by an expression of the form

$$\frac{\partial u_i}{\partial x} = \frac{a u_i + b u_{i-1} + c u_{i-2}}{\Delta x} + O(\Delta x)^2 \tag{3.9}$$

The coefficients (a, b, c) are found from a Taylor expansion. Writing

$$u_{i-1} = u_i - \frac{\Delta x}{1!}\frac{\partial u_i}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 u_i}{\partial x^2} - \frac{(\Delta x)^3}{3!}\frac{\partial^3 u_i}{\partial x^3} + \cdots \tag{3.10}$$

$$u_{i-2} = u_i - \frac{2\Delta x}{1!}\frac{\partial u_i}{\partial x} + \frac{(2\Delta x)^2}{2!}\frac{\partial^2 u_i}{\partial x^2} - \frac{(2\Delta x)^3}{3!}\frac{\partial^3 u_i}{\partial x^3} + \cdots \tag{3.11}$$

Substituting into Equation 3.9 and comparing the coefficients of u_i, $\partial u_i/\partial x$ and $\partial^2 u_i/\partial x^2$, we get

$$a + b + c = 0 \tag{3.12}$$

$$2c + b = -1 \tag{3.13}$$

$$4c + b = 0 \tag{3.14}$$

Substituting a, b and c values

$$\frac{\partial u_i}{\partial x} = \frac{3u_i - 4u_{i-1} + u_{i-2}}{2\Delta x} + O(\Delta x)^2 \tag{3.15}$$

Second order terms

$$\frac{\partial^2 u_i}{\partial x^2} = \frac{\left[\frac{\partial u}{\partial x}\right]_{i+1} - \left[\frac{\partial u}{\partial x}\right]_i}{\Delta x} \tag{3.16}$$

Substituting backward difference for gradients

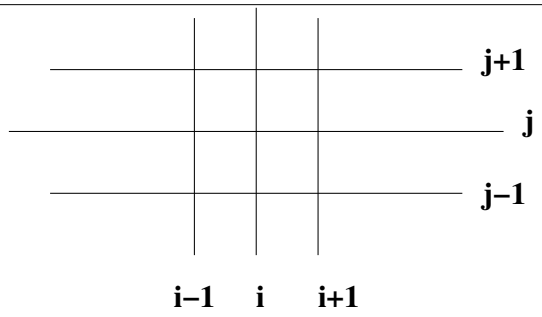

Figure 3.4: Structured grid

$$\frac{\partial^2 u_i}{\partial x^2} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + O(\Delta x)^2 \tag{3.17}$$

One sided backward formula

$$\frac{\partial^2 u_i}{\partial x^2} = \frac{u_i - 2u_{i-1} + u_{i-2}}{\Delta x^2} + O(\Delta x)^2 \tag{3.18}$$

Two dimensional FDM (Figure 3.4)

$$\left[\frac{\partial u}{\partial x}\right]_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + O(\Delta x) \tag{3.19}$$

$$\left[\frac{\partial u}{\partial y}\right]_{i,j} = \frac{u_{i,j+1} - u_{i,j}}{\Delta y} + O(\Delta y) \tag{3.20}$$

$$\left[\frac{\partial^2 u}{\partial x^2}\right]_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} + O(\Delta x) \tag{3.21}$$

Mixed derivatives backward difference

$$\left[\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right)\right]_{i,j} = \frac{\partial}{\partial x}(\Psi)_{i,j} = \frac{\Psi_{i,j} - \Psi_{i-1,j}}{\Delta x} + O(\Delta x) \tag{3.22}$$

Substitute

$$\Psi_{i,j} = \left[\frac{\partial u}{\partial y}\right]_{i,j} = \frac{u_{i,j} - u_{i,j-1}}{\Delta y} + O(\Delta y) \tag{3.23}$$

$$\Psi_{i-1,j} = \left[\frac{\partial u}{\partial y}\right]_{i-1,j} = \frac{u_{i-1,j} - u_{i-1,j-1}}{\Delta y} + O(\Delta y) \tag{3.24}$$

$$\left[\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right)\right]_{i,j} = \frac{u_{i,j} - u_{i,j-1} - u_{i-1,j} + u_{i-1,j-1}}{\Delta x \Delta y} + O(\Delta x, \Delta y) \tag{3.25}$$

Similarly forward and central differences can be done. If $\Delta x = \Delta y$, Equation 4.24 is reduced to

$$\left[\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right)\right]_{i,j} = \frac{u_{i,j} - u_{i,j-1} - u_{i-1,j} + u_{i-1,j-1}}{\Delta x^2} + O(\Delta x^2) \tag{3.26}$$

3.2.2 Finite Volume Method

The FVM takes full advantage of an arbitrary mesh, where a large number of options are open for the definition of the control volumes around which the conservation laws are expressed[1, 2]. Modifying the shape and location of the control volumes associated with a given mesh point, as well as varying the rules and accuracy for the evaluation of the fluxes through the control surfaces, gives considerable flexibility to the finite volume method. In addition, by the direct discretization of the integral form of the conservation laws we can ensure that the basic quantities mass, momentum and energy will remain conserved at the discrete level.

One dimensional approximation

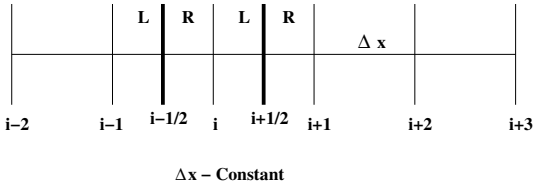

Figure 3.5: One dimensional finite volume method.

The equation in integral conservation form is (Figure 3.5)

$$\frac{d}{dt}\int_x \phi dx + \int_s \boldsymbol{n} f ds = 0 \tag{3.27}$$

$$\begin{aligned} x_{i-1/2} &= x_i - \Delta x/2 \\ x_{i+1/2} &= x_i + \Delta x/2 \\ \phi_{i\pm1/2} &= \phi(x_{i\pm1/2}) \\ f_{i\pm1/2} &= f(\phi_{i\pm1/2}) \end{aligned} \tag{3.28}$$

The conservation equation becomes

$$\frac{d}{dt}(\Delta x \bar{\phi_i}) + f_{i+1/2} - f_{i-1/2} = 0 \tag{3.29}$$

The cell average of a ϕ is calculated as

$$\bar{\phi}_i = \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \phi(x,t)dx \tag{3.30}$$

Taylor expansion of $u(x)$ is

$$\phi_x = \phi_i + \frac{\xi}{1!}\frac{\partial\phi}{\partial x} + \frac{\xi^2}{2!}\frac{\partial^2\phi}{\partial x^2} - \frac{\xi^3}{3!}\frac{\partial^3\phi}{\partial x^3} + \cdots \tag{3.31}$$

where

$$\xi = (x - x_i) \tag{3.32}$$

Now

$$\bar{\phi}_i = \frac{1}{\Delta x}\int_{x_{-\Delta x/2}}^{x_{+\Delta x/2}} \phi(x)dx \tag{3.33}$$

$$= \left[\phi_i + \frac{\Delta x^2}{24}\frac{\partial^2\phi}{\partial x^2} + \frac{\Delta x^4}{1920}\frac{\partial^4\phi}{\partial x^4}\right] + O(\Delta x^6) \tag{3.34}$$

Or

$$\bar{\phi}_i = \phi_i + O(\Delta x^2) \tag{3.35}$$

If $f = u\phi$,

$$\begin{aligned} f^L_{i+1/2} &= u\bar{\phi}_i \\ f^R_{i+1/2} &= u\bar{\phi}_{i+1} \\ f^L_{i-1/2} &= u\bar{\phi}_{i-1} \\ f^R_{i-1/2} &= u\bar{\phi}_i \end{aligned} \tag{3.36}$$

The above expressions lead to discontinuity of fluxes at faces. However, an average will avoid discontinuity, i.e.,

$$\bar{f}_{i+1/2} = \frac{1}{2}\left[f^L_{i+1/2} + f^R_{i+1/2}\right] = \frac{u}{2}\left[\bar{\phi}_i + \bar{\phi}_{i+1}\right] \tag{3.37}$$

$$\bar{f}_{i-1/2} = \frac{1}{2}\left[f^L_{i-1/2} + f^R_{i-1/2}\right] = \frac{u}{2}\left[\bar{\phi}_{i-1} + \bar{\phi}_i\right] \tag{3.38}$$

The final dicrete form of Equation 4.26 is

$$\Delta x \frac{d\bar{\phi}_i}{dt} + \frac{u}{2}\left(\bar{\phi}_{i+1} - \bar{\phi}_{i-1}\right) = 0 \tag{3.39}$$

Which is a second order central finite difference scheme. However, this is not true for mesh with different cell sizes and for unstructured meshes.

Two dimensional approximation

Lets start with the integral form of a scalar equation in two dimensions as[1]

$$\frac{d}{dt}\int_{\Omega} \phi d\Omega + \int_{s} \mathbf{f}.d\mathbf{s} = 0 \tag{3.40}$$

Cell centered approximation

$$\frac{d}{dt}\int_{\Omega} \phi d\Omega + \int_{ABCD} (f dy - g dx) = 0 \tag{3.41}$$

$$f_{AB} = \frac{1}{2}(f_A + f_B) \tag{3.42}$$

and

$$f_A = \frac{1}{4}(f_{ij} + f_{i+1,j} + f_{i+1,j-1} + f_{i,j-1}) \tag{3.43}$$

Simplification results in

$$\int_{ABCD} \mathbf{f}.d\mathbf{s} = \frac{1}{2}[(f_A - f_C)\Delta y_{DB} + (f_B - F_D)\Delta y_{AC} - (g_A - g_C)\Delta x_{DB} - (g_B - g_D)\Delta_{AC}] \tag{3.44}$$

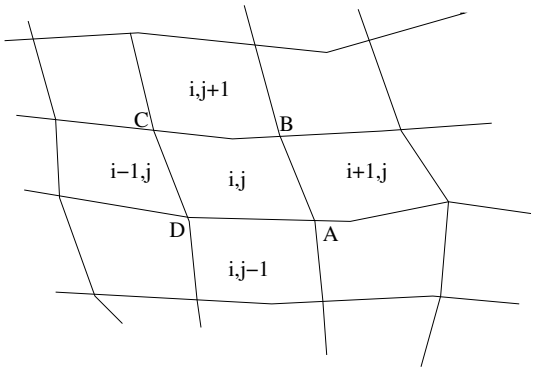

Figure 3.6: Cell centered

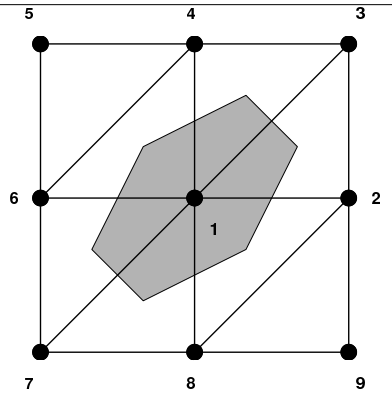

Figure 3.7: Vertex centered

3.2.3 Finite Element Method

The finite element method originated from the field of structural analysis as a result of many years of research, mainly between 1940 and 1960. The concept of 'elements' can be traced back to the techniques used in stress calculations, whereby a structure was subdivided into small substructures of various shapes and re-assembled after each 'element' had been analysed. The development of this technique and its formal elaboration led to the introduction of what is now called the finite element method.

The most widely used weighted residual for of the finite element method is the Galerkin method, in which the weighting functions are taken equal to the interpolation (or shape) function $N_i(x)$. The weighted residual form of a typical differential equation may be written as[3, 4, 5] as

$$\int_{\Omega} W \left[\frac{\partial \hat{\phi}}{\partial t} + u \frac{\partial \hat{\phi}}{\partial x} \right] d\Omega = 0 \tag{3.45}$$

The weights W are related to the approximating functions (shape functions or trail functions) of the system. In the above equation $\hat{\phi}$ is the approximate value of the function and Ω is the volume of the physical domain. For a one-dimensional problem, the weighted residual form may be written as

$$\int_{x} W \left[\frac{\partial \hat{\phi}}{\partial t} + u \frac{\partial \hat{\phi}}{\partial x} \right] dx = 0 \tag{3.46}$$

and the weights W are equal to the shape functions in the Galerkin method, i.e.,

$$\int_{x} \{\mathbf{N}\} \left[\frac{\partial \hat{\phi}}{\partial t} + u \left[\frac{\partial \mathbf{N}}{\partial x} \right] \{\bar{\phi}\} \right] dx = 0 \tag{3.47}$$

where for a set on n number of points,

$$\{\mathbf{N}\} = \left\{ \begin{array}{c} N_1 \\ N_2 \\ .... \\ .... \\ N_n \end{array} \right\}; \quad \{\bar{\phi}\} = \left\{ \begin{array}{c} \phi_1 \\ \phi_2 \\ .... \\ .... \\ \phi_n \end{array} \right\} \tag{3.48}$$

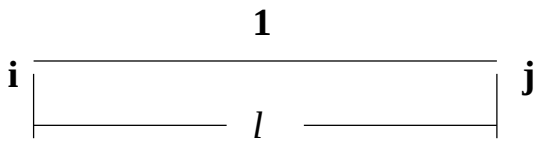

Figure 3.8: One-dimensional finite element.

At the element level, the spatial discretization of linear one-dimensional finite element may be carried out for a function ϕ as (see Figure 3.8):

$$\hat{\phi} = N_i\phi_i + N_j\phi_j \tag{3.49}$$

where subscript i and j are the two nodes of the element as shown in Figure 3.8. The linear functions may be defined as

$$N_i = \frac{x_j - x}{x_j - x_i}; N_j = \frac{x - x_i}{x_j - x_i} \tag{3.50}$$

Note the following properties of approximating or shape functions.

$$N_i + N_j = 1 \tag{3.51}$$

at node i, $N_i = 1$, $N_j = 0$ at node j, $N_i = 0$, $N_j = 1$

Derivatives of the function ϕ may now be written as

$$\frac{\partial\hat{\phi}}{\partial x} = \frac{\partial N_i}{\partial x}\phi_i + \frac{\partial N_j}{\partial x}\phi_j = \left[\begin{array}{cc} \frac{\partial N_i}{\partial x} & \frac{\partial N_j}{\partial x} \end{array} \right] \left\{ \begin{array}{c} \phi_i \\ \phi_j \end{array} \right\} \tag{3.52}$$

The integration of the second term in Equation 3.47 may be written as (assuming $u =$ constant):

$$\begin{aligned} \int_x u \left[\begin{array}{c} N_i \\ N_j \end{array} \right] \left[\begin{array}{cc} \frac{\partial N_i}{\partial x} & \frac{\partial N_j}{\partial x} \end{array} \right] \left\{ \begin{array}{c} \phi_i \\ \phi_j \end{array} \right\} dx &= u \int_x \left[\begin{array}{cc} N_i\frac{\partial N_i}{\partial x} & N_i\frac{\partial N_j}{\partial x} \\ N_j\frac{\partial N_i}{\partial x} & N_j\frac{\partial N_j}{\partial x} \end{array} \right] \left\{ \begin{array}{c} \phi_i \\ \phi_j \end{array} \right\} dx \\ &= \frac{u}{2} \left[\begin{array}{cc} -1 & 1 \\ -1 & 1 \end{array} \right] \left\{ \begin{array}{c} \phi_i \\ \phi_j \end{array} \right\} \end{aligned} \tag{3.53}$$

The elemental equations must be assembled before writing the set of simultaneous equations. Some useful integration formulae for linear approximation are:

One-dimension

$$\int_\Omega N_1^a N_2^b d\Omega = \frac{a!b!l}{(a+b+1)!} \tag{3.54}$$

where l is the length of an element.
Two-dimensions-triangular elements

$$\int_\Omega N_1^a N_2^b N_3^c d\Omega = \frac{a!b!c!2A}{(a+b+c+2)!} \tag{3.55}$$

where A is the area of a triangular element.

3.2.4 Boundary Conditions

1. *Dirichlet boundary condition:* The value of the function is given on a boundary. Implementation of Dirichlet condition is direct.
2. *Neumann boundary condition:* The flux or gradient is given on a boundary.

3.3 Temporal Discretization

The transient terms of any equation can be discretized using the same principles as spatial discretization. By suitably adjusting the time levels in space, different numerical schemes can be created. In order to demonstrate various time discretization techniques, consider the following one dimensional, transient heat conduction equation

$$\rho c_p \frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) = 0 \tag{3.56}$$

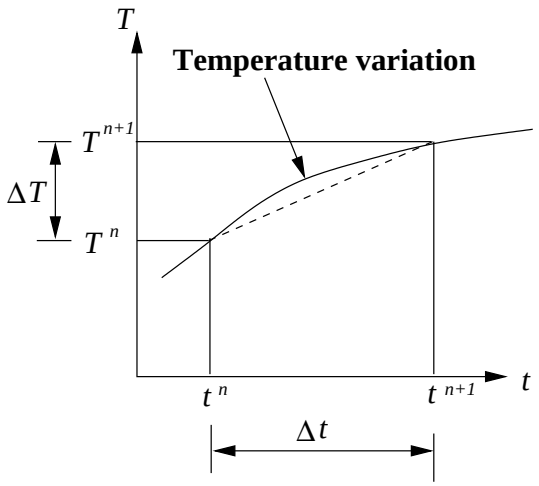

Figure 3.9: Neumann boundary conditions

where ρ is the density of material, c_p is the specific heat of the material, T is the temperature, t is the time and k is the thermal conductivity of the material. Figure 3.9 shows a typical temperature variation in time and possible time discretization methods.

3.3.1 Explicit Methods

Let us assume the thermal conductivity in the above equation is constant and the spatial term is discretized using central difference method. We therefore get a discrete form as

$$\rho c_p \frac{\Delta T}{\Delta t} = k \frac{T^n_{i+2} - T^n_i - T^n_{i+1} - T^n_{i-1}}{2\Delta x^2} \tag{3.57}$$

With reference to Figure 3.9 we can write a simple forward difference for ΔT as

$$\Delta T = T^{n+1} - T^n \tag{3.58}$$

where superscripts $n+1$ (unknown) and n (known) indicate different time levels at an interval of Δt. Substituting into Equation3.57

$$\rho c_p \frac{T^{n+1} - T^n}{\Delta t} = k \frac{T^n_{i+2} - T^n_i - T^n_{i+1} - T^n_{i-1}}{2\Delta x^2} \tag{3.59}$$

Now the question to be answered is at what time level the RHS should be considered. If we consider the RHS to be at nth time level (known), the method is called *explicit*.

3.3.2 Semi-implicit Methods

If we take

$$f = k \frac{T_{i+2} - T_i - T_{i+1} - T_{i-1}}{2\Delta x^2} \tag{3.60}$$

and define

$$f^{n+\theta} = \theta f^{n+1} + (1-\theta) f^n \tag{3.61}$$

we can rewrite Equation 3.59 as

$$\rho c_p \frac{T^{n+1} - T^n}{\Delta t} = f^{n+\theta} \tag{3.62}$$

If $\theta = 0$, we get the explicit scheme discussed in the previous section. If we take $\theta = 0.5$, the scheme is called *semi-implicit*.

3.3.3 Fully- Implicit Methods

In Equation 3.62 if $\theta = 1$, the scheme is implicit.

3.4 Exercises

E4.1. Derive the following central difference equation from Taylor series expansion

$$\frac{u_{i+1} - u_{i-1}}{2\Delta x} = \frac{\partial u_i}{\partial x} + O(\Delta x)^2 \tag{3.63}$$

E4.2. Determine coefficients a,b and c of the following formula from Taylor series of expansion

$$\frac{\partial u_i}{\partial x} = \frac{au_i - bu_{i+1} + cu_{i+2}}{2\Delta x} + O(\Delta x)^2 \tag{3.64}$$

E4.3. Derive the following one-sided backward formula for the second derivative from Taylor series expansion

$$\frac{\partial u_i^2}{\partial x^2} = \frac{u_i - 2u_{i-1} + u_{i-2}}{\Delta x} + O(\Delta x) \tag{3.65}$$

E4.4. Discretize the following equation on a uniform square mesh. Write the central difference equations for the inner points. Assume equal distance between points.

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \tag{3.66}$$

E4.5. Derive the forward and central difference formula for the following mixed derivative.

$$\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right)_{ij} \tag{3.67}$$

E4.6. Derive a second order accurate (both in space and time) finite difference scheme for the one dimensional heat conduction.

E4.7. Discretize the one dimensional heat conduction equation using the Galerkin approximation in space and finite difference approximation in time.

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Chapter 4

Numerical Algorithms

4.1 Introduction

A linear convection (or advection) equation of the type

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = 0 \tag{4.1}$$

is often used in computational fluid dynamics to understand various discretization schemes. In the above equation u is the velocity and assumed to be independent of ϕ.

Another equation commonly employed to understand the discretizations is the non-linear convection-diffusion equation. Such an equation is obtained by simplifying the compressible Navier-Stokes equations and it is often referred to as Burgers' equation, given as

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} = 0 \tag{4.2}$$

The inviscid Burgers' equation is given as

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0 \tag{4.3}$$

The non-linearity in the above inviscid equation allows a discontinuous solution to develop.

The linear convection or convection-diffusion equation is a model problem for scalar transport equations such as temperature and concentration distributions. The non-linear convection or convection-diffusion equation is a good model problem for Invisid or viscous Navier-Stokes equations. Thus, studying the properties of discretization methods for convection-diffusion problems give insight into suitable numerical schemes for solving real life fluid dynamics problems. We use only FDM in the following two sections and extension of the methods to FVM and FEM is generally possible and stright forward.

4.2 Linear Convection-Diffusion Problem

4.2.1 Forward Time Centred Space (FTCS) Scheme

The so called forward in time and central in space (FTCS) scheme in its explicit form may be written using FDM for linear convection equation as

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} = 0 \tag{4.4}$$

This equation is unconditionally unstable, i.e., this scheme will not produce any solution for ϕ at any circumstance. Thus, it is essential to avoid such schemes. The instability is developed by the negative dissipation added by the discretization[1]. Addition of the real diffusion to the equation (convection-diffusion equation) in its discrete form is sufficient to obtain conditional stability as long as a quantity referred to as Peclet number (Pe) is below unity. For convection dominated flows (flow at very high velocities), even with a diffusion term, FTCS scheme is unstable. The FTCS discretization for a convection-diffusion equation is

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} - \nu\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} = 0 \tag{4.5}$$

where ν is the diffusion coefficient. The Peclet number is defined as

$$Pe = \frac{lu}{2\nu} \tag{4.6}$$

where l is the element length (or Δx). As long as $Pe < 1$ the above equation gives a stable solution. If natural diffusion is not available, an artificial diffusion k may replace ν to obtain a conditionally stable solution. However, such an artificial diffusion can be naturally derived using the method called Lax-Wendroff scheme (see Section 4.4).

To demonstrate the instability, consider a convection-diffusion problem in one-dimension with prescribed constant ϕ boundary conditions at both inlet and exit. At inlet $\phi = 1$ and at exit $\phi = 0.0$. The Peclet number is varied for a domain with ten nodes and nine elements as shown in Figure4.1. In this figure, the solid line is generated using the exact solution

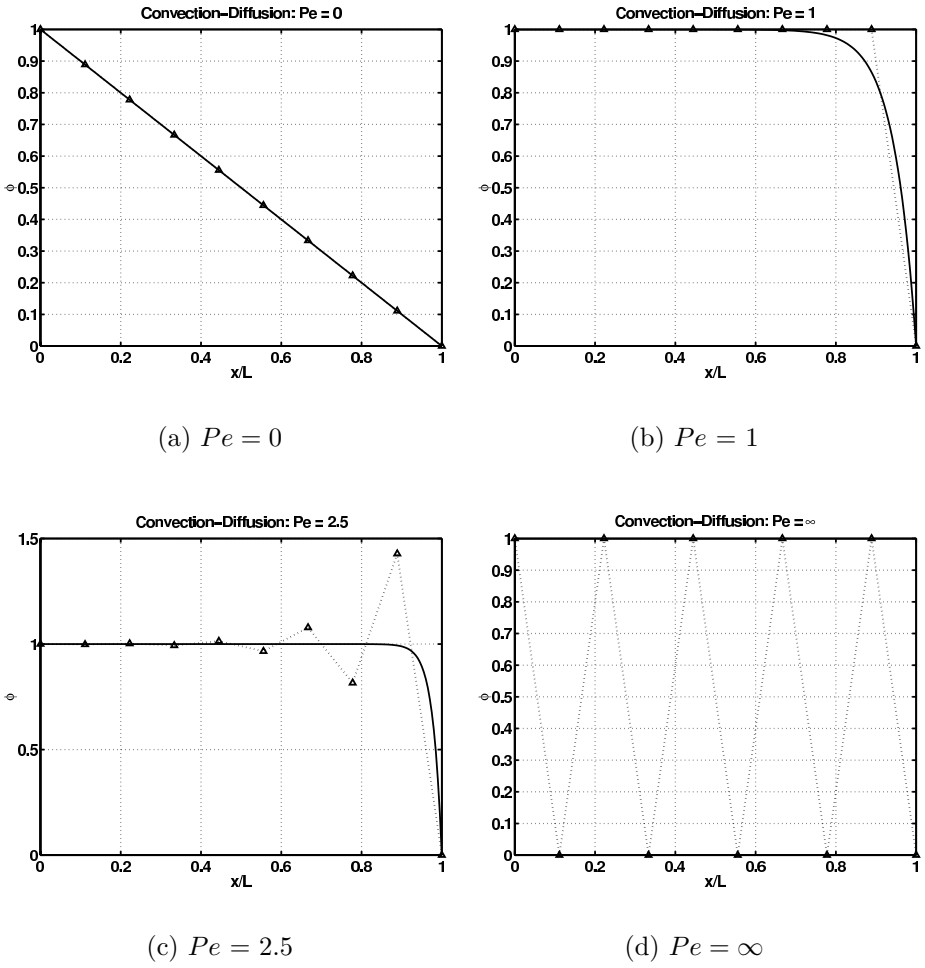
$$\phi = \frac{e^{\frac{ux}{\nu}} - e^{\frac{uL}{\nu}}}{1 - e^{\frac{uL}{\nu}}} \tag{4.7}$$

where L is the total length of the domain. The dotted line with symbols is produced using a FTCS scheme or a steady state solution method. Note that the solution given is for the steady state.

As seen in Figure 4.1, the numerical solution is smooth and accurate until a Peclet number of 1.0. Beyond this value, the solution is oscillatory and inaccurate.

The implicit FTCS scheme is given as

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u\frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} = 0 \tag{4.8}$$



(a) $Pe = 0$ (b) $Pe = 1$

(c) $Pe = 2.5$ (d) $Pe = \infty$

Figure 4.1: A linear convection-diffusion problem. ϕ distribution at different Peclet numbers.

Implicit FTCS is stable.

Von Neumann Stability analysis - Explicit FTCS for linear Convection Equation

Error in space and time may be expressed for a node i at time n using

$$\epsilon_i^n = e^{at} e^{\mathrm{i}kx} \tag{4.9}$$

where a is a constant, t is the time, $\mathrm{i} = \sqrt{-1}$, k is the wave number, x is space, subscript i represents a node and superscript n indicates time instance. Similarly, the error at nodes $i+1$ and $i-1$ may also be expressed respectively as

$$\epsilon_{i+1}^n = e^{at} e^{\mathrm{i}k(x+\Delta x)} \tag{4.10}$$

and

$$\epsilon_{i-1}^n = e^{at} e^{\mathrm{i}k(x-\Delta x)} \tag{4.11}$$

and at time instance $n+1$

$$\epsilon_i^{n+1} = e^{a(t+\Delta t)} e^{\mathrm{i}kx} \tag{4.12}$$

The error of the explicit FTCS method may be expressed using Eq. 4.4 as

$$\frac{\epsilon_i^{n+1} - \epsilon_i^n}{\Delta t} + u\frac{\epsilon_{i+1}^n - \epsilon_{i-1}^n}{2\Delta x} = 0 \tag{4.13}$$

or

$$\epsilon_i^{n+1} = \epsilon_i^n - \frac{\Delta t u}{2\Delta x}(\epsilon_{i+1}^n - \epsilon_{i-1}^n) \tag{4.14}$$

The error amplification factor is defined as

$$G = \left|\frac{\epsilon_i^{n+1}}{\epsilon_i^n}\right| = \frac{e^{a(t+\Delta t)} e^{\mathrm{i}kx}}{e^{at} e^{\mathrm{i}kx}} \tag{4.15}$$

For a stale method,

$$G = e^{a\Delta t} < 1 \tag{4.16}$$

Dividing Eq. 4.14 by ϵ_i^n gives

$$e^{a\Delta t} = 1 - \frac{u\Delta t}{\Delta x}\left(\frac{e^{\mathrm{i}k\Delta x} - e^{-\mathrm{i}k\Delta x}}{2}\right) \tag{4.17}$$

Noting

$$\mathrm{i}\ sin(k\Delta x) = \left(\frac{e^{\mathrm{i}k\Delta x} - e^{-\mathrm{i}k\Delta x}}{2}\right) \tag{4.18}$$

and defining the Courant Fridrichs Lewy (CFL) number as

$$CFL = \frac{u\Delta t}{\Delta x} \tag{4.19}$$

we can rewrite Eq. 4.17 as

$$G = \left|e^{a\Delta t}\right| = |1 - (CFL)\ \mathrm{i}\ sin(k\Delta x)| \tag{4.20}$$

Recollect, G must be less than 1 for a stable scheme, i.e.,

$$|1 - (CFL)\ \mathrm{i}\ sin(k\Delta x)| < 1 \tag{4.21}$$

or

$$|1 - (CFL)\ \mathrm{i}\ sin(k\Delta x)|^2 < 1 \tag{4.22}$$

i.e,

$$1 + (CFL)^2 sin^2(k\Delta x) < 1 \tag{4.23}$$

The above condition will never be satisfied and thus explicit FTCS method for a linear convection equation is unconditionally unstable.

4.2.2 Upwind Schemes

The first order explicit upwind scheme is given as:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u\frac{\phi_i^n - \phi_{i-1}^n}{\Delta x} = 0 \tag{4.24}$$

Explicit scheme is conditionally stable. A von Neumann stability analysis gives a ourant-Friedrichs-Lewy (CFL) condition of $0 \leq c \leq 1$, where $c = u\Delta t/\Delta x$. The implicit first order upwind scheme is given as:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u\frac{\phi_i^{n+1} - \phi_{i-1}^{n+1}}{\Delta x} = 0 \tag{4.25}$$

The implicit scheme is stable. Higher order upwind scheme for a 1D linear convection equation may be written as(with u positive)

$$\frac{\partial \phi}{\partial x} = a\phi_{i-2} + b\phi_{i-1} + c\phi_i + \phi_{i+1} \tag{4.26}$$

For negative u values

$$\frac{\partial \phi}{\partial x} = a\phi_{i+2} + b\phi_{i+1} + c\phi_i + \phi_{i-1} \tag{4.27}$$

An extension of the upwinding methods to convection-diffusion is possible by adding the central difference of the second order scheme to the above discrete forms.

The Von Neumann stability analysis of first order explicit upwind method for linear convection equation gives

$$G^2 = 1 - (CFL)(1 - CFL)[1 - cos\ (k\Delta x)] \tag{4.28}$$

The $G < 1$ condition, i.e., $\{1 - (CFL)(1 - CFL)[1 - cos\ (k\Delta x)]\} < 1$, gives $CFL \leq 1$. Thus, the first order explicit upwind method for linear convection equation is conditionally stable.

4.2.3 Lax Method

In FTCS scheme, if we replace ϕ_i^n with and averaged term

$$\frac{1}{2}(\phi_{i+1}^n + \phi_{i-1}^n) \tag{4.29}$$

we obtain the following Lax method.

$$\frac{\phi_i^{n+1} - (\phi_{i+1}^n + \phi_{i-1}^n)/2}{\Delta t} + u\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} = 0 \tag{4.30}$$

This is a first order in time and second order in space scheme with CFL condition $|c| \leq 1$.

4.2.4 Leap Frog Scheme

If both the transient and spatial derivatives are discretized using a central difference method, the resulting discretization will be second order accurate in both space and time, i.e,

$$\frac{\phi_i^{n+1} - \phi_i^{n-1}}{2\Delta t} + u\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} = 0 \tag{4.31}$$

This scheme is conditionally stable with a CFL condition of $|c| \leq 1$.

4.2.5 Lax-Wendroff Scheme

If natural diffusion ν is not available, a Lax-Wendroff scheme may be used to solve a convection equation. The Lax-Wendroff scheme for convection equation may be obtained by replacing ν with $\Delta t u^2/2$. Note that the Lax-Wendroff coefficient has a dimension of m^2/s, same as a diffusion coefficient. The Lax-Wendroff scheme may be written as

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x} - \frac{\Delta t u^2}{2}\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2} = 0 \tag{4.32}$$

The above scheme can be derived from Taylor series expansion and this scheme is second order accurate in both time and space. The Courant-Friedrichs-Lewy(CFL) number $\frac{\Delta t u}{\Delta x}$ must be maintained below unity to obtain conditional stability. To obtain an oscillation free solution, the convection should be limited to the diffusion limit, i.e.,

$$\frac{u}{2\Delta x} \leq \frac{\Delta t u^2}{2\Delta x^2} \tag{4.33}$$

Assuming, $\Delta t u^2/2 = k$ a diffusion coefficient, we have

$$\frac{u\Delta x}{2k} \leq 1 \tag{4.34}$$

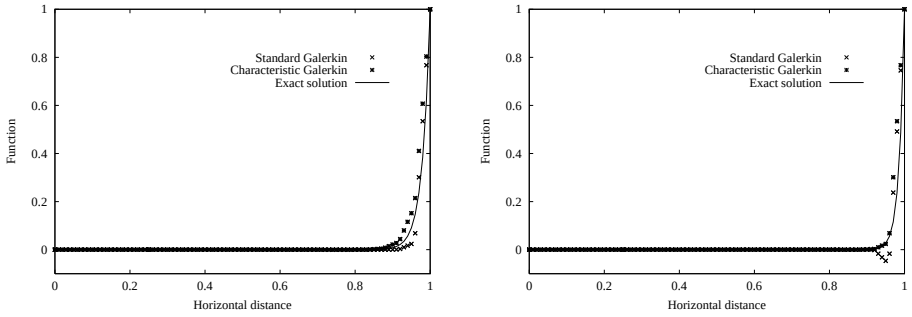
which has the same structure as the real element Peclet number defined in Equation 4.6. There are many other methods available to solve both scalar and vector equations[1, 2].

Figure 4.2 shows the ϕ distribution for the linear convection-diffusion problem discussed in Section 4.2. The number of elements used here are much higher than the ones used in Section 4.2. As seen, the solution from standard and stabilized discretizations are accurate and oscillation free at $Pe = 1$. However, at $Pe = 1.5$, only the stabilized method is oscillation free and accurate.

4.2.6 Two-Step Lax Wendroff Method

The Lax Wendroff scheme can be carried out in two steps as
Step 1:

$$\frac{\phi_{i+1/2}^{n+1/2} - (\phi_{i+1}^n + \phi_i^n)/2}{\Delta t/2} + u\frac{\phi_{i+1}^n - \phi_i^n}{\Delta x} = 0 \tag{4.35}$$



(a) $Pe = 1.0$ (b) $Pe = 1.5$

Figure 4.2: A linear convection-diffusion problem. Comparison of standard and stable discretizations. Galerkin = standard; Characteristic Galerkin ≈ Lax-Wendroff.

Step 2:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u\frac{\phi_{i+1/2}^{n+1/2} - \phi_{i-1/2}^{n+1/2}}{\Delta x} = 0 \tag{4.36}$$

The accuracy and stability conditions are identical to that of the standard Lax-Wendroff scheme discussed in Section 4.2.5.

4.2.7 MacCormack Method

This is a widely used scheme due to the fact that $i + 1/2$ or $i - 1/2$ terms are avoided but maintains same accuracy and stability conditions as the Lax-Wendroff scheme. This scheme has two steps. First step is often referred to as the predictor step and the second is the corrector step. They are given as
Predictor step:

$$\phi_i^{n+1p} = \phi_i^n - u\frac{\Delta t}{\Delta x}(\phi_{i+1}^n - \phi_i^n) \tag{4.37}$$

Corrector step:

$$\phi_i^{n+1} = \frac{1}{2}\left[\phi_i^n + \phi_i^{n+1p} - u\frac{\Delta t}{\Delta x}(\phi_i^{n+1p} - \phi_{i-1}^{n+1p})\right] \tag{4.38}$$

where superscript p indicates an intermediate quantity.

4.2.8 Crank-Nicholson Schemes (Semi-implicit)

We can write the discretization of the linear convection equation with a weighting factor θ as

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u\left[\frac{\phi_{i+1}^{n+\theta} - \phi_{i-1}^{n+\theta}}{2\Delta x}\right] = 0 \tag{4.39}$$

where

$$\phi^{n+\theta} = \theta\phi^{n+1} + (1-\theta)\phi^{n} \tag{4.40}$$

The truncation error clearly depends on a weighting factor θ. With $\theta = 0$, the explicit scheme is obtained and the truncation error is $O(\Delta t, \Delta x^2)$. As a special case, when $\theta = 1/2$ and the scheme is perfectly centred in both time and space, the error is $O(\Delta t^2, \Delta x^2)$, and hence more accurate. For $\theta = 1/2$ the scheme is second order in time and is known as the trapezium formula or the Crank-Nicholson scheme (Crank-Nicholson, 1947). The scheme is commonly employed because of its unconditional stability and inexpensive higher-order accuracy. The scheme is given as

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u\left[\frac{1}{2}\frac{\phi_{i+1}^{n+1} - \phi_{i-1}^{n+1}}{2\Delta x} + \frac{1}{2}\frac{\phi_{i+1}^{n} - \phi_{i-1}^{n}}{2\Delta x}\right] = 0 \tag{4.41}$$

As seen the RHS is equally divided between the n^{th} and $n+1^{th}$ time levels. Due to this, a matrix inversion procedure is essential to solve Equation 4.41.

4.2.9 Runge-Kutta Methods

Tunge-Kutta method is normally used in the numerical solution of ordinary differential equations. In this section, we discuss the implementation of the Runge-Kutta method for the solution of partial differential equations. From the fundamentals of numerical discretization of initial-boundary valve problems, it is often spatial derivatives of the equations are discretized first. Once the spatial terms of are discretized, the equation becomes an ordinary differential equation in time. Thus, if we assume that the convection equation can be written in terms of a residual as

$$\frac{\partial \phi}{\partial t} = R(\phi) \tag{4.42}$$

we can use the Runge-Kutta method to get a desired time integration and discretization accuracy. The second order Runge-Kutta method may be written in two steps as
Step 1:

$$\phi^{(1)} = \phi^n + \Delta t R^n \tag{4.43}$$

where

$$R^n = R(\phi^n) = -u\frac{\partial \phi}{\partial x}^n \tag{4.44}$$

Step 2:

$$\phi^{n+1} = \phi^n + \frac{\Delta t}{2}(R^n + R^{(1)}) \tag{4.45}$$

where

$$R^{(1)} = R(\phi^{(1)}) = u\frac{\partial \phi^{(1)}}{\partial x} \tag{4.46}$$

From Equation 4.43, we can write

$$\frac{\partial \phi^{(1)}}{\partial x} = \frac{\partial \phi^{n}}{\partial x} + \Delta t \frac{\partial R^n}{\partial x} \tag{4.47}$$

Substituting Equations 4.44 and 4.47 into Equation 4.46 we get

$$R^{(1)} = -u\frac{\partial \phi^{n}}{\partial x} + u^2 \Delta t \frac{\partial^2 \phi^{n}}{\partial x^2} \tag{4.48}$$

Substituting $R^{(1)}$ and R^n into Equation 4.45 gives the final form of step 2 as

$$\phi^{n+1} = \phi^n + \frac{\Delta t}{2}\left[-2u\frac{\partial \phi^{n}}{\partial x} + u^2 \Delta t \frac{\partial^2 \phi^{n}}{\partial x^2}\right] \tag{4.49}$$

If a central difference is used to discretize the derivatives, the above scheme will be second order accurate in both space and time. In a similar fashion, a fourth order Runge-Kutta scheme may be derived as
Step 1:

$$\phi^{(1)} = \phi^n + \frac{\Delta t}{2} R^n \tag{4.50}$$

Step 2:

$$\phi^{(2)} = \phi^n + \frac{\Delta t}{2} R^{(1)} \tag{4.51}$$

Step 3:

$$\phi^{(3)} = \phi^n + \Delta t R^{(2)} \tag{4.52}$$

Step 4:

$$\phi^{n+1} = \phi^n + \frac{\Delta t}{6}(R^n + 2R^{(1)} + 2R^{(2)} + R^{(3)}) \tag{4.53}$$

With central difference for spatial derivatives, the fourth order Runge-Kutta scheme gives a fourth order accuracy in time and second order accuracy in space.

4.3 Burgers Equation

The Burgers invisid equation (Equation 4.3) can be rewritten in conservation form as

$$\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} = 0 \tag{4.54}$$

with $F = 0.5u^2$. The above equation can be written in terms of a Jocobian matrix as

$$\frac{\partial u}{\partial t} + A\frac{\partial u}{\partial x} = 0 \tag{4.55}$$

where A is the Jacobian matrix and is given as $\partial F/\partial u = u$. Since the Burger' equation is one-dimensional matrix A has only one component. This matrix is large for multi-dimensional flow equations as discussed in Chapter **??**. Following sections explain a few solution methods for solving both inviscid and viscous Burgers equation.

4.3.1 FTCS Representation

FTCS representation of viscous Burgers' equation (Equation 4.2) in non-conservation form is given as

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + u_i^n \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} - \nu \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2} = 0 \tag{4.56}$$

and in conservation form

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{F_{i+1}^n - F_{i-1}^n}{2\Delta x} - \nu \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2} = 0 \tag{4.57}$$

with $F = 0.5u^2$

4.3.2 Lax method

This is a first order method and similar to the one discussed for linear convection equation in Section 4.3.2. The Lax representation of the Burgers' equation is

$$u_i^{n+1} = \frac{u_{i+1}^n + u_{i-1}^n}{2} - \frac{\Delta t}{\Delta x} \frac{F_{i+1}^n - F_{i-1}^n}{2} \tag{4.58}$$

The stability condition is $|\Delta t u_{max}/\Delta x| \leq 1$, where u_{max} is the maximum eigenvalue of matrix A. The finite volume equivalent of Lax method may be written as

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x} \left[f_{i+1/2}^n - f_{i-1/2}^n \right] \tag{4.59}$$

where f terms are the numerical fluxes at the finite volume interfaces (see Chapter 3), given as (for Lax representation)

$$f_{i+1/2} = \frac{1}{2} \left[F_i + F_{i+1} - \frac{\Delta x}{\Delta t} (u_{i+1} - u_i) \right] \tag{4.60}$$

and

$$f_{i-1/2} = \frac{1}{2} \left[F_i + F_{i-1} - \frac{\Delta x}{\Delta t} (u_i - u_{i-1}) \right] \tag{4.61}$$

The last term can be altered to increase the order of the scheme. Substituting Equations 4.60 and 4.61 into Equation 4.59 gives Equation 4.58.

4.3.3 Lax-Wendroff Scheme

The inviscid Burgers' equation in conservation form is

$$\frac{\partial u}{\partial t} = -\frac{\partial F}{\partial x} \tag{4.62}$$

Differentiate **w.r.t.** t:

$$\frac{\partial^2 u}{\partial t^2} = -\frac{\partial}{\partial x}\left[\frac{\partial F}{\partial t}\right] \tag{4.63}$$

to obtain

$$\frac{\partial F}{\partial t} = \frac{\partial F}{\partial u}\frac{\partial u}{\partial t} = A\frac{\partial u}{\partial t} = -A\frac{\partial F}{\partial x} \tag{4.64}$$

and finally

$$\frac{\partial^2 u}{\partial t^2} = -\frac{\partial}{\partial x}\left[\frac{\partial F}{\partial t}\right] = \frac{\partial}{\partial x}\left[A\frac{\partial F}{\partial x}\right] \tag{4.65}$$

with $A = \frac{\partial F}{\partial u} = u$ is Jacobian. Substituting Equations 4.62 and 4.65 into the Taylor expansion of u^{n+1} gives

$$u^{n+1} = u^n - \Delta t\frac{\partial F}{\partial x}^n + \frac{\Delta t^2}{2}\frac{\partial}{\partial x}\left[A\frac{\partial F}{\partial x}\right] \tag{4.66}$$

Finite volume disctrization gives

$$\begin{aligned} u_i^{n+1} &= u_i^n - \frac{\Delta t}{2\Delta x}\left(F_{i+1}^n - F_{i-1}^n\right) + \frac{1}{2}\left[\frac{\Delta t}{\Delta x}\right]^2\left[A_{i+1/2}\left(F_{i+1} - F_i\right)\right] \\ &\quad -\frac{1}{2}\left[\frac{\Delta t}{\Delta x}\right]^2\left[A_{i-1/2}\left(F_i^n - F_{i-1}^n\right)\right] \end{aligned} \tag{4.67}$$

where

$$\begin{aligned} A_{i+1/2} &= u_{i+1/2} = \frac{u_i + u_{i+1}}{2} \\ A_{i-1/2} &= u_{i-1/2} = \frac{u_i + u_{i-1}}{2} \end{aligned} \tag{4.68}$$

4.3.4 MacCormack Method

The predictor and corrector steps of the MacCormack method are
Predictor step:

$$u_i^{n+1p} = u_i^n - \frac{\Delta t}{\Delta x}(F_{i+1}^n - F_i^n) \tag{4.69}$$

Corrector step:

$$u_i^{n+1} = \frac{1}{2}\left[u_i^n + u_i^{n+1p} - \frac{\Delta t}{\Delta x}(F_i^{n+1p} - F_{i-1}^{n+1p})\right] \tag{4.70}$$

where superscript p indicates an intermediate quantity.

4.3.5 Semi-Implicit Method

A semi-implicit of the form

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{2}\left[\left(\frac{\partial F}{\partial x}\right)^n + \left(\frac{\partial F}{\partial x}\right)^{n+1}\right] \tag{4.71}$$

The linearisation of the flux term at $n+1$ may be carried out using

$$F^{n+1} \approx F^n + \frac{\partial F}{\partial u}^n (u^{n+1} - u^n) = F^n + A^n(u^{n+1} - u^n) \tag{4.72}$$

Substituting,

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{2}\left\{2\left(\frac{\partial F}{\partial x}\right)^n + \frac{\partial}{\partial x}\left[A^n(u_i^{n+1} - u_i^n)\right]\right\} \tag{4.73}$$

The spatial derivatives can now be discretized using central difference scheme. However, the scheme needs additional damping of the form

$$-\frac{k}{8}(u_{i+2}^n - 4u_{i+1}^n + 6u_i^n - 4u_{i-1}^n + u_{i-1}^n) \tag{4.74}$$

needs to be added to the discretization to stabilize the method. Above equation is fourth order and k is the user specified coefficient with a value between 0 and 1.

4.3.6 Other Methods

There are many other very useful and practical methods such as Roe and TVD schemes are widely used in the solution of the invisid Burgers' equation. If time permits, these methods will be discussed during the lectures.

4.4 Stabilized Finite element schemes

4.4.1 Petrov-Galerkin scheme

The first possibility is that of the use of a Petrov–Galerkin type of weighting in which $W_a \neq N_a$ [2].

$$W_a = N_a + \alpha W_a^\star \tag{4.75}$$

where $W_a^\star$ is such that (to obtain finite difference equivalent)

$$\int_{\Omega_e} W_a^\star \mathrm{d}x = \pm\frac{h}{2} \tag{4.76}$$

the sign depending on whether U is a velocity directed toward or away from the node. With this approximation discretization of a convection-diffusion equation becomes

$$\begin{aligned}\int_\Omega (N_a + \alpha W_a^\star)\left[U\,\frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} + Q\right]\mathrm{d}\Omega + \int_\Omega (\frac{\mathrm{d}N_a}{\mathrm{d}x} + \alpha\frac{\mathrm{d}W_a^\star}{\mathrm{d}x})k\frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x}\,\mathrm{d}\Omega \\ - (N_a + \alpha W_a^\star)\,\bar{q}_n\Big|_{\Gamma_q} = 0\end{aligned} \tag{4.77}$$

Various forms of $W_a^\star$ are possible, but the most convenient is the following simple definition which is, of course, a discontinuous function (continuity requirements are discussed below)

$$W_a^\star = \frac{h}{2}\,\frac{U}{|U|}\,\frac{\mathrm{d}N_a}{\mathrm{d}x} \tag{4.78}$$

where $|U|$ denotes absolute value. With the above weighting functions a typical node a becomes

$$[-Pe(\alpha+1)-1]\tilde{\phi}_{a-1} + [2+2\alpha(Pe)]\tilde{\phi}_a + [-Pe(\alpha-1)-1]\tilde{\phi}_{a+1} + \frac{Qh^2}{k} = 0 \tag{4.79}$$

where Q is assumed constant for the whole domain and equal length elements are used.

Immediately we see that with $\alpha = 0$ the standard Galerkin approximation is recovered. Now if the value of α is chosen as

$$\alpha = \alpha_{\text{opt}} = \coth|Pe| - \frac{1}{|Pe|} \tag{4.80}$$

then exact nodal values will be given *for all values of Pe*. The proof of this is given in references for the present, one-dimensional, case where it is also shown that if

$$\alpha > \alpha_{\text{crit}} = 1 - \frac{1}{|Pe|} \tag{4.81}$$

oscillatory solutions never arise.

4.4.2 Balancing diffusion in one dimension

The effect of using the Petrov–Galerkin procedure is equivalent to the use of a standard Galerkin process with the addition of a diffusion (without source)

$$k_b = \tfrac{1}{2}\alpha U h \tag{4.82}$$

to the original differential equation. One can easily verify that with this substituted into the original equation, thus writing now

$$U\frac{\mathrm{d}\phi}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left[(k+k_b)\frac{\mathrm{d}\phi}{\mathrm{d}x}\right] + Q = 0 \tag{4.83}$$

4.4.3 Galerkin least-squares scheme

Here another procedure is presented which again will produce similar results. In this a combination of the standard Galerkin and least squares approximation is made. The convection diffusion equation is re-written as

$$\mathcal{L}(\phi) + Q = 0 \qquad \phi \approx \widehat{\phi} = \mathbf{N}\tilde{\boldsymbol{\phi}} \tag{4.84a}$$

with

$$L = U\frac{\mathrm{d}}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k\frac{\mathrm{d}}{\mathrm{d}x}\right) \tag{4.84b}$$

the standard Galerkin approximation gives for the a-th equation

$$\int_\Omega N_a\left[\mathcal{L}(\widehat{\phi}) + Q\right]\mathrm{d}x = 0 \tag{4.85}$$

with boundary conditions omitted for simplicity. Similarly, a least squares minimization of the residual $R = \mathcal{L}(\widehat{\phi}) + Q$ results in

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\tilde{\phi}_a}\int_\Omega R^2\mathrm{d}x = \int_\Omega \frac{\mathrm{d}\mathcal{L}(\widehat{\phi})}{\mathrm{d}\tilde{\phi}_a}[\mathcal{L}(\widehat{\phi}) + Q]\mathrm{d}x \tag{4.86}$$

or

$$\int_\Omega\left[U\frac{\mathrm{d}N_a}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k\frac{\mathrm{d}N_a}{\mathrm{d}x}\right)\right](\mathcal{L}(\widehat{\phi}) + Q)\mathrm{d}x = \int_\Omega \mathcal{L}(N_a)\left[\mathcal{L}(\widehat{\phi}) + Q\right]\mathrm{d}x \tag{4.87}$$

If the final approximation is written as a linear combination of Eqs (4.85) and (4.87), we have

$$\begin{gathered}\int_\Omega\left[N_a + \lambda\left(U\frac{\mathrm{d}N_a}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k\frac{\mathrm{d}N_a}{\mathrm{d}x}\right)\right)\right](\mathcal{L}(\widehat{\phi}) + Q)\mathrm{d}x = 0 \\ \text{or} \\ \int_\Omega\left[N_a + \lambda\,\mathcal{L}(N_a)\right](\mathcal{L}(\widehat{\phi}) + Q)\mathrm{d}x = 0\end{gathered} \tag{4.88}$$

If the second-derivative term on N_a is omitted' Indeed, if we take

$$\lambda = \frac{\alpha h}{2|U|} \tag{4.89}$$

the approximation is identical to that of the Petrov–Galerkin method with the weighting.

4.4.4 Taylor Galerkin scheme

In the Taylor–Galerkin process, the Taylor expansion in time precedes the Galerkin space discretization. Firstly, the scalar variable ϕ is expanded by the Taylor series in time

$$\phi^{n+1} = \phi^n + \Delta t \frac{\partial \phi^n}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 \phi^n}{\partial t^2} + O(\Delta t^3) \tag{4.90}$$

From the convection-diffusion equation

$$\frac{\partial \phi^n}{\partial t} = \left[-U \frac{\partial \phi}{\partial x} + \frac{\partial}{\partial x} \left(k \frac{\partial \phi}{\partial x} \right) + Q \right]^n \tag{4.91a}$$

and

$$\frac{\partial^2 \phi^n}{\partial t^2} = \frac{\partial}{\partial t} \left[-U \frac{\partial \phi}{\partial x} + \frac{\partial}{\partial x} \left(k \frac{\partial \phi}{\partial x} \right) + Q \right]^n \tag{4.91b}$$

Substituting Eqs (4.91a) and (4.91b) into Eq. (4.90) we have

$$\phi^{n+1} - \phi^n = -\Delta t \left[U \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x} \left(k \frac{\partial \phi}{\partial x} \right) + Q \right]^n - \frac{\Delta t^2}{2} \frac{\partial}{\partial t} \left[U \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x} \left(k \frac{\partial \phi}{\partial x} \right) + Q \right]^n \tag{4.92}$$

Assuming U and k to be constant we have

$$\phi^{n+1} - \phi^n = -\Delta t \left[U \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x} \left(k \frac{\partial \phi}{\partial x} \right) + Q \right]^n - \frac{\Delta t^2}{2} \frac{\partial}{\partial x} \left[U \frac{\partial \phi}{\partial t} - \frac{\partial}{\partial x} \left(k \frac{\partial \phi}{\partial t} \right) + \frac{\partial Q}{\partial t} \right]^n \tag{4.93}$$

Rearranging and neglecting higher order terms,

$$\begin{aligned} \phi^{n+1} - \phi^n = & -\Delta t \left[U \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x} \left(k \frac{\partial \phi}{\partial x} \right) + Q \right]^n \\ & + \frac{\Delta t^2}{2} \frac{\partial}{\partial x} \left[U^2 \frac{\partial \phi}{\partial x} - U \frac{\partial}{\partial x} \left(k \frac{\partial \phi}{\partial x} \right) + UQ \right]^n + O(\Delta t^3) \end{aligned} \tag{4.94}$$

The Taylor–Galerkin procedure for the convection–diffusion equation in multi-dimensions can be written as

$$\begin{aligned} \phi^{n+1} - \phi^n = & -\Delta t \left\{ U_j \frac{\partial \phi}{\partial x_j} - \frac{\partial}{\partial x_i} \left(k \frac{\partial \phi}{\partial x_i} \right) + Q \right. \\ & \left. - \frac{\Delta t}{2} \frac{\partial}{\partial x_i} \left[U_i U_j \frac{\partial \phi}{\partial x_j} - U_i \frac{\partial}{\partial x_j} \left(k \frac{\partial \phi}{\partial x_j} \right) + U_i Q \right] \right\} \end{aligned} \tag{4.95}$$

4.5 Multi Dimensional Euler and Navier-Stokes Equations

Euler equation in two dimension can be rewritten as

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{f_x}}{\partial x} + \frac{\partial \mathbf{g_y}}{\partial y} = 0 \tag{4.96}$$

where $\mathbf{U}$ is the conservation variable vector and $\mathbf{f_x}$ and $\mathbf{g_y}$ are the invisid fluxes in x and y directions. The general 3D Navier-Stokes equation may be written as

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F^j}}{\partial x_j} + \frac{\partial \mathbf{G^j}}{\partial x_j} = 0 \tag{4.97}$$

where $\mathbf{F^j}$ and the convective fluxes and $\mathbf{G^j}$ are the diffusive fluxes. The general 3D Euler equation equation is obtained by dropping the diffusive flux term. For more details on the equations and fluxes, refer to Chapter 2.

4.5.1 One-Step Lax-Wendroff Scheme for 2D Euler Equations

The Taylor expansion of the conservation variables may be written as

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \Delta t \frac{\partial \mathbf{U}}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 \mathbf{U}}{\partial t^2} = 0 \tag{4.98}$$

Substitute

$$\frac{\partial \mathbf{U}}{\partial t} = -\frac{\partial \mathbf{f_x}}{\partial x} - \frac{\partial \mathbf{g_y}}{\partial y} \tag{4.99}$$

and

$$\frac{\partial^2 \mathbf{U}}{\partial t^2} = \frac{\partial}{\partial x}\left[\mathbf{A}\left(\frac{\partial \mathbf{f_x}}{\partial x} + \frac{\partial \mathbf{g_y}}{\partial y}\right)\right] + \frac{\partial}{\partial y}\left[\mathbf{B}\left(\frac{\partial \mathbf{f_x}}{\partial x} + \frac{\partial \mathbf{g_y}}{\partial y}\right)\right] \tag{4.100}$$

where

$$\mathbf{A} = \frac{\partial \mathbf{f_x}}{\partial \mathbf{U}}; \quad \mathbf{B} = \frac{\partial \mathbf{g_y}}{\partial \mathbf{U}} \tag{4.101}$$

are the Jocobian matrices.

4.5.2 Fractional step method (incompressible flows)

Consider the following N-S equations
Mass conservation

$$\frac{1}{\beta^2}\frac{\partial p}{\partial t} = -\frac{\partial U_i}{\partial x_i} \tag{4.102}$$

Momentum conservation

$$\frac{\partial U_i}{\partial t} = -\frac{\partial}{\partial x_j}(u_j U_i) + \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} \tag{4.103}$$

Equations (4.102) and (4.103) may be discretized in time and written in their semi-discrete form as

$$\frac{1}{\beta^2}\frac{\Delta p}{\Delta t} = \frac{1}{\beta^2}\frac{p^{n+1} - p^n}{\Delta t} = -\frac{\partial U_i}{\partial x_i}^n \tag{4.104}$$

and

$$\frac{\Delta U_i}{\Delta t} = \frac{U_i^{n+1} - U_i^n}{\Delta t} = -\frac{\partial}{\partial x_j}(u_j U_i)^n + \frac{\partial \tau_{ij}}{\partial x_j}^n - \frac{\partial p}{\partial x_i}^n \tag{4.105}$$

It is well known that the above system will be highly unstable if either appropriate upwinding treatment of convection terms is not employed or if the pressure is not stabilized. As mentioned in the introduction there are several convection and pressure stabilized schemes available in the literature but we limit our attention towards achieving stabilization via higher order time stepping and fractional steps. Assuming a Characteristic Based Split (CBS) stabilization (Taylor Galerkin) one can achieve stable and sensible solution. The explicit CBS scheme may be derived using either a semi-discrete approximation or using the fully discrete approximation. The derivation of the CBS scheme using semi-discrete form leads to a scheme very similar to the classical projection scheme.

Explicit CBS using semi-discrete form

The first order (in time) CBS scheme may be derived by assuming individual momentum component equations as convection-diffusion equations and by removing the pressure term from the momentum equations. The time discretization is carried out along the characteristic of the these equations and a Taylor expansion is employed to treat the semi-discrete equations at the same spatial position. With such an expansion, the first step of the CBS scheme in its semi-discrete form may be written as
Step1: Intermediate momentum

$$\begin{aligned} \Delta U_i^* = U_i^* - U_i^n &= \Delta t \left[-\frac{\partial}{\partial x_j}(U_i u_j) + \frac{\partial \tau_{ij}}{\partial x_j} \right]^n \\ &+ \frac{\Delta t^2}{2} u_k \frac{\partial}{\partial x_k} \left(\frac{\partial}{\partial x_j}(U_i u_j) + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} \right)^n \end{aligned} \tag{4.106}$$

where $U_i^n = U_i(t_n); \Delta t = t^{n+1} - t^n$ and $*$ indicates an intermediate quantity. In the above equation, the last term is a result of the Taylor expansion. Essentially, the second order extra term acts as a convection stabilization operator. The above intermediate stage needs a correction step, which is the third step of the CBS scheme. Substituting the correction step into the conservation of mass equation, and reorganizing we get
Step2: Pressure

$$\left(\frac{1}{\beta^2}\right)^n \Delta p = \left(\frac{1}{\beta^2}\right)^n (p^{n+1} - p^n) = \\ -\Delta t \left[\frac{\partial U_i^n}{\partial x_i} + \theta_1 \frac{\partial \Delta U_i^*}{\partial x_i} - \Delta t \theta_1 \left(\frac{\partial^2 p^n}{\partial x_i \partial x_i} + \theta_2 \frac{\partial^2 \Delta p}{\partial x_i \partial x_i}\right)\right] \tag{4.107}$$

As seen two parameters, θ_1 and θ_2, are introduced in the above equation. θ_1 is a stabilization parameter, which is introduced by treating the right hand side of Equation (4.102) at $n+\theta_1$ level. The stabilization parameter θ_1 must be above zero to get any pressure stability. The parameter θ_2 is introduced to move between explicit and implicit treatment of the RHS pressure term. In this paper we adopt $\theta_2 = 0$, which means that the RHS pressure terms are treated explicitly at step 2.

Selection of artificial compressible wave speed β for an explicit scheme is crucial. Constant values are commonly employed in the literature. However, we prefer to use a variable β value which is linked to the time step of the scheme. Since the time step values are determined from the convection and diffusion wave velocities, we employ the following relation for the artificial compressibility parameter

$$\beta = max(\epsilon, u_{conv}, u_{diff}) \tag{4.108}$$

where ϵ is a constant, u_{conv} and u_{diff} are convection and diffusion wave speeds respectively calculated as $u_{conv} = \sqrt{u_i u_i}$ and $u_{diff} = 2\nu/h$. The parameter ϵ should be smaller than the maximum wave speeds expected. For the non-dimensional scales discussed in the previous section, the reference u_{conv} value would be unity. Hence, the non-dimensional ϵ value in this study is chosen to be 0.5. Determining an exact value for this parameter is not important for the present discussion.

It is also important to note here that we employ local time steps, calculated at nodes. The local time steps are calculated as

$$\Delta t = \frac{h}{|\mathbf{u}_{conv}| + \beta} \tag{4.109}$$

Due to the fully explicit nature of the presented scheme, Equation (4.109) needs to be multiplied by a safety factor mostly below unity to keep this value below the critical time step. The element size h is calculated on the nodes by taking the minimum element size surrounding a node.

Once the the relation between the pressure and intermediate momentum is established, we can return to the correction stage, where the actual velocity is computed at the third step as shown below.

Step3: Momentum correction

$$\Delta U_i = U_i^{n+1} - U_i^n = \Delta U_i^* - \Delta t \frac{\partial p}{\partial x_i}^n \tag{4.110}$$

The standard Galerkin approximation can now be applied to all the three steps. The fully discrete matrix form of the three steps may be written as

Step 1

$$\mathbf{M}\Delta\mathbf{U}^* = -\Delta t\mathbf{C}\mathbf{U}^n + \Delta t\mathbf{K}\mathbf{U}^n + \mathbf{F}^n + conv.stabilization \tag{4.111}$$

assuming $\theta_2 = 0$,
Step 2

$$\tilde{\mathbf{M}}\Delta p = -\theta_1\Delta t\mathbf{D}\mathbf{U}^n - \theta_1\Delta t\mathbf{D}\Delta\mathbf{U}^* + \theta_1\Delta t\mathbf{L}p^n \tag{4.112}$$

where $\tilde{\mathbf{M}}$ is equal to $(1/\beta^2)\mathbf{M}$ and finally
Step 3

$$\mathbf{M}\Delta\mathbf{U} = \tilde{\mathbf{M}}\Delta\mathbf{U}^* - \Delta t\mathbf{G}p^n \tag{4.113}$$

In the above equations $\mathbf{C}$, $\mathbf{G}$, $\mathbf{D}$, $\mathbf{L}$ and $\mathbf{K}$ are discrete convection, gradient, divergence, Laplacian and viscous operators and $\mathbf{M}$ is the mass matrix. To obtain a matrix free formulation we lump the mass matrix by summing up the rows for linear elements.

It should be noted that the Dirichlet conditions for velocity are applied only at step 3.

4.5.3 Explicit CBS using fully discrete form

Here, we discuss the explicit CBS scheme derived from a fully discrete approximation. The discrete form of the conservation of mass and momentum equations may be written as

$$\tilde{\mathbf{M}}\Delta p = -\mathbf{D}\mathbf{U}^{n+\theta_1} = -\theta_1\mathbf{D}\mathbf{U}^{n+1} - (1-\theta_1)\mathbf{D}\mathbf{U}^n \tag{4.114}$$

and

$$\mathbf{M}\Delta\mathbf{U} = -\Delta t\mathbf{C}\mathbf{U}^n + \Delta t\mathbf{K}\mathbf{U}^n \quad - \quad \Delta t\mathbf{G}p^n + \mathbf{F}^n + conv.stabilization \tag{4.115}$$

Now, employing the fractional step approach to the above two equations we get the following steps
Step 1

$$\mathbf{M}\Delta\mathbf{U}^* = -\Delta t\mathbf{C}\mathbf{U}^n + \Delta t\mathbf{K}\mathbf{U}^n + \mathbf{F}^n + conv.stabilization \tag{4.116}$$

This step is identical to the one discussed in the previous subsection. The step 2 is derived by substituting the momentum correction (step 3),

$$\mathbf{U}^{n+1} = \mathbf{U}^* - \mathbf{M}^{-1}\mathbf{G}p^n \tag{4.117}$$

into Equation (4.114) as
Step 2

$$\tilde{\mathbf{M}}\Delta p^n = -\theta_1\Delta t\mathbf{D}\mathbf{U}^n \quad - \quad \theta_1\Delta t\mathbf{D}\Delta\mathbf{U}^* + \theta_1\Delta t\mathbf{D}\mathbf{M}^{-1}\mathbf{G}p^n \tag{4.118}$$

The difference from the step 2 of the previous subsection lies in the pressure term on the RHS. The operator $\mathbf{L}$ is replaced here by $\mathbf{D}\mathbf{M}^{-1}\mathbf{G}$. The third step remains identical to the one discussed in the previous subsection. It appears, therefore, the difference is caused by the the inverse mass matrix in the RHS pressure term. The step 2 of the previous subsection may therefore be treated as an approximation of Equation (4.118) with $\mathbf{M}^{-1}$ replaced with an identity matrix.

4.6 Pressure stability

Assuming incompressible flow equations, following discrete form of the direct Galerkin scheme could be written

Discrete continuity

$$[\mathbf{D}]u_i^{n+1} = 0$$

Discrete momentum

$$[\mathbf{M}]u_i^{n+1} + \frac{\Delta t}{\rho}[\mathbf{G}]p^{n+1} - \Delta t\,\nu[\mathbf{L}]u_i^{n+1} = \{\mathbf{F}\}^n$$

Discrete matrix form

$$\begin{bmatrix} [\mathbf{M}] - \nu[\mathbf{L}] & \frac{1}{\rho}[\mathbf{G}] \\ [\mathbf{D}] & 0 \end{bmatrix} \begin{bmatrix} u_i^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} \{\mathbf{F}\} \\ 0 \end{bmatrix}^n$$

Figure 4.3: Diagonal zero if direct Galerkin is employed

4.7 Artificial compressibility method

When the real compressibility is small, it is often assumed that the fluid is incompressible with the speed of sound approaching infinity. Even if the speed of sound is finite, its value will have to be large and hence a very sever time step limitation arises. However, an artificial compressibility method can be employed to eliminate the restrictions posed by the speed of sound at step 2 by taking an artificial value for the speed of sound which is sufficiently low. This of course only possible if steady state conditions exist and therefore in that limit the transient term dis-appears. The step 2 of the CBS scheme may be rewritten in its semi-discrete form as [3]

$$(\frac{1}{c^2})^n \Delta p \approx (\frac{1}{\beta^2})^n \Delta p = -\Delta t \left[\frac{\partial U_i^n}{\partial x_i} + \theta_1 \frac{\partial \Delta U_i^\star}{\partial x_i} - \Delta t \theta_1 \left(\frac{\partial^2 p^n}{\partial x_i \partial x_i} + \theta_2 \frac{\partial^2 \Delta p}{\partial x_i \partial x_i} \right) \right] \tag{4.119}$$

where β is an artificial parameter with the dimensions of speed. This parameter may be either given as a constant throughout the domain or determined based on the convective or diffusive time step restrictions. We recommend the latter option, as this results in manageable local and global time step sizes. The β value may be locally computed using the following relation so that the convective and viscous time steps are represented.

$$\beta = max(\epsilon, u_{conv}, u_{diff}) \tag{4.120}$$

where ϵ is a small constant and it make sure that the β is not approaching zero at any circumstances. u_{conv} and u_{diff} are respectively the convection and diffusion velocities given as

$$\begin{aligned} u_{conv} &= |\mathbf{u}| = \sqrt{u_i u_i} \\ u_{diff} &= \frac{\nu}{h} \end{aligned} \tag{4.121}$$

where h is the element size and ν is the kinematic viscosity.

The three steps of the CBS scheme follow exactly the procedure discussed in the preceding sections. However, the difference here is that no coupling exists between the energy and rest of the governing equations. Note that the time step limitation for the artificial compressibility method may be written as

$$\Delta t = \frac{h}{|\mathbf{u}| + \beta} \tag{4.122}$$

The above relation includes the viscous effect via the artificial parameter. The artificial compressibility method explained here is valid for steady flows. However, an appropriate dual time stepping method, explained in the following subsection, should be employed to recover true transient solution.

4.8 Determination of time step limits

4.8.1 Fully explicit form

In fully explicit forms, $\frac{1}{2} \leq \theta_1 \leq 1$ and $\theta_2 = 0$. In general the time step limitations explained for the convection–diffusion equations are applicable i.e.

$$\Delta t \leq \frac{h}{c + |\mathbf{u}|} \tag{4.123}$$

if the viscosity effects are negligible. In the above equation h is the element size. Assuming linear elements only and one-dimensional behaviour. For two and three dimensional flow problems determination of the element size is difficult.

This particular form is very successful in compressible flow computations and has been widely used by the authors for solving many complex problems. More recently the algorithm has also been successfully used in conjunction with artificial compressibility to solve many other flow situations, including those in which incompressibility is involved.

4.8.2 Semi-implicit form

In semi-implicit form the following values apply

$$\frac{1}{2} \leq \theta_1 \leq 1 \qquad \text{and} \qquad \frac{1}{2} \leq \theta_2 \leq 1 \quad . \tag{4.124}$$

Again the CBS algorithm is conditionally stable. The permissible time step is governed by the critical step of the characteristic–Galerkin explicit relation solved in Step 1 of the

algorithm. This is the standard convection–diffusion problem and the same stability limits apply, i.e.

$$\Delta t \leq \Delta t_u = \frac{h}{|\mathbf{u}|} \tag{4.125a}$$

and/or

$$\Delta t \leq \Delta t_\nu = \frac{h^2}{2\nu} \tag{4.125b}$$

where ν is the kinematic viscosity. A convenient form incorporating both limits can be written as

$$\Delta t \leq \frac{\Delta t_u \Delta t_\nu}{\Delta t_u + \Delta t_\nu} \quad . \tag{4.126}$$

The reader can verify that the above relation will give appropriate time step limits with and without the domination of viscosity.

4.9 Neumann Boundary Conditions

At a boundary note where a boundary flux $q = \partial\phi/\partial x$ is given, we can discretize the first order derivative using a central difference scheme as:

$$\frac{\partial \phi}{\partial x} = \frac{\phi_2^n - \phi_0^n}{2\Delta x} + O(\Delta x)^2 \tag{4.127}$$

Where ϕ_0 is a node outside the domain. Substituting ϕ_0 into explicit FTCS scheme of

$$\frac{\partial \phi}{\partial t} + \alpha \frac{\partial^2 \phi}{\partial x^2} = 0 \tag{4.128}$$

with

$$\frac{\partial \phi}{\partial x} = q \tag{4.129}$$

we get,

$$\phi_1^{n+1} = (1 - 2\eta)\phi_1^n + 2\eta\phi_2^n - 2\eta q^n \Delta x \tag{4.130}$$

with

$$\eta = \frac{\alpha \Delta t}{\Delta x^2} \tag{4.131}$$

Application of the flux condition using finite element discretization is natural. Normally a boundary integral from integration by parts appears as

$$\int_{\Gamma}\{\mathbf{N}\}\frac{\partial\phi}{\partial\mathbf{x}}\mathbf{d\Gamma\bar{n}} \tag{4.132}$$

Replacing

$$\frac{\partial\phi}{\partial x}=q \tag{4.133}$$

in Equation 4.133, completes the application of flux boundary condition. $\mathbf{n}$ is outward boundary normal.

4.10 Consistency, Stability and Convergence

Consistency
Consistency expresses that the discretized equations should tend to the differential equation to which they are related when Δx and Δt tend to zero.
Stability
Any component of the initial solution should not be amplified without bound.
Convergence
The numerical solution should approach the exact solution of differential equation at any point and time when Δx and Δt tend to zero.

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Chapter 5

Special Topics

5.1 Introduction

This chapter introduces some special topics of interest to CFD scientists. Consideration is given to two topics of special interest. They are turbulence and free surface flows. Turbulence is one of the major challenges facing the CFD community. This challenge is being addressed as the computing power is increasing. Free surface flows are found in many of the incompressible flow problems such as sea water and mould filling. Studying such flows can be very useful in designing off-shore structures, casting of machine parts etc.

5.2 Turbulence

Turbulent flow is defined as a flow with random variation of various flow quantities such as velocity, pressure and density. Turbulence is a property of the flow, not the property of a fluid. Despite serious progress on the topic of turbulence modelling over the last century, one has to admit that the turbulence presents an unresolved problem, which will remain so for a foreseeable future. At this point, it is worth noting that a turbulent flow is always three dimensional and occurs at high Reynolds numbers. The turbulent flow is marked by random variation of quantities as shown in Figure5.1.

The Navier-Stokes equations are sufficient to resolve all turbulent scales if adequate mesh resolution is used. However, this requires extremely large computer resources. With the present day computers, this is possible only for relatively low Reynolds numbers. Until sufficiently fast computing power is available it is essential to employ Reynolds decomposition and turbulence models.

In a real turbulent flow, the kinetic energy is transferred from larger scales to smaller scales. At smallest scale, the kinetic energy is transformed into internal energy and this process is called dissipation and the process of energy transfer between the scales is called 'the cascade process'. The smallest turbulent length scale is determined by the molecular viscosity and dissipation rate. Such a length scale is often referred to as *Kolmogorov length scale* and given as

$$\left(\frac{\nu^3}{\epsilon}\right)^{1/4} \tag{5.1}$$

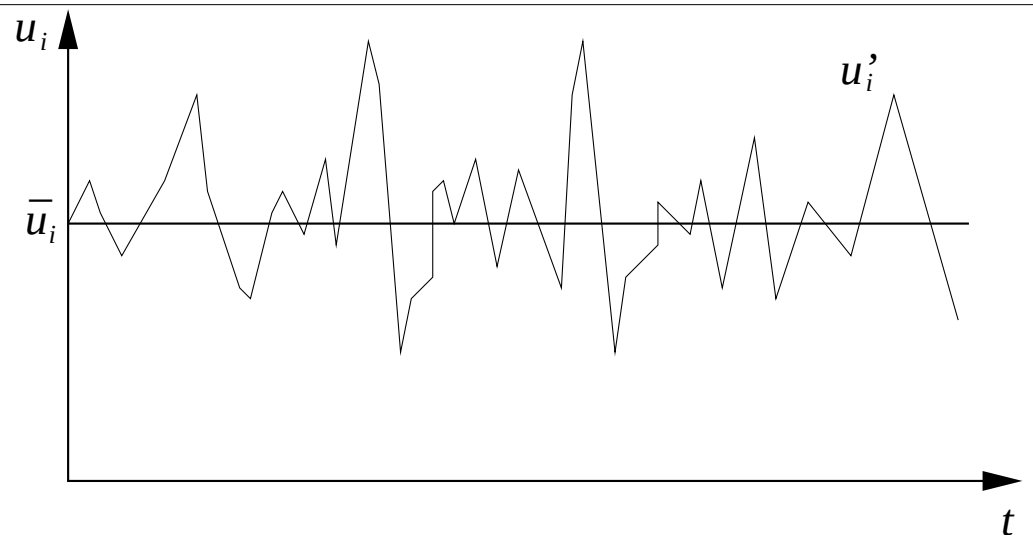


Figure 5.1: Random variation of velocity in a turbulent flow with respect to time

Similarly Kolmogorov velocity and time scales are determined as

$$v = (\nu\epsilon)^{1/4} \tag{5.2}$$

and

$$\tau = \left(\frac{\nu}{\epsilon}\right)^{1/2} \tag{5.3}$$

The dissipation rate can be linked to the energy of large eddies as

$$\epsilon = \frac{U^3}{l} \tag{5.4}$$

where U is the large eddy velocity scale and l is the large eddy length scale. The turbulent kinetic energy of a flow is defined as

$$\kappa = \frac{1}{2}\overline{u_i' u_i'} \tag{5.5}$$

where u_i' is the fluctuating component of the velocity as shown in Figure 5.1. The above relations are given to make the readers aware that the length scales, turbulent kinetic energy and dissipation are closely related. Various turbulence modelling procedures are developed based on these relationships.

5.2.1 Time averaging

As mentioned previously, extremely high mesh resolution is required to solve molecular level turbulence and is very expensive and presently not possible for high Reynolds number flows. It is, therefore, obvious that other alternatives are necessary to get an approximate solution. The standard procedure is to employ time averaged Navier-Stokes equations along with a turbulence modelling approach to determine the essential time averaged quantities which

reduces the excessive grid resolution otherwise needed. With reference to Figure 5.1 any turbulence quantity of interest may be expressed as

$$\phi = \overline{\phi} + \phi' \tag{5.6}$$

The time averaged quantity may be obtained as

$$\overline{\phi} = \frac{1}{2T}\int_{-T}^{T} \phi(t)dt \tag{5.7}$$

Let us consider a one dimensional steady state incompressible momentum equation to demonstrate time averaging

$$\frac{du^2}{dx} + \frac{1}{\rho}\frac{dp}{dx} - \frac{d}{dx}\left(\nu\frac{du}{dx}\right) = 0 \tag{5.8}$$

Substituting variation of the form of Equation 5.6 for velocity u and pressure p into Equation 5.7 and time averaging, we have

$$\frac{d}{dx}\left[\overline{(\overline{u}+u')(\overline{u}+u')}\right] + \frac{1}{\rho}\frac{d}{dx}\overline{(\overline{p}+p')} - \frac{d}{dx}\left[\nu\frac{d}{dx}\overline{(\overline{u}+u')}\right] = 0 \tag{5.9}$$

In the above equation the average of fluctuating components $\overline{u'}$ and $\overline{p'}$ are equal to zero. Now the simplified form of the above equation may be written as

$$\frac{d}{dx}\left[(\overline{u}^2 + \overline{u'^2})\right] + \frac{1}{\rho}\frac{d\overline{p}}{dx} - \frac{d}{dx}\left[\nu\frac{d}{dx}(\overline{u})\right] = 0 \tag{5.10}$$

Rearranging and rewriting the above momentum equation in multi-dimensions and including the time term, we have

$$\frac{\partial(\rho\bar{u}_i)}{\partial t} + \frac{\partial}{\partial x_j}(\rho\bar{u}_j\bar{u}_i) = -\frac{\partial\bar{p}}{\partial x_i} + \rho\frac{\partial\bar{\tau}_{ij}}{\partial x_j} - \frac{\partial}{\partial x_j}(\rho\overline{u_i u_i}) \tag{5.11}$$

where

$$\bar{\tau}_{ij} = \nu\left(\frac{\partial\bar{u}_i}{\partial x_j} + \frac{\partial\bar{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial\bar{u}_k}{\partial x_k}\delta_{ij}\right) \tag{5.12}$$

is the time averaged deviatoric stress and $\rho\overline{u_i u_i}$ is a new unknown referred to as *Reynolds stress*. The *Boussinesq assumption* gives the Reynolds stress as

$$-\rho\overline{u_i u_i} = \mu_T\left(\frac{\partial\bar{u}_i}{\partial x_j} + \frac{\partial\bar{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial\bar{u}_k}{\partial x_k}\delta_{ij}\right) \tag{5.13}$$

or

$$\bar{\tau_i j}^R = -\overline{u_i u_i} = \nu_T\left(\frac{\partial\bar{u}_i}{\partial x_j} + \frac{\partial\bar{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial\bar{u}_k}{\partial x_k}\delta_{ij}\right) \tag{5.14}$$

Thus, the unknown quantity to be modelled is the turbulent kinematic viscosity ν_T.

5.2.2 Relation between κ, ϵ and ν_T

The turbulent kinematic viscosity or turbulent eddy viscosity ν_T has the same dimensions as the laminar viscosity. Thus, we can express the turbulent eddy viscosity in terms of velocity and length scales of a large eddy, i.e.,

$$\nu_T = CUl \tag{5.15}$$

where C is a constant. The definitions of U and l are discussed in Section 5.2. In the above equation U may be replaced with $\sqrt{\kappa}$. With such a substitution the turbulent eddy viscosity may be determined by solving a scalar transport equation for κ and assuming an appropriate turbulence length scale l ($\kappa - l$ or one equation models). However, a better expression for turbulent eddy viscosity may be obtained by substituting Equation 5.4 into Equation 5.15 as

$$\nu_T = c_\mu \frac{\kappa^2}{\epsilon} \tag{5.16}$$

where c_μ is a constant. To employ the above equation, we need to solve two transport equations, one for κ and another for ϵ ($\kappa - \epsilon$ or two equation model). Details of many one and two equation models are provided in the following sections.

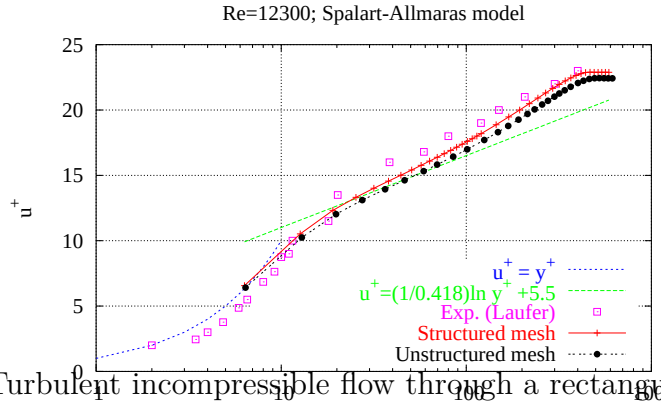


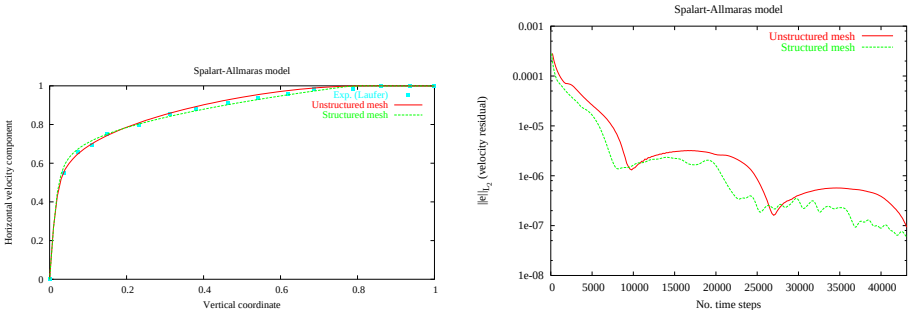
Figure 5.2: Turbulent incompressible flow through a rectangular channel using the Spalart-Allmaras model at Re=12300. Logarithmic representation of time-averaged velocity profile.

5.3 Treatment of Incompressible Turbulent Flows

5.3.1 Reynolds Averaged Navier-Stokes Equations (RANS)

For turbulent flow computations, Reynolds averaged Navier-Stokes equations of motion are written in conservation form as follows

Mean-continuity



(a) (b)

Figure 5.3: Turbulent incompressible flow in a rectangular channel using the Spalart-Allmaras model at Re=12300. (a) Comparison of fully developed velocity profiles; (b) Convergence to the steady state.

$$\frac{1}{\beta^2}\frac{\partial \bar{p}}{\partial t} + \frac{\partial \rho \bar{u}_i}{\partial x_i} = 0 \tag{5.17}$$

Mean-momentum

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\bar{u}_j \bar{u}_k) = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} + \frac{\partial \bar{\tau}^R_{ij}}{\partial x_j} \tag{5.18}$$

where β is an artificial compressibility parameter, $\bar{u}_i$ are the mean velocity components, p is the pressure, ρ is the density, $\bar{\tau}_{ij}$ is the laminar shear stress tensor given as

$$\bar{\tau}_{ij} = \nu\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial \bar{u}_k}{\partial x_k}\delta_{ij}\right) \tag{5.19}$$

The Reynolds stress tensor, $\bar{\tau}^R_{ij}$, is introduced by Boussinesq's assumption as

$$\bar{\tau}^R_{ij} = -\overline{u'_i u'_j} = \nu_T\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial \bar{u}_k}{\partial x_k}\delta_{ij}\right) - \frac{2}{3}\kappa\delta_{ij} \tag{5.20}$$

In the above equations, ν is the kinematic viscosity of the fluid, ν_T is the turbulent eddy viscosity and δ_{ij} is the Kroneker delta.

5.3.2 Turbulent Flow Through a Channel

Figure 5.2 shows the results. The first node of the structured mesh was placed at a distance of 0.005 and the unstructured mesh was placed roughly around 0.01. As seen the logarithmic representation of time averaged velocity variation is close to the experimental data of Laufer [1]. The small difference between the structured and unstructured meshes is attributed to the slightly larger elements of the unstructured mesh used close to the wall. The point we are trying to prove here is that the turbulence model and the artificial compressibility based CBS schemes together can predict the time averaged turbulence quantities satisfactorily. In several ways these results allow us to present the unstructured mesh results with confidence. We also

show the comparison of fully developed velocity profiles with the experimental data of Laufer [1] in Figure 5.3(a). As seen the agreement between the numerical and experimental data is excellent. Figure 5.3(b) shows the convergence histories of structured and unstructured meshes to steady state. As seen the convergence is rapid and it took only about 5000 time steps to reach an L_2 norm velocity residual of 10^{-5}. We use local time steps to accelerate the solution to steady state.

Bibliography

[1] J. Laufer. Investigation of turbulent flow in a two-dimensional channel. *NACA Report 1053*, 1951.

Chapter 6

Projects

6.1 Introduction

The continuous assessment is carried out via two mini-projects each carrying 15% of the total marks. Submission deadlines for the first and second projects are **5PM 01 March 2024** and **5PM 22 March 2024** respectively. The projects should be submitted in the form of typed documents via blackboard. Any pictures used to describe the project must be appropriately placed within the text. The computer codes developed as a part of the projects should be listed in the report. The maximum **number of pages allowed for each project is 10**, excluding computer code listing. The mini-projects given in the following sections are not group projects. Discussion between participating students are allowed but all the computer programs and reports must be written independently. The assessment of the projects may include an interview.

6.2 Project 1

Various finite difference projects will be distributed during the first/second week of teaching.

Suggested contents of the report: (1) Introduction (why this project is important for CFD, why this method, etc.) (2) Governing equations and discretization (detailed explanation of the equation, boundary conditions, stabilized FE discretization) and stability analysis (3) Code structure (refer to the code listing and indicate pre- , main- and post- processing components in the code) (4) Results and discussion and (5) Conclusions (lessons learned from this assignment) (6) References

Mark distribution: (a) Report style, structure, clarity - 20% (b) Comprehensive mathematics and discretization - 15% (c) Results and discussion, explanation for the behaviour of the method and comparisons in detail - 50% and (d) Robust conclusions derived - 15%

6.3 Project 2

In this project you are asked to develop a one-dimensional finite element program for steady-state convection-diffusion equation using the balancing-diffusion or Petrov-Galerkin approach. You need to demonstrate the stabilization properties of the code developed by solving a one-dimensional convection-diffusion problem with the scalar variable values given at the inlet (= 1) and exit (= 0). Assume a total domain length of unity. Draw the variation of the the scalar variable for different element Peclet numbers starting with a Peclet number value of 0 and increasing the value to 10,000. Also discuss why you need special schemes such as Petrov-Galerkin method to solve convection-diffusion equations and compare against standard Galerkin results.

Suggested contents of the report: (1) Introduction (why this project is important for CFD, why this method, etc.) (2) Governing equations and discretization (detailed explanation of the equation, boundary conditions, stabilized FE discretization) (3) Code structure (refer to the code listing and indicate pre- , main- and post- processing components in the code) (4) Results and discussion and (5) Conclusions (lessons learned from this assignment) (6) References

Results and discussions should contain at least the following graphs

- Standard Galerkin discretization is oscillatory beyond an element Peclet number of unity. Plot the scalar variable value at different Peclet numbers along the domain length,
- Stabilized finite element scheme reduces or eliminates spatial oscillations. Plot the scalar variable value at different Peclet numbers along the domain length,
- Compare the standard Galerkin and stabilized method results to the given analytical solution,
- Plot the stabilized solution for different degrees of mesh refinement,

All graphs presented must be discussed in the report.

Mark distribution: (a) Report style, structure, clarity - 20% (b) Comprehensive mathematics and discretization - 15% (c) Results and discussion, explanation for the behaviour of the method and comparison with analytical solution in detail - 50% and (d) Robust conclusions derived - 15%

6.4 Optional Project on Navier-Stokes Equations

Please check with Professor Nithiarasu if you want to develop a 2D FDM code to solve Navier-Stokes equations. This is optional for those with strong interest in CFD and programming.