LECTURE NOTE 2

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MCE 521

CFD

Computational Fluid Dynamics (CFD) is the branch of fluid dynamics providing a cost-effective means of simulating real flows by the numerical solution of the governing equations. The governing equations for Newtonian fluid dynamics, namely the Navier-Stokes equations, have been known for over 150 years. However, the development of reduced forms of these equations is still an active area of research, in particular, the turbulent closure problem of the Reynolds-averaged Navier-Stokes equations. For non-Newtonian fluid dynamics, chemically reacting flows and two phase flows, the theoretical development is at less advanced stage.

Experimental methods has played an important role in validating and exploring the limits of the various approximations to the governing equations, particularly wind tunnel and rig tests that provide a cost-effective alternative to full-scale testing. The flow governing equations are extremely complicated such that analytic solutions cannot be obtained for most practical applications.

Computational techniques replace the governing partial differential equations with systems of algebraic equations that are much easier to solve using computers. The steady improvement in computing power, since the 1950's, thus has led to the emergence of CFD. This branch of fluid dynamics complements experimental and theoretical fluid dynamics by providing alternative potentially cheaper means of testing fluid flow systems. It also can allow for the testing of conditions which are not possible or extremely difficult to measure experimentally and are not amenable to analytic solutions

PREDICTION METHODS.

Engineers are interested in predicting the behaviour of systems to understand the relationship between the system variables. This allows for better design of systems or understanding of their behaviour for optimising their operation. Typically, engineers used to perform experiments which either allows them to understand the system directly, or construct mathematical models that represent their systems.

Another approach to understand the system is to construct a mathematical model based on the understanding of the basic physical phenomena that govern its behaviour and then trying to solve these models for a given set of conditions by finding a mathematical solution to the resulting system of equations. This is termed the analytical approach.

The third approach is the use of CFD methods mentioned above, where the differential equations governing the system are converted to a set of algebraic equations at discrete points, and then solved using digital computers. We will now shed some light on these three approaches highlighting their advantages and limitations.

EXPERIMENTAL TECHNIQUES.

The most reliable information about physical phenomena is usually given by measurements. In certain situations, an experimental investigation involving full-scale equipment can be used to predict how the equipment would perform under given conditions. However, in most practical engineering applications, such full scale tests are either difficult or very expensive to perform, or not possible at all.

A common alternative is to perform experiments on small scale models. The resulting information however, needs to be extrapolated to the full scale and general rules for doing this are often unavailable. The small scale models do not usually simulate all the features of the full scale system. This sometimes limits the usefulness of the test results.

In many situations, there are serious difficulties in measurements and the measuring equipment can have significant errors. For example, the performance of an aircraft engine at high altitude conditions is a difficult, expensive and sometimes a risky undertaking, and is usually done at the later stages of the process where major changes to the design can result in significant costs.

Although the above discussion implies that the need for reliable computational models is of paramount importance, it is should be stressed that these numerical models require validation using reliable experimental data before they can be put to good use. This indicates that experimental methods will remain to play an important rule in engineering.

ANALYTICAL METHODS

Analytical models work out the consequences of a mathematical model which represents the behaviour of a system. The mathematical model representing the physical process mainly consists of a set of differential equations. If classical mathematics were used to solve these equations, we call the approach as the analytical or theoretical approach.

In most practical engineering applications, various assumptions and simplifications need to be made to enable the analytical solution of the differential equations representing the physical situation. This at one hand limits the applicability of these methods to simple type problems, or limits the validity of the solutions if too many assumptions and simplifications are made.

Despite that, analytical methods played significant role in the past and they still play an important role. They have helped engineers and scientists in the understanding of the fundamental rules controlling the behaviour of many engineering systems. In addition, they are used to help understand and interpret experimental results. Furthermore, they can be used as a first stage in the validation of CFD models.

CFD TECHNIQUES

CFD techniques have emerged with the advent of digital computers. Since then, a large number of numerical methods were developed to solve flow problems using this approach. The basic approach is outlined below.

The purpose of a flow simulation is to find out how the flow behaves in a given system for a given set of inlet and outlet conditions. These conditions are usually termed boundary conditions.

For example, in a boiler required to raise the temperature of water for heating purposes, it may be required to calculate, for a given mass inflow of water and energy input using the gas fire, what is the temperature and velocity of the water coming out of the boiler. It might be also required to know the flow pattern and temperature distribution within the boiler if design improvements need to be made to improve mixing or reduce energy loss through the walls.

Since the geometry in most boilers is complex, it is difficult to find an analytical solution to the flow equations. For all engineering purposes, it will be useful to know the basic flow quantities at a large number of discrete points spread around the boiler geometry. This will give enough understanding of the flow behaviour and will enable engineers to get the required information either for operation or design purposes.

The basic concept of CFD methods is then to find the values of the flow quantities at a large number of points in the system. These points are usually connected together in what is called numerical grid or mesh. The system of differential equations representing the flow is converted, using some procedure, to a system of algebraic equations representing the interdependency of the flow at those points and their neighbouring points.

If the flow is unsteady, either due to varying boundary conditions, or due to inherent unsteadiness. The solution procedure is repeated at discrete time intervals to predict the evolution in time of the flow variables at the grid points.

With the development of fast and validated numerical procures, and the continuous increase in computer speed and availability of cheap memory, larger and larger problems are being solved using CFD methods at cheaper cost and quicker turn around times. In many design and analysis applications, CFD methods are quickly replacing experimental and analytical methods.

It should be noted that there are certain levels of numerical approximations and assumptions made during the development of CFD models. Hence, good understanding of the applicability range and the limitation of a CFD tools is essential to enable the correct use of these tools.

In addition to the speed and reduced cost of CFD methods, compared to experimental procedures in most engineering applications, they also offer a more complete set of information. They usually provide all relevant flow information throughout the domain of interest. Experimental methods are mostly limited to measurements of some flow quantities at certain locations accessible by the measuring equipment.

CFD simulations also enable flow solutions at the true scale of the engineering systems with the actual operating conditions, while experimental measurements mostly require either scaling up or down. In most cases, realistic conditions cannot be economically represented and thus results need to be extrapolated. This problem does not exit in CFD simulations.

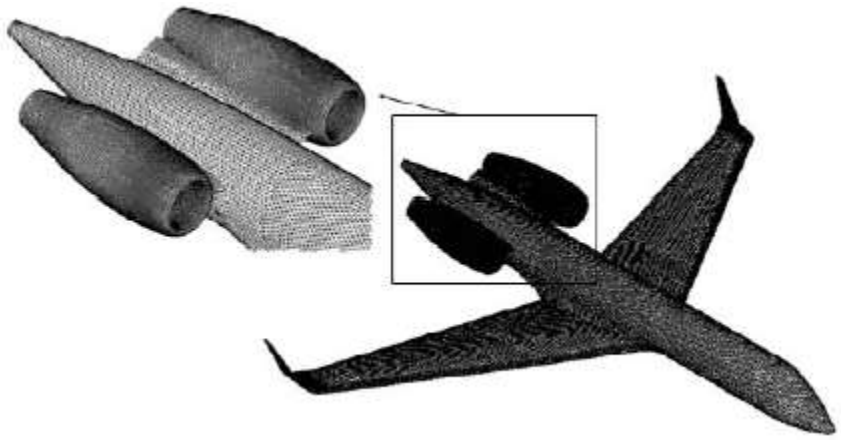
TYPICAL PROBLEMS.

AEROSPACE APPLICATIONS.

CFD methods are now widely used in most aerospace applications for the purpose of predicting component performance and as an integral part of the design cycle. The applications are numerous and we will only list few examples here.

The first example is flow around an aircraft. Wind tunnel tests require substantial scaling which leads to some difficulties of matching the important flow parameters. If we attempt to model the correct Mach number, the Reynolds number will be substantially lower than the full scale Reynolds number leading to errors in the modelled shear stress and other flow features. It is also very expensive to replicate altitude conditions within a wind tunnel.

On the other hand, full scale flight tests are extremely expensive and are not without risk. For these reasons, CFD provides a useful tool in predicting the performance of the airframe components under various conditions and this leads to substantial cuts in the time and cost of the design process. An example of a flow around a complete aircraft is shown in Figure 1.



Mach number

It may be seen that the speed of sound is the thermodynamic property that varies from point to point. When there is a large relative speed between a body and the compressible fluid surrounds it, then the compressibility of the fluid greatly influences the flow properties. Ratio of the local speed (V) of the gas to the speed of sound (a) is called as local Mach number. M

$$M = \frac{V}{a} = \frac{V}{\sqrt{\gamma RT}}$$

There are few physical meanings for Mach number;

(a) It shows the compressibility effect for a fluid i.e. M < 0.3 implies that fluid is incompressible.

(b) It is a measure of directed motion of a gas compared to the random thermal motion of the molecules.

(c) It can be shown that Mach number is proportional to the ratio of kinetic to internal energy.

$$\frac{(V^2/2)}{e} = \frac{V^2/2}{c_v T} = \frac{V^2/2}{RT/(\gamma-1)} = \frac{(\gamma/2)V^2}{a^2/(\gamma-1)} = \frac{\gamma(\gamma-1)}{2}M^2$$

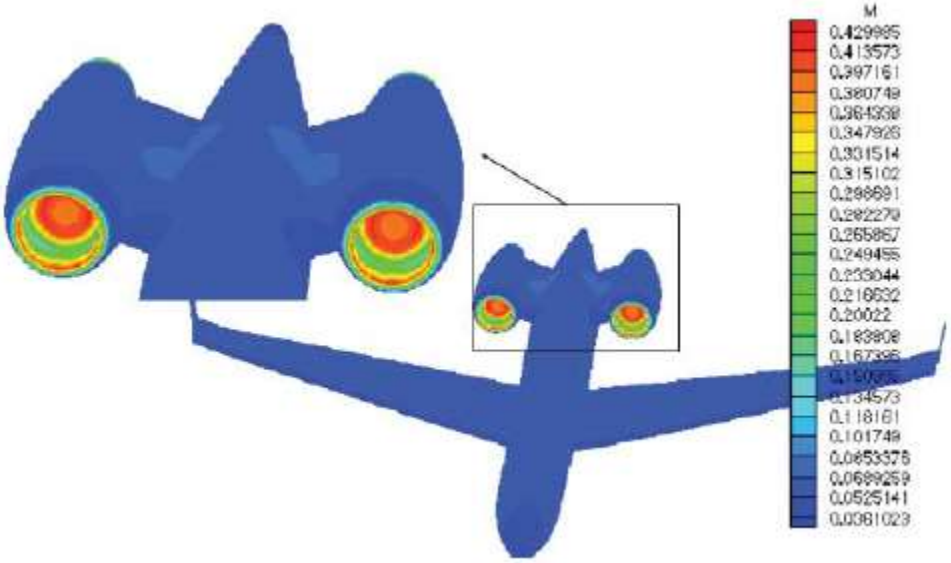
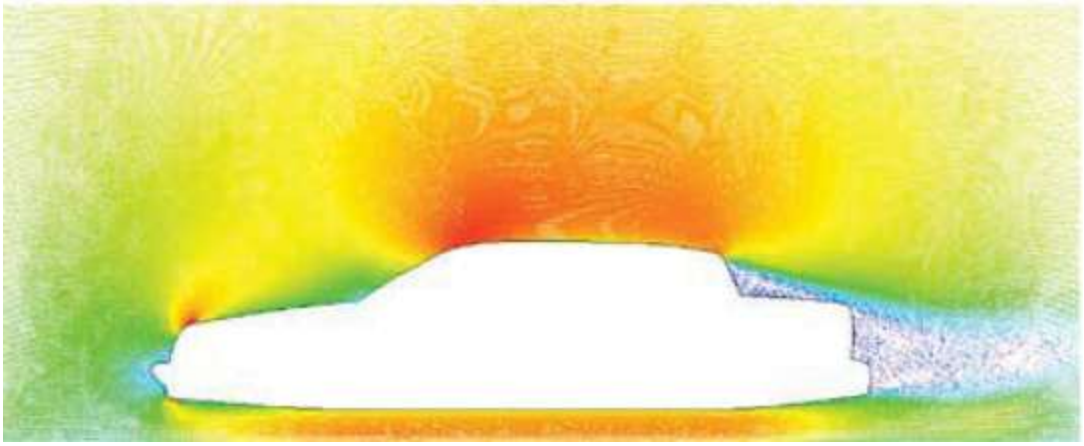


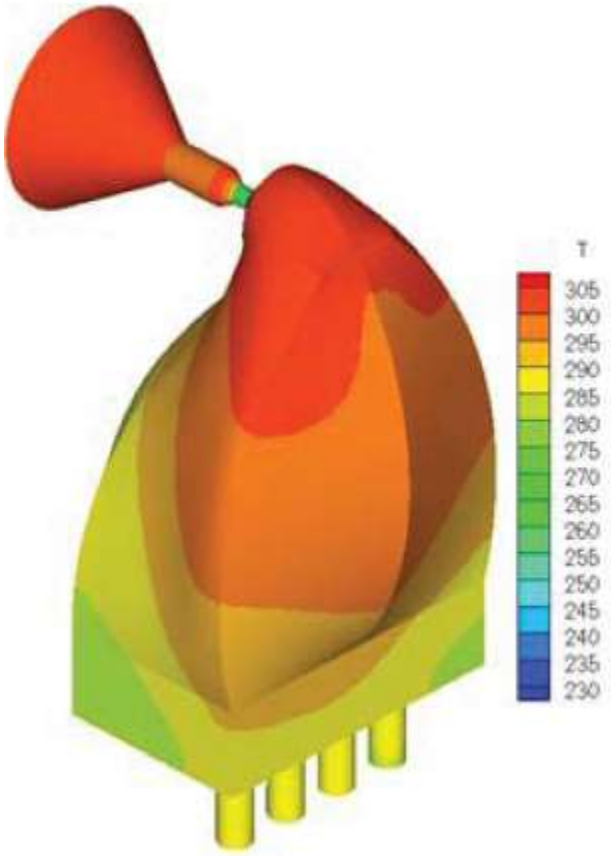
Figure 1: Grid and flow solution for a civil aircraft with nacelles.

AUTOMOTIVE APPLICATIONS

In automotive applications CFD is nowadays used in a large number of areas including engine components, auxiliary systems and also for modeling the aerodynamics of the car to minimise drag and optimise the down force under various operating conditions. Figure [redacted] shows two examples of automotive applications. Figure [redacted]a shows the flow field around a family car obtained using CFD methods. Figure [redacted]b shows the flow in the induction duct for a formula student racing car. The objectives of this analysis are to understand the flow pattern within the induced during the process of design optimisation to minimise pressure losses and ensure uniformity of air ducted to the cylinders.



(a) Flow around a car.



(b) Formula student racing car induction duct.

Figure 2a, b: Examples of automotive applications.

BASIC EQUATIONS OF FLUID FLOW AND LEVELS OF APPROXIMATIONS.

Fluid flow equations are made essentially of differential equations representing the interrelationship between the flow variables and their evolution in time and space. These equations are complemented by algebraic relations such as the equation of state for compressible flow as we will see below.

To help the student understand the physical meaning of the terms in these equations, we will illustrate the basic concepts using a simple differential equation before presenting the system of differential equations representing the flow.

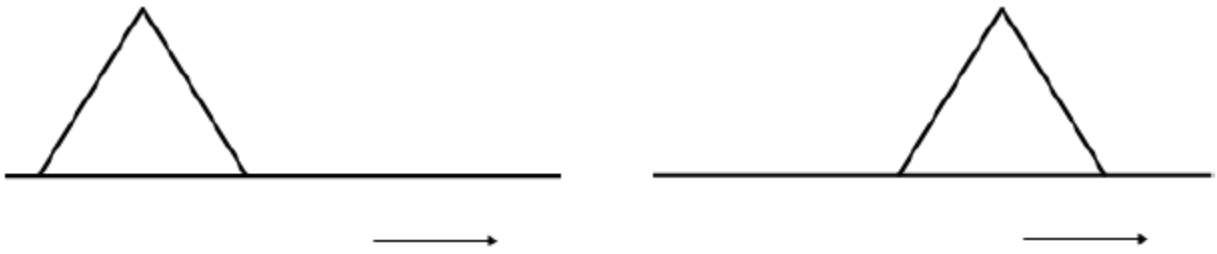
Let us take for example, the temperature distribution of a flow in straight a pipe, where the velocity is fixed by pumping a fixed volume flow rate into the pipe, Assume also that the flow velocity is not altered by the change in temperature. The temperature distribution $T(x,t)$ in the pipe as a function of the pipe axial coordinate x is given by the following differential equation:

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} - \alpha\frac{\partial^2 T}{\partial x^2} = 0 \qquad \ldots\ldots. 1$$

where u is the flow velocity which is assumed constant across the pipe, t is time and α is the thermal diffusivity. In Equation 1, the first term is the time derivative expressing the temperature gradient with time. The second term is called the advection term which is responsible for the transport of any temperature disturbance with the flow without any distortion.

The third term is called the diffusion term, which is responsible for the spread of any disturbance in all directions. To illustrate these concepts, let us take these terms one by one. If the thermal diffusivity is assumed to be negligible, Equation 1 reduces to:

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} = 0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots 2$$



(a) x (b)

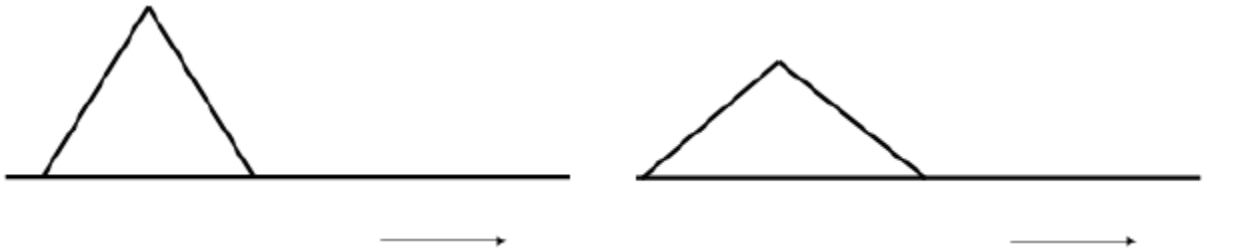
x

Figure 3: Convection of a disturbance in a pipe.

A temperature disturbance entering the pipe from the left (Figure 1(a)) at time t = 0 will be convected without any distortion after a while to the right as shown in Figure 1(b). If the flow velocity is zero, Equation 1 reduces to:

$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = 0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots 3$$

A temperature disturbance shown in Figure 4(a) will be diffused to the right and left and reduced in amplitude after a while as shown in Figure 4(b). The action of both convection and diffusion can now be added together to represent the behaviour described by equation 3 as shown in Figure 5, where a disturbance introduced at the left, will both be convected and diffused as shown in Figure 5(b).



(a) x (b)

x

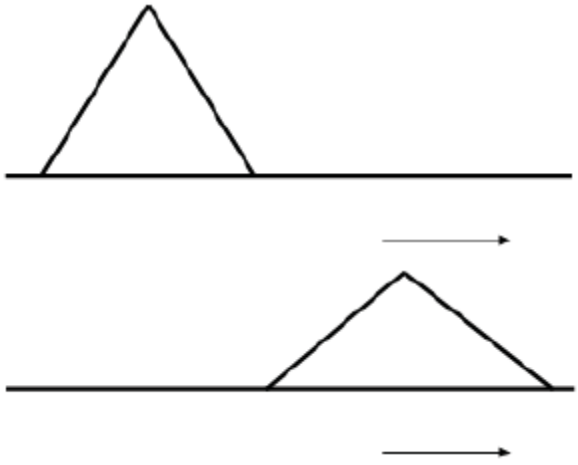
Figure 4: Diffusion of a wave in a pipe.

The simplicity of this system enabled a straightforward interpretation of the various terms. Equation 3 is said to be linear because the velocity is assumed constant and does not depend on temperature. Hence there is only one dependent variable, which is the temperature.

A system which might include a nonlinear convective term is shown in the equation below:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \alpha \frac{\partial^2 u}{\partial x^2} = 0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots 4$$

This equation represents the transport of momentum along the pipe. In this case, velocity is the dependent variable and it is not assumed to be constant. The nonlinearity arises in the convective term where the velocity, which is the sought variable, is being convected by the action of the velocity itself.



(a) x (b)
x

Figure 5: Convective and diffusion of a wave in a pipe.

THE NAVIER - STOKES EQUATIONS.

The Navier – Stokes and continuity equations provide the foundations for modeling fluid motion.

The laws of motion that apply to solids are valid for all matter including liquids and gases. A principal difference, however, between fluids and solids is that fluids distort without limit. For example, if a shear stress is applied to a fluid, then layers of fluid particles will move relative to each other and the particles will not return to their original position if application of the shear force is stopped. Analysis of a fluid needs to take account of such distortions.

A fluid particle will respond to a force in the same way that a solid particle will. If a force is applied to a particle, acceleration will result as governed by Newton's second law of motion, which states that the rate of change of momentum of a body is proportional to the unbalanced force acting on it and takes place in the direction of the force. It is useful to consider the forces that a fluid particle can experience. These include:

body forces such as gravity and electromagnetism;
forces due to pressure;
forces due to viscous action;
forces due to rotation.

Assuming that the shear rate in a fluid is linearly related to shear stress, and that the fluid flow is laminar, Navier (1823) derived the equations of motion for a viscous fluid from molecular considerations. Stokes (1845) also derived the equations of motion for a viscous fluid in a slightly different form and the basic equations that govern fluid flow are now generally known as the Navier-Stokes equations of motion. The Navier-Stokes equations can also be used for turbulent flow, with appropriate modifications.

The Navier – Stokes equation can be derived by considering the dynamic equilibrium of a fluid element.

They state that the inertial forces acting on a fluid element are balanced by the surface and body forces

We are not going to derive the Navier-Stokes and continuity equations here as this can be found in most standard text books. However, we will state the equations here and briefly give the physical interpretation of the terms as this will help us understand the numerical schemes used to solve those equations. It will also allow us to introduce the various levels of approximations used to simplify the equations to reduce the numerical solution costs.

COMPRESSIBLE FLOW.

The flow governing equations are the continuity equation, momentum equation (Navier – Stokes) and energy equation:

$$-\frac{\partial \rho}{\partial t} = \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad 5$$

THE NAVIER – STOKES EQUATION.

$$\underbrace{\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z}\right)}_{\text{Inertial terms}} = \underbrace{-\frac{\partial p}{\partial x}}_{\text{Pressure gradient}} + \underbrace{\mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right)}_{\text{Viscous terms}} + \underbrace{F_x}_{\text{Body force terms}} \quad \ldots 6$$

$$\rho\left(\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z}\right) = -\frac{\partial p}{\partial y} + \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2}\right) + F_y \quad \ldots\ldots\ldots \quad 7$$

$$\rho\left(\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z}\right) = -\frac{\partial p}{\partial z} + \mu\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) + F_z \quad \ldots\ldots\ldots \quad 8$$

THE ENERGY EQUATION.

$$\rho c_p\left(\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} + w\frac{\partial T}{\partial z}\right) = \Phi + \frac{\partial}{\partial x}\left[k\frac{\partial T}{\partial x}\right] + \frac{\partial}{\partial y}\left[k\frac{\partial T}{\partial y}\right] + \frac{\partial}{\partial z}\left[k\frac{\partial T}{\partial z}\right] + \left(u\frac{\partial p}{\partial x} + v\frac{\partial p}{\partial y} + w\frac{\partial p}{\partial z}\right) \quad \ldots\ldots\ldots\ldots\ldots\ldots 9$$

Where Φ is the dissipation function given by:

$$\Phi = 2\mu\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2 + 0.5\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2 + 0.5\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)^2 + 0.5\left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}\right)^2 - \frac{2}{3}\mu\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right)^2\right]$$

In these equations, *u,v,w* are the velocity components in the x, y, z directions, ρ is the density, T is the temperature, p is the pressure, μ is the viscosity and c_p is the specific heat at constant pressure.

The continuity equation applies to all fluids, compressible and incompressible flow, Newtonian and non-Newtonian fluids. It expresses the law of conservation of mass at each point in a fluid and must therefore be satisfied at every point in a flow field.

It is worthwhile to offer brief comment on the physical significance of Equations (2.6-2.8). The terms on the left side are often referred to as inertial terms, and arise from the momentum changes. These are countered by the pressure gradient, $\partial p/\partial x$, viscous forces which always act to retard the flow, and if present, body forces.

The inertial term gives a measure of the change of velocity of one fluid element as it moves about in space. The term $\partial/\partial t$ gives the variation of velocity at a fixed point and is known as the local derivative. The remaining three terms of the inertial term are grouped together and known as the convective terms or convective differential.

Assuming constant properties of viscosity and specific heat, the above system of equations contains 6 unknowns. With only five equations available, a further equation is needed to close the system. Usually, this is provided by a constitutive relation for the pressure. For example, for an ideal gas, the relation between temperature and pressure is given by: $p = \rho RT$, where R is the gas constant.

INCOMPRESSIBLE FLOW.

The above system of equation can be simplified if the density is constant. If the temperature is also is assumed constant, the system reduces to (for simplicity, body forces are also neglected, but they can be retained if needed):

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \quad \ldots\ldots\ldots\ldots \quad 10$$

$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right)=-\frac{\partial p}{\partial x}+\mu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right) \quad \ldots\ldots\ldots\ldots \quad 11$$

$$\rho\left(\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}\right)=-\frac{\partial p}{\partial y}+\mu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right) \quad \ldots\ldots\ldots\ldots \quad 12$$

$$\rho\left(\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}\right)=-\frac{\partial p}{\partial z}+\mu\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right) \quad \ldots\ldots\ldots\ldots \quad 13$$

For incompressible flows with temperature variation, the energy equation need to be solved to obtain the temperature variation, but its effect on the continuity and momentum equations are neglected.

BASIC COMPUTATIONAL TECHNIQUES

In this Chapter, basic computational techniques will be introduced. We will start first by describing how the typical terms in a fluid flow differential equation, namely first and second derivatives are converted to approximate discrete expressions which can be used in the construction of numerical schemes. We will briefly talk about time discretisation, leaving more details about this later on as further concepts are developed.

A general description of the most common discretisation techniques for fluid flow will then be given, namely the Finite Difference Method, The Finite Element Method and The Finite Volume Method.

- DISCRETISATION

Converting Derivatives to Discrete Expressions.

The process of obtaining a numerical solution to a differential equation can be viewed in the same way as conducting a lab experiment. In a lab experiment, the physical quantity, flow velocity for example, is measured at discrete points in the domain of interest using a measurement device. A picture of the flow variation then can be constructed by connecting the measurement points allowing us to visualise the flow.

If we require the flow quantities between the measurement points, some interpolation technique can be used which may be linear or a higher order interpolation. This will depend on how far the points from each other, or how accurate we require these intermediate quantities.

In the same manner, numerical techniques convert the continuous differential equation to that of finding the solution at discrete points in space which we call grid points. A full picture of the flow then can be constructed from the solution at those points.

- SPATIAL DISCRETISATION.

Let us assume that we want to represent a variation of a function θ, such as the one shown in Figure 6 using a polynomial in x of degree n. The function then can be expressed as:

$$\theta(x) = a_0 + a_1 x + a_2 x^2 + \cdots \ldots \ldots \ldots + a_n x^n \quad \ldots\ldots\ldots\ldots \quad 14$$

We need then to employ a numerical method to find the coefficients $a_0, a_1 \ldots\ldots a_n$. Once these coefficients are determined, we are able to evaluate the function θ at any given value of x.

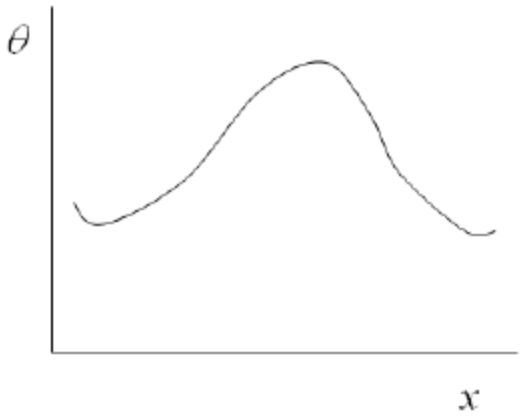


Figure 6: One dimensional function with x – coordinate.

However, this procedure is inconvenient as every time we need the value of the function at a point, we need to substitute into the polynomial. The values of the coefficients themselves have no physical meaning and it is not easy to judge their validity by inspection.

A rather more convenient way is to employ the value of the dependent variable θ at the discrete points as the unknown which need to be determined numerically. The numerical methods to do that include providing a set of algebraic equations of these unknowns and finding an algorithm to solve those equations. This leads us to the concept of discretisation of the differential equation.

By focussing our attention on the values of the dependent variable at a set of grid points, we can replace the continuous information contained in the differential equation with discrete values. We thus can say that we have discretised the distribution of θ in the domain of interest.

The algebraic equations that involve the unknown values of the function θ at the grid points are derived from the governing differential equation by transferring the spatial derivatives to their discrete approximations as we shall see below.

We can thus view the discretised equations as algebraic relations connecting the approximations of the values of the dependent variable at the grid points. Since these algebraic equations are derived from the differential equation, they express the same physical information as that differential equation.

DISCRETISATION METHODS.

We turn our attention now to the process of deriving the discretization equations. The discretized form of a differential equation can be derived in many ways. We shall concentrate in this lecture on the most common methods used. These methods are explained in the following three subsections.

- The Finite Difference Method.

The simplest procedure used to derive the discrete from of a differential equation, which we call here the Finite Difference equations consists of approximating the derivatives in the differential equation using a truncated Taylor series.

The Finite Difference Method is the simplest method to apply, particularly on uniform grids. However it requires high degree of mesh regularity. The mesh needs to be set up in a structured way where mesh points sould to be located at the intersection points of families of rectilinear curves.

Let us consider a one dimensional situation where the independent variable θ is a function of the space coordinate x as shown in Figure 6. We will discretise the spatial domain using equal space intervals of Δx and concentrate on three neighbouring points in the domain shown by the enlarged part of the domain in Figure 7. The three points are numbered arbitrarily as shown in the figure.

For grid point 2 in the middle between points 1 and 3, the Taylor series expansion gives the value of the field variable at point 1 as a function of the field variable and its derivatives at point 2 as follows:

$$\theta_1 = \theta_2 - \Delta x\left(\frac{d\theta}{dx}\right)_2 + \frac{1}{2}(\Delta x)^2\left(\frac{d^2\theta}{dx^2}\right) - \ldots\ldots + \frac{1}{n}(\Delta x)^n\left(\frac{d^n\theta}{dx^n}\right) - \ldots\ldots \quad \ldots\ldots 15$$

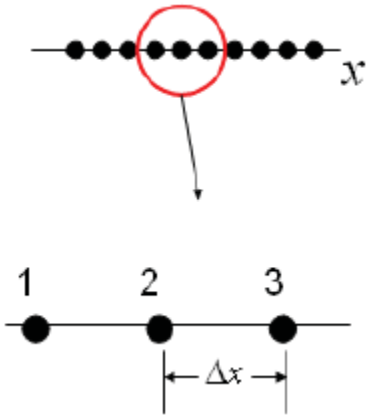


Figure 7: Finite Difference discretization.

Similarly, the expansion gives the field variable at point 3 as:

$$\theta_3 = \theta_2 + \Delta x\left(\frac{d\theta}{dx}\right)_2 + \frac{1}{2}(\Delta x)^2\left(\frac{d^2\theta}{dx^2}\right) + \ldots\ldots + \frac{1}{n}(\Delta x)^n\left(\frac{d^n\theta}{dx^n}\right) + \ldots\ldots \quad \ldots\ldots 16$$

By truncating the series in equation 15 after the 2nd term and rearranging, we obtain this expression for the first derivative at point 2:

$$\left(\frac{d\theta}{dx}\right)_2 = \frac{\theta_2 - \theta_1}{2\Delta x} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 17$$

This is called the first order backward difference approximation of the first derivative.

Similarly, a first order forward difference can be obtained from equation 16. By subtracting equation 16 from equation 15, a second order central difference approximation for the first derivative is obtained:

$$\left(\frac{d\theta}{dx}\right)_2 = \frac{\theta_3 - \theta_1}{2\Delta x} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 18$$

By adding equations 16 and 17, we obtain an expression for the second derivative at point 2:

$$\left(\frac{d^2\theta}{dx^2}\right)_2 = \frac{\theta_1 - 2\theta_2 + \theta_3}{(\Delta x)^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 19$$

If we substitute the expressions for the approximate derivatives into a differential equation, we obtain what is called the finite difference equation [redacted] Note that this leads to the transformation of the differential equation to an algebraic equation at point 2. Similar expressions can be obtained for all the points in the domain leading to a set of discrete algebraic equations.

Boundary conditions are applied by setting the known values at the end points. The system of algebraic equations can then be solved for the unknown quantities at the grid points.

THE FINITE ELEMENT METHOD.

The Finite Element Method is based on the so called 'Method of Weighted Residuals'. This is a powerful method for solving partial differential equations which was developed between 1940 and 1960, mainly for structural dynamics problems. This was extended later to the field of fluid flow.

This method has a distinct advantage over the Finite Difference method in the fact that it allows naturally for handling complex arbitrary geometries as it can be easily applied using irregular grids of various shapes. It also provides a set of functions that give the variation of the differential equations between grid points, whereas Finite Difference method provides information for the values at grid points only.

Assume that the differential equation at hand is of the general convection diffusion form as given in Equation [redacted]1. Taking the steady state version of this equation, to focus on the spatial discretisation, the equation becomes:

$$\mu\frac{\partial T}{\partial X} - \alpha\frac{\partial^2 T}{\partial X^2} = 0 \quad \ldots\ldots\ldots\ldots\ldots \quad 20$$

For simplicity of presentation, this equation will be expressed in symbolic form as:

$$Q(T) = 0 \quad \ldots\ldots\ldots\ldots\ldots \quad 21$$

Note that equation 20 is given here for illustration purposes and the principle can be applied for any other differential equation.

If we assume that we are seeking an approximate solution T' using a trial function of some form. Then substituting this into the differential equation will not satisfy the equation. Thus a residual appears on the right hand side instead of zero. That is:

$$Q(T') = R \quad \ldots\ldots\ldots\ldots\ldots \quad 21$$

Because $Q(T')$ is an approximation, residual R does not vanish in most of the domain. The 'Weighted Residual Method' is based on the concept of introducing a weighting function W and then requiring that the integral of the weighted residual vanishes over the whole solution domain. That is:

$$\int_{\Omega} WQ(T')d\Omega = 0 \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 22$$

For the sake of argument, if we assume that the trial function is a polynomial with a number of unknown coefficients, then by selecting a succession of trial functions and integrating, a number of equations can be created which can be solved simultaneously to obtain the coefficients of the polynomial thus resulting in the solution.

This implies that the finite element method can be used to obtain analytic solutions to differential equations provided suitable trial and weighting functions can be found.

Now we turn our attention on how to use this method to solve differential equations numerically. The first step is to assume local trial functions over the discretised domain. The solution domain is subdivided into non-overlapping cells, called elements. For example, in one dimension, these can be line segments between grid points. The trial functions are then interpolation functions which assume the shape of the variation of the variable between the grid points comprising the cell. The simplest of which are the linear shape functions that assume that the field variable has a linear variation between grid points. We then can express the solution as:

$$T'(x) = T_i N_i(x) \quad \ldots\ldots\ldots\ldots\ldots \quad 23$$

where N_i is the interpolation function at node i and T_i is the sought solution at that node. By choosing a series of weighting functions that have the value of W^i at node i and zero elsewhere for each node in the domain in turn, we can get an expression of the discrete weighted residual form by substituting into equation 22.

Substituting in equation, we obtain:

$$\int_{\Omega} W'Q\big(T_i N_i(x)\big)d\Omega = 0 \quad \ldots\ldots\ldots\ldots\ldots \quad 24$$

Integrating at all the domain cells produces a system of algebraic equations of the form

$$K \bullet T_i = r \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad 25$$

Which can be solved for the coefficients T_i representing the field function at the nodal points. The matrix K is called the Jacobean or Mass matrix and the right hand side usually contains boundary conditions and source terms if there is any.

There are several possible choices for the approximation function and the weighting function. The most widely used choice is that weighting function is the same as the approximation function. This method is called the Galerkin Method.

THE FINITE VOLUME METHOD.

This method was developed in the early 1970's. It can be viewed as a special case of the Weighted Residual Method described in the previous Section, where the weighting function takes the form:

$$W^I = 1 \qquad \ldots\ldots\ldots\ldots \quad 26$$

For this, a number of weighted residual equations are generated by dividing the solution domain into sub-domains called 'control volumes' and setting the weighting function to be unity over the control volumes one at a time, and zero elsewhere. This implies that the residual over each volume must become zero.

Another way of deriving a finite volume discretisation is by starting from the integral form of the flow equations. Recall [redacted] that we expressed the flow equations in their differential form. An alternative way of expressing the flow equations is the so called integral form.

For example, the continuity equation (Equation 1.5) can be expressed for a control volume Ω with a surface boundary Γ as:

$$\frac{\partial}{\partial t}\int_{\Omega} \rho d\Omega + \oint_{\Gamma} \rho \vec{U} d\vec{\Gamma} = 0 \qquad \ldots\ldots\ldots\ldots \quad 27$$

where $U = \vec{u} + \vec{v} + \vec{w}$. This essentially states that the rate of accumulation of matter within domain Ω equals to the rate of the flux through its boundaries.

Similarly, integral formulations can be obtained for the momentum equations. For example, the integral form of the x-momentum equation takes the form:

$$\frac{\partial}{\partial t}\int_{\Omega} \rho u d\Omega + \oint_{\Gamma} \left(\rho u \vec{U} + p - \tau\right) d\Gamma \qquad \ldots\ldots\ldots\ldots\ldots \quad 28$$

where τ is the viscous flux given by:

$$\tau = \mu\left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} + \frac{\partial u}{\partial z}\right)$$ …….. 29

Similar integral forms can be written for the y and z momentum equations.

The finite volume formulation can start from this integral form. The fact that the variation of any quantity within a volume depends entirely on the surface values of the fluxes presents the basis of the Finite Volume formulation

The Finite Volume formulation starts by subdividing the solution domain into small volumes. We can then write the integral form of the conservation laws for each volume separately. The global conservation can be recovered by adding up the fluxes of the sub-volumes.

Let's take for example the volume in Figure 8, which is divided to 4 sub-volumes

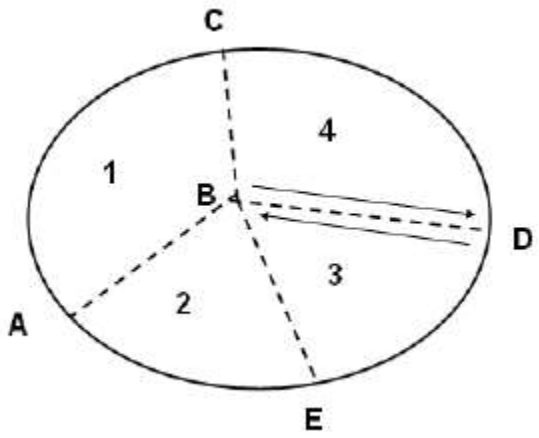


Figure 8: Finite Volume Subdivisions.

The flux through the internal subdivisions cancels out. For example the flux going through boundary BD of volume 3 is equal in magnitude and opposite in sign to the flux going through boundary DB of volume 4.

By working out the fluxes through all the boundaries on each sub-volume in terms of the field variable either at the volume centre point or at the vertices, a system of algebraic equations is constructed which can be solved for the unknown field variables.

EXAMPLE 1

We will use here the solution of a simple equation to illustrate the use of the Finite Difference Method to solve a differential equation in one dimension. The problem at hand is that of heat transfer in a cylindrical fin given in Figure 9, where both the base and the tip have fixed temperatures.

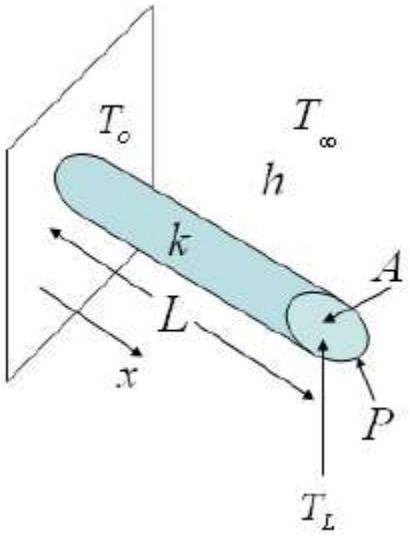


Figure 9: Heat transfer from a circular fin.

If we define the non-dimensional temperature as:

$$\theta = \frac{T - T_\infty}{T_o - T_\infty}$$

and the axial coordinate as:

$$\zeta = \frac{x}{L}$$

Additionally, the characteristic convection conduction parameter is defined as:

$$\psi^2 = \frac{hP}{kA} L^2$$

where h is the convective heat transfer coefficient of the fluid around the fin, k is the conductivity of the fin material and P and A are the perimeter and cross sectional area of the fin respectively. It can be shown that the differential equation governing the temperature distribution along the fin is given by:

$$\frac{\partial^2 \theta}{\partial \zeta^2} - \psi^2 \theta = 0$$

We are required to obtain a solution for this equation for the following conditions:

$\psi^2 = 3$

$\theta_{base} = 1$

$\theta_{tip} = 0$

Let us discretise the one dimensional domain using 5 cells of equal spacing resulting in 6 grid points as shown in Figure 10

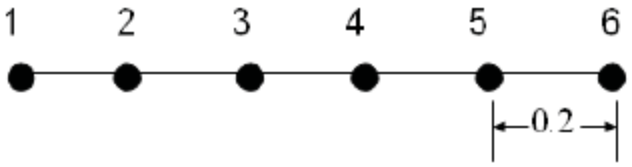


Figure 10: Grid used for the fin problem.

Boundary conditions are given for points 1 and 6 as above. So for internal points, using equation 18 for the second derivative, a discrete form for each point can be written as follows:

$$\frac{\theta_{i-1} - 2\theta_i + \theta_{i+1}}{(0.2)^2} - 3\theta_i = 0$$

Rearranging:

$$25\theta_{i-1} - 53\theta_i + 25\theta_{i+1} = 0 \qquad \ldots\ldots\ldots\ldots\ldots \quad 31$$

Thus if we use the boundary conditions for the end nodes and equation 31 for the inner nodes, we obtain the following set of algebraic equations for the discrete system:

$\theta_1 = 1$

$25\theta_1 - 53\theta_2 + 25\theta_3$

$25\theta_2 - 53\theta_3 + 25\theta_4$

$25\theta_3 - 53\theta_4 + 25\theta_5 \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad 32$

$25\theta_4 - 53\theta_5 + 25\theta_6$

$\theta_6 = 0$

This is a system of six equations containing six unknowns, which can be easily solved for the unknown temperatures. The solution for this systems and comparison with analytical solution will be left for the student as an exercise.

Assignment.

Discuss the three basic properties of Numerical schemes:

a. Consistency.
b. Stability
c. Convergence

THE FINITE DIFFERENCE METHOD.

During the lecture we presented a brief overview of the most popular methods used for the discretization of differential equations. The finite difference method was introduced and it was mentioned it is the simplest one conceptually. However, this method is difficult to apply when we are encountered with complex geometries. For this reason, this method is of limited use for practical applications and only a very small number of engineering codes rely on this method.

However, the simplicity of the method allows us to explore the properties of various numerical discretisations and compare their degree of accuracy. It also allows us to have a better grasp of numerical procedures. Additionally, for solution procedures which require higher order derivatives or high order of accuracy, this method can be better suited than other methods despite the limitation of mesh regularity.

THE FINITE DIFFERENCE METHOD BASICS.

During the lecture we have used the Taylor's series expansion to transform the terms in a differential equation to their discrete counterpart at grid points. We will start with this to build an understanding of the accuracy of the various formulations.

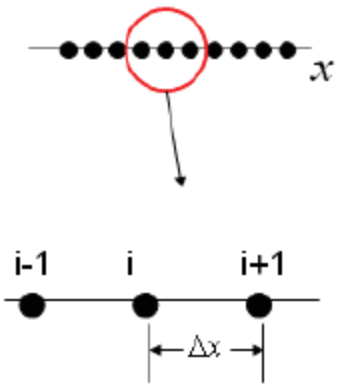


Figure 1: Finite difference stencil.

Let's start with the Finite Difference stencil shown in Figure 1. A Taylor's series expansion around point i in terms point $i-1$ gives:

$$\theta_{i-1} = \theta_i - \Delta x\left(\frac{d\theta}{dx}\right)_i + \frac{1}{2}(\Delta x)^2\left(\frac{d^2\theta}{dx^2}\right)_i - \frac{1}{3}(\Delta x)^3\left(\frac{d^3\theta}{dx^3}\right)_i + \ldots\ldots \quad \ldots\ldots\ldots\ldots\ldots\ldots\ 1$$

Rearranging equation 1 gives:

$$\left(\frac{d\theta}{dx}\right)_i = \frac{\theta_i - \theta_{i-1}}{\Delta x} + \frac{1}{2}\Delta x\left(\frac{d^2\theta}{dx^2}\right)_i - \frac{1}{3}(\Delta x)^2\left(\frac{d^3\theta}{dx^3}\right)_i + \ldots\ldots \quad \ldots\ldots\ldots\ldots\ 2$$

If we truncate the right hand side after the first term, we obtain the expression:

$$\left(\frac{d\theta}{dx}\right)_i = \frac{\theta_i - \theta_{i-1}}{\Delta x} \quad \ldots\ldots\ldots\ldots\ldots\ 3$$

The expression in Equation 3 is called the backward difference and it is first order accurate. The order of accuracy is related to the power of Δx in the first truncated term of the Taylor's series, which is one in this case.

Similarly, a first order accurate forward difference can be obtained by a Taylor's series expansion in terms of point $i+1$ as follows:

$$\theta_{i+1} = \theta_i + \Delta x\left(\frac{d\theta}{dx}\right)_i + \frac{1}{2}(\Delta x)^2\left(\frac{d^2\theta}{dx^2}\right)_i + \frac{1}{3}(\Delta x)^3\left(\frac{d^3\theta}{dx^3}\right)_i + \ldots\ldots \quad \ldots\ldots\ldots\ldots\ 4$$

$$\left(\frac{d\theta}{dx}\right)_i = \frac{\theta_{i+1} - \theta_i}{\Delta x} + \frac{1}{2}\Delta x\left(\frac{d^2\theta}{dx^2}\right)_i + \frac{1}{3}(\Delta x)^2\left(\frac{d^3\theta}{dx^3}\right)_i + \ldots\ldots \quad \ldots\ldots\ldots\ldots\ 5$$

$$\left(\frac{d\theta}{dx}\right)_i = \frac{\theta_{i+1} - \theta_i}{\Delta x} \quad \ldots\ldots\ldots\ldots\ldots\ 6$$

If we add Equations 2 and 4 and divide both sides by 2 gives:

$$\left(\frac{d\theta}{dx}\right)_i = \frac{\theta_{i+1} - \theta_{i-1}}{2\Delta x} + 0 + \frac{1}{3}(\Delta x)^2\left(\frac{d^3\theta}{dx^3}\right)_i + \ldots\ldots \quad \ldots\ldots\ldots\ldots\ 7$$

Truncating equation 7 after the first term gives:

$$\left(\frac{d\theta}{dx}\right)_i = \frac{\theta_{i+1} - \theta_{i-1}}{2\Delta x} \quad \ldots\ldots\ldots\ldots\ 8$$

Equation 8 is a central difference scheme of 2nd order accuracy because the first truncated term is in the order of $(\Delta x)^2$. That is the power of Δx for the first truncated term is two. A geometrical interpretation of the three difference schemes is shown in Figure 2. It can be seen that the central difference approximation provides a better representation of the slope of the curve at the point of interest which is the first derivative.

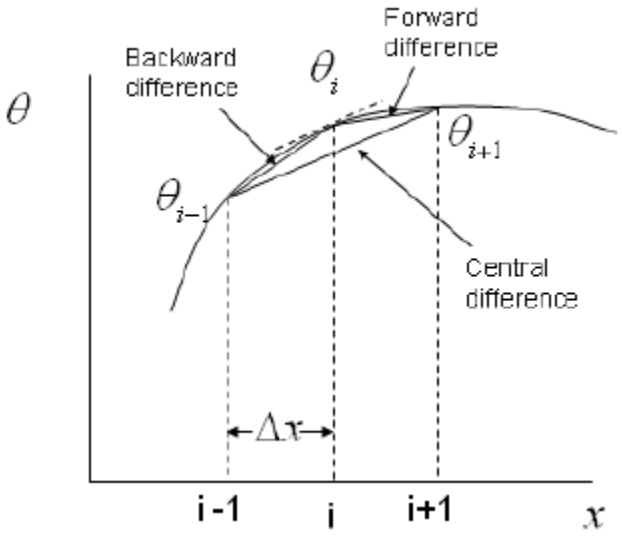


Figure 2: Geometric interpretation of difference formulae.

Example 2.

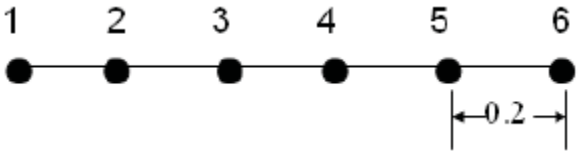
In this example, we will revisit the fin example presented earlier. The objective is to show how the finite difference gradient boundary condition can be applied. Let's solve the equation:

$$\frac{\partial^2\theta}{\partial\zeta^2} - \psi^2\theta = 0 \qquad \text{..... 9}$$

with the boundary condition $\frac{\partial\theta}{\partial\zeta} = 0$ at $x = L$, that is at $\zeta = 1$. This is a more realistic boundary condition than prescribed temperature. It indicates that the heat flux at the tip of the fin is zero, indicating that temperature gradient is zero.

SOLUTION.

Let's use the same discretization of 6 grid points earlier introduced, and use the central difference scheme for all internal nodes (node 2 – 5) as before giving the discrete equation of



$$25\theta_{i-1} - 53\theta_i + 25\theta_{i+1} = 0$$

At point 1, the temperature is specified by the base temperature and thus we do not need to elaborate further as we have:

$$\theta_1 = 1$$

However, for point 6, there is a problem if we attempt to use the central difference scheme as there is no grid point to the right of point 6. Remember that we need to apply the gradient boundary condition at this point. We could be tempted to use a backward difference formula (Equation 13). At the first instance, this might seem a good idea. Let's examine that.

Applying Equation 13 to point 6 and imposing the condition of $\frac{\partial \theta}{\partial \zeta} = 0$ gives:

$$\frac{\theta_6 - \theta_5}{0.2} = 0$$

This leads to the equation $\theta_6 = \theta_5$

This can be used with the other set of equations to solve the problem, however, an error is found near that point which propagates to the rest of the domain. This error results from the fact that the discretisation at point 6 is first order accurate which is not consistent with the second order accurate scheme for the internal nodes. Figure 13 shows the solution compared to the analytic solution for this case.

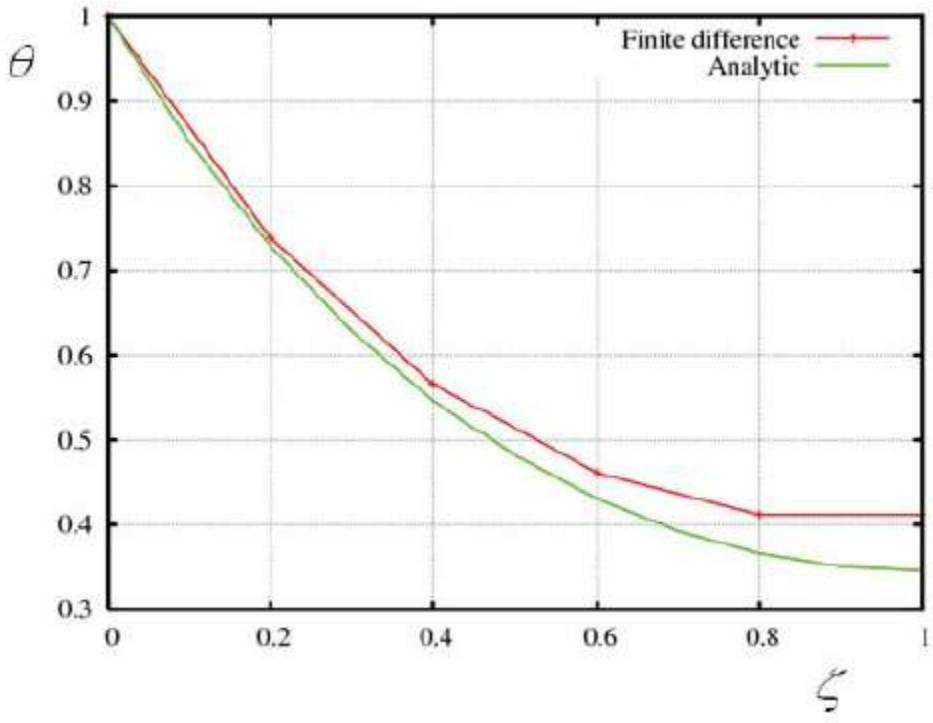


Figure 3: Solution with first order discretization of boundary conditions.

overcome this problem, the boundary conditions equation needs to be discretised with the same order of accuracy as the internal points. To enable this, we add an imaginary point after nodes 6, lets say node 7, and we work out the value of the field variable at this node in terms of the values at nodes 5 and 6. This then allows us to formulate a central difference equation. Thus, with reference to Figure 4:

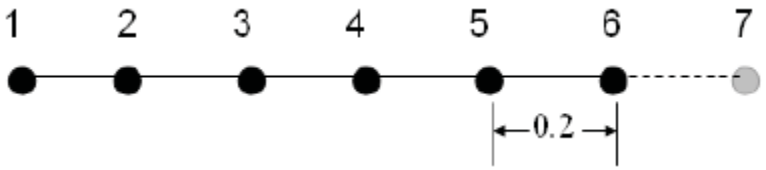


Figure 5: Applying gradient boundary condition at point 6.

The central difference formula at point 6 is then:

$$25\theta_5 - 53\theta_6 + 25\theta_7 = 0$$

which can be solved for θ_7 to give:

$$\theta_7 = \frac{53\theta_6 - 25\theta_5}{25} \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad 10$$

The second order gradient boundary condition for point 6 is then:

$$\frac{\partial\theta}{\partial\zeta} = \frac{\theta_7 - \theta_5}{0.4} = 0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad 11$$

Substituting from 10 into 11:

$$\frac{\frac{53\theta_6 - 25\theta_5}{25} - \theta_5}{0.4} = 0$$

which can be rearranged to give:

$$53\theta_6 - 50\theta_5 = 0$$

Which is clearly different from that obtained using the first order backward formula above. Using this equation together with the other equations for the rest of the nodes leads to the solution shown in Figure 5 which is in a much better agreement with the analytic solution.

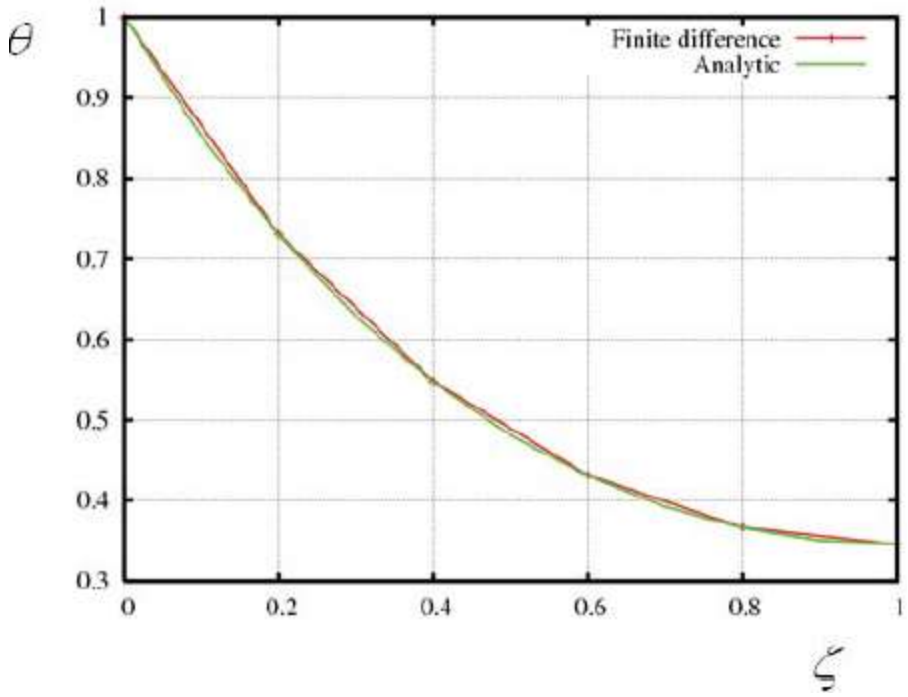


Figure 5: Solutions with second order discretization of boundary conditions.

OTHER DIFFERENCE FORMULAE

We have seen that difference formulae for the first derivative can be formulated using one or two adjacent points. However, finite difference formulae for the first derivative can be formulated using any number of adjacent points with the order of approximation increasing with the number of points.

In a particular numerical scheme, a balance need to be found between the order of accuracy and the number of grid points involved in the computation. This will dictate the computational memory and effort both need to be kept to a minimum for a given overall solution accuracy.

It is usually difficult to devise rules that govern the optimum combination of discretisation accuracy and number of grid points as these vary from problem to problem and only experience with a large number of cases can produce guidance in this respect.

Let's now examine the process of finding formulae involving more grid points for a given accuracy. Consider the stencil shown in Figure 6.

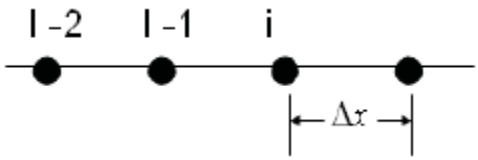


Figure 6: Stencil for second order backward difference formula.

If we are required to formulate a second order backward difference formula, we use the following procedure:

$$\frac{d\theta}{dx} = \frac{a\theta_i + b\theta_{i-1} + c\theta_{i-2}}{\Delta x} + O\left[(\Delta x)^2\right] \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 12$$

where O in the last term on the right ha
expansions to create a system of equati

$$\theta_{i-1} = \theta_i - \Delta x\left(\frac{d\theta}{dx}\right)_i + \frac{1}{2}(\Delta x)^2\left(\frac{d^2\theta}{dx^2}\right)_i - \frac{1}{3}(\Delta x)^3\left(\frac{d^3\theta}{dx^3}\right)_i + \ldots\ldots \quad \ldots\ldots\ldots\ldots \quad 13$$

$$\theta_{i-2} = \theta_i - 2\Delta x\left(\frac{d\theta}{dx}\right)_i + (2\Delta x)^2\left(\frac{d^2\theta}{dx^2}\right)_i - \frac{1}{3}(2\Delta x)^3\left(\frac{d^3\theta}{dx^3}\right)_i + \ldots\ldots \quad \ldots\ldots\ldots\ldots \quad 14$$

Multiplying Equation 13 by b and Equation 14 by c and adding $a\theta_i$ we get:

$$a\theta_i + b\theta_{i-1} + c\theta_{i-2} =$$

$$(a+b+c)\theta_i + \Delta x(2c+b)\left(\frac{d\theta}{dx}\right)_i + \frac{(\Delta x)^2}{2}(4c+b)\left(\frac{d^2\theta}{dx^2}\right)_i - O\left[(2\Delta x)^3\right] \quad \ldots\ldots 15$$

Comparing this to Equation 12, we find that only the coefficients of the term containing the first derivative will not vanish. This gives the following three Equations:

$$a + b + c = 0$$

$$-(2c + b) = 1$$

$$4c + b = 0$$

Solving simultaneously gives:

$$a = \frac{3}{2}, \quad b = -2, \quad c = \frac{1}{2}$$

Thus the second order difference formula becomes:

$$\frac{d\theta}{dx} = \frac{1.5\theta_i - 2\theta_{i-1} + 0.5\theta_{i-2}}{\Delta x} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad 16$$

The above procedure with undetermined coefficients can by systematically used to obtain finite difference formulae for all derivatives at any required degree of accuracy. As an exercise for the student, try to derive a second order forward formula using a three point stencil to give the following:

$$\frac{d\theta}{dx} = \frac{-1.5\theta_i + 2\theta_{i+1} - 0.5\theta_{i+2}}{\Delta x} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 17$$

MULTI – DIMENSIONAL FINITE DIFFERENCE FORMULAE

One of the advantages of the finite difference method is its straight forward extension to multi-dimensions. The way that partial derivatives of a function of several variables can be discretised using the same methods of the previous sections for each variable and for each coordinate direction.

To illustrate this lets consider the thermal conduction problem in two dimensions, which is also know as Laplace's equations.

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 18$$

Our objective is to discretise this equation for a two dimensional domain. Let's first consider internal nodes. Figure 7 shows part of the two dimensional finite difference grid with a stencil centred on point m, n. The index m is incremented in the x-direction, while the index n is incremented in the y direction

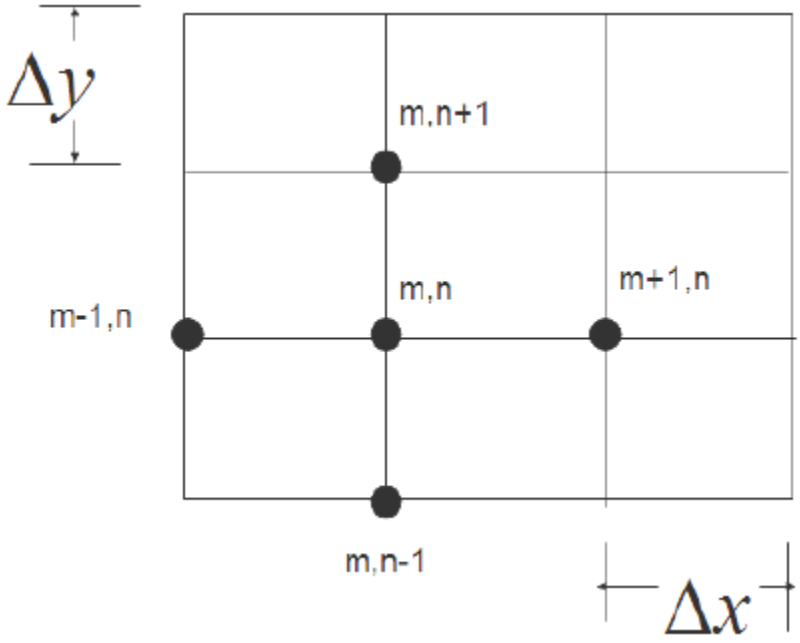


Figure 7: Two dimensional Finite Difference Stencil.

If we apply the second order difference formula of equation 19 (shown below) from the previous lecture for both x and y direction separately, we obtain the following discrete form for node m, n:

$$\left(\frac{d^2\theta}{dx^2}\right)_2 = \frac{\theta_1 - 2\theta_2 + \theta_3}{(\Delta x)^2}$$

$$\frac{T_{m+1,n} - 2T_{m,n} + T_{m-1,n}}{(\Delta x)^2} + \frac{T_{m,n+1} - 2T_{m,n} + T_{m,n-1}}{(\Delta y)^2} = 0 \quad \ldots\ldots\ldots\ldots\ 19$$

If we assume that the grid spacing is equal in both x and y directions, that is $\Delta x = \Delta y$, then Equation 19 reduces to:

$$T_{m+1,n} + T_{m-1,n} + T_{m,n+1} + T_{m,n-1} - 4T_{m,n} = 0 \quad \ldots\ldots\ldots\ldots\ 20$$

A similar equation can be obtained for each internal grid node. For boundary nodes, the discretisation will depend on the type of boundary conditions applied. If a given temperature boundary conditions is to be applies, then the equation for that node is deleted and replaced by the given value for the temperature.

If a flux boundary condition is to be applied, then a procedure similar to that explained above under "OTHER DIFFERENCE FORMULAE" is applied. In this case a fictious node is added and the value of the temperature at that node is computed as a function of the internal nodes. The same central difference scheme then can be used at boundary nodes. The resulting discretization leads to a number of equations, which equals the number of unknown temperatures. These equations can then be solved simultaneously for the unknown nodal temperatures.

The case described here illustrates the simplicity of extension of the finite difference method to two dimensions. Extension to three-dimensions is equally simple and follows the same logic.

THE FINITE ELEMENT METHOD.

The Finite Element Method was briefly introduced earlier. We also outlined the history of the method and its advantages. We also outlined the theoretical background and the framework by which the Galerkin weighted residual method is used to discretize differential equations. In this lecture, we will present the method in more detail.

The concept of the Finite Element Method can be traced back to the technique used in stress calculations whereby a structure was divided into small sub-structures of various shapes called 'elements'. The structure is then re-assembled after each element has been analysed.

The technique was developed further in what is now known as the Finite Element Method between 1940 and 1960, mainly in the field of structural dynamics. The technique was then expanded to solve field problems in the 1960's (Zeinkiewicz, 1977).

Nowadays, the Finite Element Method has been put in an engineering rigorous framework with precise mathematical conditions for existence, convergence and error bounds. In this lecture, we will not concentrate on the mathematical derivation of the method, but rather on its application for the discretization of differential equations.

THE FINITE ELEMENT METHOD BASICS.

As discussed earlier in the lecture, a numerical model for fluid flow starts with a physical model of the problem. We could choose a model of the full Navier – Stokes equations or any of the approximation levels. We then require solving the mathematical model over a given physical domain with some boundary conditions.

The first step is to discretise the spatial domain into non-overlapping elements or sub-regions. The Finite Element Method allows a variety of element shapes, for example, triangles, quadrilaterals in two dimensions and tetrahedral, hexahedral, pentahedral, and prisms in three dimensions. Each element is formed by the connection of a certain number of nodes, with the number of nodes in an element depending on the type of the element (Figure 1).

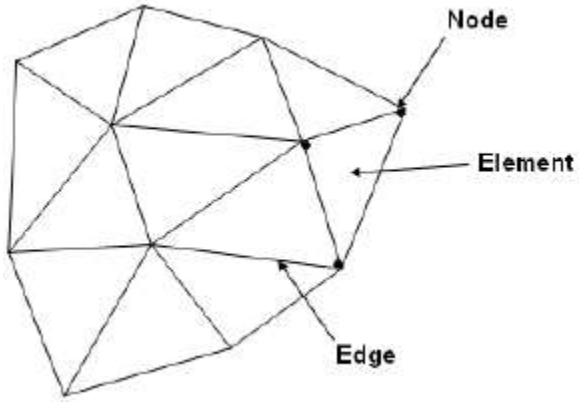


Figure 1:Typical two dimensional Finite Element Mesh.

The number of nodes in each element does not depend only on the number of corner points in the element, but also on the type of the element interpolation function as we will explain later.

Once a mesh is generated, we choose the type of interpolation function that represents the variation of the field variable over the element. A clear distinction can be seen here from the Finite Difference Method. In the Finite Difference Method, we were only interested in the values of the field variable at grid nodes, and no information was required for the behaviour between the nodes. We may have implicitly assumed that it is linear, but we did not have to do that.

The next stage is to determine the matrix equations that express the properties of the individual element by forming a left hand side matrix and a load vector. A typical left hand side matrix and a load vector for a one dimensional element may look like:

$$[K]_e = A\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 1$$

$$\{f\}_e = \begin{Bmatrix} q_i \\ q_j \end{Bmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 2$$

where A contains some geometric and/or physical parameters of the element.

The next stage is to assemble the element equations to obtain a system of simultaneous equations that can be solved for the unknown field variables at the mesh nodes. The final system of equations will be represented in matrix notation as:

$$[K]\{U\} = \{f\} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 3$$

The vector $\{U\}$ is the vector of the unknown field variables at the nodes.

In the next section, we will illustrate those steps using a simple example. But before we do that, we will present more information about the element shape functions and the Finite Element discretisation process of differential equations.

ELEMENTS AND SHAPE FUNCTIONS.

The Finite Element Method involves both the discretisation of the computational domain and the discretisation of the differential equations. In this process, the variables are represented in a piece-wise manner over the domain. By dividing the solution domain into elements, and approximating the solution over these elements using a suitable known function, a relationship between the elements and the differential equation is established.

The functions used to represent the variation of the solution within each element are called shape functions, or interpolation functions or basis functions. Typically, polynomial functions are used because they can be easily integrated or differentiated. The accuracy of the results can be improved by increasing the order of the polynomial used.

1. One - dimensional elements.

These are the simplest elements and their discussion will help illustrate the basic principles. The simplest element has a piece – wise linear interpolation function and contains two nodes. Let's consider the function shown in Figure 2. If the x-coordinate is discretised to a set of elements each containing two nodal points, and the function is approximated using linear variation between each nodes, then the variation for a typical element is shown in figure 3.

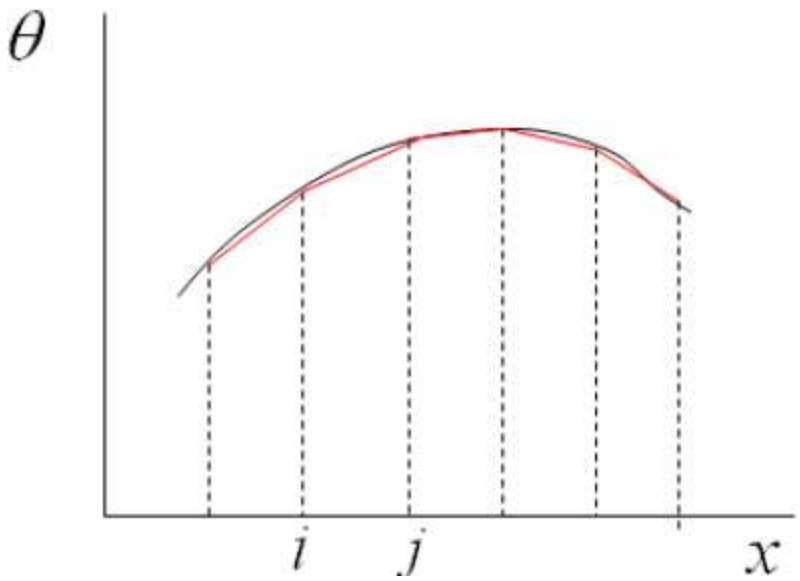


Figure 2: Linear piece-wise representation

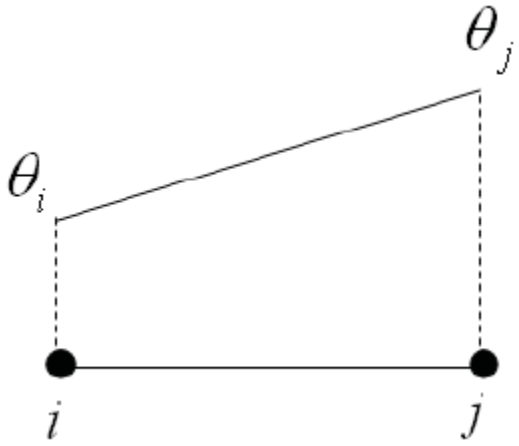


Figure 3: Linear variation over one element.

The linear variation over the element of Figure 3 can be represented using the summation of two shape functions N_i and N_j at nodes i and j respectively. Each shape function will have a maximum of unity and the corresponding point and varies linearly to zero at the other point as shown in Figure 4.

The shape functions can be expressed mathematically as:

$$N_i = \frac{x_j - x}{x_j - x_i} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 4$$

$$N_j = \frac{x - x_i}{x_j - x_i} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad 5$$

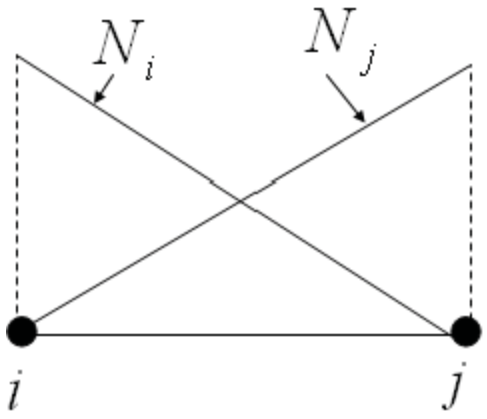


Figure 4: Linear shape functions in one dimension.

The field function is then represented over the element using the shape function as:

$$\theta_e = N_i\theta_i + N_j\theta_j \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 6$$

This is essentially the same as the linear variation in Figure 3. We can use the expression in equation 6 to get the first derivative of the field variable within the element. That is:

$$\frac{d\theta_e}{dx} = \frac{dN_i}{dx}\theta_i + \frac{dN_j}{dx}\theta_j \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 7$$

$$\frac{d\theta_e}{dx} = \frac{-1}{x_j - x_i}\theta_i + \frac{1}{x_j - x_i}\theta_j \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 8$$

Noting that $x_j - x_i$ is the length of the element. Let's give this length the symbol l.

Then equation 8 can be written in the following compact matrix notation:

$$\frac{d\theta_e}{dx} = \frac{1}{l}\begin{bmatrix}-1 & 1\end{bmatrix}\begin{bmatrix}\theta_i \\ \theta_j\end{bmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 9$$

We can observe from this also that the first derivative of the field variable is constant over the element. This indicates that the first derivative of the function over the domain will be stepwise constant over the entire domain indicating that it is not a continuous function.

Higher order shape functions can be obtained by using more nodes within the element. For example a quadratic shape function can be obtained by using three nodes in the element as shown in Figure 5. Using a quadratic polynomial, the shape functions can be derived to give (with the length of the element $l = x_k - x_i$):

$$N_i = 1 - \frac{3x}{l} + \frac{2x^2}{l^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 10$$

$$N_j = \frac{4x}{l} + \frac{4x^2}{l^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots 11$$

$$N_k = -\frac{x}{l} + \frac{2x^2}{l^2} \quad \ldots\ldots\ldots\ldots\ldots 12$$

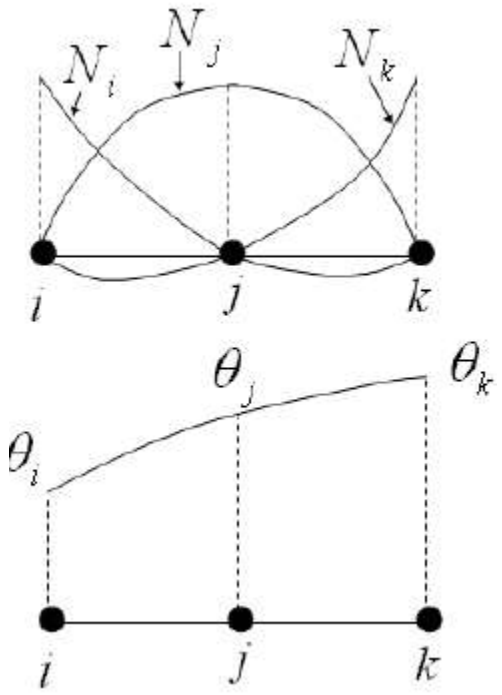


Figure 5: Quadratic element and shape functions.

And the field variable is represented over the element by:

$$\theta_e = N_i\theta_i + N_j\theta_j + N_k\theta_k \quad \ldots\ldots\ldots\ldots\ldots\ldots 13$$

TWO – DIMENSIONAL TRIANGULAR ELEMENTS.

The most popular element for arbitrary two dimensional geometries is the triangular element. This is mainly because triangular meshes are relatively easier to generate and to control their quality. In this lecture we will discuss the shape functions for these elements. A two dimensional linear element is shown in Figure 6. We can represent the variation of the field function on this element using a linear polynomial as follows:

$$\theta_e(x, y) = a + bx + cy \quad \ldots\ldots\ldots\ldots\ldots\ldots 14$$

If the field functions at the three grid point are labelled θ_1, θ_2 and θ_3, then the three coefficients a, b and c can be determined as follows:

$$\theta_1 = a + bx_1 + cy_1 \quad \ldots\ldots\ldots\ldots \quad 15$$

$$\theta_2 = a + bx_2 + cy_2 \quad \ldots\ldots\ldots\ldots \quad 16$$

$$\theta_3 = a + bx_3 + cy_3 \quad \ldots\ldots\ldots\ldots\ldots 17$$

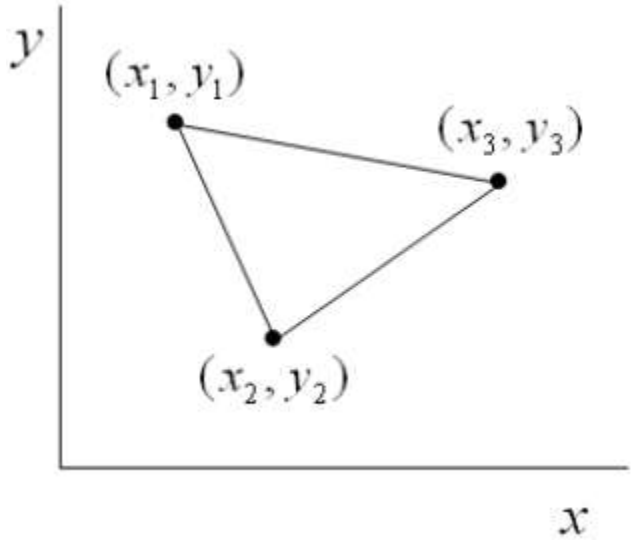


Figure 6: Two dimensional linear triangular element.

Equations 15 – 17 can be solved simultaneously to get the shape function coefficients in terms of the nodal coordinates to give:

$$a = \frac{1}{2A}\left[(x_2y_3 - x_3y_2)\theta_1 + (x_3y_1 - x_1y_3)\theta_2 + (x_1y_2 - x_2y_1)\theta_3\right] \quad \ldots\ldots\ldots\ldots \quad 18$$

$$b = \frac{1}{2A}\left[(y_2 - y_3)\theta_1 + (y_3 - y_1)\theta_2 + (y_1 - y_3)\theta_3\right] \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 19$$

$$c = \frac{1}{2A}\left[(x_3 - x_2)\theta_1 + (x_1 - x_3)\theta_2 + (x_2 - x_1)\theta_3\right] \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 20$$

where A is the area of the triangle given by:

$$A = \frac{1}{2}\left[(x_1y_2 - x_2y_1) + (x_3y_1 - x_1y_3) + (x_2y_3 - x_3y_2)\right] \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 21$$

Substituting the values of the three coefficients from equations 18 – 20 into equations 15 – 17 and gathering coefficients we obtain the following expression for equation 14:

$$\theta_e(x,y) = N_1\theta_1 + N_2\theta_2 + N_3\theta_3 \quad \ldots\ldots\ldots\ldots \; 22$$

where the shape functions are given by:

$$N_1 = \frac{1}{2A}\left[(x_2y_3 - x_3y_2) + (y_2 - y_3)x + (x_3 - x_2)y\right] \quad \ldots\ldots\ldots\ldots\ldots \; 23$$

$$N_2 = \frac{1}{2A}\left[(x_3y_1 - x_1y_3) + (y_3 - y_1)x + (x_1 - x_3)y\right] \quad \ldots\ldots\ldots\ldots \; 24$$

$$N_3 = \frac{1}{2A}\left[(x_1y_2 - x_2y_1) + (y_1 - y_2)x + (x_2 - x_1)y\right] \quad \ldots\ldots\ldots\ldots\ldots\ldots \; 25$$

Equation 22 can be written using the following matrix notation:

$$\theta_e(x,y) = \begin{bmatrix} N_1 & N_2 & N_3 \end{bmatrix} \begin{Bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{Bmatrix} \quad \ldots\ldots\ldots\ldots \; 25a$$

The shape functions have some properties that are worth noticing. The first is that if we evaluate the shape function at its corresponding node, for example if we evaluate N_1 at node 1, we obtain $2A/2A = 1$ and if we evaluate N_1 at nodes 2 or 3, we get zero. Additionally, at any point in the triangle:

$$N_1 + N_2 + N_3 = 1 \quad \ldots\ldots\ldots\ldots\ldots \; 26$$

The gradient of the field variable over the element can be calculated as follows:

$$\frac{\partial\theta}{\partial x} = \frac{\partial N_1}{\partial x}\theta_1 + \frac{\partial N_2}{\partial x}\theta_2 + \frac{\partial N_3}{\partial x}\theta_3$$

$$\frac{\partial\theta}{\partial y} = \frac{\partial N_1}{\partial y}\theta_1 + \frac{\partial N_2}{\partial y}\theta_2 + \frac{\partial N_3}{\partial y}\theta_3 \quad \ldots\ldots\ldots\ldots \; 27$$

which can be written as follows after getting the derivatives of the shape functions:

$$\frac{\partial \theta}{\partial x} = \frac{y_2 - y_3}{2A}\theta_1 + \frac{y_3 - y_1}{2A}\theta_2 + \frac{y_1 - y_2}{2A}\theta_3$$
$$\frac{\partial \theta}{\partial y} = \frac{x_3 - x_2}{2A}\theta_1 + \frac{x_1 - x_3}{2A}\theta_2 + \frac{x_3 - x_2}{2A}\theta_3 \quad \ldots\ldots\ldots\ldots \ 28$$

Equation 28 can be written using the following compact matrix notation:

$$\begin{bmatrix} \frac{\partial \theta}{\partial x} \\ \\ \frac{\partial \theta}{\partial y} \end{bmatrix} = \frac{1}{2A}\begin{bmatrix} (y_2 - y_3) & (y_3 - y_1) & (y_1 - y_2) \\ \\ (x_3 - x_2) & (x_1 - x_3) & (x_3 - x_2) \end{bmatrix}\begin{Bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{Bmatrix} \quad \ldots\ldots\ldots\ldots\ldots \ 29$$

It should be noted, as in the linear one dimensional element, that the first derivative of the field function is constant within the triangular two dimensional element.

WEIGHTED RESIDUAL METHOD.

It was explained in the lecture that there are several methods to derive a Finite Element formulation for differential equations. It was also mentioned that the method of weighted residuals, particularly the Galerkin method is the most popular one.

We are not interested in the theoretical derivation of this method. Our interest here is mainly on how to apply this method to transform a given differential equation into its equivalent discrete form over a Finite Element grid. We will illustrate this by way of an example for a one-dimensional problem that we address earlier in the class; that is the fin problem.

The choice of this example serves at least two purposes. The first is the illustration of the Finite Element discretisation using the Galerkin method. The second, if we use the same regular grid that was used for the Finite Difference Discretisation, we can compare the two discretisations.

We want to discretise the equation:

$$\frac{\partial^2 \theta}{\partial \zeta^2} - \psi^2 \theta = 0 \quad \ldots\ldots\ldots\ldots\ldots \ 30 \ (53)$$

Using the 5 element grid shown in figure 12 with the boundary conditions:

$\theta_1 = 1$ and $\theta_6 = 0$

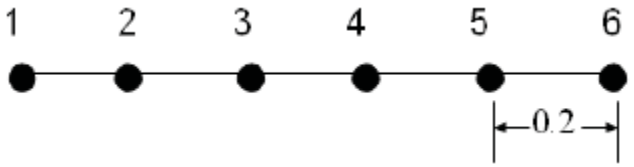


Figure 12: Finite element grid for equation 30

We can start the discretisation using the shape functions of the linear one-dimensional element of Equations 5 and 6. However to follow a more general procedure that can be used in two and three-dimensional isoprametric elements, we will express the one-dimensional shape functions using isoparametric one-dimensional element.

If we pick any of the elements in figure 13 and map it to a local coordinate system as shown in figure 14, the origin is defined at the mid-point of the element, then substituting $x_i = -1$ and $x_j = 1$ in equations 5 and 6, we get the following shape functions:

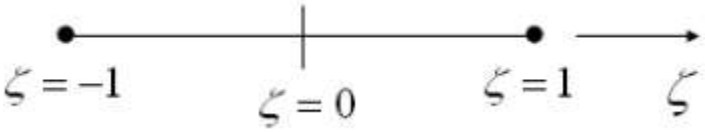


Figure 13: Isoparametric one-dimensional linear element.

$$N_i = \frac{\zeta - 1}{-1 - 1} = \frac{1}{2}(1 - \zeta) \quad \ldots\ldots\ldots\ldots\ldots \quad 31$$

$$N_i = \frac{\zeta - (-1)}{-1 - (-1)} = \frac{1}{2}(1 + \zeta) \quad \ldots\ldots\ldots\ldots\ldots \quad 32$$

Thus the approximate field function expressed over the element is given by:

$$\theta_e = N_i\theta_i + N_j\theta_j \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 33$$

And the gradient over the element is given by:

$$\frac{d\theta_e}{d\zeta} = \frac{dN_i}{d\zeta}\theta_i + \frac{dN_j}{d\zeta}\theta_j = -\frac{1}{\zeta}\theta_i + \frac{1}{\zeta}\theta_j \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 34$$

The next stage is to use the Galerkin formulation earlier, by which we substitute the approximation of the field variable from equation 33 into the differential equation, multiply this

by a weighting function which is of the same form as the field shape function and require that the integral of this weighted residual to equal zero over the solution domain. Hence:

$$\int_{\Omega} N_k \left(\frac{d^2\theta_e}{d\zeta^2} - \psi^2 \theta_e \right) d\zeta = 0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad 35$$

The subscript k indicates the nodes in the domain. This means that by using the shape functions at all nodes one at a time, we obtain a set of equations which equals the number of nodes. Since the first derivative of the linear shape function (Equation 33) is constant, then the second derivative is zero. To be able to represent the second derivative, we need to obtain the so called weak formulation, by which the first term of equation 35 is integrated by parts. So for the first node of the above element:

$$\int_{\Omega} N_i \left(\frac{d^2\theta_e}{d\zeta^2} \right) d\zeta = \vec{n} \left[N_i \frac{d\theta}{d\zeta} \right]_0^{\zeta_e} - \int_0^{\zeta_e} \frac{dN_i}{d\zeta} \frac{d\theta}{d\zeta} d\zeta \qquad \ldots\ldots\ldots\ldots\ldots \quad 36$$

where $\vec{n}$ is the outward normal to the boundary which equals 1, with appropriate sign. The end result when the equations are assembled together is that this term cancels out for all internal nodes and will be either 1 or -1 at the boundary nodes.

Substituting into equation 35, and replacing the field function and its derivative by their approximate representations from equations 33 and 34, we get:

$$\int_{\Omega} N_i \left(\frac{d^2\theta_e}{d\zeta^2} - \psi^2 \theta_e \right) d\zeta = \vec{n} \left[N_i \frac{d\theta}{d\zeta} \right]_0^{\zeta_e} - \int_0^{\zeta_e} \left(\frac{dN_i}{d\zeta} \frac{dN_i}{d\zeta} \theta_i + \frac{dN_i}{d\zeta} \frac{dN_j}{d\zeta} \theta_j \right) d\zeta$$
$$- \int_0^{\zeta_e} \psi^2 \left(N_i N_i \theta_i + N_i N_j \theta_j \right) d\zeta \qquad \ldots.. \quad 37$$

Substituting the values of the shape function and its derivative in terms of ζ and integrating, we obtain an equation for node i which can be written in the following matrix notation; with the outward normal at node 1 is 1.

$$\frac{1}{\zeta_e} \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{Bmatrix} \theta_i \\ \theta_j \end{Bmatrix} + \frac{\psi^2 \zeta_e}{6} \begin{bmatrix} 2 & 1 \end{bmatrix} \begin{Bmatrix} \theta_i \\ \theta_j \end{Bmatrix} + \begin{Bmatrix} \frac{d\theta}{d\zeta} \\ 0 \end{Bmatrix} \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad 38$$

If we weight the equation with N_j and repeat the integration, we obtain the following equation for the second node of element 1, where the outward normal here is -1 because it is in the opposite direction:

$$\frac{1}{\zeta_e}\begin{bmatrix}-1 & 1\end{bmatrix}\begin{Bmatrix}\theta_i\\ \theta_j\end{Bmatrix}+\frac{\psi^2\zeta_e}{6}\begin{bmatrix}2 & 1\end{bmatrix}\begin{Bmatrix}\theta_i\\ \theta_j\end{Bmatrix}+\begin{Bmatrix}0\\ -\frac{d\theta}{d\zeta}\end{Bmatrix} \quad \ldots\ldots\ldots\ldots\ldots\ 39$$

We can now assemble the contributions of nodes 1 and 2 of the first element in one matrix representing the element to give:

$$\frac{1}{\zeta_e}\begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix}\begin{Bmatrix}\theta_i\\ \theta_j\end{Bmatrix}+\frac{\psi^2\zeta_e}{6}\begin{bmatrix}2 & 1\\ 1 & 2\end{bmatrix}\begin{Bmatrix}\theta_i\\ \theta_j\end{Bmatrix}+\begin{Bmatrix}\frac{d\theta}{d\zeta}\\ -\frac{d\theta}{d\zeta}\end{Bmatrix} \quad \ldots\ldots\ldots\ldots\ 40$$

The same matrix can be assembled for all remaining elements. Note that the only metric in the matrix is the element length ζ_e. No assumption was made so far that this should be equal for all elements. Thus, this formulation is general for arbitrary distribution of grid nodes. Once we have chosen the grid, we can substitute the length of each element in equation 40 and obtain the specific matrix for the particular element. Those matrices can then be assembled in the global system matrix as we will see next. But first, let's take the specific case of figure 12 where the domain was divided into equal elements of length 2 and using $\psi^2 = 3$ as stated earlier, we obtain the following matrix for each element:

$$\begin{bmatrix}5.2 & -4.9\\ -4.9 & 5.2\end{bmatrix}\begin{Bmatrix}\theta_1\\ \theta_2\end{Bmatrix}=\begin{Bmatrix}-\frac{d\theta}{d\zeta}\\ \frac{d\theta}{d\zeta}\end{Bmatrix} \quad \ldots\ldots\ldots\ldots\ 41$$

The contributions from all elements can be assembled by placing the matrix for each element in the global matrix. This means that for internal nodes where the node is shared between two elements, the contributions need to be overlapped, or in other words added together. The process is explained schematically in Figure 14 for a system containing three elements with their contributions which are labelled a, b and c. Each colour represents a column of the assembled matrix. Note that the two middle columns and rows each containing contributions from two neighbouring elements.

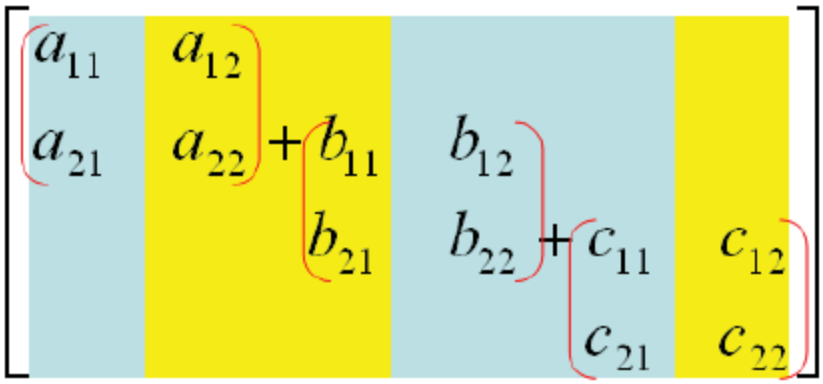


Figure 14: Schematic of system matrix assembly.

Following the same procedure, the system matrix can be assembled for the six nodes from the contribution matrices of equation 41 to give the following system matrix:

$$\begin{bmatrix} 5.2 & -4.9 & 0.0 & 0.0 & 0.0 & 0.0 \\ -4.9 & 10.4 & -4.9 & 0.0 & 0.0 & 0.0 \\ 0.0 & -4.9 & 10.4 & -4.9 & 0.0 & 0.0 \\ 0.0 & 0.0 & -4.9 & 10.4 & -4.9 & 0.0 \\ 0.0 & 0.0 & 0.0 & -4.9 & 10.4 & -4.9 \\ 0.0 & 0.0 & 0.0 & 0.0 & -4.9 & 5.2 \end{bmatrix} \begin{Bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \\ \theta_5 \\ \theta_6 \end{Bmatrix} = \begin{Bmatrix} -\frac{d\theta}{d\zeta} \\ 0.0 \\ 0.0 \\ 0.0 \\ 0.0 \\ \frac{d\theta}{d\zeta} \end{Bmatrix} \quad \ldots\ldots \ 42$$

Multiplying across and using the boundary conditions $\theta_1 = 1$ and $\theta_6 = 0$ we obtain the following system of linear equations:

$$\begin{aligned} &\theta_1 = 1 \\ &-4.9\theta_1 + 10.4\theta_2 - 4.9\theta_3 = 0 \\ &-4.9\theta_2 + 10.4\theta_3 - 4.9\theta_4 = 0 \\ &-4.9\theta_3 + 10.4\theta_4 - 4.9\theta_5 = 0 \\ &-4.9\theta_4 + 10.4\theta_5 - 4.9\theta_6 = 0 \\ &\theta_6 = 0 \end{aligned} \quad \ldots\ldots\ldots\ldots\ldots\ 43$$

Comparing the systems of Equations in Equation 32 under the finite volume method section and Equation 43 in this section, we notice that they are essentially the same set of equations. This can be assured multiplying all terms on the left and right of Equation 43 by (-5.1); we obtain Equation 32. This means that the solution for this system is the same as Equation 32. This leads

to the verification of equations 43 as the solution for equations 32 was equivalent to the analytic solution. It also leads us to the conclusion that the discretization using linear one-dimensional

elements is equivalent to the second order accurate central difference scheme of the Finite Difference formulation if we used equal grid spacing. However, the important point is that the Finite Element scheme can be used in a straight forward manner using irregular grids. In additions, the incorporation of higher order schemes by using higher order elements is straightforward.

You might think that the derivation of the Finite Element formulation is cumbersome compared to the Finite Difference formulation, and at the end, we obtained the same results as the simple finite difference scheme. That is correct. However, the advantages of the Finite Element formulations become more apparent in two and three dimensional problems when arbitrary geometries are handled.

THE FINITE VOLUME METHOD.

The finite volume method was introduced earlier in the lecture. It was mentioned that it can be viewed as a special case of the weighted residual method, where the function is 1. We also presented an alternative way of obtaining a finite volume discretization using the integral form of the differential equation.

The solution domain needs to be divided into non-overlapping cells surrounded by boundary edges in two-dimensions or boundary faces in three-dimensions. Integrating by parts leads the volume integral to equal a flux through the volume boundary. Working out these fluxes in terms of the unknown field variables at grid points either at the cell corners or centres leads to a system of algebraic equations which can be solved for the unknown field variables.

In the lecture, we will explain the principles of the finite difference method through worked examples that start by one-dimensional simple models. We will build these up gradually to more complex models and multiple dimensions. We will also compare the discretization resulting from the Finite Volume formulation to that of the Finite Difference and Finite Element formulations to the fin problem.

1. THE DIFFUSION EQUATION.

To illustrate the basic concepts of the Finite Volume discretisation for fluid flow problems. Let's consider the diffusion equation. This equation is known as the Stokes equation, which contains the pressure and viscous terms in the Navier-Stokes equations. In one-dimensional steady state formulation, it takes the form:

$$\frac{d}{dx}\left(\mu\frac{du}{dx}\right)-\frac{dp}{dx}=F \qquad \ldots\ldots\ldots 1$$

where F is the body force. To simplify matters further, we will ignore the pressure term for the moment. Once this is done, the equation resembles the heat conduction equation which also includes a source term. To be more physically meaningful in this analysis, let's consider the heat conduction equation instead which takes the form:

$$\frac{d}{dx}\left(k\frac{dT}{dx}\right)+S=0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ 2$$

Here, k is the thermal conductivity, S is the source or internal heat generation per unit volume and T is the temperature.

To derive a Finite Volume discretisation, we will use a three point stencil as shown in Figure 1. We are seeking to derive the discretisation for the middle point P. We have also used the conventional Finite Volume notation for the surrounding point of E and W for east and west.

The next stage is to integrate Equation 2 over the cell (volume) which is highlighted in Figure 1, this gives:

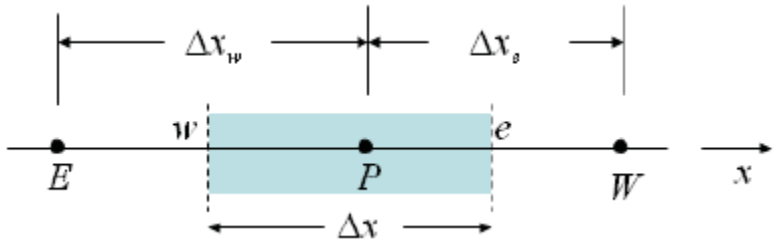


Figure 1: Finite Volume stencil for the 1D conduction equation.

$$\int_w^e \frac{d}{dx}\left(k\frac{dT}{dx}\right)dx+\int_w^e S\,dx=0 \qquad \ldots\ldots\ldots\ldots\ldots\ 3$$

Giving:

$$\left(k\frac{dT}{dx}\right)_e-\left(k\frac{dT}{dx}\right)_w+\int_w^e S\,dx=0 \qquad \ldots\ldots\ldots\ldots\ldots\ 4$$

To enable the calculation of the temperature gradient at the east and west boundaries of the cell, we need to make an assumption of the temperature profiles within the grid. A reasonable assumption would be that the temperature is varying linearly between grid points as shown in Figure 2. This allows a straight forward evaluation of the first two terms of Equation 4.

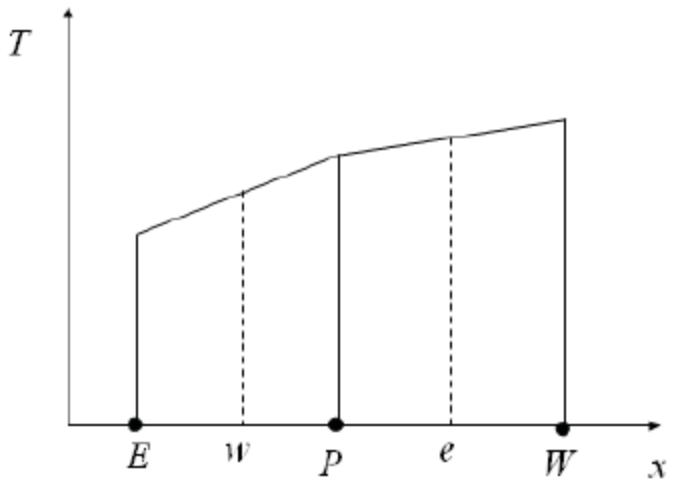


Figure 2: Piecewise linear profile.

For the source term, we will assume that the average value $\bar{S}$ prevails over the control volume. Thus:

$$\frac{k_e(T_E - T_P)}{\Delta x_e} - \frac{k_w(T_P - T_W)}{\Delta x_w} + \bar{S}\Delta x = 0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad 5$$

Example.

Applying the discretization used in equation 5 for equation 9 under the finite difference method basics:

$$\frac{\partial^2\theta}{\partial\zeta^2} - \psi^2\theta = 0 \text{ for } \psi^2 = 3$$

and equal grid spacing of 0.2.

Solution.

The discretization applied to equation 9 gives:

$$\frac{(\theta_E - \theta_P)}{\Delta x_e} - \frac{(\theta_P - \theta_W)}{\Delta x_w} - 3\theta_p\Delta x = 0$$

For equal grid spacing, $\Delta x = \Delta x_e = \Delta x_w = 0.2$, thus dividing by Δx and rearranging gives:

$$\frac{(\theta_E - 2\theta_P + \theta_W)}{(\Delta x)^2} - 3\theta_p = 0$$

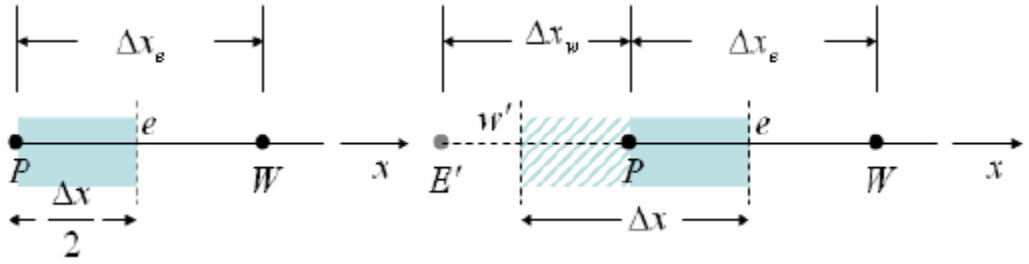
$$\frac{(\theta_E - 2\theta_P + \theta_W)}{(0.2)^2} - 3\theta_p = 0$$

$$25\theta_E - 53\theta_P + 25\theta_W = 0 \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad 6$$

Equation 6 is the same as Equation 31(The finite volume method). Thus the finite volume discretization in Equation 6 is equivalent to the 2nd order Finite Difference discretization on the same stencil. We also found in the lecture, for the same example, that this is also equivalent to the Finite Element discretization over the same grid size.

In general, in the Finite Volume discretisation, it is not necessary that the distances Δx_e and Δx_w be equal. In fact, the use of non-uniform grid spacing is often desirable as it enables the effective use of computing power. In general, an accurate solution will be obtained when the grid is sufficiently fine. However, there is no need to use fine grids in regions where the field variable changes slowly with the space coordinate. On the other hand, fine grids are required when the variation is steep.

Similar equations can be formulated for all internal cells as discussed above. For boundary points, the last cell is not complete as shown in Figure 3a. Boundary conditions need to be applied. This is done depending on the type of boundary conditions.



(a) (b)

Figure 3a: Application of boundary conditions.

If the value of the field variable is given, then there is no need to formulate a flux calculation there as the equation for that cell will be replaced by the given temperature for the end node. For a given gradient of the flow field, a treatment similar to that performed with the Finite Difference methods was done earlier.

The approach proposed here, which ensures second order accuracy of the boundary conditions discretisation is to extend the domain by an additional virtual node which completes the cell as shown in Figure 3b. The value of the field variable at the virtual node is computed in terms of the two neighbouring internal nodes using the inner cell scheme.