School of Mechanical Aerospace and Civil Engineering

TPFE MSc CFD-1

Finite Difference Schemes

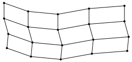
T. J. Craft
George Begg Building, C41

Reading:
J. Ferziger, M. Peric, *Computational Methods for Fluid Dynamics*
H.K. Versteeg, W. Malalasekara, *An Introduction to Computational Fluid Dynamics: The Finite Volume Method*
S.V. Patankar, *Numerical Heat Transfer and Fluid Flow*
Notes: http://cfd.mace.manchester.ac.uk/tmcfd
- People - T. Craft - Online Teaching Material

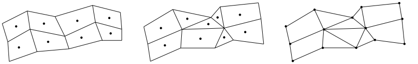
Introduction

- In this lecture we consider the process of discretizing the governing partial differential equations of a fluid flow.
- Discretization is the process of approximating the differential equations by a system of algebraic ones linking the (discrete) nodal values of velocity, pressure, etc.
- There are three broad methods employed for discretizing the governing partial differential equations of a fluid flow:
  - Finite Difference (FD)
  - Finite Element (FE)
  - Finite Volume (FV)
- Although there are obvious similarities in the resulting set of discretized algebraic equations, the methods employ different approaches to obtaining these. As a result, there can be differences in both the accuracy and ease of application of the various methods.

- Finite difference schemes can generally be applied to regular-shaped domains using body-fitted grids (curved grid lines, following domain boundaries).



- Large grid distortions need to be avoided, and the schemes cannot easily be applied to very complex flow geometry shapes.
- Finite element and finite volume schemes are both based on dividing the flow domain into a (large) number of small cells, or volumes. These can be of any shape (triangles, quadrilaterals, etc. in 2-D; tetrahedra, prisms, cubes, etc. in 3-D). They are thus more suitable for application to complex flow geometries.



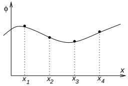
- Finite element approaches are traditionally used in solid mechanics. These can be adapted to fluid problems, but finite volume schemes tend to be the more popular choice in CFD (and are currently used in most, if not all, of the major commercial packages).
- We will examine finite volume schemes later. However, to begin with we consider how finite difference schemes can be devised.
- Despite not being generally used in industrial codes, finite difference schemes are useful for introducing the ideas of accuracy, truncation error, stability and boundedness in a well-defined and fairly transparent way.

Approximating Derivatives

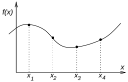
- For illustration, a simple equation to consider, related to the more complex Navier-Stokes system, is the 1-D convection-diffusion problem:

$$\frac{\partial \rho U \phi}{\partial x} = \frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right) \qquad (1)$$

- ϕ is the variable transported by the flow (ie. the quantity we need to solve for), U is the convective velocity and Γ the diffusivity.
- If, for example, ϕ represents fluid temperature, this equation describes the 1-D problem of temperature changes due to convection by the fluid and diffusion by molecular action.
- We store ϕ at a number of fixed grid points (x_1, x_2, x_3, etc).
- To approximate equation (1) by a set of algebraic equations relating the values of ϕ at x_1, x_2, etc. we need to approximate the various derivatives in terms of these nodal values of ϕ.



- Many problems involve rather more complex expressions than simply derivatives of ϕ itself.
- We therefore consider some arbitrary function $f(x)$, and suppose we can evaluate it at the uniformly spaced grid points x_1, x_2, x_3, etc. as shown.

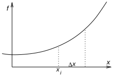


Taylor Series Approximation

- Taylor series expansions can often be used to develop and/or analyse the accuracy of numerical approximations for derivatives.
- Writing a Taylor series expansion to evaluate f at positions x close to x_i:

$$f(x_i+\Delta x) = f(x_i) + \Delta x f'(x_i) + \frac{(\Delta x)^2}{2!} f''(x_i) + \frac{(\Delta x)^3}{3!} f'''(x_i) + O(\Delta x^4) \qquad (2)$$

where f' denotes the derivative df/dx, f'' the second derivative d^2f/dx^2 etc.



- Rearranging gives

$$\begin{aligned} f'(x_i) &= \frac{f(x_i+\Delta x) - f(x_i)}{\Delta x} - \frac{\Delta x}{2!} f''(x_i) - \frac{(\Delta x)^2}{3!} f'''(x_i) + O(\Delta x^3) \\ &= \frac{f(x_i+\Delta x) - f(x_i)}{\Delta x} + O(\Delta x) \qquad (3) \end{aligned}$$

where $O(\Delta x)$ means the leading term is proportional to Δx.

- If we take Δx as the uniform grid spacing, so $\Delta x = x_{i+1} - x_i$, then we get the approximation

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{\Delta x} + O(\Delta x) \qquad (4)$$

which we will write in shorthand form as

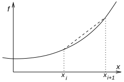
$$f'_i = \frac{f_{i+1} - f_i}{\Delta x} + O(\Delta x) \qquad (5)$$

where f_i represents f evaluated at x_i, etc.

- The approximation suggested by equation (5),

$$f'_i \approx (f_{i+1} - f_i)/\Delta x \qquad (6)$$

is known as a *forward difference*.



- This is a *first order* scheme, since the error is proportional to Δx, so decreases linearly with grid spacing.

- Alternatively, we could use equation (2) to evaluate f at a point $x_i - \Delta x$:

$$f(x_i - \Delta x) = f(x_i) - \Delta x f'(x_i) + \frac{(\Delta x)^2}{2!} f''(x_i) - \frac{(\Delta x)^3}{3!} f'''(x_i) + O(\Delta x^4) \quad (7)$$

- Taking Δx as the grid spacing now leads to

$$f(x_{i-1}) = f(x_i) - \Delta x f'(x_i) + \frac{(\Delta x)^2}{2!} f''(x_i) - \frac{(\Delta x)^3}{3!} f'''(x_i) + O(\Delta x^4) \quad (8)$$

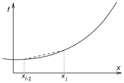
- Rearranging leads to the approximation

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{\Delta x} + O(\Delta x) \quad (9)$$

- This approximation,

$$f'_i \approx (f_i - f_{i-1})/\Delta x \quad (10)$$

is referred to as a *backward differencing* scheme.



- It is again a first order scheme.

- We could combine the two Taylor series approximations above:

$$f(x_{i+1}) = f(x_i) + \Delta x f'(x_i) + \frac{(\Delta x)^2}{2!} f''(x_i) + \frac{(\Delta x)^3}{3!} f'''(x_i) + O(\Delta x^4) \quad (11)$$

$$f(x_{i-1}) = f(x_i) - \Delta x f'(x_i) + \frac{(\Delta x)^2}{2!} f''(x_i) - \frac{(\Delta x)^3}{3!} f'''(x_i) + O(\Delta x^4) \quad (12)$$

- Subtracting one from the other results in

$$f(x_{i+1}) - f(x_{i-1}) = 2\Delta x f'(x_i) + 2\frac{(\Delta x)^3}{3!} f'''(x_i) + O(\Delta x^5) \quad (13)$$

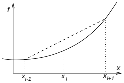
- Rearranging gives the approximation

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} + O(\Delta x^2) \quad (14)$$

- This approximation

$$f'_i \approx (f_{i+1} - f_{i-1})/(2\Delta x) \quad (15)$$

is referred to as a *centred difference*.



- This is a second order approximation, since the error reduces as $(\Delta x)^2$: if the grid spacing is halved, the error goes down by a factor of 4.

Order of Approximation

- At this point it is worth considering exactly what is meant by the order of accuracy of a discretization approximation.
- As we refine the grid, for any useful scheme, errors associated with the discretization approximation can be expected to reduce.
- We reach a *grid independent* solution when any further grid refinement produces no significant difference in the computed solution. At this stage the discretization errors are small enough that they can be neglected.
- We have defined the order of a scheme in terms of the leading order error term in the Taylor series expansion.
- This should, therefore, determine at what rate the error reduces as the grid is refined.
- For a first order scheme, if the grid spacing is halved the error is halved; for a second order scheme the error would reduce by a factor of 4.

- Note this does not mean a second order solution on one particular grid will always be more accurate than a first order one (although this will usually be the case for a sufficiently fine grid).
- It does, however, imply that as we refine the grid the error in the higher order scheme goes down more rapidly, so we expect the higher order scheme to reach a grid independent solution on a coarser grid than would be required for a lower order scheme.
- It is worth noting that the behaviour described above for a particular scheme can only be expected on a reasonably fine grid.
- The reason for this can be seen from the Taylor series expansion. For example, in the first order backward difference scheme we have

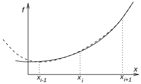
$$f'_i = \frac{f_i - f_{i-1}}{\Delta x} + \frac{\Delta x}{2!} f''(x_i) - \frac{(\Delta x)^2}{3!} f'''(x_i) + O(\Delta x^3) \quad (16)$$

If the first term in the truncation is to be the leading error term, then Δx has to be small enough so that

$$\frac{(\Delta x)^2}{3!} |f'''(x_i)| << \frac{\Delta x}{2!} |f''(x_i)| \qquad \text{or} \qquad \Delta x << 3 \left| \frac{f''(x_i)}{f'''(x_i)} \right| \quad (17)$$

Polynomial Approximation

- The above approximations for the derivatives could also have been derived by fitting a polynomial to the function f through x_i and surrounding points and then differentiating this polynomial to get its gradient.
- The forward and backward difference schemes arise from fitting a first order polynomial (a straight line) through the points (x_i, x_{i+1}) and (x_{i-1}, x_i) respectively.
- The centred difference scheme can be obtained by fitting a quadratic curve through the points x_{i-1}, x_i and x_{i+1}. The resulting polynomial approximation for f can be written as



$$f(x) = \frac{(x-x_i)(x-x_{i+1})f_{i-1}}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})} + \frac{(x-x_{i-1})(x-x_{i+1})f_i}{(x_i-x_{i-1})(x_i-x_{i+1})} + \frac{(x-x_i)(x-x_{i-1})f_{i+1}}{(x_{i+1}-x_i)(x_{i+1}-x_{i-1})} \tag{18}$$

- On a uniform grid with $x_{i+1}-x_i = x_i - x_{i-1} = \Delta x$ and $x_{i+1}-x_{i-1} = 2\Delta x$ this becomes

$$f(x) = \frac{(x-x_i)(x-x_{i+1})}{2(\Delta x)^2}f_{i-1} - \frac{(x-x_{i-1})(x-x_{i+1})}{(\Delta x)^2}f_i + \frac{(x-x_i)(x-x_{i-1})}{2(\Delta x)^2}f_{i+1} \tag{19}$$

- Differentiating with respect to x then gives

$$f'(x) = \frac{(x-x_i+x-x_{i+1})}{2(\Delta x)^2}f_{i-1} - \frac{(x-x_{i-1}+x-x_{i+1})}{(\Delta x)^2}f_i + \frac{(x-x_i+x-x_{i-1})}{2(\Delta x)^2}f_{i+1} \tag{20}$$

and thus

$$f'(x_i) = \frac{-\Delta x}{2(\Delta x)^2}f_{i-1} - \frac{0}{(\Delta x)^2}f_i + \frac{\Delta x}{2(\Delta x)^2}f_{i+1} = \frac{(f_{i+1}-f_{i-1})}{2\Delta x} \tag{21}$$

- The above procedure does not immediately show us what order the truncation error is.
- However, the order of the scheme can be determined by expressing f_{i+1} and f_{i-1} as Taylor series expansions about x_i as before, and substituting these into the right hand side expression of equation (21).

Approximating Higher Order Derivatives

- Taylor series expansions or polynomial fits can also be used to derive approximations to higher order derivatives.
- For example, to approximate the second derivative d^2f/dx^2 we could, as before, write:

$$f(x_{i+1}) = f(x_i) + \Delta x f'(x_i) + \frac{(\Delta x)^2}{2!}f''(x_i) + \frac{(\Delta x)^3}{3!}f'''(x_i) + O(\Delta x^4) \tag{22}$$

$$f(x_{i-1}) = f(x_i) - \Delta x f'(x_i) + \frac{(\Delta x)^2}{2!}f''(x_i) - \frac{(\Delta x)^3}{3!}f'''(x_i) + O(\Delta x^4) \tag{23}$$

- Adding the two equations and rearranging now results in

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{(\Delta x)^2} + O((\Delta x)^2) \tag{24}$$

- This gives the central difference approximation for the second derivative

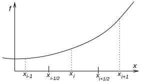
$$f''_i \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{(\Delta x)^2} \tag{25}$$

which is again second order accurate when applied on a uniform grid.

- Note the *computational stencil* (the nodal points used) is now larger, because we need more points to give information about curvature etc.
- In many fluids related problems the second derivative that requires approximation is a diffusion term of the form

$$\frac{\partial}{\partial x}\left(\Gamma \frac{\partial f}{\partial x}\right) \tag{26}$$

- This can be approximated using central differences to estimate df/dx at the mid-points $x_{i+1/2}$ and $x_{i-1/2}$, followed by a central difference between these values to estimate the second derivative term:



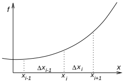
$$\left.\frac{df}{dx}\right|_{i-1/2} \approx \frac{f_i - f_{i-1}}{\Delta x} \qquad \left.\frac{df}{dx}\right|_{i+1/2} \approx \frac{f_{i+1} - f_i}{\Delta x} \tag{27}$$

$$\frac{\partial}{\partial x}\left(\Gamma \frac{\partial f}{\partial x}\right) \approx \frac{\Gamma_{i+1/2}(f_{i+1}-f_i) - \Gamma_{i-1/2}(f_i - f_{i-1})}{(\Delta x)^2} \tag{28}$$

- Note that interpolation may be required to estimate values of Γ at the midpoints $x_{i+1/2}$ and $x_{i-1/2}$.

Non-Uniform Grids

- In most CFD applications non-uniform grids are employed, allowing the grid to be more refined in regions where strong gradients are expected.
- In such a case, the simple forward/backward differences are clearly still first order.
- Analysis of the central difference scheme, however, is a little different.



- Using Taylor series expansions we can now write:

$$f(x_{i+1}) = f(x_i) + \Delta x_i f'(x_i) + \frac{(\Delta x_i)^2}{2!} f''(x_i) + \frac{(\Delta x_i)^3}{3!} f'''(x_i) + O((\Delta x_i)^4) \quad (29)$$

$$f(x_{i-1}) = f(x_i) - \Delta x_{i-1} f'(x_i) + \frac{(\Delta x_{i-1})^2}{2!} f''(x_i) - \frac{(\Delta x_{i-1})^3}{3!} f'''(x_i) + O((\Delta x_{i-1})^4) \quad (30)$$

- Subtracting gives

$$f(x_{i+1}) - f(x_{i-1}) = (\Delta x_i + \Delta x_{i-1}) f'(x_i) + (\Delta x_i^2 - \Delta x_{i-1}^2) f''(x_i) + O(\Delta x^3) \quad (31)$$

- Hence we obtain

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{\Delta x_i + \Delta x_{i+1}} + \frac{f''(x_i)}{2!}(\Delta x_i - \Delta x_{i-1}) + O(\Delta x^2) \quad (32)$$

- Note that formally the central difference $f_i' = (f_{i+1} - f_{i-1})/(\Delta x_i + \Delta x_{i-1})$ is now only first order accurate.
- In practice, one should avoid using rapidly expanding grids, so typically $\Delta x_i = r \Delta x_{i-1}$ with grid expansion ratio r not too far from unity. The factor $(\Delta x_i - \Delta x_{i-1}) = \Delta x_i (1 - r)$ in the leading order error can then still be essentially second order.
- The approximation derived from the polynomial fit of equation (18) still gives a formally second order approximation.
- In this case we get

$$f(x) = \frac{(x - x_i)(x - x_{i+1}) f_{i-1}}{(\Delta x_{i-1})(\Delta x_i + \Delta x_{i-1})} - \frac{(x - x_{i-1})(x - x_{i+1}) f_i}{\Delta x_i \Delta x_{i-1}} + \frac{(x - x_i)(x - x_{i-1}) f_{i+1}}{(\Delta x_i)(\Delta x_i + \Delta x_{i-1})} \quad (33)$$

- Differentiating leads to

$$f'(x_i) = \frac{(x - x_i + x - x_{i+1}) f_{i-1}}{(\Delta x_{i-1})(\Delta x_i + \Delta x_{i-1})} + \frac{(x - x_{i-1} + x - x_{i+1}) f_i}{\Delta x_i \Delta x_{i-1}} + \frac{(x - x_i + x - x_{i-1}) f_{i+1}}{(\Delta x_i)(\Delta x_i + \Delta x_{i-1})} \quad (34)$$

- Hence we obtain the approximation

$$f_i' \approx \frac{-\Delta x_i}{(\Delta x_{i-1})(\Delta x_i + \Delta x_{i-1})} f_{i-1} + \frac{\Delta x_i - \Delta x_{i-1}}{\Delta x_i \Delta x_{i-1}} f_i + \frac{\Delta x_{i-1}}{(\Delta x_i)(\Delta x_i + \Delta x_{i-1})} f_{i+1} \quad (35)$$

- If we express f_{i+1} and f_{i-1} as Taylor series expansions about x_i the above approximation implies

$$\begin{aligned} f_i' \approx & \frac{-\Delta x_i}{(\Delta x_{i-1})(\Delta x_i + \Delta x_{i-1})} \left[f_i - \Delta x_{i-1} f_i' + \frac{(\Delta x_{i-1})^2}{2!} f_i'' - \frac{(\Delta x_{i-1})^3}{2!} f_i''' + O(\Delta x^4) \right] \\ & + \frac{\Delta x_i - \Delta x_{i-1}}{\Delta x_i \Delta x_{i-1}} f_i \\ & + \frac{\Delta x_{i-1}}{(\Delta x_i)(\Delta x_i + \Delta x_{i-1})} \left[f_i + \Delta x_i f_i' + \frac{(\Delta x_i)^2}{2!} f_i'' + \frac{(\Delta x_i)^3}{2!} f_i''' + O(\Delta x^4) \right] \\ = & f_i' + \frac{\Delta x_i \Delta x_{i-1}}{3!} f_i''' + O(\Delta x^3) \end{aligned}$$

Thus showing that the approximation of equation (35) is indeed second order.

The Convection-Diffusion Problem

- The 1-D convection-diffusion equation for a transported variable is sufficient to demonstrate some of the advantages and weaknesses that can be encountered with the numerical approximations outlined above.
- It can be written as

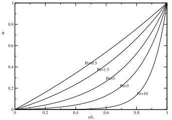
$$\frac{\partial \rho U \phi}{\partial x} = \frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right) \quad (36)$$

- ϕ is the variable being transported by the flow, which could be temperature, chemical species concentration, etc. U is the fluid velocity which, for simplicity, we take as constant.
- The fluid density, ρ, and Γ, the diffusivity of ϕ, are also taken as constants.
- The left hand side of the equation represents the transport effect of ϕ being convected by the fluid. The right hand side represents the molecular diffusion of ϕ.

- As an example, we consider the above equation, applied on the interval $0 \le x \le L$, with boundary conditions $\phi = 0$ at $x = 0$ and $\phi = 1$ at $x = L$.
- The exact solution to this problem is given by

$$\phi(x) = \frac{\exp(xPe/L) - 1}{\exp(Pe) - 1} \qquad (37)$$

where $Pe = \rho UL/\Gamma$ is the Peclet number.



- Notice that the Peclet number gives a measure of the ratio of convective effects to diffusive ones.
- As the Peclet number increases (diffusive effects become weaker), the region over which most of the variation in ϕ occurs becomes thinner, and the gradients of ϕ across it become correspondingly larger.

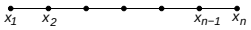
- Discretizing this convection-diffusion equation on a uniform grid using central differences for both convective and diffusive terms, we get

$$\rho U \left(\frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} \right) = \Gamma \left(\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} \right) \qquad (38)$$

or, on rearranging:

$$\phi_{i-1} \left(-\frac{\rho U}{2\Delta x} - \frac{\Gamma}{\Delta x^2} \right) + \frac{2\Gamma}{\Delta x^2}\phi_i + \phi_{i+1} \left(\frac{\rho U}{2\Delta x} - \frac{\Gamma}{\Delta x^2} \right) = 0 \qquad (39)$$

- ϕ_1 and ϕ_n are known from the boundary conditions ($\phi_1 = 0$ and $\phi_n = 1$). Hence the discretized equations at nodes 2 and $n-1$ can be simplified to



$$\frac{2\Gamma}{\Delta x^2}\phi_2 + \phi_3 \left(\frac{\rho U}{2\Delta x} - \frac{\Gamma}{\Delta x^2} \right) = 0 \qquad (40)$$

$$\phi_{n-2} \left(-\frac{\rho U}{2\Delta x} - \frac{\Gamma}{\Delta x^2} \right) + \frac{2\Gamma}{\Delta x^2}\phi_{n-1} = -\left(\frac{\rho U}{2\Delta x} - \frac{\Gamma}{\Delta x^2} \right) \qquad (41)$$

- The discretized form of equations can thus be represented in the tri-diagonal matrix form:

$$\begin{pmatrix} b_1 & c_1 & 0 & \cdots & & & \cdots \\ a_2 & b_2 & c_2 & 0 & & & \cdots \\ 0 & a_3 & b_3 & c_3 & 0 & & \cdots \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ \cdots & 0 & a_{n-3} & b_{n-3} & c_{n-3} & 0 & \\ \cdots & & & 0 & a_{n-2} & b_{n-2} & c_{n-2} \\ \cdots & & & & 0 & a_{n-1} & b_{n-1} \end{pmatrix} \begin{pmatrix} \phi_2 \\ \phi_3 \\ \vdots \\ \vdots \\ \vdots \\ \phi_{n-2} \\ \phi_{n-1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \vdots \\ \vdots \\ 0 \\ \frac{\Gamma}{(\Delta x)^2} - \frac{\rho U}{2\Delta x} \end{pmatrix} \qquad (42)$$

where $a_i = -\frac{\rho U}{2\Delta x} - \frac{\Gamma}{(\Delta x)^2}$, $b_i = \frac{2\Gamma}{(\Delta x)^2}$, $c_i = \frac{\rho U}{2\Delta x} - \frac{\Gamma}{(\Delta x)^2}$.

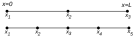
- This system of equations can be solved by a variety of methods, some of which will be examined later.

- In this case, rearranging equation (39) to solve for ϕ_i gives

$$\phi_i = \frac{\phi_{i+1}}{2}\left[1 - \frac{\rho U \Delta x}{2\Gamma}\right] + \frac{\phi_{i-1}}{2}\left[1 + \frac{\rho U \Delta x}{2\Gamma}\right]$$
$$= \frac{\phi_{i+1}}{2}\left[1 - \frac{Pe_x}{2}\right] + \frac{\phi_{i-1}}{2}\left[1 + \frac{Pe_x}{2}\right] \qquad (43)$$

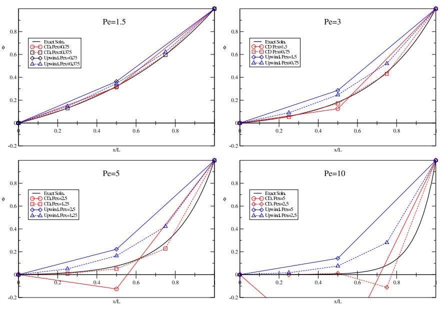
where Pe_x is the *cell Peclet number*, $Pe_x = \rho U \Delta x/\Gamma$.

- For a given bulk Peclet number, $\rho UL/\Gamma$, as we divide the domain into a larger number of intervals, the cell Peclet number $\rho U \Delta x/\Gamma$ decreases.
- For uniform grids with 3 gnd 5 grid nodes, the cell Peclet numbers, Pe_x, at different bulk Peclet numbers, Pe, are given in the table.



	Δx	$Pe = 0.5$	$Pe = 1.5$	$Pe = 3$	$Pe = 5$	$Pe = 10$
3 nodes	$L/2$	0.25	0.75	1.5	2.5	5
5 nodes	$L/4$	0.125	0.375	0.75	1.25	2.5

- The values of ϕ at the nodes can be found by solving equation (43) at each node, and the results are shown in the following graphs.



- At $Pe = 1.5$ both the 3 node and 5 node central difference solutions give a good approximation to the exact result.
- At $Pe = 3$ the coarser grid solution (with $Pe_x = 1.5$) is becoming less accurate.
- At $Pe = 5$ the finer grid solution (with $Pe_x = 1.25$) is still satisfactory, but with $Pe_x = 2.5$ the estimated value of ϕ at $x/L = 0.5$ is now negative.
- At $Pe = 10$ both solutions with $Pe_x = 2.5$ and 5 give negative values of ϕ at some nodes.
- This is an example of an *unbounded* scheme. If ϕ represented a species concentration, for example, or some other physically positive quantity, then the under/overshoots would imply a solution returning physically unrealizable results.
- It can be shown that $Pe_x < 2$ is a *sufficient* condition to ensure the centred difference scheme does not produce under/overshoots in this problem.

- However, this is not a *necessary* condition. If a non-uniform grid were used, large cells with $Pe_x > 2$ could be placed towards the left hand side of the domain (where $d\phi/dx$ is small) without having an adverse effect on the solution.
- Generally, the centred convection scheme will produce under and overshoots when the cell Peclet number is large *and* the solution has steep gradients.
  (What exactly is large, or steep, can be problem-dependent).

Upwinding

- A similar set of solutions can be generated using the first order upwind scheme (a backward difference) for approximating the convective terms.
- The discretized equation is then

$$\rho U \left(\frac{\phi_i - \phi_{i-1}}{\Delta x} \right) = \Gamma \left(\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} \right) \qquad (44)$$

- Rearranging leads to

$$\phi_{i-1} \left(-\frac{\rho U}{\Delta x} - \frac{\Gamma}{\Delta x^2} \right) + \phi_i \left(\frac{\rho U}{\Delta x} + \frac{2\Gamma}{\Delta x^2} \right) + \phi_{i+1} \left(-\frac{\Gamma}{\Delta x^2} \right) = 0 \qquad (45)$$

  and introducing the cell Peclet number, Pe_x, results in

$$\phi_i = \frac{\phi_{i-1}(1 + Pe_x) + \phi_{i+1}}{2 + Pe_x} \qquad (46)$$

- The results of solving these equations on the same grids as those used earlier for the central difference scheme are also shown in the graphs.

- As might be expected, once the grid is reasonably fine (Pe_x not too large) the first order upwind solution is not as accurate as the second order central difference one.
- However, the upwind solution is always bounded.
- Whereas the central difference gives under/overshoots when the cell Peclet number is large, the upwind scheme does not. Instead, it appears to underestimate the gradients in ϕ.

Numerical Diffusion

- As seen in the above example, the first order upwind scheme always returns a bounded solution. However, it is not particularly accurate.
- The Taylor series expansions examined earlier show that

$$\frac{\phi_i - \phi_{i-1}}{\Delta x} = \phi_i' - \frac{\Delta x}{2!}\phi_i'' + \frac{\Delta x^2}{3!}\phi_i''' + O(\Delta x^3) \quad (47)$$

$$\frac{\phi_{i-1} - 2\phi_i + \phi_{i+1}}{\Delta x^2} = \phi_i'' + \frac{2\Delta x^2}{4!}\phi_i'''' + O(\Delta x^4) \quad (48)$$

- Hence the differential equation actually being solved when using the first order upwind scheme is

$$\rho U \left(\frac{d\phi}{dx} - \frac{\Delta x}{2!}\frac{d^2\phi}{dx^2} + \frac{\Delta x^2}{3!}\frac{d^3\phi}{dx^3} \right) = \Gamma \left(\frac{d^2\phi}{dx^2} + \frac{2\Delta x^2}{4!}\frac{d^4\phi}{dx^4} \right) + O(\Delta x^4) \quad (49)$$

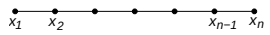
- If we retain only leading order error terms, this can be written as

$$\rho U \frac{d\phi}{dx} = \left(\Gamma + \frac{\rho U \Delta x}{2!} \right) \frac{d^2\phi}{dx^2} = \Gamma \left(1 + \frac{Pe_x}{2!} \right) \frac{d^2\phi}{dx^2} \quad (50)$$

- The error introduced by the upwind scheme is seen to be equivalent to increasing the diffusivity.
- The error is thus referred to as diffusive, and generally acts to "smear" the solution. This tends to exert a stabilizing influence on the numerical solution, although as seen it has an adverse effect on accuracy.

Boundary Conditions

- As in the example examined earlier, the form of the difference equation to be solved often has to be modified at the edges of the domain to account for boundary conditions.
- *Dirichlet* boundary conditions (where the value of the variable is fixed) can usually be implemented by simply setting the appropriate value at the boundary node.



- Terms involving this boundary node in the discretized equations at neighbouring nodes can then be moved to the source term on the right hand side, as was done in the example earlier. The values of ϕ to be solved for are then ϕ_2, ϕ_3,...,ϕ_{n-1}.
- If high order schemes with computational stencils covering more than three points are used, it may be necessary to modify these at the near-boundary nodes (to avoid referencing non-existent nodes).

- *Neumann* boundary conditions (the gradient of ϕ being prescribed) can be implemented by using a discretized form of the boundary condition.
- Suppose, for example, we have the condition $d\phi/dx = 0$ at $x = 0$.
  - A first order one-sided difference would give

$$\left.\frac{d\phi}{dx}\right|_1 \approx \frac{\phi_2 - \phi_1}{\Delta x} \qquad \text{so} \qquad \phi_1 = \phi_2 \tag{51}$$

  - A quadratic fit through the boundary and two neighbouring points on a uniform grid would give

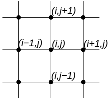
$$\left.\frac{d\phi}{dx}\right|_1 \approx \frac{-3\phi_1 + 4\phi_2 - \phi_3}{2\Delta x} \qquad \text{so} \qquad \phi_1 = (4/3)\phi_2 - (1/3)\phi_3 \tag{52}$$

  - Note the above expressions both use one-sided differences. Central differences can sometimes be applied by adding 'imaginary' nodes beyond the domain boundary (see problem sheet example).
- These expressions can then be used to modify the discretized equation at the near-boundary nodes.

Extension to Multiple Dimensions

- Although the finite difference methods outlined have been presented in terms of 1-D problems, the extension to 2 or 3 dimensions is fairly straightforward.
- If, for example, we discretize the 2-D Poisson equation

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = f(x,y) \tag{53}$$

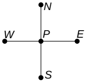


on a uniform grid as shown, using central differences for the derivatives, we obtain

$$\frac{\phi_{i-1,j} - 2\phi_{i,j} + \phi_{i+1,j}}{(\Delta x)^2} + \frac{\phi_{i,j-1} - 2\phi_{i,j} + \phi_{i,j+1}}{(\Delta y)^2} = f_{i,j} \tag{54}$$

- Note that we now have a five point stencil, with a difference equation of the form

$$a_p\phi_P = a_e\phi_E + a_w\phi_W + a_n\phi_N + a_s\phi_S + S_u \tag{55}$$



where the subscripts P, E, W, N, S denote the nodal positions and the coefficients and source term are:

$$a_e = a_w = 1/(\Delta x)^2 \qquad a_n = a_s = 1/(\Delta y)^2$$
$$a_p = a_e + a_w + a_n + a_s \qquad S_u = -f_{i,j}$$