

Review of Basic Finite Volume Methods

T. J. Craft

George Begg Building, C41

Contents:

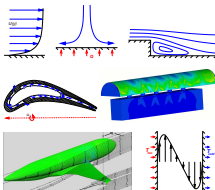
- ▶ **Review of basic FV method**
- ▶ Pressure-velocity coupling
- ▶ Body-fitted coordinate systems
- ▶ Unsteady problems
- ▶ Turbulence and other physical modelling

Reading:

J. Ferziger, M. Peric, *Computational Methods for Fluid Dynamics*
 H.K. Versteeg, W. Malalasekera, *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/tmcfid>
 - People - T. Craft - Online Teaching Material

Overview of CFD in Advanced Modelling & Simulation

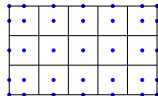
- ▶ Material builds on that covered in Modelling & Simulation III.
- ▶ Our general aim in CFD is to be able to simulate a wide range of flows:
 - ▶ Boundary layers, impingement, separation/reattachment, streamline curvature, ...
 - ▶ Complex flow geometries; often turbulent flow
 - ▶ Heat/mass transfer
 - ▶ Buoyancy, system rotation, etc. ...
- ▶ Most general purpose CFD codes employ Finite Volume (FV) discretization methods.



- ▶ Modelling & Simulation III covered
 - ▶ Basic FV discretization on rectangular grids.
 - ▶ Examining the order of accuracy of numerical schemes.
 - ▶ The importance of convection terms, and some different schemes for these (1st order upwind, higher order schemes: QUICK, etc)
 - ▶ The general trade-off between accuracy and stability.
- ▶ In Advanced Modelling & Simulation we will cover
 - ▶ Revision of the basic FV schemes.
 - ▶ Pressure-velocity coupling on staggered and collocated grids.
 - ▶ Extension of FV to non-orthogonal, body-fitted, grids.
 - ▶ Time-dependent problems.
 - ▶ Modelling considerations for turbulent flows.
- ▶ CFD element of the course consists of 12 hours of lectures/examples and one laboratory session.
- ▶ Rather than teach how to use a particular CFD code, the course aims to give an understanding of the approximations and numerical treatments found in most general CFD codes.

The Basic Finite Volume Method

- ▶ One important feature of finite volume schemes is their conservation properties. Since they are based on applying conservation principles over each small control volume, global conservation is also ensured.
- ▶ Initially we consider how they are applied on rectangular Cartesian grids. In later lectures we see how to adapt them to non-orthogonal and even unstructured grids.
- ▶ The method starts by dividing the flow domain into a number of small control volumes.
- ▶ The grid points where variables are stored are typically defined as being at the centre of each control volume.
- ▶ Extra boundary nodes are often added, as shown in the figure.
- ▶ The transport equation(s) are then integrated over each control volume.



- ▶ We consider a general (steady) transport equation for some quantity ϕ :

$$\frac{\partial(U\phi)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\gamma \frac{\partial \phi}{\partial x_j} \right) + S_\phi \quad (1)$$

or

$$\nabla \cdot (\underline{U}\phi) = \nabla \cdot (\gamma \nabla \phi) + S_\phi \quad (2)$$

- ▶ Integrating this over the control volume Ω gives:

$$\int_{\Omega} \frac{\partial(U\phi)}{\partial x_j} dV = \int_{\Omega} \frac{\partial}{\partial x_j} \left(\gamma \frac{\partial \phi}{\partial x_j} \right) dV + \int_{\Omega} S_\phi dV \quad (3)$$

or

$$\int_{\Omega} \nabla \cdot (\underline{U}\phi) dV = \int_{\Omega} \nabla \cdot (\gamma \nabla \phi) dV + \int_{\Omega} S_\phi dV \quad (4)$$

- ▶ The convection and diffusion terms can be combined:

$$\int_{\Omega} \nabla \cdot (\underline{U}\phi - \gamma \nabla \phi) dV = \int_{\Omega} S_\phi dV \quad (5)$$



- ▶ The divergence theorem can be used to convert the left hand side volume integral to an integral around the boundary, $\partial\Omega$, of the control volume:

$$\int_{\partial\Omega} (\underline{U}\phi - \gamma \nabla \phi) \cdot \underline{n} dS = \int_{\Omega} S_\phi dV \quad (6)$$

- ▶ $\underline{U}\phi \cdot \underline{n} dS$ is the convective flux of ϕ across the part of the boundary edge dS , and $\gamma \nabla \phi \cdot \underline{n} dS$ is the diffusive flux across the same boundary part.
- ▶ The left hand side of equation (6) is thus simply the total net convective and diffusive flux of ϕ into the control volume.
- ▶ Equation (6) is thus a statement of conservation for the control volume. In the case of the momentum equation, where $\phi = U$ for example, it is simply the force-momentum principle applied over the control volume.
- ▶ Provided the same expressions are used for fluxes across faces in neighbouring cells, this approach ensures that the conservation properties will also be satisfied globally over the flow domain.

- ▶ The surface integral is approximated in a discretized form by

$$\int_{\partial\Omega} (\underline{U}\phi - \gamma \nabla \phi) \cdot \underline{n} dS \approx \sum_k (\underline{U}\phi - \gamma \nabla \phi)_k \cdot (\underline{n} \Delta S)_k \quad (7)$$

where $(\underline{U}\phi - \gamma \nabla \phi)_k$ is evaluated at the centre of edge k of the cell, and $(\Delta S)_k$ and \underline{n}_k are the area and unit vector normal to this edge.



- ▶ This approximation of the surface integral can be shown to be of second order accuracy; for some function f a Taylor series expansion gives:

$$\int f(s) ds = \int \left(f(\xi) + (s - \xi)f'(\xi) + \frac{(s - \xi)^2}{2!} f''(\xi) + \dots \right) ds \quad (8)$$

for any point ξ lying somewhere on the line being integrated along.

- ▶ The integration of terms on the right hand side of equation (8) can then be carried out, using a suitable change of variable, to give

$$\begin{aligned} \int f(s) ds &= f(\xi) \int ds + f'(\xi) \int (s - \xi) ds + \dots \\ &= f(\xi) \Delta S + O((\Delta S)^2) \end{aligned}$$

- ▶ In fact, when ξ is taken as the mid-point of the face then the above approximation has leading order term of $O((\Delta S)^3)$, and the approximation is third order.

- ▶ The source terms in the volume integral of equation (6) are approximated as

$$\int_{\Omega} S_\phi dV \approx \overline{S_\phi} Vol \approx (S_\phi)_P Vol \quad (9)$$

where $\overline{S_\phi}$ is the "average" value of S_ϕ over the control volume and $(S_\phi)_P$ is simply its value at the cell centre node P .

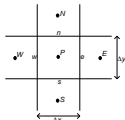
- ▶ This approximation can also be shown to be generally of second order accuracy.

Finite-Volume Method on a 2-D Rectangular Grid

- To complete the discretization, one needs to consider how to approximate the convective and diffusive fluxes at the cell faces and, if necessary, the source terms at the cell centre.

- To simplify the explanation for now, consider the steady U momentum equation in 2-D and a uniform rectangular grid.

- The velocity U is stored at the nodes P, N, S, E, W , located at control volume centres; cell faces are denoted by lower case n, s, e, w .



- The finite-volume method starts by integrating the momentum equation over the P control volume:

$$\iint_V \frac{\partial}{\partial x} (\rho U^2) + \frac{\partial}{\partial y} (\rho UV) dx dy = - \iint_V \frac{\partial P}{\partial x} dx dy + \iint_V \frac{\partial}{\partial x} \left(\mu \frac{\partial U}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial U}{\partial y} \right) dx dy \quad (10)$$

- This leads to

$$\left[\int \rho U^2 dy \right]_w^e + \left[\int \rho UV dx \right]_s^n = \left[\int \mu \frac{\partial U}{\partial x} dy \right]_w^e + \left[\int \mu \frac{\partial U}{\partial y} dx \right]_s^n - \iint_V \frac{\partial P}{\partial x} dx dy \quad (11)$$

Evaluating Source Terms

- The source terms can be approximated by evaluating them at the cell centre and multiplying by the volume of the cell:

$$- \iint_V \frac{\partial P}{\partial x} dx dy \approx \left(\frac{\partial P}{\partial x} \right)_P \Delta x \Delta y \quad (12)$$

- In the example considered, the pressure gradient at the cell centre, $(\partial P / \partial x)_P$, is evaluated by interpolating pressure values from surrounding nodes, if necessary. This will be addressed in more detail in later lectures.
- Other source terms can be evaluated similarly, interpolating where necessary to estimate cell centre values.

Evaluating Diffusive Fluxes

- The diffusive flux integrals can be approximated by

$$\left[\int \mu \frac{\partial U}{\partial x} dy \right]_w^e + \left[\int \mu \frac{\partial U}{\partial y} dx \right]_s^n \approx \left[\mu \frac{\partial U}{\partial x} \Delta y \right]_w^e + \left[\mu \frac{\partial U}{\partial y} \Delta x \right]_s^n \quad (13)$$

- The gradients $\partial U / \partial x$ and $\partial U / \partial y$ at the cell faces can be evaluated using central differences, so that the diffusion terms become

$$(\mu \Delta y)_e \frac{U_E - U_P}{\Delta x} - (\mu \Delta y)_w \frac{U_P - U_W}{\Delta x} + (\mu \Delta x)_n \frac{U_N - U_P}{\Delta y} - (\mu \Delta x)_s \frac{U_P - U_S}{\Delta y} \quad (14)$$

- This is again a second order, centered, approximation.

- The discretized diffusion terms can thus be written as

$$a_e^d U_E + a_w^d U_W + a_n^d U_N + a_s^d U_S - a_P^d U_P \quad (15)$$

where

$$a_e^d = (\mu \Delta y / \Delta x)_e \quad a_w^d = (\mu \Delta y / \Delta x)_w \quad a_n^d = (\mu \Delta x / \Delta y)_n \quad a_s^d = (\mu \Delta x / \Delta y)_s$$

$$\text{and } a_P^d = a_e^d + a_w^d + a_n^d + a_s^d.$$

Evaluating Convective Fluxes

- The convection terms can be approximated as

$$\begin{aligned} \left[\int \rho U^2 dy \right]_w^e + \left[\int \rho UV dx \right]_s^n &\approx \left[\rho U^2 \Delta y \right]_w^e + \left[\rho UV \Delta x \right]_s^n \\ &= (\rho U \Delta y)_e U_E - (\rho U \Delta y)_w U_W + (\rho V \Delta x)_n U_N - (\rho V \Delta x)_s U_S \\ &= C_{xe} U_E - C_{xw} U_W + C_{yn} U_N - C_{ys} U_S \end{aligned} \quad (16)$$

where C_{xe} , C_{xw} , C_{yn} and C_{ys} are simply the mass fluxes through the east, west, north and south faces.

- The values of U at the cell faces, U_e , U_w , U_n and U_s need to be obtained by interpolation between nodal values.

- The scheme used to interpolate these values affects both the stability and accuracy of the overall solution, and a few commonly-used alternatives are outlined below.

First Order Upwind Scheme

- A very simple scheme for approximating cell face values for the convective terms is the first-order upwind convection scheme:

$$U_e = \begin{cases} U_P & \text{for } C_{xe} > 0 \\ U_E & \text{for } C_{xe} \leq 0 \end{cases} \quad (17)$$


- This gives a convection contribution to the discretized equation of

$$-a_e^c U_E - a_w^c U_W - a_n^c U_N - a_s^c U_S + a_p^c U_P \quad (18)$$

where

$$\begin{aligned} a_e^c &= \max(-C_{xe}, 0) & a_w^c &= \max(C_{xw}, 0) \\ a_n^c &= \max(-C_{yn}, 0) & a_s^c &= \max(C_{ys}, 0) \end{aligned}$$

and $a_p^c = a_e^c + a_w^c + a_n^c + a_s^c + (C_{xe} - C_{xw} + C_{yn} - C_{ys})$

- Note that the coefficients a_e^c , etc are all positive, as is a_p^c . The final set of terms in a_p^c is the net mass flux into the cell, which should be zero, so in practice a_p^c can simply be taken as the sum $a_e^c + a_w^c + a_n^c + a_s^c$.

- Combining the convection and diffusion terms results in a discretized equation of the form

$$a_p U_P = a_e U_E + a_w U_W + a_n U_N + a_s U_S + s_u \quad (19)$$

where $a_e = a_e^d + a_e^c$, etc, $a_p = a_p^d + a_p^c$, and s_u represents the source terms arising from the pressure gradient.

- We thus get a set of equations relating U_P to the values of U at surrounding nodes.
- Having obtained the coefficients and source terms for each grid cell, the resulting system of equations can be solved by a suitable numerical algorithm.
- The above upwind scheme is always bounded. However, as implied by its name, it is only first order accurate.
- To illustrate this, we assume that $C_{xe} > 0$. Then the scheme approximates

$$C_{xe} U_e \approx C_{xe} U_P = C_{xe} \left(U_e + (x_P - x_e) \left(\frac{\partial U}{\partial x} \right)_e + O((x_P - x_e)^2) \right) \quad (20)$$

- The leading error term in this can thus be written as

$$C_{xe} (\Delta x / 2) \left(\frac{\partial U}{\partial x} \right)_e = (\Gamma_u)_e \left(\frac{\partial U}{\partial x} \right)_e \Delta y$$

where the 'numerical viscosity' $(\Gamma_u)_e = C_{xe} \Delta x / (2 \Delta y)$.

- The error is therefore diffusive in nature, and so tends to make the solution stable, but inaccurate.
- The order of accuracy gives information on how rapidly numerical errors decrease as the grid is refined. Since the error in the above scheme decreases only linearly with grid spacing, a very fine grid can be needed to obtain a grid independent solution.
- For this reason, whilst first order schemes are often used, it is usually preferable to employ a higher order scheme.
- Note, however, that in practical applications it is common practice to begin a calculation with a first order scheme, for its stability, and then switch to a higher order one once the solution is closer to convergence.

Central Difference Scheme

- This scheme simply interpolates linearly between U_P and U_E to approximate U_e . For a uniform grid this gives

$$U_e = 0.5(U_E + U_P) \quad (21)$$

- This is a second order approximation, which can be seen by writing Taylor series expansions for U_P and U_E around U_e :

$$U_P = U_e + (x_P - x_e) \left(\frac{\partial U}{\partial x} \right)_e + O(\Delta x^2) = U_e - 0.5 \Delta x \left(\frac{\partial U}{\partial x} \right)_e + O(\Delta x^2) \quad (22)$$

$$U_E = U_e + (x_E - x_e) \left(\frac{\partial U}{\partial x} \right)_e + O(\Delta x^2) = U_e + 0.5 \Delta x \left(\frac{\partial U}{\partial x} \right)_e + O(\Delta x^2) \quad (23)$$

- Adding equations (23) and (22) then leads to

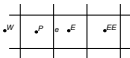
$$U_e = 0.5(U_E + U_P) + O(\Delta x^2) \quad (24)$$

- The central difference scheme is thus more accurate than the first order upwind scheme, although it can produce oscillatory solutions.

QUICK Scheme

- The QUICK (Quadratic Upwind Interpolation for Convection Kinetics) scheme fits a parabola between three points to approximate U_ϕ .

- If $C_{xe} > 0$ a parabola is fitted through the points W , P and E .



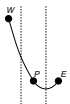
- If $C_{xe} < 0$ a parabola is fitted through the points P , E and EE .

- For $C_{xe} > 0$, on a regular grid we get

$$\phi_e = \phi_P + \frac{\phi_E - \phi_P}{2} - \frac{1}{8}(\phi_E - 2\phi_P + \phi_W) \quad (25)$$

- The QUICK scheme can be shown to be third order accurate.

- However, it is not bounded, and can produce undershoots and overshoots in regions of steep gradients.



- Note that the discretization stencil associated with the QUICK scheme is larger than that of the first and second order schemes outlined earlier, since contributions from U_{EE} , U_{WW} , U_{NN} and U_{SS} now appear.

- QUICK (and other) schemes are often coded as "deferred corrections". This means that the upwind scheme contributions are included in the coefficients a_E , a_W , etc. whilst the additional contributions from the QUICK (or other) scheme are simply placed in the source term S_U .

- This maintains the five point stencil of points treated implicitly, and the positivity of the coefficient matrix.

- Higher order schemes can also be devised and employed. However, in order to benefit significantly from them the simple formulations introduced earlier for approximating surface and volume integrals (which are only second order accurate) should also be replaced by a higher order method.

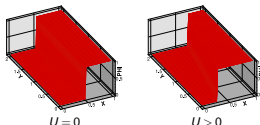
Convection Scheme Performances

- As an example, we consider the pure convection problem:

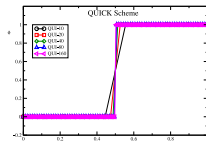
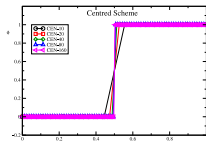
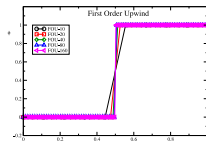
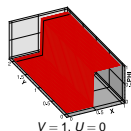
$$\frac{\partial U \phi}{\partial x} + \frac{\partial V \phi}{\partial y} = 0 \quad (26)$$

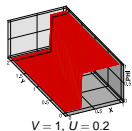
on the box $0 < x < 1$ and $0 < y < 2$ with velocities U and V constant and ϕ prescribed as a step function at $y = 0$ and $\partial \phi / \partial x = 0$ at $x = 0$ and $x = 1$.

- The exact solution is the step function simply convected with the velocity.

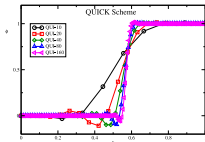
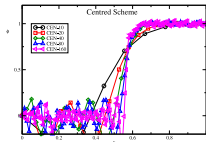
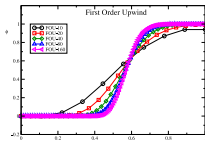


- The following slides show profiles of ϕ , close to the top boundary $y = 2$, with $U = 0$ and $U \neq 0$, using the three convection schemes outlined earlier on uniform grids ranging from 10 to 160 points in the x direction.





$$V = 1, U = 0.2$$



- ▶ In the $U = 0$ case the flow is aligned with the grid lines and all the schemes perform reasonably well (obviously resolving the step change better as the grid is refined).
- ▶ When $U \neq 0$ the flow is not aligned with the grid lines.
- ▶ In this case the numerical diffusion introduced by the first order upwind scheme is clearly present.
- ▶ The centred scheme captures the steep gradient better, but shows significant oscillations.
- ▶ The QUICK scheme also represents the steep gradients quite well, and improves rapidly as the grid is refined. However, it does show some over- and under-shoots at the base and crest of the step.

Boundary Condition Treatments

- ▶ For illustration we consider a cell at the east boundary of the flow domain.
- ▶ Typical boundary conditions might be one of

$$\phi = 0 \text{ at } x_E \text{ or } \partial\phi/\partial x = 0 \text{ at } x_E$$

- ▶ The discretized form of the transport equation can be written as

$$a_P \phi_P = a_E \phi_E + a_W \phi_W + a_N \phi_N + a_S \phi_S + S_P \quad (27)$$

where the coefficients a_E , a_W , a_N and a_S contain the convective and diffusive contributions, and $a_P = a_E + a_W + a_N + a_S$.

- ▶ The first type of boundary condition above can be simply implemented by setting the value of ϕ_E to zero.
- ▶ The zero gradient condition can be implemented by setting $a_E = 0$; the contributions $a_E \phi_P$ and $a_P \phi_E$ are then effectively removed from the left and right hand sides of equation (27) respectively.
- ▶ Fixed flux conditions (eg. prescribed heat flux) can also be implemented by setting a_E to zero and adding the desired flux to the source term S_P .



Numerical Flow Solver Strategy

- ▶ Each momentum equation can be discretized as described, leading to a set of algebraic equations relating the nodal values of U , V and W .
- ▶ Other transport equations (for temperature, mass fraction, etc.) can be treated similarly.
- ▶ However, the equations are coupled in a non-linear fashion, through the convection terms (and sometimes source terms).
- ▶ An often-used practice is to solve the equations in an iterative, segregated, manner:
 - ▶ Assemble the discretized equations for U , and hence update U .
 - ▶ Assemble the discretized equations for V , and hence update V .
 - ▶ Assemble the discretized equations for W , and hence update W .
 - ▶ Update the pressure field.
 - ▶ Repeat until the solution has converged.
- ▶ At this stage it is not clear how the pressure field is updated, since we do not have a transport equation for the pressure. This issue is addressed in the following section.