Numerical ThermoFluid Dynamics

Contents

By A.M.

Part I

Introduction

CFD codes are structured around the numerical algorithms. All codes contains three main elements:

1. **Pre-Processor**

   Consist of the input of a flow problem to a CFD program. The user activities at the pre-processing stage involve:

   (a) To define the geometry of the region of interest (computational domain);

   (b) Grid generation, the subdivision of the domains into a number of smaller sub domain of subdomain by grid (or mesh);

   (c) Gelection of the physical phenomena that need to be modeled;

   (d) Definition of the fluid properties;

   (e) Specification of appropriate boundary condition at cells.

   The solution of a flow problem is defined at **nodes** inside each cell.

   Accuracy of CFD is proportional to the number of cell: optimal meshes are often non uniform.

2. **Solver**

   We have almost 3 kind of numerical techniques: (i) Finite difference; (ii) Finite element; (iii) Special methods.

   We use **finite volume method** that is a special finite difference formulation.

   Numerical algorithm follow this steps

   (a) **Integration of the governing equations** of fluid all over the control volume of the domain; item **Discretisation** or conversion of the resulting integral equations into a system of algebraic equations;

   (b) **Solution** of algebraic equations by an *iterative method.*

   CFD codes contains discretisation techniques suitable for the tratment of the key transport phenomena:

   - *Convection*: transport of the fluid flow;
   - *Diffusion*: transport due to variations of ϕ from point to point;

   The most popular solution procedures are the TDMA and SIMPLE algorithm to ensure the correct linkage between pressure and velocity.

3. **Post-Processor**

   We need to make assumptions to reduce the complexity of the problem (3d model into 2d model, exclude some effect of $T, \Delta p, \rho \dots$)

Two aspects that characterize a simulation results are convergence and grid independence.

Classification of physical behavior

In order to construct a well mathematical model of fluid flow, initial and boundary conditions are needed in conjunction with the governing equations.

We have two categories of physical behavior

- Equilibrium problems
- Marching problems

Equilibrium problems

Problems in this category are steady state. These problems are governed by **elliptic equations**.

A prototype of elliptic equations in Laplace's equation, which describes irrotational flow af an uncompressible fluid and steady state conductive heat transfer.
In 2D we have:

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

a unique solution in all the elliptic problems can be obtained by specifying conditions on the dependent value on all the boundaries of the solution domain.

Whenever is present a disturbance in the interior of the solution region, this change the solution everywhere else, for this reason the solution of elliptic equations are always smooth even if the boundary conditions are discontinuous.

Marching problems

These problem are typical of transient cases, unsteady flow and wave phenomena.
This problems are governed bu **parabolic** o **hyperbolic** equations.

- **Parabolic equations**

  Describe time-dependent problems which involute significant amounts of diffusion.

  $$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2}$$

  A disturbance at one point in the interior of the solution region can only influence events al later time $t > t_1$.

  Solution can be obtained specifying initial and boundary conditions.

- **Hyperbolic equations**

  Dominate the analysis of vibration problems. Appear in time dependent problems with negligible energy dissipation.

  $$\frac{\partial^2 \phi}{\partial^2 t} = c^2 \frac{\partial^2 \phi}{\partial x^2}$$

  Solution can be obtained specifying two initial conditions and one conditions on all the boundaries.

Part II

Turbulence

At low Reynolds numbers flows are laminar; at higher Reynolds numbers flows become turbulent: a chaotic and random state of motion develops in which the velocity and pressure change continuously with time and space.

Flows in the laminar regime are completely described by the continuity and Navier Stokes equations.

These velocity fluctuations are found to give rise to additional stresses on the fluid: the **Reynolds stresses**, so additional models for these extra stress terms are needed for solving turbulent flows.
The Reynolds number gives a measure of the relative importance of inertia forces and viscous forces, At values of the Reynolds number above Re_{crit} a complicated series of events takes place which leads to a radical change of the flow characteristics. In the final state the flow behavior is random and chaotic, the motion becomes intrinsically unsteady even with constant imposed boundary conditions and the velocity and all other flow properties vary in a random and chaotic way.
This regime is called **turbulent**.

Because of the random nature of a turbulent flow, the velocity is decomposed into a steady mean value U with a fluctuating component $u(t)$ superimposed on it

$$u(t) = U + u'(t)$$

This is called the **Reynolds decomposition**.
In this way a turbulent flow can be characterized by its mean values and by some statistical fluctuation.

Nevertheless, by its nature, the turbulence problem has a 3d spacial character.
This by observing that in the turbulent flows there is a creation of rotational flow structures: the turbulent eddies, of a wide range on length scales.

These eddies leads particle of fluid initially separated by long distance, brought close, giving rise to an exchange of heat, mass and momentum.
The largest turbulent eddies interact with the mean flow extracting its energy, in a process called **vortex stretching**. Smaller eddies are themselves stretched by largest in a way that eddies get smaller in an **energy cascade**.

The turbulence extract energy from the mean flow to supply the eddies and the small eddies extract the kinetic energy from the largest eddies, in a cascade of dissipation up to a certain dimension of these eddies, under the Kolmogorov scale eddy motions is dissipated and converted into thermal internal energy.

The turbulent flows are associated with a increase energy losses.

Simple characteristics

From the study of the flat plate boundary layer, it is observed that in flow along solid boundaries there is a region of inertia-dominated flow far away from the wall and a thin layer with a viscous-dominated flow.
In this thin layer the flow is influenced by viscous effects and does not depend on free stream parameters.
Dimensional analysis show that

$$u^+ = \frac{U}{u_\tau} = f\left(\frac{\rho u_\tau u}{\mu}\right) = f(y^+)$$

This formula, the **law of the wall** contains, over the friction velocity $u_\tau = \sqrt{\frac{\tau_w}{\rho}}$, two important dimensionless groups u^+, y^+.

The turbulent boundary layer adjacent to a solid surface is composed of mainly two regions:

1. The **inner region** which consist of about the 10 -20% of the total thickness of the wall layer, where the shear stress is constant and almost equal to the wall shear stress.

   Inside this region there are three zone:

   (a) The **linear sub-layer**: $y^+ < 5$ where the viscous stresses dominate the flow adjacent the surface;

   (b) The **buffer layer** where viscous and turbulent stresses are of similar magnitude;

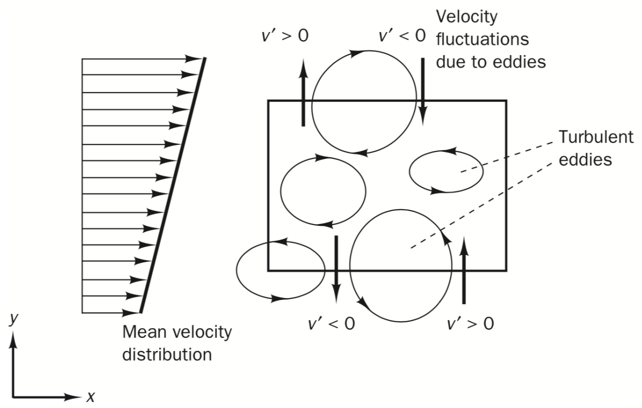
   (c) The **log-law layer**: $30 < y^+ < 500$ where the viscous and turbulent effects are both important:

   $$u^+ = \frac{1}{k}\ln(y^+)$$

2. The **outer region**, a layer of inertia dominated flow far from wall and free from direct viscous effects.

Effect of the fluctuations

The presence eddies in motions creates strong mixing: fluid parcels can be transported by the eddies carrying momentum and energy into and out of the control volume.



$v' > 0$
$v' < 0$
Velocity fluctuations due to eddies
Turbulent eddies
$v' < 0$
$v' > 0$
Mean velocity distribution
y
x

The net result of this mixing is momentum exchange due to convective transport by the eddies, which causes the faster moving fluid layers to be decelerated and the slower moving layers to be accelerated.

Consequently, the fluid layers experience additional turbulent shear stresses, which are known as the **Reynolds stresses**.
This proves that the equations for momentum and energy are affected by these fluctuations.

RANS equations

By the instantaneous continuity and Navier Stokes equations we can investigate the effects of fluctuations on the mean flow using the Reynolds decomposition and replace the flow variables by the sum of a mean and fluctuating component.

We discover that arise some terms that's involve the products of fluctuating velocities and are associated with convective momentum transfer due to turbulent eddies.

$$\cdots + \left[\frac{\partial(-\overline{u'w'})}{\partial x} + \frac{\partial(-\overline{v'w'})}{\partial y} + \frac{\partial(-\overline{w'^2})}{\partial z} \right]$$

This result in six additional stresses:

- Three normal stresses

$$\tau_{xx} \sim \overline{u'^2} \qquad \tau_{yy} \sim \overline{v'^2} \qquad \tau_{zz} \sim \overline{w'^2}$$

- Three shear stresses:

$$\tau_{yx} \sim \overline{u'v'} \qquad \tau_{zy} \sim \overline{v'x'} \qquad \tau_{zx} \sim \overline{w'u'}$$

The extra turbulent stresses terms, are the Reynolds stresses.

The normal stresses involve the respective variances of the x y and z velocity fluctuations they are always non zero because they contain squared velocity fluctuations

Turbulent flow calculations

The numerical methods developed to capture the important effects due to turbulence can be grouped into the following three categories:

1. **Turbulence models** for Reynolds averaged Navier Stokes (RANS) equations:

   The k-ε model and the Reynolds stress model, which computing resources required for reasonably accurate flow computations are modest.

2. **LES**, Large eddy simulation:

   An intermediate form of turbulence calculations which tracks the behavior of the larger eddies. The method involves space filtering of the unsteady Navier Stokes equations prior to the computations, which passes the larger eddies and rejects the smaller eddies. Large computing demand.

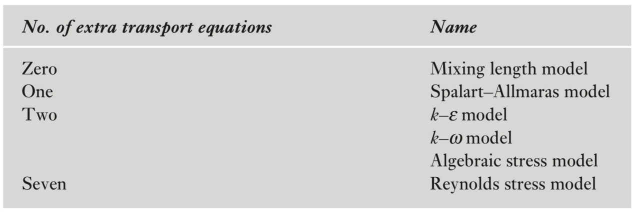
3. **DNS**, Direct numerical simulation:

   These simulations compute the mean flow and all turbulent velocity fluctuations. The grids comprehend the Kolmogorov scales with extra fine time steps. Very high costly method.

Classical turbulence models

In order to be able to compute turbulent flows with the RANS equations it is necessary to develop turbulence models to predict the Reynolds stresses and the scalar transport terms and close the system of mean flow equations.

The most common RANS turbulence models are classified on the basis of the number of additional transport equations that need to be solved along with the RANS flow equations.



No. of extra transport equations	*Name*
Zero	Mixing length model
One	Spalart–Allmaras model
Two	k–ε model
	k–ω model
	Algebraic stress model
Seven	Reynolds stress model

The mixing length and k-ε models are the most widely used and validated They are based on the presumption that there exists an analogy between the action of viscous stresses and Reynolds stresses on the mean flow.

Both stresses appear on the right hand side of the momentum equation, and in Newton's law of viscosity the viscous stresses are taken to be proportional to the rate of deformation of fluid elements.
Boussinesq proposed in 1877 that Reynolds stresses might be proportional to mean rates of deformation:

$$\tau_{ij} \sim \overline{u_i' u_j'} = \mu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3}\rho k \delta_{ij}$$

where k is the turbulent kinetic energy per unit mass.

Turbulent transport of heat, mass and other scalar properties can be modelled similarly taken to be proportional to the gradient of the mean value of the transported quantity':

$$\overline{u_i' \varphi'} = \Gamma_t \frac{\partial \Phi}{\partial x_i}$$

where Γ_t is the turbulent or eddy diffusivity.

Since turbulent transport of momentum and heat or mass is due to the same mechanism - eddy mixing - we expect that the value of the turbulent diffusivity Γ_t is fairly close to that of the turbulent viscosity μ_t.
This assumption is better known as the Reynolds analogy.
We can now introduce a turbulent Prandtl/Schmidt number

$$\sigma_t = \frac{\mu_t}{\Gamma_t} \approx 1$$

The **k-ε model** is a more sophisticated and general, but also more costly, description of turbulence which allows for the effects of transport of turbulence properties by convection and diffusion and for production and destruction of turbulence.
Two transport equations, one for the turbulent kinetic energy k and one for the rate of dissipation of turbulent kinetic energy ε are solved.
The underlying assumption of both these models is that the turbulent viscosity μ_t is isotropic: the ratio between Reynolds stress and mean rate of deformation is the same in all directions.
However, this assumption fails in many complex flows: the six transport equations, one for each Reynolds stress, contain diffusion, pressure strain and dissipation terms whose individual effects are unknown and cannot be measured.

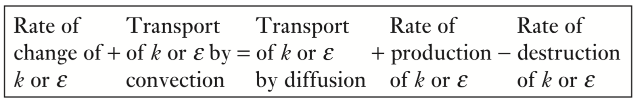
In **Reynolds stress equation models** assumptions are made about these unknown terms, and the resulting PDEs are solved in conjunction with the transport equation for the rate of dissipation of turbulent kinetic energy ε.

K-ε model

The standard k-ε model (1974) has two model equations, one for k and one for ε based on our best understanding of the relevant processes causing changes to these variables.
We use k and ε to define velocity scale ϑ and length scale ℓ representative of the large scale turbulence:

$$\vartheta = k^{\frac{1}{2}} \qquad \ell = \frac{k^{\frac{3}{2}}}{\varepsilon}$$

In words, the equations that leads are:



Rate of change of k or ε	+	Transport of k or ε by convection	=	Transport of k or ε by diffusion	+	Rate of production of k or ε	−	Rate of destruction of k or ε

Production and destruction of turbulent kinetic energy are always closely linked: dissipation rate ε is large where production of k is large.
The model equation for ε assumes that its production and destruction terms are proportional to the production and destruction terms of the k equation.

The model equations for k and ε are elliptic by virtue of the gradient diffusion term Their behavior is similar to the other elliptic flow equations, which gives rise to the need for the following boundary conditions:

- Inlet;
- Outlet, Symmetry;
- Free stream;
- Solid Walls:
  - $\uparrow$ *Re* the turbulence production equals the rate of dissipation: wall functions;
  - $\downarrow$ *Re* viscous effect are predominant: wall damping functions needs to be applied.

Spalart-Allmaras model

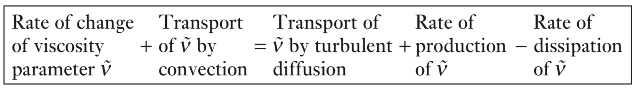
The Spalart Allmaras model involves one transport equation for kinematic eddy viscosity parameter $\widetilde{\nu}$ and a specification of a length scale by means of an algebraic formula, and provides economical computations of boundary layers in external aerodynamics.

The dynamic eddy viscosity is related to $\widetilde{v}$ by:

$$\mu_t = \rho\widetilde{\nu} f_{\nu 1}$$

This equation contains the wall damping function $f_{\nu 1} = f_{\nu 1}\left(\frac{\widetilde{\nu}}{\nu}\right)$ which tends to unity for high Reynolds numbers, so the kinematic eddy viscosity parameter $\widetilde{\nu}$ is just equal to the kinematic eddy viscosity ν_t in this case.
At the wall the damping function $f_{\nu 1}$ tends to zero.

In words ew always have:



Rate of change of viscosity parameter $\tilde{\nu}$	+	Transport of $\tilde{\nu}$ by convection	=	Transport of $\tilde{\nu}$ by turbulent diffusion	+	Rate of production of $\tilde{\nu}$	−	Rate of dissipation of $\tilde{\nu}$

In the k ε model the length scale is found by combining the two transported quantities k and ε.
In this one-equation turbulence model the length scale cannot be computed, but must be specified to determine the rate of dissipation of the transported turbulence quantity.

So, the product ky (with y distance to the solid wall) will be used as the length scale.

In complex geometries it is difficult to define the length scale, so the model is unsuitable for more general internal flows Moreover, it lacks sensitivity to transport processes in rapidly changing flows

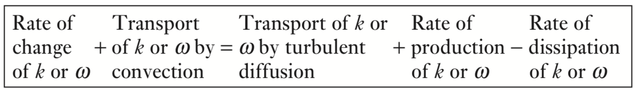
Wilcox k-ω model

In the k -ε model the kinematic eddy viscosity ν_t is expressed as the product of a velocity scale ϑ and a length scale ℓ.
The rate of dissipation of turbulence kinetic energy ε is not the only possible length scale determining variable: many other two equation models have been postulated.

The most prominent alternative is the k-ω model proposed by Wilcox ('88, '93, '94)which uses the turbulence frequency $\omega = \dfrac{\varepsilon}{k}$ as the second variable.
If we use this variable the length scale is $\ell = \dfrac{\sqrt{k}}{\omega}$.
The eddy viscosity is given by:

$$\mu_t = \frac{\rho k}{\omega}$$

So, in words:



Rate of change of k or ω	+	Transport of k or ω by convection	=	Transport of k or ω by turbulent diffusion	+	Rate of production of k or ω	−	Rate of dissipation of k or ω

The k-ω model initially attracted attention because integration to the wall does not require wall damping functions in low Reynolds number applications.
At inlet boundaries the values of k and ω must be specified, and at outlet boundaries the usual zero gradient conditions are used.
The boundary condition of ω in a free stream, where turbulence kinetic energy $k \to 0$ and turbulence frequency $\omega \to 0$ is the most problematic one.
Equation for μ_t shows that the eddy viscosity is indeterminate or infinite as $\omega \to 0$ so a small non zero value of ω must be specified.
Unfortunately, results of the model tend to be dependent on the assumed free stream value of ω which is a serious problem in external aerodynamics and aerospace applications where free stream boundary conditions are used as a matter of routine.

Menter SST k-ω model

Menter (1992) noted that the results of the k-ε model are much less sensitive to the assumed values in the free stream, but its near wall performance is unsatisfactory for boundary layers with adverse pressure gradients.

This led him to suggest a hybrid model using:

- A transformation of the k-ε model into a k-ω model in the near wall region;
- The standard k-ε model in the fully turbulent region far from the wall;

The Reynolds stress computation and the k equation are the same as in Wilcox's original k-ω model, but the ε equation is transformed into an ω equation by substituting $\varepsilon = k\omega$.

This arise an extra source term in the model PDEs: the cross-diffusion term, which arises during the $\varepsilon = k\omega$ transformation of the diffusion term in the ε-equation.

Menter (2003) summarize a series of modifications to optimize the performance of the SST k-ω model based on experience with the model in general purpose computation:

- **Revised model constants**;
- **Blending functions**: used to achieve a smooth transition between the two models;
- **Limiters**: the turbulent kinetic energy production is limited to prevent the build up of turbulence in stagnation regions.

Turbulence models performance

The k-ε model gives good results for simple flows and some recirculating flows, but research over a period of three decades has highlighted a number of shortcomings in low Reynolds number flows, rapidly changing flows, strong adverse pressure gradients and re-circulation regions.

External aerodynamics: the Spalart-Allmaras, k-ω and SST k-ω models are all suitable.
The SST k-ω model is most general, and tests suggest that it gives superior performance for zero pressure gradient and adverse pressure gradient boundary layers, free shear layers and a NACA 4412 aerofoil.

General purpose CFD:the k-ω and SST k-ω models can both be applied. They both have a similar range of strengths and weaknesses as the k-ε model and fail to include accounts of more subtle interactions between turbulent stresses and mean flow when compared with the RSM.

Large Eddy Simulation (LES)

In a turbulent flow the smaller eddies are nearly isotropic and have a universal behavior.

On the other hand, the larger eddies, which interact with and extract energy from the mean flow, are more an-isotropic and their behavior is dictated by the geometry of the problem domain, the boundary conditions and body forces.

A different approach to the computation of turbulent flows accepts that the larger eddies need to be computed for each problem with a time dependent simulation. The universal behavior of the smaller eddies, on the other hand, should hopefully be easier to capture with a compact model.

This is the essence of the large eddy simulation approach to the numerical treatment of turbulence.

Instead of time averaging, LES uses a spatial filtering operation to separate the larger and smaller eddies.
The method starts with the selection of a filtering function and a certain cutoff width with the aim of resolving in an unsteady flow computation all those eddies with a length scale greater than the cutoff width.

In the next step the spatial filtering operation is performed on the time dependent flow equations. During spatial filtering information relating to the smaller, filtered-out turbulent eddies is destroyed.

The interaction effects between the larger, resolved eddies and the smaller unresolved ones, gives rise to sub-grid-scale stresses or SGS stresses: their effect on the resolved flow must be described by means of an SGS model.

The inherent unsteady nature of LES suggests that the computational requirements should be much larger than those of classical turbulence models.

Direct Numerical Simulation (DNS)

Direct numerical simulation of turbulent flow takes the Navier-Stokes equations set as a starting point and develops a transient solution on a sufficiently fine spatial mesh with sufficiently small time steps to resolve even the smallest turbulent eddies and the fastest fluctuations.

This leads to:

- Precise details of turbulence parameters;
- Instantaneous results can be generated that are not measurable with instrumentation;
- Advanced experimental techniques can be tested and evaluated.

On the other side, is extremely computer demanding: Moin and Kim (1997) estimated computing times of 100 hours to 300 years for turbulent flows at Reynolds numbers in the range 10^4 to 10^6 based on high performance computer speeds of 150 Mflops available at that time.

Part III

Finite Volume Method

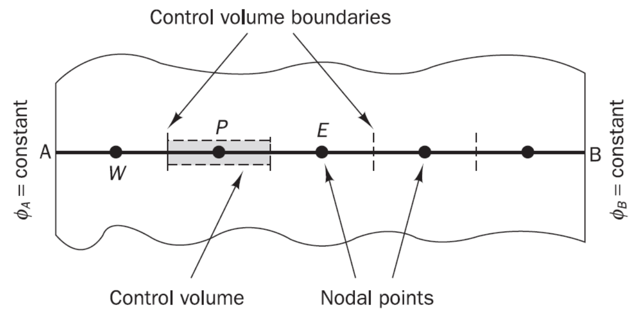
Diffusion problems

In this part we develop the numerical method based on the integration of transport equations governing fluid flow and heat transfer, the **finite volume method** by considering the simplest transport process of all pure diffusion in the steady state.

The control volume integration, which forms the key step of the finite volume method that distinguishes it from all other CFD techniques, yields to an integrated formula of the governing equations.

1-Dimensional diffusion problems

Consider the steady state diffusion of a property φ in a one dimensional domain defined in figure:



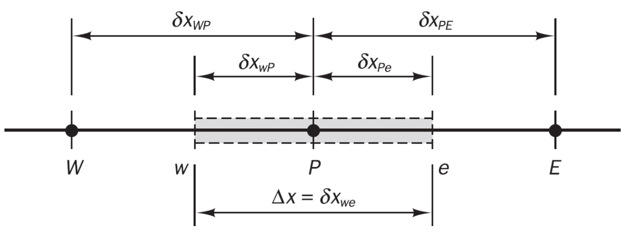
The finite volume method consists into three fundamental steps for producing a solution:

1. **Grid Generation**

   We have to divide the domain into discrete control volumes.

   Let us place a number of nodal points in the space between A and B.

   The boundaries (or faces) of control volumes are positioned mid way between adjacent nodes.

   Thus, each node is surrounded by a control volume or cell.

   It is common practice to set up control volumes in such a way that the physical boundaries coincide with the control volume boundaries.

   A general nodal point is identified by P and its neighbors in a one dimensional geometry, the nodes to the west and east, are identified by W and E respectively.

   The west side face of the control volume is referred by w and the east side control volume face by e.

2. **Discretization**

The key step of the finite volume method is the integration of the governing equation over a control volume to yield a discretised equation at its nodal point P.

NB: the discretised equation has a clear physical interpretation:

The diffusive flux of φ leaving the east face minus the diffusive flux of φ entering the west face is equal to the generation of φ, long story short, it constitutes a balance equation for φ over the control volume.

The values of the property φ and the diffusion coefficient are defined and evaluated at nodal points.

To calculate gradients (and hence fluxes) at the control volume faces an approximate distribution of properties between nodal points is used: the linear approximations seem to be the obvious and simplest way of calculating interface values and the gradients.

This practice is called central differencing:

$$\Gamma_w = \frac{\Gamma_W + \Gamma_P}{2} \qquad \Gamma_e = \frac{\Gamma_P + \Gamma_E}{2}$$

3. **Solution**

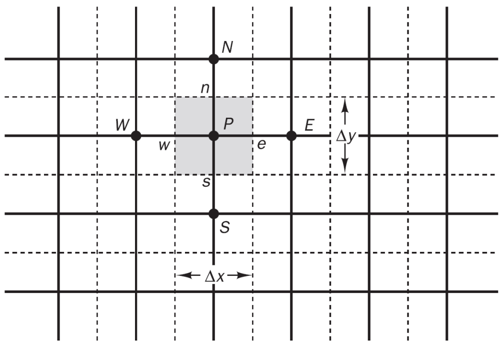
   Discretised equations must be set up at each of the nodal points in order to solve a problem.

   For control volumes that are adjacent to the domain boundaries the general discretised equation is modified to incorporate boundary conditions.

   The resulting system of linear algebraic equations is then solved to obtain the distribution of the property φ at nodal points.

2-Dimensional diffusion problems

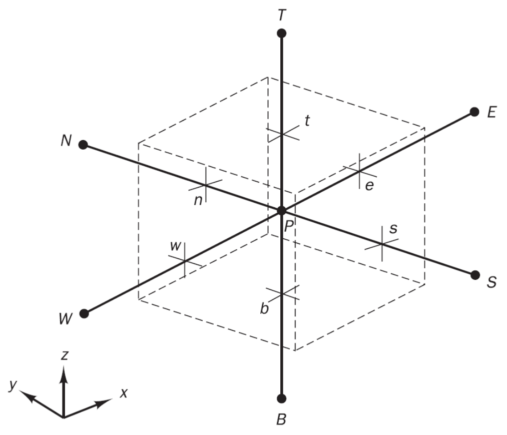
The methodology used in deriving discretised equations in the one dimensional case can be easily extended to two dimensional problems.



In addition to the east E and west W neighbours a general grid node P now also has north N and south S neighbours.

3-Dimensional diffusion problems

Now a three dimensional grid is used to sub divide the domain A typical control volume is shown in figure



A cell containing node P now has six neighbouring nodes identified as west, east, south, north, bottom and top W, E, S, N, B, T.
As before, the notation w e s n b and t is used to refer to the west, east, south, north, bottom and top cell faces respectively.

Convection-Diffusion problems

Diffusion always occurs alongside convection in nature so here we examine methods to predict combined convection and diffusion.
The steady convection diffusion equation can be derived from the transport equation for a general property φ by deleting the transient term, in integral form:

$$\int_A \mathbf{n} \cdot (\rho\varphi\mathbf{u})dA = \int_A \mathbf{n} \cdot (\Gamma\nabla\varphi)dA + \int_{CV} S_\varphi dV$$

This equation represents the flux balance in a control volume.

The LHS gives the net convective flux and the RHS contains the net diffusive flux and the generation or destruction of the property φ within the control volume.

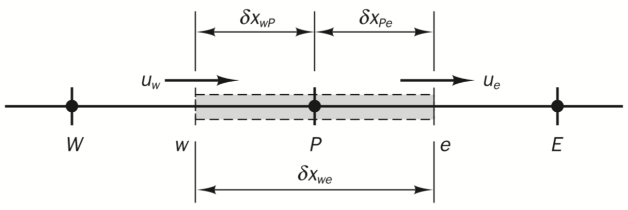
Take Home Message

The main problem in the discretisation of the convective terms is the calculation of the value of transported property φ at control volume faces and its convective flux across these boundaries.

It would seem obvious to try out the central differencing method, which worked so well for diffusion problems also on the convective terms for obtaining discretised equations, however, the diffusion process affects the distribution of a transported quantity along its gradients in all directions.
In this way the grid size become dependent on the relative strength of convection and diffusion.

In a simple way, in this current analysis we assume that the velocity is "somehow" known.

Let us consider absence of source and a 1D control volume as it follows:



Our attention is focused on a general node P.
Steady convection and diffusion of property φ is governed by:

$$\frac{d}{dx}(\rho u \varphi) = \frac{d}{dx}\left(\Gamma \frac{d\varphi}{dx}\right)$$

The flow must also satisfy the continuity equation:

$$\frac{d(\rho u)}{dx} = 0$$

The Integration fo these equation leads to, respectively

$$(\rho u A \varphi)_e - (\rho u A \varphi)_w = \left(\Gamma A \frac{d\varphi}{dx}\right)_e - \left(\Gamma A \frac{d\varphi}{dx}\right)_w$$

$$(\rho u A)_e - (\rho u A)_w = 0$$

It is convenient to define two variables F and D to represent the convective mass flux per unit area and diffusion conductance at cell faces:

$$F = \rho u \qquad D = \frac{\Gamma}{\delta x}$$

Assuming that $A_w = A_e = A$:

$$F_e \varphi_e - F_w \varphi_w = D_e(\varphi_E - \varphi_P) - D_w(\varphi_P - \varphi_W)$$

$$F_e - F_w = 0$$

In order to solve the convection diffusion equation we need to calculate the transported property φ at the e and w faces.

The central differencing approximation has been used to represent the diffusion terms and it seems logical to try linear interpolation to compute the cell face values for the convective terms on the left hand side of the transport equation

$$\varphi_e = \frac{\varphi_P + \varphi_E}{2} \qquad \varphi_w = \frac{\varphi_W + \varphi_P}{2}$$

After some mathematical passages and after identifying the coefficients of φ_W and φ_E as a_W and a_E the central differencing expressions for the discretised convection diffusion equation are

$$a_P \varphi_P = a_W \varphi_W + a_E \varphi_E$$

It can be easily recognised that the equation for steady convection diffusion problems takes the same general form as equation for pure diffusion problems.

The difference is that the coefficients of the former contain additional terms to account for convection.
To solve a one dimensional convection diffusion problem we write discretised equations for all grid nodes. This yields a set of algebraic equations that is solved to obtain the distribution of the transported property φ.

Otherwise, central differencing scheme produces a solution that appears to oscillate around the exact solution, these oscillations are often called "wiggles" and show that often the analytical solution is clearly not very good.

Discretisation scheme properties

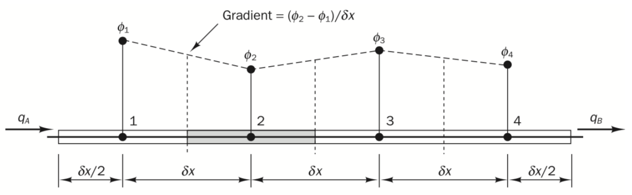
The failure of central differencing scheme in certain cases involving combined convection and diffusion forces.

in practical calculations we can only use a finite sometimes quite small number of cells, and our numerical results will only be physically realistic when the discretisation scheme has certain fundamental properties

1. Conservativeness;
2. Boundedness;
3. Transportiveness.

Conservativeness

Integration of the convection diffusion equation over a finite number of control volumes yields a set of discretised conservation equations involving fluxes of the transported property φ through control volume faces; to ensure conservation of φ for the whole solution domain, the flux of φ leaving a control volume across a certain face must be equal to the flux of φ entering the adjacent control volume through the same face.
To achieve this, the flux through a common face must be represented in a consistent manner by one and the same expression in adjacent control volumes.

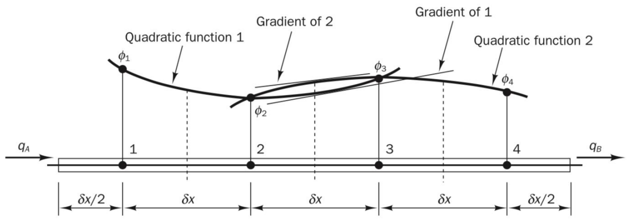


The fluxes across the domain boundaries are denoted by q_A and q_B. Let us consider four control volumes and apply central differencing to calculate the diffusive flux across the cell faces.

$$\begin{aligned}&\left[\Gamma_{e_1}\frac{(\phi_2-\phi_1)}{\delta x}-q_A\right]+\left[\Gamma_{e_2}\frac{(\phi_3-\phi_2)}{\delta x}-\Gamma_{w_2}\frac{(\phi_2-\phi_1)}{\delta x}\right]\\&+\left[\Gamma_{e_3}\frac{(\phi_4-\phi_3)}{\delta x}-\Gamma_{w_3}\frac{(\phi_3-\phi_2)}{\delta x}\right]+\left[q_B-\Gamma_{w_4}\frac{(\phi_4-\phi_3)}{\delta x}\right]\\&=q_B-q_A\end{aligned}$$

Since $\Gamma_{e1} = \Gamma_{w2}, \Gamma_{e2} = \Gamma_{w3}, \Gamma_{e3} = \Gamma_{w4}$ the fluxes across control volume faces are expressed in a consistent manner and cancel out in pairs when summed over the entire domain: only the two boundary fluxes remain in the overall balance, so the equation expresses overall conservation of property φ.

Inconsistent flux interpolation formulae give rise to unsuitable schemes that do not satisfy overall conservation. For example, let us consider the situation where a quadratic interpolation formula:



the flux values calculated at the east face of control volume 2 and the west face of control volume 3 may be unequal if the gradients of the two curves are different at the cell face: this is the case when two fluxes do not cancel out when summed and overall conservation is not satisfied.

Boundedness

The discretised equations at each nodal point represent a set of algebraic equations that needs to be solved.

Normally iterative numerical techniques are used to solve large equation sets: these techniques start the solution process from a guessed distribution of the variable φ and perform successive updates until a converged solution is obtained.

Scarborough (1958) has shown that a sufficient condition for a **convergent iterative method** can be achieved if the differencing scheme produces coefficients which put into a matrix, this is **diagonally dominant**.

Take Home Message

This states that in the absence of sources the internal nodal values of property φ should be bounded by its boundary values

Another essential requirement for boundedness is that all coefficients of the discretised equations should have the same sign (usually all positive).
Physically this implies that an increase in the variable φ at one node should result in an increase in φ at neighbouring nodes.

If the discretisation scheme does not satisfy the boundedness requirements it is possible that the solution does not converge at all, or, if it does, contains "wiggles".

Transportiveness

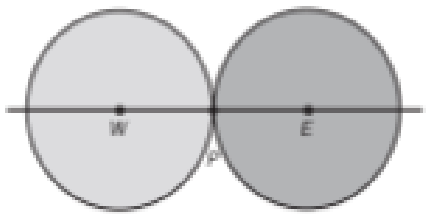
The transportiveness property of a fluid flow can be illustrated by considering the effect at a point P due to two constant sources of φ at nearby points W and E
We define the non-dimensional cell Peclet number as a measure of the relative strengths of convection and diffusion

$$Pe = \frac{F}{D}$$

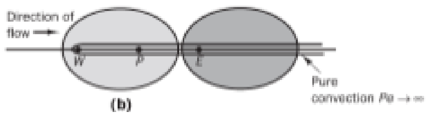
The lines in figure indicate the general shape of contours of constant φ due to both sources for different values of Pe.
The value of φ at any point can be thought of as the sum of contributions due to the two sources.
Let us consider two extreme cases to identify the extent of the influence at node P due to the sources at W and E

- No convection and pure diffusion $Pe \to 0$
- No diffusion and pure convection $Pe \to \infty$

In the case of pure diffusion, the fluid is stagnant $Pe \to 0$ and the contours of constant φ will be concentric circles centred around W and E since the diffusion process tends to spread φ equally in all directions.
Conditions at this point are influenced by both sources at W and E.



As Pe increases the contours change shape from circular to elliptical and are shifted in the direction of the flow



Influencing becomes increasingly biased towards the upstream direction at large values of Pe.
In the case of pure convection $Pe \to \infty$ the elliptical contours are completely stretched out in the flow direction all of property φ emanating from the sources at W and E is immediately transported downstream.

Conditions at P are now unaffected by the downstream source at E and completely dictated by the upstream source at W.

Take Home Message

The relationship between directionality of influencing (based on the flow direction) and magnitude of the Peclet number in the discretisation scheme is known as the **transportiveness**

Central Differencing Scheme

- **Conservativeness**:

  The central differencing scheme uses consistent expressions to evaluate convective and diffusive fluxes.

  The scheme is conservative.

- **Boundedness**:

  1. The coefficients of the central differencing scheme satisfy the Scarborough criterion.
  2. If the convection dominates it is possible for a_E to be negative, for this coefficient to be positive, must be
     $$Pe_e < 2$$
     If this condition is not respected, will be the violation of a boundedness requirements, leading to maybe not physical solutions.

- **Transportiveness**:

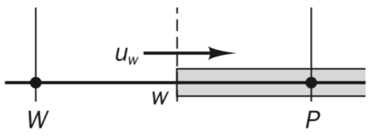
  The central differencing scheme introduces influencing at node P from the directions of all its neighbours to calculate the convective and diffusive flux. Thus, the scheme does not recognise the direction of the flow or the strength of convection relative to diffusion it does not possess the transportiveness property at high Pe.

- **Accuracy**:

  The Taylor series truncation error of the central differencing scheme is second order.

Upwinding Differencing Scheme

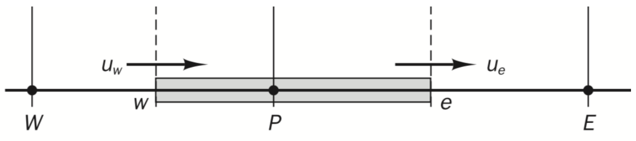
The upwind differencing scheme takes into account the flow direction when determining the value at a cell face.



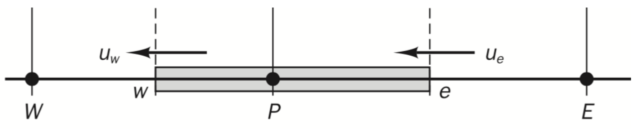
Take Home Message

The convected value of φ at a cell face is taken to be equal to the value at the upstream node.

When the flow is in the positive direction:



When the flow is in the negative direction:



- **Conservativeness**:

  The upwind differencing scheme utilises consistent expressions to calculate fluxes through cell faces.

- **Boundedness**:

  The coefficients of the discretised equation are always positive and satisfy the requirements for boundedness.

  All the coefficients are positive and the coefficient matrix is diagonally dominant, hence no "wiggles" occur in the solution.

- **Transportiveness**:

  The scheme accounts for the direction of the flow so transportiveness is built into the formulation

- **Accuracy**:

  The scheme is based on the backward differencing formula so the accuracy is only first order on the basis of the Taylor series truncation error

A major **drawback** of the scheme is that it produces erroneous results when the flow is not aligned with the grid lines: the resulting error has a diffusion like appearance and is referred to as false diffusion.

Hybrid Differencing Scheme

The hybrid differencing scheme is based on a combination of central and upwind differencing schemes.

The central differencing scheme, which is second-order accurate, is employed for small Peclet numbers and the upwind scheme, which is first-order accurate but accounts for transportiveness, is employed for large Peclet numbers.
The hybrid differencing scheme uses piecewise formulae based on the local Peclet number to evaluate the net flux through each control volume face.

The scheme is fully **conservative** and since the coefficients are always positive it is unconditionally **bounded**, satisfies the **transportiveness** requirement by using an upwind formulation for large values of Peclet number.

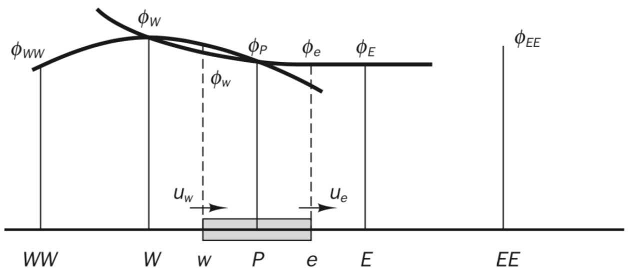
The **disadvantage** is that the **accuracy** in terms of Taylor series truncation error is only first-order, and makes it prone to diffusion errors.

QUICK Scheme

Formulations that do not take into account the flow direction are unstable and, therefore, more accurate higher-order schemes, which preserve upwinding for stability and sensitivity to the flow direction, are needed.

The quadratic upstream interpolation for convective kinetics (QUICK) scheme uses a three-point upstream-weighted quadratic interpolation for cell face values.

The face value of φ is obtained from a quadratic function passing through two bracketing nodes (on each side of the face) and a node on the upstream side:



The diffusion terms may be evaluated using the gradient of the approximating parabola.
It is interesting to note that on a uniform grid this practice gives the same expressions as central differencing for diffusion, since the slope of the chord between two points on a parabola is equal to the slope of the tangent to the parabola at its midpoint.

The scheme uses consistent quadratic profiles – the cell face values of fluxes are always calculated by quadratic interpolation between two bracketing nodes and an upstream node – and is therefore **conservative**.

Since the scheme is based on a quadratic function its **accuracy** in terms of Taylor series truncation error is third-order on a uniform mesh.

The **transportiveness** property is built into the scheme as the quadratic function is based on two upstream and one downstream nodal values. If the flow field satisfies continuity the coefficient a_P equals the sum of all neighbour coefficients, which is desirable for **boundedness**.

On the **downside**, the main coefficients (E and W) are not guaranteed to be positive and the coefficients a_{WW} and a_{EE} are negative.
This gives rise to stability problems and unbounded solutions under certain flow conditions.
The QUICK scheme is therefore conditionally stable.

Another notable feature is the fact that the discretised equations involve not only immediate neighbour nodes but also nodes further away. Tri-diagonal matrix solution methods are not directly applicable.

The resultant false diffusion is small, and solutions achieved with coarse grids are often considerably more accurate than those of the upwind or hybrid schemes.

Part IV
Pressure - velocity coupling

Steady flows

The convection of a scalar variable φ depends on the magnitude and direction of the local velocity field.
To develop our methods in the previous parts we assumed that the velocity field was somehow known.

In general the velocity field is, however, not known and emerges as part of the overall solution process along with all other flow variables.

Every velocity component appears in each momentum equation, and the velocity field must also satisfy the continuity equation.

The solution of these equations is bounded with a series of intrinsic problems:

- The convective terms of the momentum equations contain non linear quantities;
- All three equations are intricately coupled: every velocity component appears in each momentum equation and in the continuity equation.

  The most complex issue to resolve is the role-played by the pressure: it appears in both momentum equations, but there is evidently no equation for knowing the filed of pressure.

In general purpose flow computations we also wish to calculate the pressure field as part of the solution, so its gradient is not normally known.

We can separate this study into two principal cases:

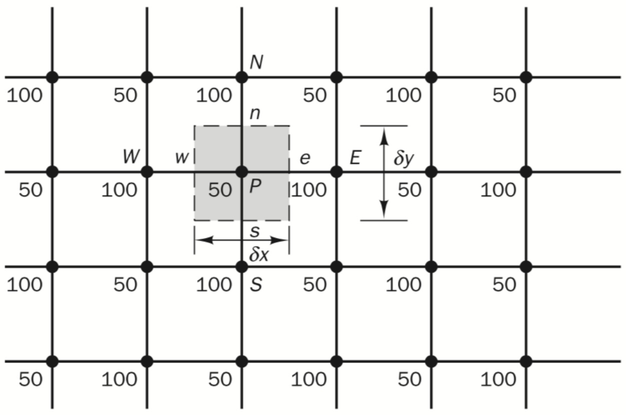
1. If the flow is **compressible** the continuity equation may be used as the transport equation for density and, in addition to momentum equations, the energy equation is the transport equation for temperature, in this way the pressure may be obtained from density and temperature by using the equation of state.
2. If the flow is **incompressible** the density is constant and hence by definition not linked to the pressure.

   In this case coupling between pressure and velocity introduces a constraint in the solution of the flow field and the pressure-velocity linkage can be resolved by adopting an iterative solution strategy such as the SIMPLE.

Staggered grid

The finite volume method starts, as always, with the discretisation of the flow domain and of the relevant transport equations.

First we need to decide where to store the velocities and it seems logical to define these at the same locations as the scalar variables such as pressure, temperature...
However, if velocities and pressures are both defined at the nodes of an ordinary control volume a highly non uniform pressure field can act like a uniform field in the discretised momentum equations.



If pressures at e and w are obtained by linear interpolation the pressure gradient terms in the u and v momentum equation are given by

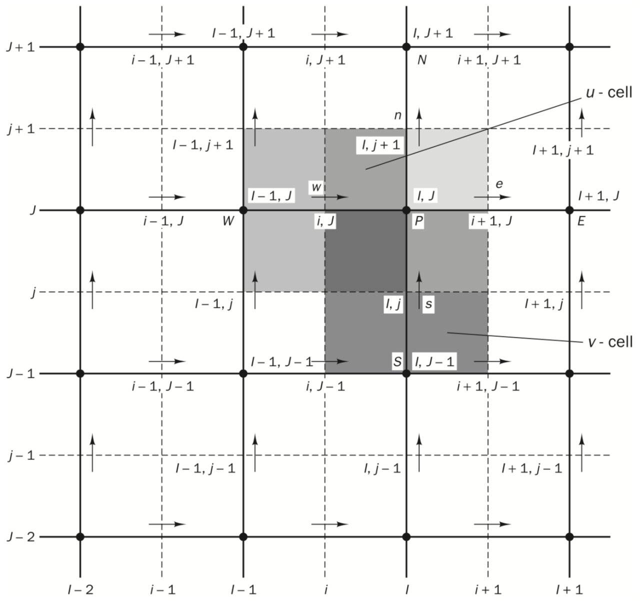
$$\frac{\partial p}{\partial x} = \frac{p_E - p_W}{2\delta x} \qquad \frac{\partial p}{\partial y} = \frac{p_N - p_S}{2\delta y}$$

Substituting the appropriate values from the obtained pressure field, we find that all the discretised gradients are zero at all the nodal points even though the pressure field exhibits spatial oscillations in both directions. As a result, this pressure field would give the same (null) momentum source in the discretised equations as a uniform pressure field: this behaviour is obviously non physical.

A remedy for this problem is to use a **staggered grid**.

Take Home Message

The idea is to evaluate scalar variables, such as pressure, density, temperature etc at ordinary nodal points but to calculate velocity components on staggered grid centered around the cell faces



The scalar variables, including pressure, are stored at the nodes marked • The velocities are defined at the (scalar) cell faces in between the nodes and are indicated by arrows: horizontal → arrows indicate the locations for u velocities and vertical ↑ ones denote those for v velocity.

In the staggered grid arrangement, the pressure nodes coincide with the cell faces of the u and v control volumes.

The pressure gradient terms are given by

$$\frac{\partial p}{\partial x} = \frac{p_P - p_W}{\delta x_u} \qquad \frac{\partial p}{\partial y} = \frac{p_P - p_S}{2\delta y_v}$$

If we consider the "chessboard" pressure field again, substitution of the appropriate nodal pressure values into these equations now yields very significant non zero pressure gradient terms.

The staggering of the velocity avoids the unrealistic behaviour of the discretised momentum equation for spatially oscillating pressures.

A further **advantage** of the staggered grid arrangement is that it generates velocities at exactly the locations where they are required for the scalar convection diffusion transport computations, hence, no interpolation is needed to calculate velocities at the scalar cell faces.

Always remembering that the values of single coefficients may be calculated with any of the differencing methods (hybrid, QUICK. . .) suitable for convection diffusion problems.

If the pressure field is correct the resulting velocity field will satisfy continuity. As the pressure field is unknown, we need a method for calculating pressure

SIMPLE algorithm

The acronym SIMPLE stands for Semi Implicit Method for Pressure Linked Equations and is essentially a guess and correct procedure for the calculation of pressure on the staggered grid arrangement.

To initiate the SIMPLE calculation process a pressure field p^* is guessed.
Discretised momentum equations are solved using the guessed pressure field to yield velocity components u^* and v^*, at this point we define the correction p' as the difference between correct pressure field p and the guessed pressure field p^* so that

$$p = p^* + p'$$

Similarly we define velocity corrections u' and u' to relate the correct velocities u and v to the guessed velocities u^* and v^*.

The pressure correction equation is susceptible to divergence unless some under relaxation is used during the iterative process:

$$p^{new} = p^* + \alpha_p p'$$

Taking α_p between 0 and 1 allows us to add to guessed field p^* a fraction of the correction field p' that is large enough to move the iterative improvement process forward, but small enough to ensure stable computations. Also the velocities are under relaxed.

A correct choice of under relaxation factors α is essential for cost effective simulations, too large value may lead to oscillatory or even divergent iterative solutions, and too small values will cause extremely slow convergence. Unfortunately, the optimum values of under relaxation factors are flow dependent and must be sought on a case by case basis.

The SIMPLE algorithm gives a method of calculating pressure and velocities.
The method is iterative, and when other scalars are coupled to the momentum equations the calculation needs to be done sequentially.

SIMPLER algorithm

The SIMPLER (SIMPLE Revised) algorithm is an improved version of SIMPLE.

In this algorithm the discretised continuity equation is used to derive a discretised equation for pressure, instead of a pressure correction equation as in SIMPLE.
Thus the intermediate pressure field is obtained directly without the use of a correction.
Velocities are, however, still obtained through the velocity corrections of SIMPLE, in this way, not using a guessed pressure, we obtain a sort of pseudo-velocities.

From the discretised momentum equations, the velocity components u^* and $v*$ are obtained.

The velocity correction equations of the SIMPLE algorithm are used in the SIMPLER algorithm to obtain corrected velocities.
Therefore, the p'-equation must also be solved to obtain the pressure corrections needed for the velocity corrections.

SIMPLEC algorithm

The SIMPLEC (SIMPLE-Consistent) algorithm follows the same steps as the SIMPLE algorithm.

The difference is that the momentum equations are manipulated so that the SIMPLEC velocity correction equations omit terms that are less significant than those in SIMPLE.

The discretised pressure correction equation is the same as in SIMPLE, except that the d-terms are calculated as above.

The sequence of operations of SIMPLEC is identical to that of SIMPLE.

PISO algorithm

The PISO algorithm, which stands for Pressure Implicit with Splitting of Operators, is a pressure-velocity calculation procedure developed originally for non iterative computation of unsteady compressible flows.

PISO involves **one** predictor step and **two** corrector steps and it can be seen as an extension of SIMPLE, with a further corrector step to enhance it.

Predictor Step
Discretised momentum equations are solved with a guessed or intermediate pressure field p^* to give velocity components $u*$ and v^* using the same method as the SIMPLE algorithm.

Corrector Step 1
The $u*$ and v^* fields will not satisfy continuity unless the pressure field p^* is correct.

The first corrector step of SIMPLE is introduced to give a velocity field (u^{**}, v^{**}) which satisfies the discretised continuity equation.

The resulting equations are the same as the velocity correction equations of SIMPLE but, since there is a further correction step in the PISO algorithm, we use a slightly different notation:

$$p^{**} = p^* + p' \qquad u^{**} = u^* + u' \qquad v^{**} = v^* + v'$$

As in the SIMPLE algorithm, these equations are substituted into the discretised continuity equation to yield pressure correction equation.
In the context of the PISO method, this pressure correction equation is called the *first* pressure correction equation and it's solved to yield the first pressure correction field p'.
Once these the pressure corrections are known, the velocity components u^{**} and v^{**} can be obtained.

Corrector Step 2
To enhance the SIMPLE procedure PISO performs a second corrector step.

A twice corrected velocity field (u^{***}, v^{***}) may be obtained by solving the momentum equations once more, using in this step the u^{**} and v^{**} velocities calculated in the previous step.

Substitution of u^{***} and v^{***} in the discretised continuity equation yields a second pressure correction equation, by solving this equation, a second pressure correction field p" is obtained, and the twice-corrected pressure field is calculated from:

$$p^{***} = \underbrace{p^{**}}_{=p^*+p'} + p" = p^* + p' + p"$$

The PISO algorithm solves the pressure correction equation twice so the method requires additional storage for calculating the source term of the second pressure correction equation.

Although this method implies a considerable increase in computational effort it has been found to be efficient and fast.

Final remarks

- The **SIMPLE** algorithm is relatively straightforward and has been successfully implemented in numerous CFD procedures.

  the pressure correction p' is satisfactory for correcting velocities but not so good for correcting pressure.

- The improved procedure **SIMPLER** uses the pressure corrections to obtain velocity corrections only.

  A separate, more effective, pressure equation is solved to yield the correct pressure field, by the way, no terms are omitted to derive the discretised pressure equation in SIMPLER, the obtained correct pressure field results in the correct velocity field.

  Consequently, the method is highly effective in calculating the pressure field correctly.

- **SIMPLEC** and **PISO** have proved to be as efficient as SIMPLER in certain types of flows, but it is not clear whether it can be categorically stated that they are better than SIMPLER.

Comparisons have shown that the performance of each algorithm depends on the flow conditions, the degree of coupling between the momentum equation and scalar equations, the amount of under relaxation used, and sometimes even on the details of the numerical technique used for solving the algebraic equations.

Part V

Solution of discretised equations

In the previous parts we have discussed methods of discretising the governing equations of fluid flow and heat transfer.

This process results in a system of linear algebraic equations which needs to be solved.

The complexity and size of the set of equations depends on:

- The dimensionality of the problem;
- The number of grid nodes;
- The discretisation practice

There are two families of solution techniques for linear algebraic equations

1. **Direct methods**: Cramer's rule matrix inversion and Gaussian elimination
2. **Iterative methods**: Jacobi and Gauss Seidel point iterative methods

The total number of operations cannot be predicted in advance, and it is not possible to guarantee convergence unless the system of equations satisfies some defined criteria.

- The **TDMA** is a direct method for 1 D situations, but it can be applied iteratively to solve multi dimensional problems.

  TDMA is computationally inexpensive and has the advantage that it requires a minimum amount of storage.
- The **Jacobi** and **Gauss Seidel** methods are general purpose point iterative algorithms that are easily implementable, but their convergence rate can be slow when the system of equations is large.
- More recently **multigrid** acceleration techniques have improved the convergence rates of iterative solvers to such an extent that they are now the method of choice in commercial CFD codes.

Thomas algorithm (TDMA)

Consider a system of equations that has a tri-diagonal form, the general form of **any** single equation is:

$$-\beta_j \phi_{j-1} + D_J \phi_j - \alpha_j \phi_{j+1} = C_j$$

And it can be rewritten as

$$\phi_j = \frac{\alpha_j}{D_J}\phi_{j+1} + \frac{\beta_j}{D_j}\phi_{j-1} + \frac{C_j}{D_j}$$

These equations can be solved by **forward elimination** and **back substitution**.

This process starts by eliminating of the ϕ_{j-1} value in the ϕ_{j+1} formula by substituting this value with the ϕ_j formula previously obtained.

$$\phi_2 = \frac{\alpha_2}{D_2}\phi_3 + \frac{\beta_2}{D_2}\phi_1 + \frac{C_2}{D_2}$$

$$\phi_3 = \frac{\alpha_3}{D_3}\phi_4 + \frac{\beta_3}{D_3}\phi_2 + \frac{C_3}{D_3}$$

$$\phi_4 = \frac{\alpha_4}{D_4}\phi_5 + \frac{\beta_4}{D_4}\phi_3 + \frac{C_4}{D_4}$$

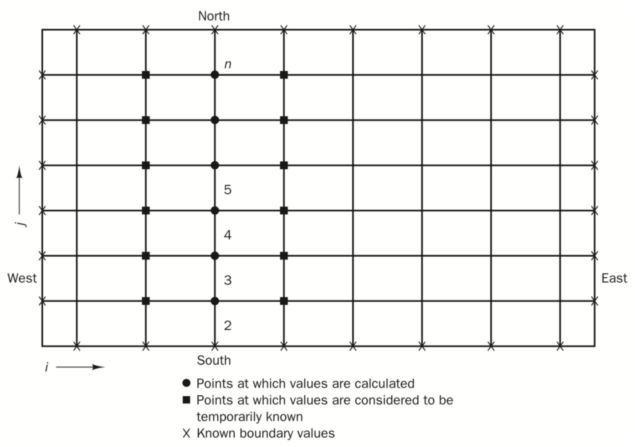
$$\vdots$$

$$\phi_n = \frac{\alpha_n}{D_n}\phi_{n+1} + \frac{\beta_n}{D_n}\phi_{n-1} + \frac{C_n}{D_n}$$

In the above derivation of the TDMA we assumed that boundary values ϕ_1 and ϕ_{n+1} were given.

Thomas algorithm 2D

The TDMA can be applied iteratively to solve a system of equations for two dimensional problems.


North
n
5
4
3
2
j
West
East
South
i
● Points at which values are calculated
■ Points at which values are considered to be temporarily known
X Known boundary values

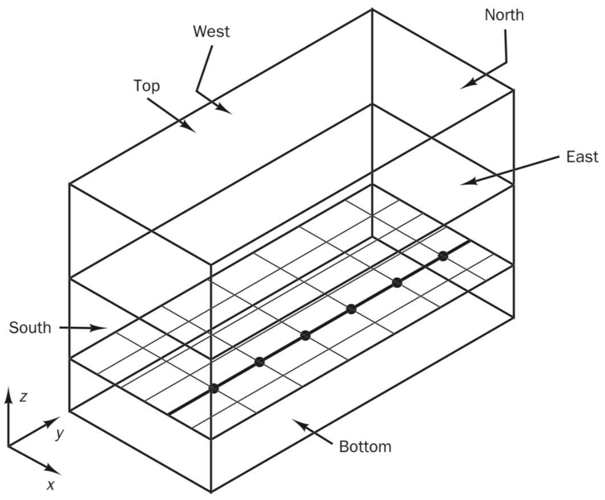
To solve the system, the TDMA is applied along chosen path, e. g. north south (n-s) lines.
Subsequently the calculation is moved to the next north south line.

The sequence in which lines are moved is known as the **sweep direction**.
If we sweep from west to east the values of ϕ_W to the west of a point P are known from the calculations made on the previous line.
Values of ϕ_E to its east, however, are unknown so the solution process must be iterative.
At each iteration cycle ϕ_E is taken to have its value at the end of the previous iteration or a given initial/guessed value at the first iteration.

The line by line calculation procedure is repeated several times until a converged solution is obtained.

Thomas algorithm 3D

For three dimensional problems the TDMA is applied line by line on a selected plane and then the calculation is moved to the next plane, scanning the domain plane by plane.



In two and three dimensional computations the convergence can often be accelerated by alternating the sweep direction so that all boundary information is fed into the calculation more effectively, sweeping from upstream to downstream along the flow direction produces faster convergence than sweeping against the flow or parallel to the flow direction.

The TDMA algorithm may cause problems in unsteady flow calculations because can only be applied by incorporating several neighbouring contributions in the source term.

A generalised version of the TDMA, known as the penta diagonal matrix algorithm, is available Basically a sequence of operations is carried out on the original matrix to reduce it to upper triangular form, and subsequently the back substitution is performed to obtain the solution.

Point-iterative methods

Point iterative techniques consists to isolate the unknown value in the respective equation en substitute the remaining unknowns with some guessed initial values.
After obtaining the first solution, this is substitute in place of the last guessed initial values.
This process is repeated until there is no more change in the solution.

One condition for the iteration process to be convergent is that the matrix must be diagonally dominant When general systems of equations are solved it is sometimes necessary to rearrange the equations, but the finite volume method yields diagonally dominant systems as part of the discretisation process, so this aspect does not require special attention.

Jacobi Method

In the Jacobi method, the unknown values at the k iteration $(x_1^k \dots n_n^k)$ in the LHS are evaluated by substituting in the RHS the last known values at the previous iteration $k-1$.

To generalize, a $n \times n$ system of equation can be written as

$$\sum_{j=1}^{n} a_{ij} x_j = b_i$$

The single equation who leds a solution can be written as

$$a_{ii}x_i = b_i - \sum_{j=1}^{n} a_{ij}x_j$$

By introducing the iterations, the Jacobi method consists in:

$$x_i^k = \sum_{j=1}^{n} \left(\frac{-a_{ij}}{a_{ii}} \right) x_j^{k-1} + \frac{b_i}{a_{ii}}$$

In matrix form:

$$X^k = T \cdot X^{k-1} + C$$

Where the iteration matrix is

$$T = T_{ij} = \begin{cases} -\dfrac{a_{ij}}{a_i i} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

Gauss - Seidel Method

In the Jacobi method the right hand side is evaluated using the results of the previous iteration level or from the initial guess.
If all the right hand sides could be evaluated simultaneously there would be no further discussion, **but in most computing machines the calculations are performed sequentially**.

Take Home Message

The Gauss Seidel method proceeds by making direct use of the recently available solution value and calculates by this, the next.

$$x_i^k = \sum_{j=1}^{n} \left(\frac{-a_{ij}}{a_{ii}} \right) x_j^k \qquad \underbrace{+ \sum_{j=1}^{n} \left(\frac{-a_{ij}}{a_{ii}} \right) x_j^{k-1} + \frac{b_i}{a_{ii}}}_{\text{solution obtained by the previous iteration}}$$

The convergence rate of the Jacobi and Gauss Seidel methods depends on the properties of the iteration matrix. It has been found that these can be improved by the introduction of a so called relaxation parameter α.
When we choose $0 < \alpha < 1$ the procedure is an under relaxation method, whereas $\alpha > 1$ is called over relaxation.
The introduction of the relaxation parameter α changes the iteration path without changing the final solution.

We define the residual r_i^k of the i^{th} equation after k iterations as the difference:

$$r_i^k = b_i - \sum_{j=1}^{n} a_{ij}x_j^k$$

As the iteration process is convergent the intermediate solution vector x_j^k should get progressively closer to final solution vector $x_j^{k\to\infty}$, at the same time, the $r_i^k \underset{k\to\infty}{\to} 0$.
The relaxation may be advantageous if we select an optimum value of α that minimises the number of iterations required to reach the converged solution.
Unfortunately, the optimum value of the relaxation parameter is problem and mesh dependent, and it is difficult to give precise guidance.

Multigrid methods

The convergence rate of iterative methods such as the Jacobi and Gauss Seidel, rapidly reduces as the mesh is refined.

The concept of residual already introduced can be used to obtain a measure of the closeness to the true solution of an intermediate solution in an iteration sequence.

The average residual $\bar{r}$ over all n equations in the system is a useful indicator of iterative convergence for a given problem

$$\bar{r} = \frac{1}{n} \sum_{i=1}^{n} |r_i|$$

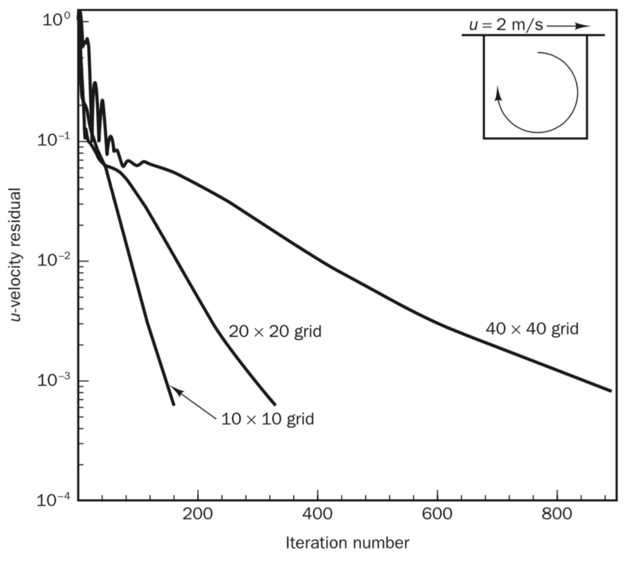
If the iteration process is convergent the average residual $\bar{r} \to 0$.

The average residual for a given solution parameter, is usually normalised to make it easier to interpret its value from case to case and to compare it with residuals relating to other solution parameters.
The most common normalisation is to consider the ratio of the average residual after k iterations and its value at the first iteration

$$R^k_{norm} = \frac{\bar{r}^k}{\bar{r}^1}$$

As we said, within the CFD code it is possible to improve the convergence rate by adjusting solution parameters, including relaxation parameters, but for the sake of consistency all solution parameters were kept constant in this case.

The pattern of residual reduction is evident from the diagram After a rapid initial reduction of the residuals their rate of decrease settles to a more modest final value



It is also clear that the final convergence rate is lowest for the finest mesh. If we tried an even finer mesh, it would take even longer to converge.

It has been established that the solution error has components with a range of wavelengths that are multiples of the mesh size. Iteration methods cause rapid reduction of error components with short wavelengths up to a few multiples of the mesh size.
However, long wavelength components of the error tend to decay very slowly as the iteration count increases.

In figure can be seen that for the coarse mesh, the longest possible wavelengths of error components (those of the order of the domain size) are just within the short wavelength range of the mesh and all error components reduce rapidly. On the finer meshes, however, the longest error wavelengths are progressively further outside the short wavelength range for which decay is rapid.

Multigrid methods are designed to exploit these inherent differences of the error behaviour and use iterations on meshes of different size.

The short wavelength errors are effectively reduced on the finest meshes, whereas the long wavelength errors decrease rapidly on the coarsest meshes. Moreover, the computational cost of iterations is larger on finer meshes than on coarse meshes, so the extra cost due to iterations on the coarse meshes is offset by the benefit of much improved convergence rate.

Multigrid procedure

1. **Fine grid iterations**

   Perform iterations on the finest grid with mesh spacing h to generate an intermediate solution Y^h.

   The number of iterations is chosen sufficiently large that the short wavelength oscillatory component of the error is effectively reduced, but no attempt is made to eliminate the long wavelength error component.

   The residual vector R^h for the solution on this mesh satisfies

   $$R^h = B - A^h \cdot Y^h$$

   And the error vector E^h is given by

   $$E^h = X - Y^h$$

   We have also established that the error and residual are related as follows

   $$A^h \cdot E^h = R^h$$

2. **Restriction**

   The solution is transferred from the fine mesh with spacing h onto a coarse mesh with spacing ch where $c > 1$.

   Due to the larger mesh spacing of the coarse mesh the long wavelength error (on the fine mesh) appears as a short wavelength error on the new mesh and will reduce rapidly.

3. **Prolongation**

   After obtaining the converged solution of error vector E^{ch} for the coarse mesh we need to transfer it back to the fine mesh but note that we have fewer data than points in the fine mesh.

   We use a convenient interpolation operator to generate values for the prolonged error vector $E^{'h}$ at intermediate points in the fine mesh.

4. **Correction & final iterations**

   Once we have calculated the prolonged error vector $E^{'h}$ we may correct the intermediate fine grid solution

   $$Y^{impro} = Y^h + E^{'h}$$

   Because the long wavelength error has been eliminated, this improved solution is closer to the true solution vector.

   However, several approximations were made, so we perform a few more iterations with the improved solution to iron out any errors that may have been introduced during restriction and prolongation.

Part VI

Finite volume method - Unsteady flows

The conservation law for the transport of a scalar in an unsteady flow has the general form:

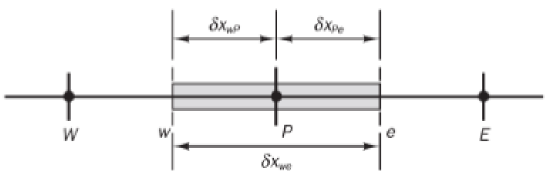
$$\frac{\partial}{\partial t}(\rho\phi) + \nabla \cdot (\rho \mathbf{u} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S_\phi$$

The first term of the equation represents the rate of change term and is zero for steady flows to predict transient problems we must retain this term in the discretisation process.
The finite volume integration of this equation over a control volume must be augmented with a further integration over a finite time step Δt.

The control volume integration is essentially the same as in steady flows and the same measures are again adopted to ensure successful treatment of convection, diffusion and source terms Here we focus our attention on methods necessary for the time integration.

1-Dimension flows

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + S$$



If the temperature at a node is assumed to prevail over the whole control volume, the LHS can be written as - using a first order (backward) differencing scheme:

$$\int_{CV} \left[\int_t^{t+\Delta t} \rho c \frac{\partial T}{\partial t} \right] dV = \rho c (T_P - T_P^0) \Delta V$$

Applying central differencing scheme to the RHS

$$\int_t^{t+\Delta t} \left[\left(k_e A \frac{T_E - T_P}{\delta x_{PE}} \right) - \left(k_w A \frac{T_P - T_W}{\delta x_{WP}} \right) \right] dt + \int_t^{t+\Delta t} \bar{S} dV dt$$

To evaluate the right hand side of this equation we need to make an assumption about the variation of $T_P T_E$ and T_W with time.
We may generalise the approach by means of a weighting parameter ϑ between 0 and 1 and write the integral I_T of temperature T_P with respect to time as:

$$I_T = \int_t^{t+\Delta t} T_P dt = [\vartheta T_P + (1 + \vartheta) T_P^0] \Delta t$$

We have highlighted the following values of integral I_T

- If $\vartheta = 0$ the temperature at old time level t is used and the resulting scheme is called **explicit**;
- If $0 < \vartheta \leq 1$ temperatures at the new time level are used on both sides of the equation and the resulting schemes are called **implicit**;

- If $\vartheta = 1$ the temperature at new time level $t + \Delta t$ is used and the scheme if **fully implicit**;
- If $\vartheta = \frac{1}{2}$ the temperatures at t and $t+\Delta t$ are equally weighted and the scheme is called **Crank-Nicolson** scheme.

So the exact form of the final discretised equation depends on the value of ϑ

$$\boxed{\begin{aligned} a_P T_P = {} & a_W[\theta T_W + (1-\theta)T_W^o] + a_E[\theta T_E + (1-\theta)T_E^o] \\ & + [a_P^o - (1-\theta)a_W - (1-\theta)a_E]T_P^o + b \end{aligned}}$$

The substitution of $\vartheta = 0$ gives the **explicit** discretisation of the unsteady conductive heat transfer equation:

$$\boxed{a_P T_P = a_W T_W^o + a_E T_E^o + [a_P^o - (a_W + a_E - S_P)]T_P^o + S_u}$$

where

$$\boxed{a_P = a_P^o}$$

and

$$\boxed{a_P^o = \rho c \frac{\Delta x}{\Delta t}}$$

a_W	a_E
$\dfrac{k_w}{\delta x_{WP}}$	$\dfrac{k_e}{\delta x_{PE}}$

For boundedness requirements, all coefficients need to be positive in the discretised equation.
For the coefficient of T_P^0 to be positive we must have $a_P^0 - a_w - a_e > 0$, which for constant k and uniform grid spacing ($\delta x = \Delta x$) can be written as

$$\Delta t < \rho c \frac{\Delta x^2}{2k}$$

This inequality sets a stringent maximum limit to the time step size and represents a serious limitation for the explicit scheme It becomes very expensive to improve spatial accuracy because the maximum possible time step needs to be reduced as the square of Δx Consequently, this method is not recommended for general transient problems.

Using instead the **Crank Nicolson** scheme leads to:

$$\Delta t < \rho c \frac{\Delta x^2}{k}$$

This time step limitation is only slightly less restrictive than that of the explicit method.
The Crank Nicolson method is based on central differencing and hence it is second order accurate in time.

With **fully implicit** scheme both sides of the equation contain temperatures at the new time step, and a system of algebraic equations must be solved at each time level.
It can be seen that all coefficients are positive, which makes the implicit scheme unconditionally stable for any size of time step.
Since the accuracy of the scheme is only first order in time, small time steps are needed to ensure the accuracy of results.
The implicit method is recommended for general purpose transient calculations because of its robustness and unconditional stability.

The extension to unsteady 2D and 3D diffusion problems is made by quoting the fully implicit method due to its superior stability.

Transient SIMPLE

Algorithms such as SIMPLE, for the calculation of steady flows, may be extended to transient calculations. The discretised momentum equations will now include transient terms formulated with the procedure described until now. An additional term is also required in the pressure correction equation.

The pressure correction equation is derived from the continuity equation and should therefore contain terms representing its transient behaviour.

In transient flow calculations with the implicit formulation, the iterative procedures described for steady state calculations employing SIMPLE, SIMPLER or SIMPLEC are applied at each time level until convergence is achieved.

Transient PISO

The PISO algorithm is a non iterative calculation procedure in its transient version all time dependent terms are retained in the momentum and continuity equations: the basic equations and steps involved in the transient version of the PISO algorithm are the same as those for steady state version.

Its shows that the temporal accuracy achieved by the predictor corrector process for pressure and momentum is third order (Δt^3) and fourth order (Δt^4) respectively.

Therefore, the pressure and velocity fields obtained at the end of the PISO process with a suitably small time step are considered to be accurate enough to proceed to the next time step immediately.
Since the algorithm relies on the higher order temporal accuracy gained by the splitting technique, small time steps are recommended to ensure accurate results.

Since the PISO method does not require iterations within a time level it is less expensive than the implicit SIMPLE algorithm.

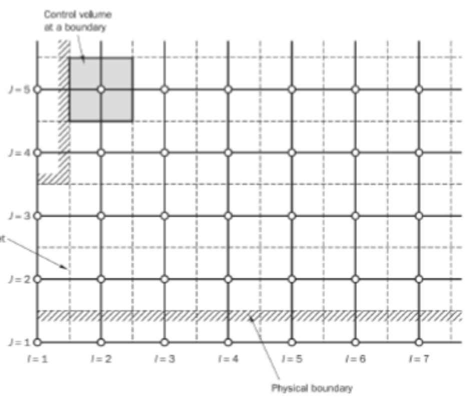
Part VII
Boundary conditions

All CFD problems are defined in terms of initial and boundary conditions It is important that the user specifies these correctly and understands their role in the numerical algorithm.
In transient problems the initial values of all the flow variables need to be specified at all solution points in the flow domain.

The most commons boundary conditions are:

- Inlet;
- Outlet;
- Wall;
- Prescribed pressure;
- Symmetry.

In constructing a staggered grid arrangement, we set up additional nodes surrounding the physical boundary:



The calculations are performed at internal nodes only.

Two notable features of the arrangement are

1. The physical boundaries coincide with scalar control volume boundaries;
2. The nodes just outside the inlet of the domain are available to store the inlet conditions.

We make the following assumptions (i) the flow is always subsonic,(ii) k-ε turbulence modelling is used (iii) the hybrid differencing method is used for discretisation and (iv) the SIMPLE solution algorithm is applied.

Inlet

The distribution of all flow variables needs to be specified at inlet boundaries.
As mentioned, the grid extends outside the physical boundary and the nodes along the line are used to store the inlet values of flow variables; just downstream of this extra node we start to solve the discretised equation for the first internal cell.

Since the velocity is known at inlet, it is also not necessary to make a velocity correction here.

Reference pressure
The pressure field obtained by solving the pressure correction equation does not give absolute pressures, so its common practice to fix the absolute pressure at one inlet node and set the pressure correction to zero at that node, once having specified a reference value, the absolute pressure field inside the domain can now be obtained.

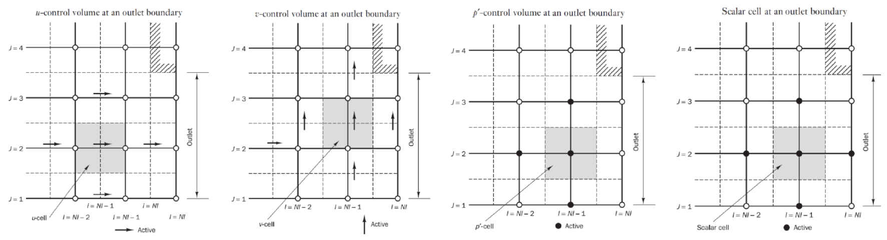
Estimation of k & ε
The most accurate simulations can only be achieved by supplying measured inlet values of turbulent kinetic energy k and dissipation rate ε However, such data are often not available in this case commercial CFD codes often estimate k and ε with approximate formulae based on a turbulence intensity.

Outlet

If the location of the outlet is selected far away from geometrical disturbances the flow eventually reaches a fully developed state where no change occurs in the flow direction.
In such a region we can place an outlet surface and state that the gradients of all variables (except pressure) are zero in the flow direction.
It is normally possible to make a reasonably accurate prediction of the flow direction far away from obstacles.

Figures show grid arrangements near such an outlet boundary. The last cells upstream of the outlet, for which a discretised equation is solved, have been shaded and, as before, active neighbours and faces have been highlighted.

This gives us the opportunity to locate the outlet surface perpendicular to the flow direction and take gradients in the direction normal to the outlet surface equal to zero.


u-control volume at an outlet boundary
v-control volume at an outlet boundary
p'-control volume at an outlet boundary
Scalar cell at an outlet boundary
J = 4
J = 3
J = 2
J = 1
Outlet
u-cell
v-cell
p'-cell
Scalar cell
I = NI − 2
I = NI − 1
I = NI
i = NI − 1
i = NI
Active

If NI is the total number of nodes in the x direction, equations are solved for cells up to I (or i) $=$ NI-1
Before the relevant equations are solved the values of flow variables at the next node NI just outside the domain, are determined by extrapolation from the interior on the assumption of zero gradient at the outlet plane.
For the v and scalar equations this implies setting $v_{NI} = v_{NI-1}, \varphi_{NI} = \varphi_{NI-1}$
Special care should be taken in the case of the u velocity: during the iteration cycles of the SIMPLE algorithm there is no guarantee that these velocities will conserve mass over the computational domain; to ensure that overall continuity is satisfied the total mass flux going out of the domain M_{out} is first computed by summing all the extrapolated outlet velocities.

To make the mass flux out equal to the mass flux M_{in} coming into the domain all the outlet velocity components u_{NI} are multiplied by the ratio $\dfrac{M_{in}}{M_{out}}$

$$u_{NI,f} = u_{NI-1,f} \times \frac{M_{in}}{M_{out}}$$

These values are subsequently used as the east neighbor velocities in the discretised momentum equations for u_{NI-1}

Wall

The wall is the most common boundary encountered in confined fluid flow problems.

The no slip condition $u = v = 0$ is the appropriate condition for the velocity components at solid walls.

The normal component of the velocity can simply be set to zero at the boundary and the discretised momentum equation at the next v cell in the flow can be evaluated without modification.

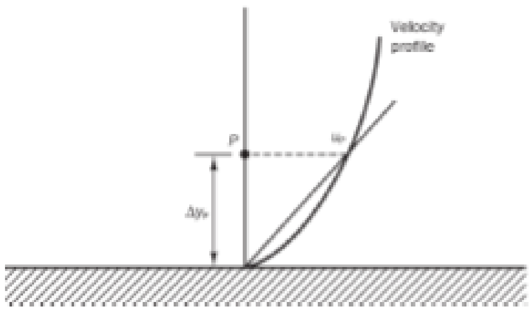
We already studied the multi layered structure of the near wall turbulent boundary layer: immediately adjacent to the wall we have an extremely thin viscous sub layer followed by the buffer layer and the turbulent core, the number of mesh points required to resolve all the details on this turbulent boundary layer would be prohibitively large, and normally we employ 'wall functions' to represent the effect of the wall boundaries.

By the evaluation of y^+ it can be possible to place the changeover from laminar to turbulent near wall flow in the buffer layer between the linear and log law regions of a turbulent wall layer.

The wall conditions for laminar flow or linear sub layer apply in two cases:

1. For solutions of laminar flow equations

2. For solutions of turbulent flow equations when $y^+ \leq 11.63$



In both cases the near wall flow is taken to be laminar it is assumed that the velocity varies linearly with distance from the wall in a laminar flow.

When $y^+ > 11.63$ node P is considered to be in the log law region of a turbulent boundary layer, in this region wall function formulae associated with the log law are used to calculate shear stress, heat flux and other variables.

Moving walls
Wall movement in the x direction is felt by the fluid by a change in the wall shear stress: its value is adjusted by replacing the absolute velocity by the relative velocity.

Constant Pressure

The constant pressure condition is used in situations where exact details of the flow distribution are unknown but the boundary values of pressure are known.

A convenient way of dealing with a constant pressure boundary condition is to fix pressure at the nodes just inside the physical boundary.

The main problem is the unknown flow direction, which is governed by the conditions inside the calculation domain

Symmetry

The conditions at a symmetry boundary are i no flow across the boundary and no scalar flux across the boundary.

In the implementation, normal velocities are set to zero at a symmetry boundary, and the values of all other properties just outside the solution domain are equated to their values at the nearest node just inside the domain.

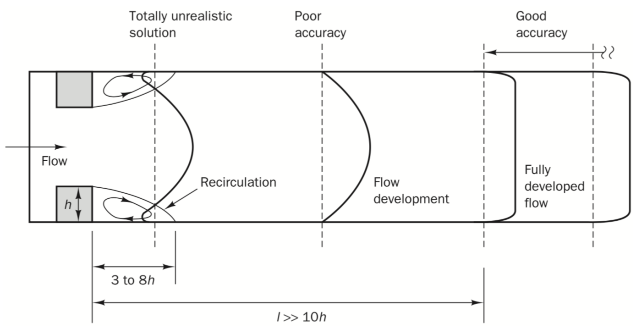
Final remarks

Flows inside a CFD solution domain are driven by the boundary conditions. In a certain way the process of solving a fluid flow problem is nothing more than the extrapolation of a set of data defined on a boundary contour or surface into the domain interior.
It is, therefore, of paramount importance that we supply physically realistic, well posed boundary conditions, otherwise severe difficulties are encountered in obtaining solutions.

Particular care must be taken in applying the outlet boundary condition: physically the exit pressures govern the flow split between multiple outlets so it is better to specify this quantity at exits than (zero gradient) outlet conditions.

It is **not permitted** to combine an outlet condition with one or more constant pressure boundaries, because the zero gradient outlet condition specifies neither the flow rate nor the pressure at the exit, thus leaving the problem under specified.

If outlet boundaries are placed too close to solid obstacles it is possible that the flow has not yet reached a fully developed state (zero gradients in the flow direction), which may lead to errors.



It is imperative that the outlet boundary is placed much further downstream than 10 heights of the last obstacle to give accurate results.

For high accuracy it is necessary to demonstrate that the interior solution is unaffected by the choice of location of the outlet by means of a sensitivity study for the effect of different downstream distances.