

Lecture 5 - Solution Methods

Applied Computational Fluid Dynamics

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Solution methods

- Focus on finite volume method.
- Background of finite volume method.
- Discretization example.
- General solution method.
- Convergence.
- Accuracy and numerical diffusion.
- Pressure velocity coupling.
- Segregated versus coupled solver methods.
- Multigrid solver.
- Summary.

Overview of numerical methods

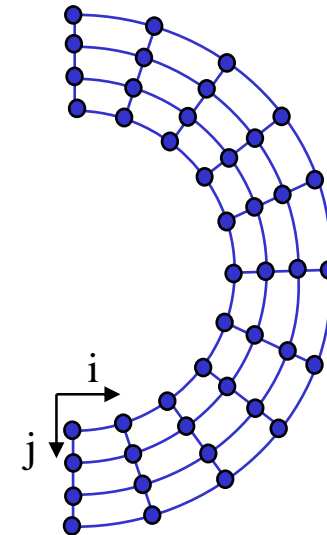
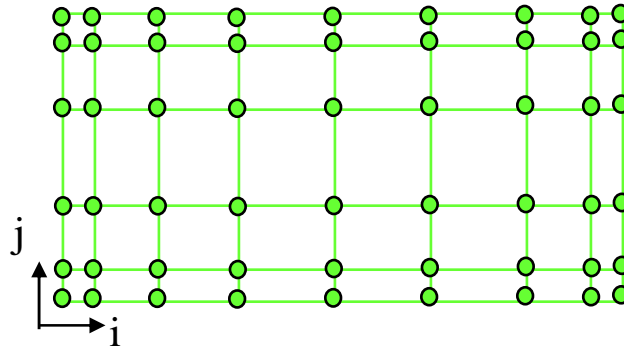
- Many CFD techniques exist.
- The most common in commercially available CFD programs are:
 - The finite volume method has the broadest applicability (~80%).
 - Finite element (~15%).
- Here we will focus on the finite volume method.
- There are certainly many other approaches (5%), including:
 - Finite difference.
 - Finite element.
 - Spectral methods.
 - Boundary element.
 - Vorticity based methods.
 - Lattice gas/lattice Boltzmann.
 - And more!

Finite difference method (FDM)

- Historically, the oldest of the three.
- Techniques published as early as 1910 by L. F. Richardson.
- Seminal paper by Courant, Fredrichson and Lewy (1928) derived stability criteria for explicit time stepping.
- First ever numerical solution: flow over a circular cylinder by Thom (1933).
- Scientific American article by Harlow and Fromm (1965) clearly and publicly expresses the idea of “computer experiments” for the first time and CFD is born!!
- Advantage: easy to implement.
- Disadvantages: restricted to simple grids and does not conserve momentum, energy, and mass on coarse grids.

Finite difference: basic methodology

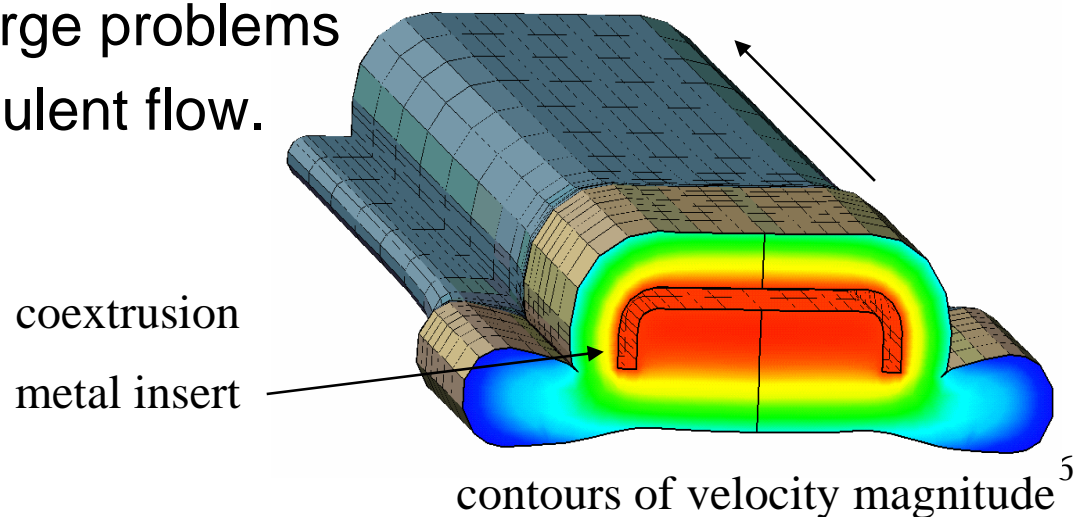
- The domain is discretized into a series of grid points.
- A “structured” (ijk) mesh is required.



- The governing equations (in differential form) are discretized (converted to algebraic form).
- First and second derivatives are approximated by truncated Taylor series expansions.
- The resulting set of linear algebraic equations is solved either iteratively or simultaneously.

Finite element method (FEM)

- Earliest use was by Courant (1943) for solving a torsion problem.
- Clough (1960) gave the method its name.
- Method was refined greatly in the 60's and 70's, mostly for analyzing structural mechanics problem.
- FEM analysis of fluid flow was developed in the mid- to late 70's.
- Advantages: highest accuracy on coarse grids. Excellent for diffusion dominated problems (viscous flow) and viscous, free surface problems.
- Disadvantages: slow for large problems and not well suited for turbulent flow.

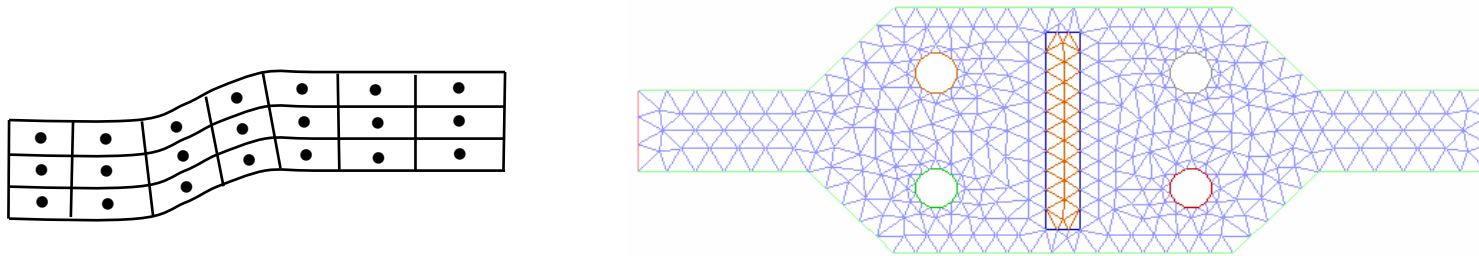


Finite volume method (FVM)

- First well-documented use was by Evans and Harlow (1957) at Los Alamos and Gentry, Martin and Daley (1966).
- Was attractive because while variables may not be continuously differentiable across shocks and other discontinuities mass, momentum and energy are always conserved.
- FVM enjoys an advantage in memory use and speed for very large problems, higher speed flows, turbulent flows, and source term dominated flows (like combustion).
- Late 70's, early 80's saw development of body-fitted grids. By early 90's, unstructured grid methods had appeared.
- Advantages: basic FV control volume balance does not limit cell shape; mass, momentum, energy conserved even on coarse grids; efficient, iterative solvers well developed.
- Disadvantages: false diffusion when simple numerics are used.

Finite volume: basic methodology

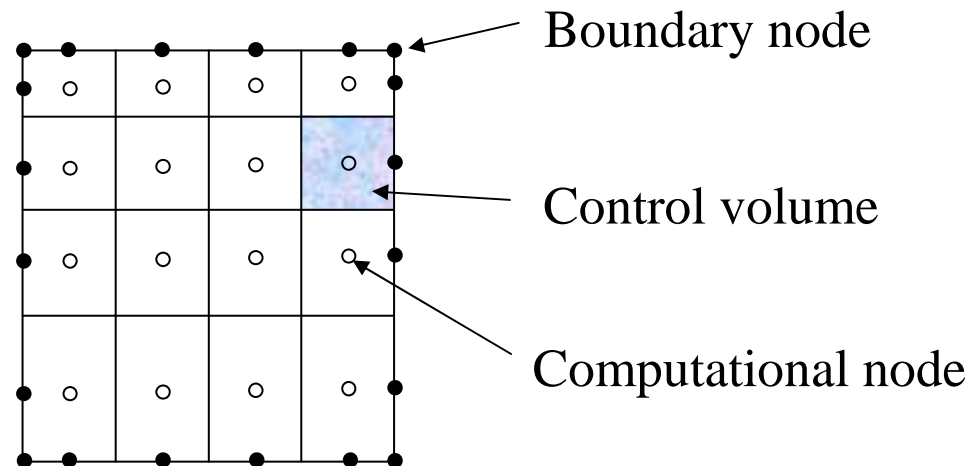
- Divide the domain into control volumes.



- Integrate the differential equation over the control volume and apply the divergence theorem.
- To evaluate derivative terms, values at the control volume faces are needed: have to make an assumption about how the value varies.
- Result is a set of linear algebraic equations: one for each control volume.
- Solve iteratively or simultaneously.

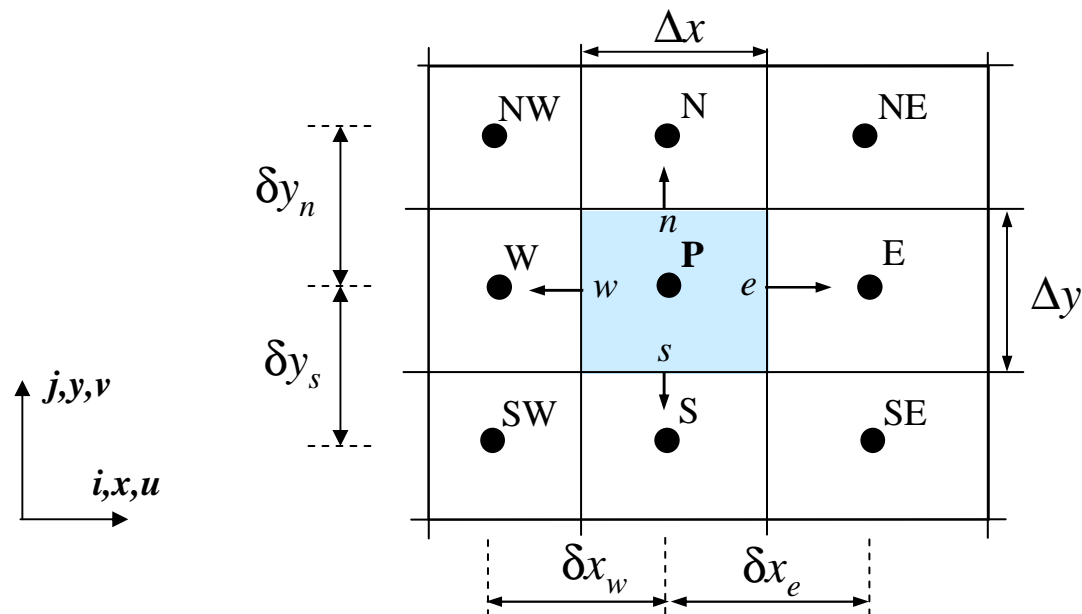
Cells and nodes

- Using finite volume method, the solution domain is subdivided into a finite number of small control volumes (cells) by a grid.
- The grid defines the boundaries of the control volumes while the computational node lies at the center of the control volume.
- The advantage of FVM is that the integral conservation is satisfied exactly over the control volume.



Typical control volume

- The net flux through the control volume boundary is the sum of integrals over the four control volume faces (six in 3D). The control volumes do not overlap.
- The value of the integrand is not available at the control volume faces and is determined by interpolation.

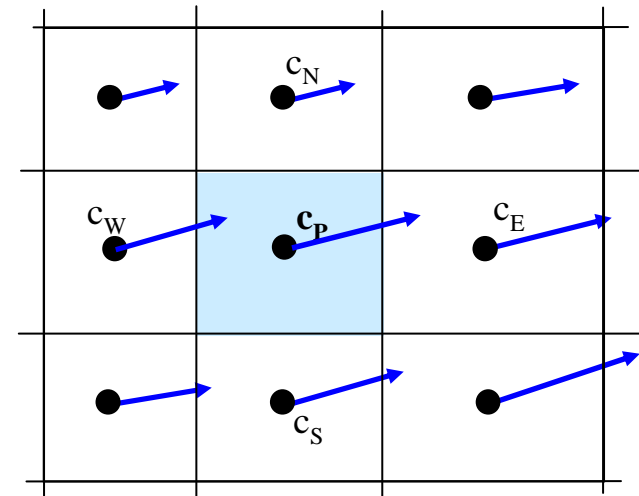


Discretization example

- To illustrate how the conservation equations used in CFD can be discretized we will look at an example involving the transport of a chemical species in a flow field.
- The species transport equation (constant density, incompressible flow) is given by:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i} (u_i c) = \frac{\partial}{\partial x_i} \left(\mathbf{D} \frac{\partial c}{\partial x_i} \right) + S$$

- Here c is the concentration of the chemical species and \mathbf{D} is the diffusion coefficient. S is a source term.
- We will discretize this equation (convert it to a solveable algebraic form) for the simple flow field shown on the right, assuming steady state conditions.



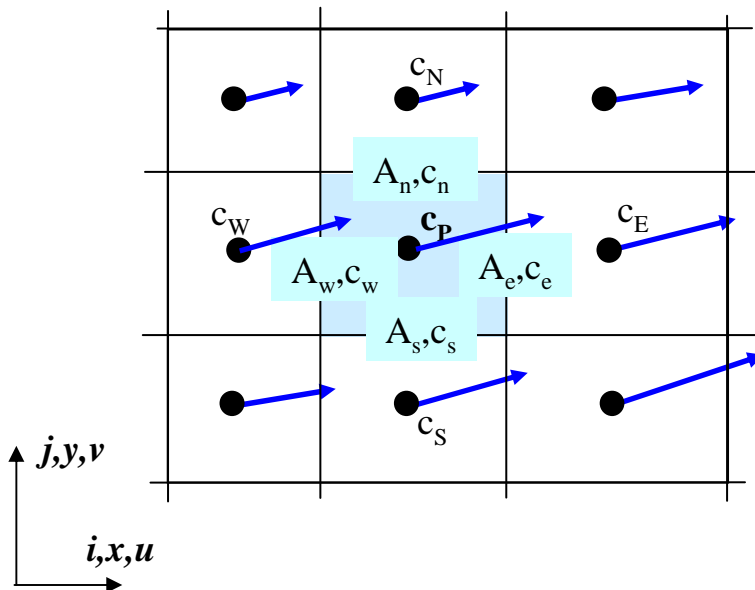
Discretization example - continued

- The balance over the control volume is given by:

$$A_e u_e c_e - A_w u_w c_w + A_n v_n c_n - A_s v_s c_s =$$

$$\mathbf{D}A_e \left. \frac{dc}{dx} \right|_e - \mathbf{D}A_w \left. \frac{dc}{dx} \right|_w + \mathbf{D}A_n \left. \frac{dc}{dy} \right|_n - \mathbf{D}A_s \left. \frac{dc}{dy} \right|_s + S_p$$

- This contains values at the faces, which need to be determined from interpolation from the values at the cell centers.



Notation

A_w, A_n, A_e, A_s : areas of the faces

c_w, c_n, c_e, c_s : concentrations at the faces

c_w, c_n, c_e, c_s : concentrations at the cell centers

$u_w, u_n, u_e, u_s, v_w, v_n, v_e, v_s$: velocities at the faces

$u_w, u_n, u_e, u_s, v_w, v_n, v_e, v_s$: velocities at the cell centers

S_p : source in cell P

\mathbf{D} : diffusion coefficient

Discretization example - continued

- The simplest way to determine the values at the faces is by using first order upwind differencing. Here, let's assume that the value at the face is equal to the value in the center of the cell upstream of the face. Using that method results in:

$$A_e u_P c_P - A_w u_W c_W + A_n v_P c_P - A_s v_S c_S = \mathbf{D}A_e (c_E - c_P) / \delta x_e \\ - \mathbf{D}A_w (c_P - c_W) / \delta x_w + \mathbf{D}A_n (c_N - c_P) / \delta y_n - \mathbf{D}A_s (c_P - c_S) / \delta y_s + S_P$$

- This equation can then be rearranged to provide an expression for the concentration at the center of cell P as a function of the concentrations in the surrounding cells, the flow field, and the grid.

Discretization example - continued

- Rearranging the previous equation results in:

$$c_P(A_n v_P + A_e u_P + \mathbf{D}A_w / \delta x_w + \mathbf{D}A_n / \delta y_p + \mathbf{D}A_e / \delta x_e + \mathbf{D}A_s / \delta y_s) = c_W(A_w u_W + \mathbf{D}A_w / \delta x_w) + c_N(\mathbf{D}A_n / \delta y_n) + c_E(\mathbf{D}A_e / \delta x_e) + c_S(A_s v_S + \mathbf{D}A_s / \delta y_s) + S_P$$

- This equation can now be simplified to:

$$\begin{aligned} a_P c_P &= a_W c_W + a_N c_N + a_E c_E + a_S c_S + b \\ &= \sum_{nb} a_{nb} c_{nb} + b \end{aligned}$$

- Here nb refers to the neighboring cells. The coefficients a_{nb} and b will be different for every cell in the domain at every iteration. The species concentration field can be calculated by recalculating c_P from this equation iteratively for all cells in the domain.

General approach

- In the previous example we saw how the species transport equation could be discretized as a linear equation that can be solved iteratively for all cells in the domain.
- This is the general approach to solving partial differential equations used in CFD. It is done for all conserved variables (momentum, species, energy, etc.).
- For the conservation equation for variable ϕ , the following steps are taken:
 - Integration of conservation equation in each cell.
 - Calculation of face values in terms of cell-centered values.
 - Collection of like terms.
- The result is the following discretization equation (with nb denoting cell neighbors of cell P):

$$a_P \phi_P = \sum_{nb} a_{nb} \phi_{nb} + b$$

General approach - relaxation

- At each iteration, at each cell, a new value for variable ϕ in cell P can then be calculated from that equation.
- It is common to apply relaxation as follows:

$$\phi_P^{new, used} = \phi_P^{old} + U(\phi_P^{new, predicted} - \phi_P^{old})$$

- Here U is the relaxation factor:
 - $U < 1$ is underrelaxation. This may slow down speed of convergence but increases the stability of the calculation, i.e. it decreases the possibility of divergence or oscillations in the solutions.
 - $U = 1$ corresponds to no relaxation. One uses the predicted value of the variable.
 - $U > 1$ is overrelaxation. It can sometimes be used to accelerate convergence but will decrease the stability of the calculation.

Underrelaxation recommendation

- Underrelaxation factors are there to suppress oscillations in the flow solution that result from numerical errors.
- Underrelaxation factors that are too small will significantly slow down convergence, sometimes to the extent that the user thinks the solution is converged when it really is not.
- The recommendation is to always use underrelaxation factors that are as high as possible, without resulting in oscillations or divergence.
- Typically one should stay with the default factors in the solver.
- When the solution is converged but the pressure residual is still relatively high, the factors for pressure and momentum can be lowered to further refine the solution.

General approach - convergence

- The iterative process is repeated until the change in the variable from one iteration to the next becomes so small that the solution can be considered converged.
- At convergence:
 - All discrete conservation equations (momentum, energy, etc.) are obeyed in all cells to a specified tolerance.
 - The solution no longer changes with additional iterations.
 - Mass, momentum, energy and scalar balances are obtained.
- Residuals measure imbalance (or error) in conservation equations.
- The absolute residual at point P is defined as:

$$R_P = \left| a_P \phi_P - \sum_{nb} a_{nb} \phi_{nb} - b \right|$$

Convergence - continued

- Residuals are usually scaled relative to the local value of the property ϕ in order to obtain a relative error:

$$R_{P,scaled} = \frac{|a_P \phi_P - \sum_{nb} a_{nb} \phi_{nb} - b|}{|a_P \phi_P|}$$

- They can also be normalized, by dividing them by the maximum residual that was found at any time during the iterative process.
- An overall measure of the residual in the domain is:

$$R^\phi = \frac{\sum_{all\ cells} |a_P \phi_P - \sum_{nb} a_{nb} \phi_{nb} - b|}{\sum_{all\ cells} |a_P \phi_P|}$$

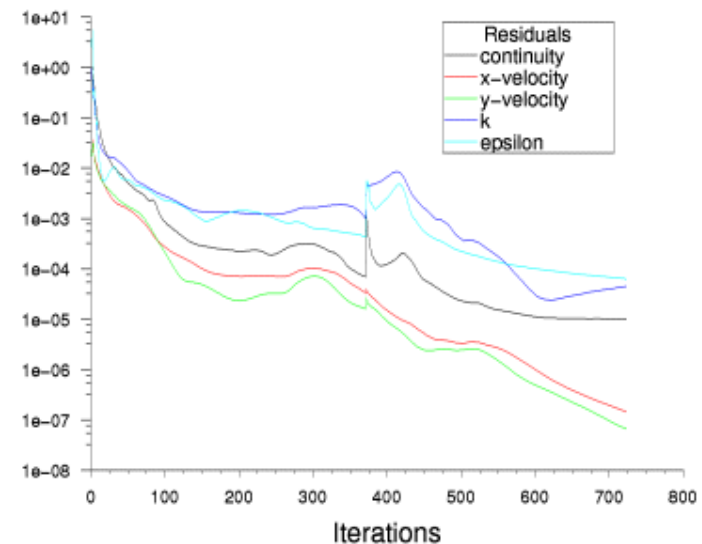
- It is common to require the scaled residuals to be on the order of 1E-3 to 1E-4 or less for convergence.

Notes on convergence

- Always ensure proper convergence before using a solution: unconverged solutions can be misleading!!
- Solutions are converged when the flow field and scalar fields are no longer changing.
- Determining when this is the case can be difficult.
- It is most common to monitor the residuals.

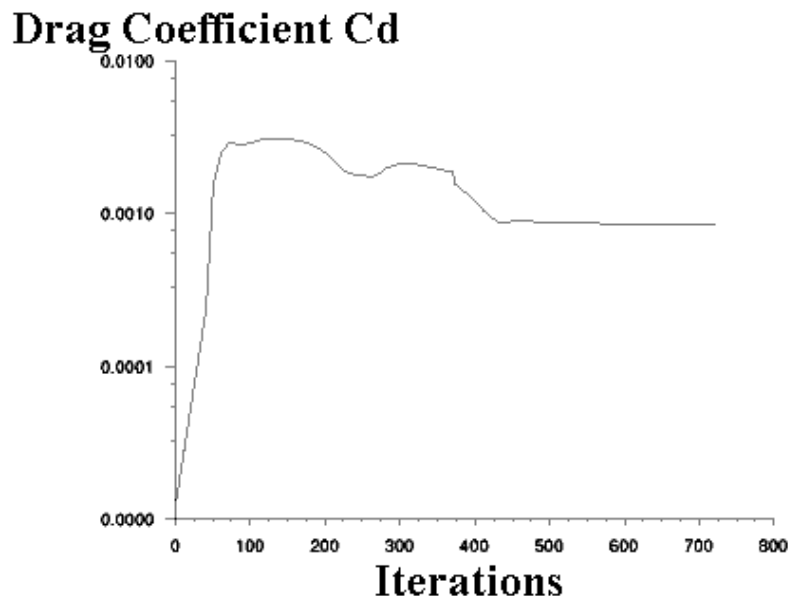
Monitor residuals

- If the residuals have met the specified convergence criterion but are still decreasing, the solution may not yet be converged.
- If the residuals never meet the convergence criterion, but are no longer decreasing and other solution monitors do not change either, the solution is converged.
- Residuals are not your solution! Low residuals do not automatically mean a correct solution, and high residuals do not automatically mean a wrong solution.
- Final residuals are often higher with higher order discretization schemes than with first order discretization. That does not mean that the first order solution is better!
- Residuals can be monitored graphically also.



Other convergence monitors

- For models whose purpose is to calculate a force on an object, the predicted force itself should be monitored for convergence.
- E.g. for an airfoil, one should monitor the predicted drag coefficient.



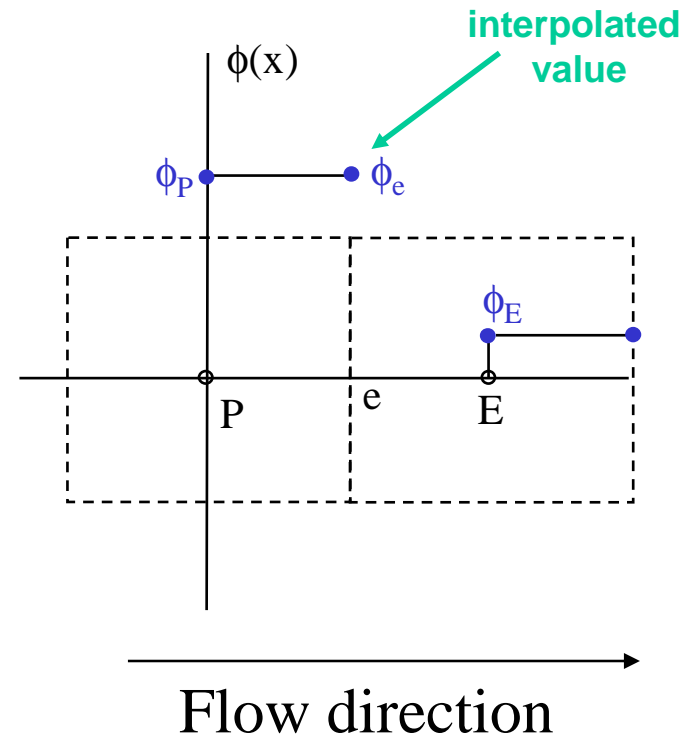
- Overall mass balance should be satisfied.
- When modeling rotating equipment such as turbofans or mixing impellers, the predicted torque should be monitored.
- For heat transfer problems, the temperature at important locations can be monitored.
- One can automatically generate flow field plots every 50 iterations or so to visually review the flow field and ensure that it is no longer changing.

Numerical schemes: finding face values

- Face values of ϕ and $\partial\phi/\partial x$ are found by making assumptions about variation of ϕ between cell centers.
- Number of different schemes can be devised:
 - First-order upwind scheme.
 - Central differencing scheme.
 - Power-law scheme.
 - Second-order upwind scheme.
 - QUICK scheme.
- We will discuss these one by one.

First order upwind scheme

- This is the simplest numerical scheme. It is the method that we used earlier in the discretization example.
- We assume that the value of ϕ at the face is the same as the cell centered value in the cell upstream of the face.
- The main advantages are that it is easy to implement and that it results in very stable calculations, but it also very diffusive. Gradients in the flow field tend to be smeared out, as we will show later.
- This is often the best scheme to start calculations with.

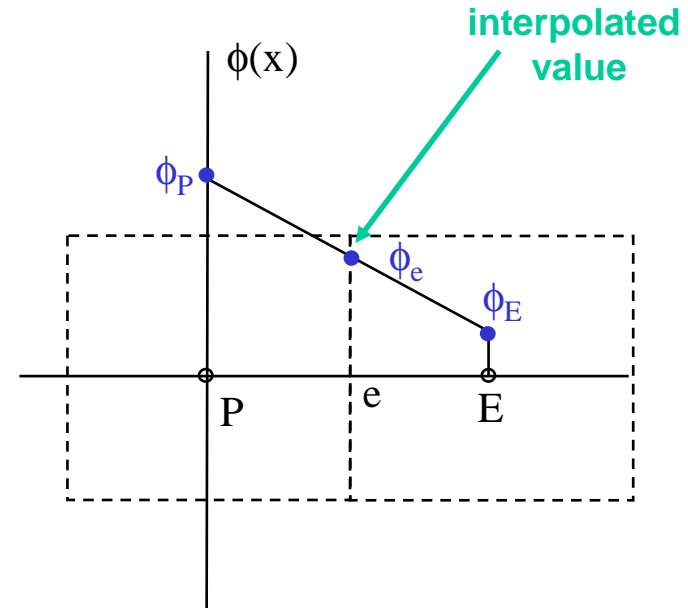


Central differencing scheme

- We determine the value of ϕ at the face by linear interpolation between the cell centered values.
- This is more accurate than the first order upwind scheme, but it leads to oscillations in the solution or divergence if the local Peclet number is larger than 2. The Peclet number is the ratio between convective and diffusive transport:

$$Pe = \frac{\rho u L}{\mathbf{D}}$$

- It is common to then switch to first order upwind in cells where $Pe > 2$. Such an approach is called a hybrid scheme.

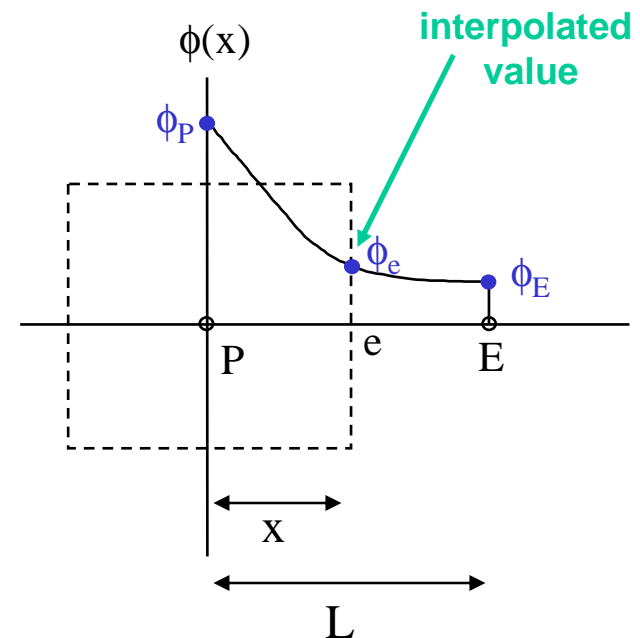


Power law scheme

- This is based on the analytical solution of the one-dimensional convection-diffusion equation.
- The face value is determined from an exponential profile through the cell values. The exponential profile is approximated by the following power law equation:

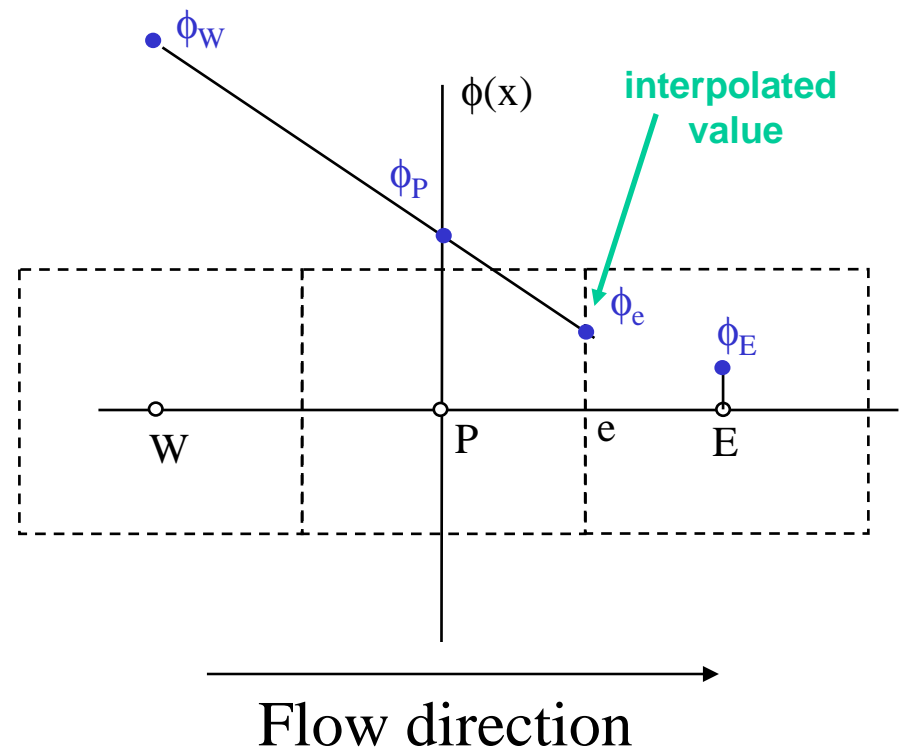
$$\phi_e = \phi_P - \frac{(1 - 0.1Pe)^5}{Pe} (\phi_E - \phi_P)$$

- Pe is again the Peclet number.
- For $Pe > 10$, diffusion is ignored and first order upwind is used.



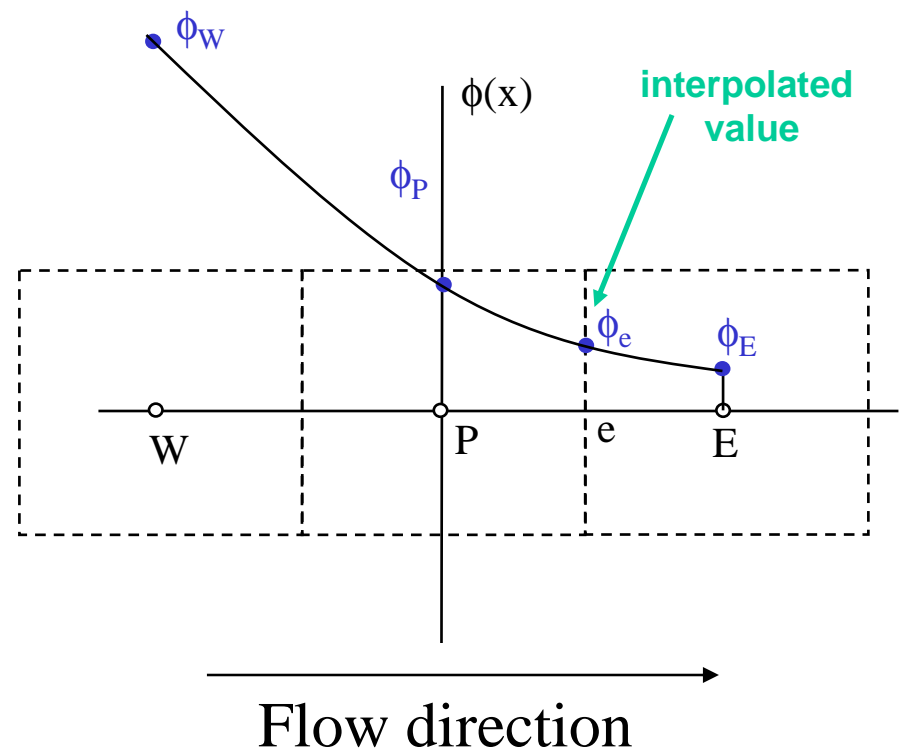
Second-order upwind scheme

- We determine the value of ϕ from the cell values in the two cells upstream of the face.
- This is more accurate than the first order upwind scheme, but in regions with strong gradients it can result in face values that are outside of the range of cell values. It is then necessary to apply limiters to the predicted face values.
- There are many different ways to implement this, but second-order upwind with limiters is one of the more popular numerical schemes because of its combination of accuracy and stability.



QUICK scheme

- QUICK stands for Quadratic Upwind Interpolation for Convective Kinetics.
- A quadratic curve is fitted through two upstream nodes and one downstream node.
- This is a very accurate scheme, but in regions with strong gradients, overshoots and undershoots can occur. This can lead to stability problems in the calculation.



Accuracy of numerical schemes

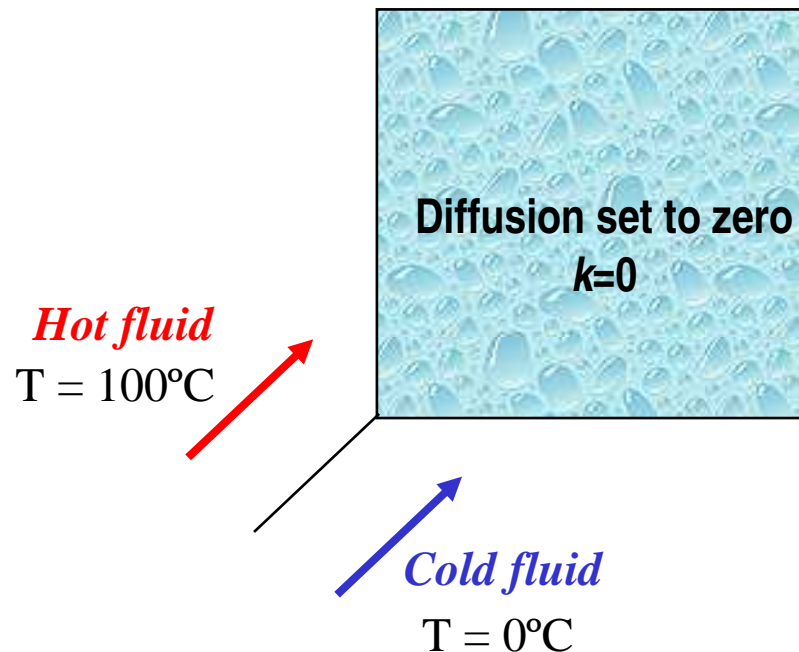
- Each of the previously discussed numerical schemes assumes some shape of the function ϕ . These functions can be approximated by Taylor series polynomials:

$$\phi(x_e) = \phi(x_p) + \frac{\phi'(x_p)}{1!}(x_e - x_p) + \frac{\phi''(x_p)}{2!}(x_e - x_p)^2 + \dots + \frac{\phi^n(x_p)}{n!}(x_e - x_p)^n + \dots$$

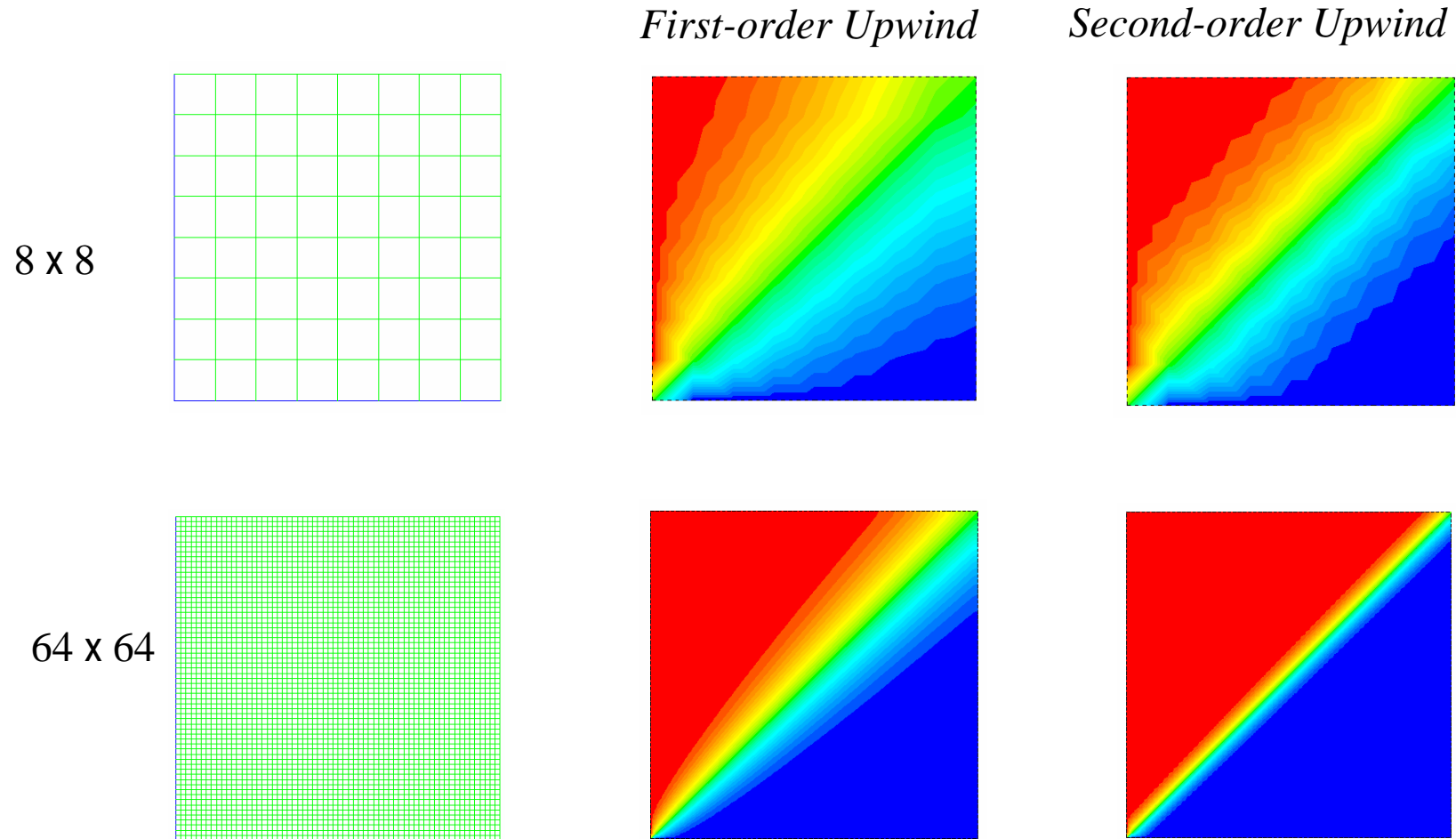
- The first order upwind scheme only uses the constant and ignores the first derivative and consecutive terms. This scheme is therefore considered first order accurate.
- For high Peclet numbers the power law scheme reduces to the first order upwind scheme, so it is also considered first order accurate.
- The central differencing scheme and second order upwind scheme do include the first order derivative, but ignore the second order derivative. These schemes are therefore considered second order accurate. QUICK does take the second order derivative into account, but ignores the third order derivative. This is then considered third order accurate.

Accuracy and false diffusion (1)

- False diffusion is numerically introduced diffusion and arises in convection dominated flows, i.e. high Pe number flows.
- Consider the problem below. If there is no false diffusion, the temperature will be exactly 100 °C everywhere above the diagonal and exactly 0 °C everywhere below the diagonal.
- False diffusion will occur due to the oblique flow direction and non-zero gradient of temperature in the direction normal to the flow.
- Grid refinement coupled with a higher-order interpolation scheme will minimize the false diffusion as shown on the next slide.



Accuracy and false diffusion (2)



Properties of numerical schemes

- All numerical schemes must have the following properties:
 - Conservativeness: global conservation of the fluid property ϕ must be ensured.
 - Boundedness: values predicted by the scheme should be within realistic bounds. For linear problems without sources, those would be the maximum and minimum boundary values. Fluid flow is non-linear and values in the domain may be outside the range of boundary values.
 - Transportiveness: diffusion works in all directions but convection only in the flow direction. The numerical scheme should recognize the direction of the flow as it affects the strength of convection versus diffusion.
- The central differencing scheme does not have the transportiveness property. The other schemes that were discussed have all three of these properties.

Solution accuracy

- Higher order schemes will be more accurate. They will also be less stable and will increase computational time.
- It is recommended to always start calculations with first order upwind and after 100 iterations or so to switch over to second order upwind.
- This provides a good combination of stability and accuracy.
- The central differencing scheme should only be used for transient calculations involving the large eddy simulation (LES) turbulence models in combination with grids that are fine enough that the Peclet number is always less than one.
- It is recommended to only use the power law or QUICK schemes if it is known that those are somehow especially suitable for the particular problem being studied.

Pressure

- We saw how convection-diffusion equations can be solved. Such equations are available for all variables, except for the pressure.
- Gradients in the pressure appear in the momentum equations, thus the pressure field needs to be calculated in order to be able to solve these equations.
- If the flow is compressible:
 - The continuity equation can be used to compute density.
 - Temperature follows from the enthalpy equation.
 - Pressure can then be calculated from the equation of state $p=p(\rho,T)$.
- However, if the flow is incompressible the density is constant and not linked to pressure.
- The solution of the Navier-Stokes equations is then complicated by the lack of an independent equation for pressure.

Pressure - velocity coupling

- Pressure appears in all three momentum equations. The velocity field also has to satisfy the continuity equation. So even though there is no explicit equation for pressure, we do have four equations for four variables, and the set of equations is closed.
- So-called pressure-velocity coupling algorithms are used to derive equations for the pressure from the momentum equations and the continuity equation.
- The most commonly used algorithm is the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations). An algebraic equation for the pressure correction p' is derived, in a form similar to the equations derived for the convection-diffusion equations:

$$a_p p' = \sum_{nb} a_{nb} p' + b'$$

- Each iteration, the pressure field is updated by applying the pressure correction. The source term b' is the continuity imbalance. The other coefficients depend on the mesh and the flow field.

Principle behind SIMPLE

- The principle behind SIMPLE is quite simple!
- It is based on the premise that fluid flows from regions with high pressure to low pressure.
 - Start with an initial pressure field.
 - Look at a cell.
 - If continuity is not satisfied because there is more mass flowing into that cell than out of the cell, the pressure in that cell compared to the neighboring cells must be too low.
 - Thus the pressure in that cell must be increased relative to the neighboring cells.
 - The reverse is true for cells where more mass flows out than in.
 - Repeat this process iteratively for all cells.
- The trick is in finding a good equation for the pressure correction as a function of mass imbalance. These equations will not be discussed here but can be readily found in the literature.

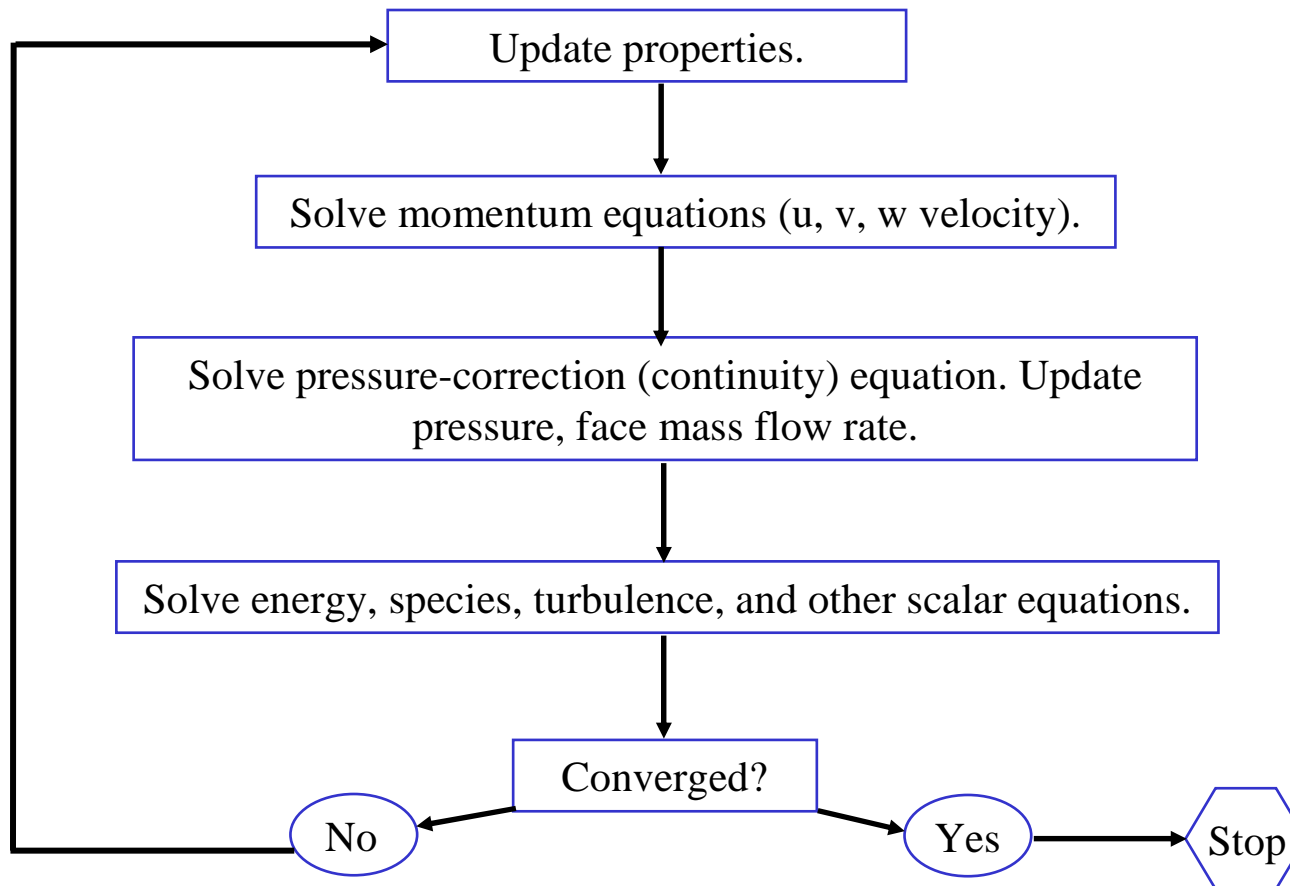
Improvements on SIMPLE

- SIMPLE is the default algorithm in most commercial finite volume codes.
- Improved versions are:
 - SIMPLER (SIMPLE Revised).
 - SIMPLEC (SIMPLE Consistent).
 - PISO (Pressure Implicit with Splitting of Operators).
- All these algorithms can speed up convergence because they allow for the use of larger underrelaxation factors than SIMPLE.
- All of these will eventually converge to the same solution. The differences are in speed and stability.
- Which algorithm is fastest depends on the flow and there is no single algorithm that is always faster than the other ones.

Finite volume solution methods

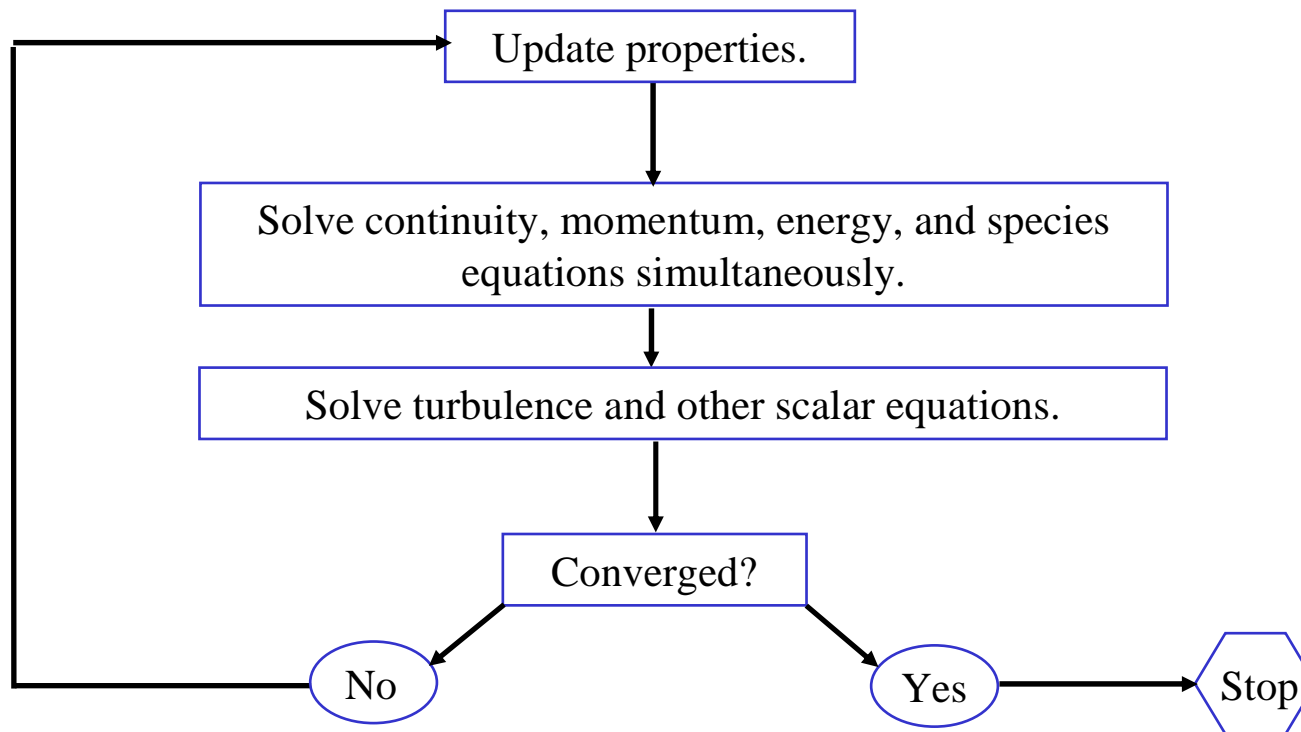
- The finite volume solution method can either use a “segregated” or a “coupled” solution procedure.
- With segregated methods an equation for a certain variable is solved for all cells, then the equation for the next variable is solved for all cells, etc.
- With coupled methods, for a given cell equations for all variables are solved, and that process is then repeated for all cells.
- The segregated solution method is the default method in most commercial finite volume codes. It is best suited for incompressible flows or compressible flows at low Mach number.
- Compressible flows at high Mach number, especially when they involve shock waves, are best solved with the coupled solver.

Segregated solution procedure



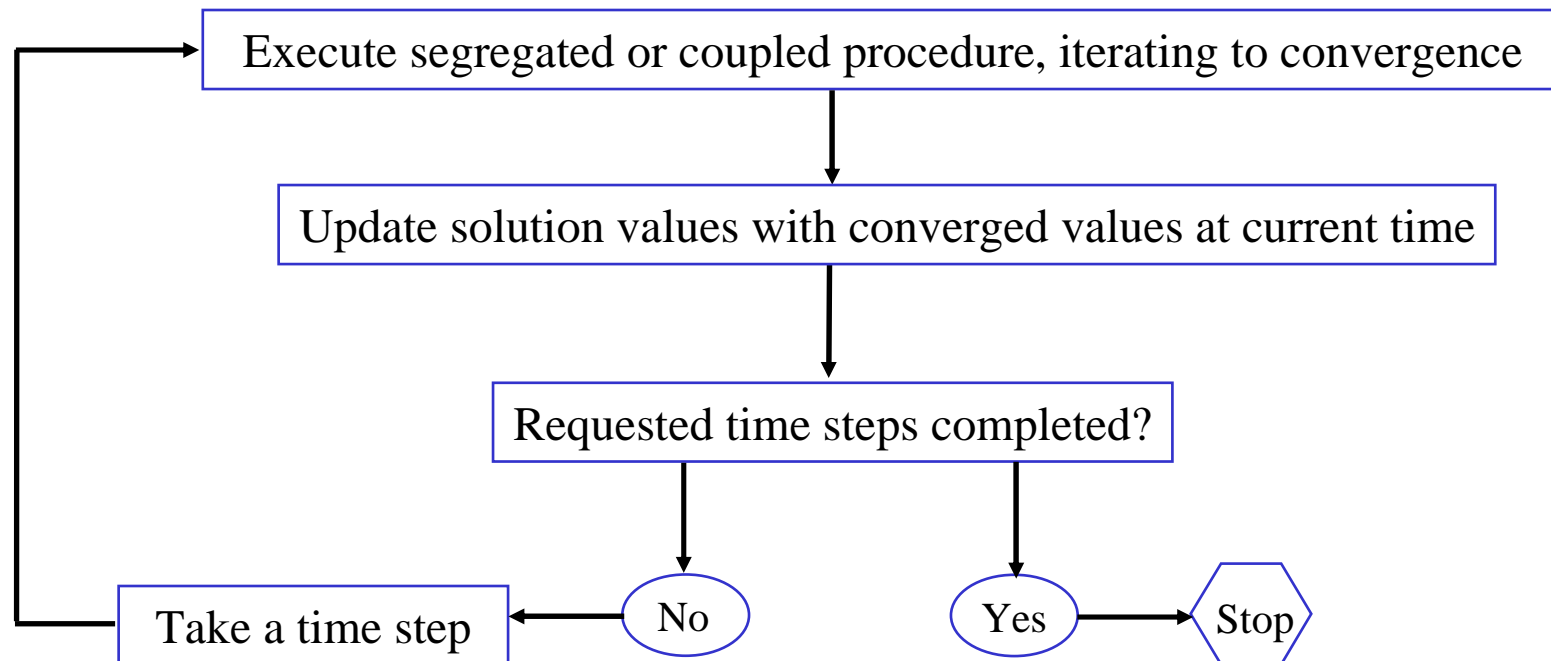
Coupled solution procedure

- When the coupled solver is used for steady state calculations it essentially employs a modified time dependent solution algorithm, using a time step $\Delta t = CFL/(u/L)$ with CFL being the user specified Courant-Friedrich-Levy number, L being a measure of the size of the cell, and u being a measure of the local velocities.



Unsteady solution procedure

- Same procedure for segregated and coupled solvers.
- The user has to specify a time step that matches the time variation in the flow.
- If a time accurate solution is required, the solution should be converged at every time step. Otherwise, convergence at every time step may not be necessary.

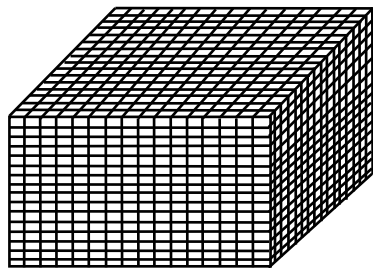


The multigrid solver

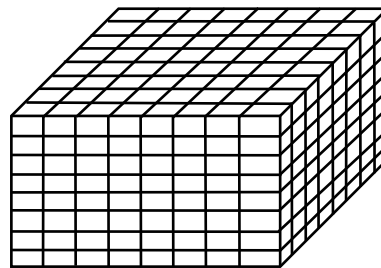
- The algebraic equation $a_P \phi_P = \sum_{nb} a_{nb} \phi_{nb} + b$ can be solved by sweeping through the domain cell-by-cell in an iterative manner.
- This method reduces local errors quickly but can be slow in reducing long-wavelength errors.
- On large grids, it can take a long time to see the effect of far away grid points and boundaries.
- Multigrid acceleration is a method to speed up convergence for:
 - Large number of cells.
 - Large cell aspect ratios (e.g. $\Delta x/\Delta y > 20$).
 - Large differences in thermal conductivity such as in conjugate heat transfer problems.

The multigrid solver

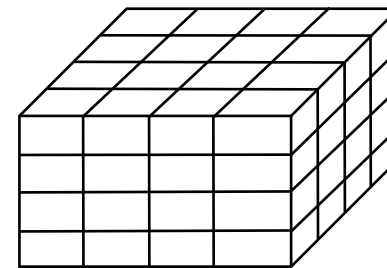
- The multigrid solver uses a sequence of grids going from fine to coarse.
- The influence of boundaries and far-away points is more easily transmitted to the interior on coarse meshes than on fine meshes.
- In coarse meshes, grid points are closer together in the computational space and have fewer computational cells between any two spatial locations.
- Fine meshes give more accurate solutions.



original grid



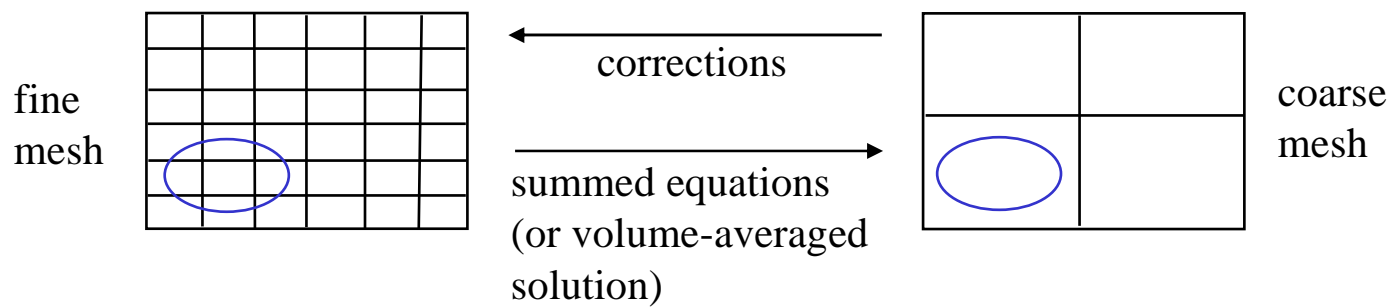
coarse grid
level 1



coarse grid
level 2

The multigrid solver

- The solution on the coarser meshes is used as a starting point for solutions on the finer meshes.
- The coarse-mesh solution contains the influence of boundaries and far neighbors. These effects are felt more easily on coarse meshes.
- This accelerates convergence on the fine mesh.
- The final solution is obtained for the original (fine) mesh.
- Coarse mesh calculations only accelerate convergence and do not change the final answer.



Finite volume method - summary

- The FVM uses the integral conservation equation applied to control volumes which subdivide the solution domain, and to the entire solution domain.
- The variable values at the faces of the control volume are determined by interpolation. False diffusion can arise depending on the choice of interpolation scheme.
- The grid must be refined to reduce “smearing” of the solution as shown in the last example.
- Advantages of FVM: integral conservation is exactly satisfied and the method is not limited to grid type (structured or unstructured, Cartesian or body-fitted).
- Always ensure proper convergence.