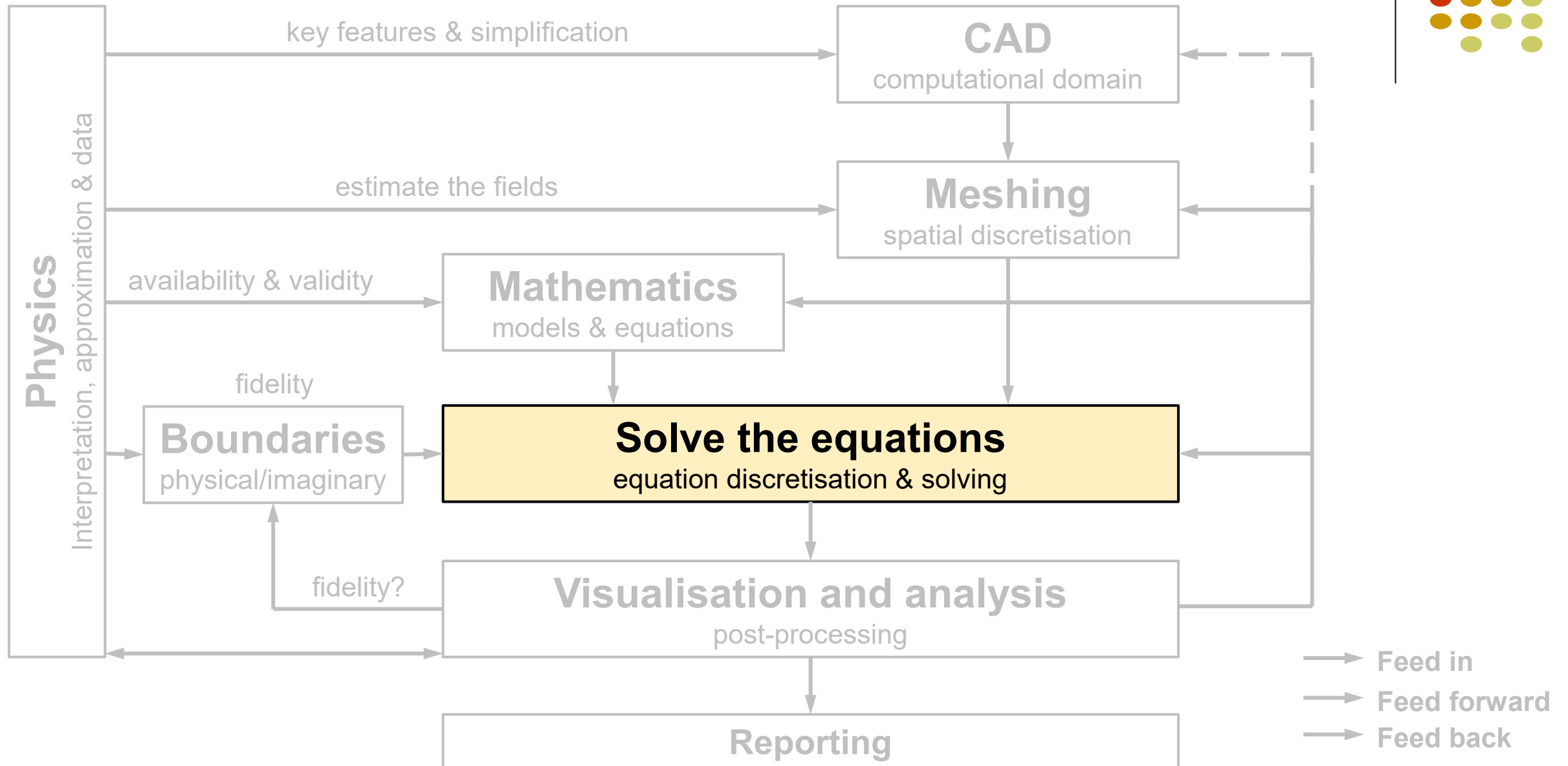
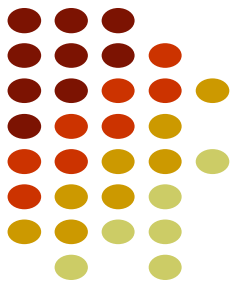
The background of the slide features a 3D visualization of a fighter jet, likely an F-35, with a complex flow field around it. The flow field is represented by a color gradient from blue (low velocity) to red (high velocity), with streamlines indicating the flow direction. The jet is shown from a side-on perspective, angled upwards.

ENGINEERING COMPUTATIONAL FLUID DYNAMICS (ECFD)

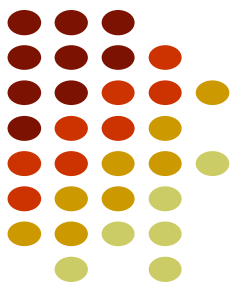
Dr Xiangdong Li

Module 6 – Solving the equations

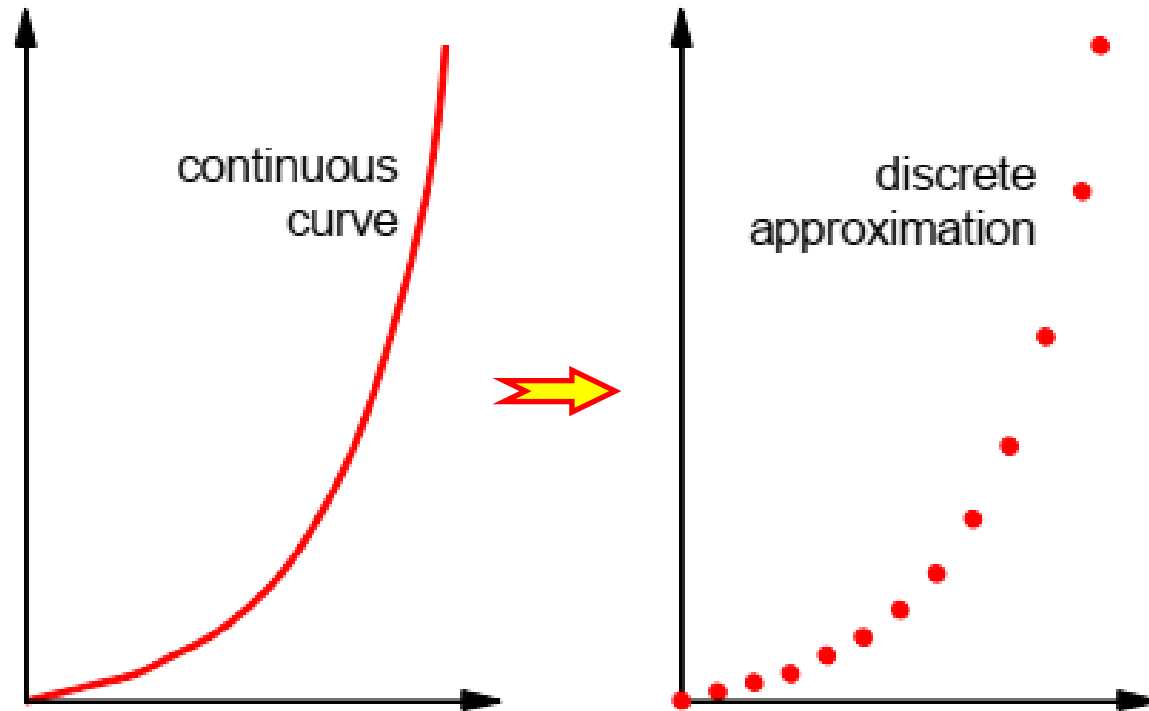
CFD workflow



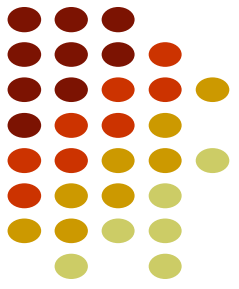
Discretisation



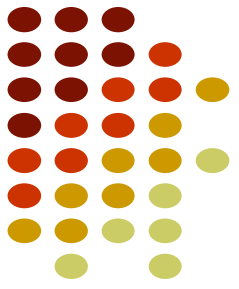
Field variables:



This module



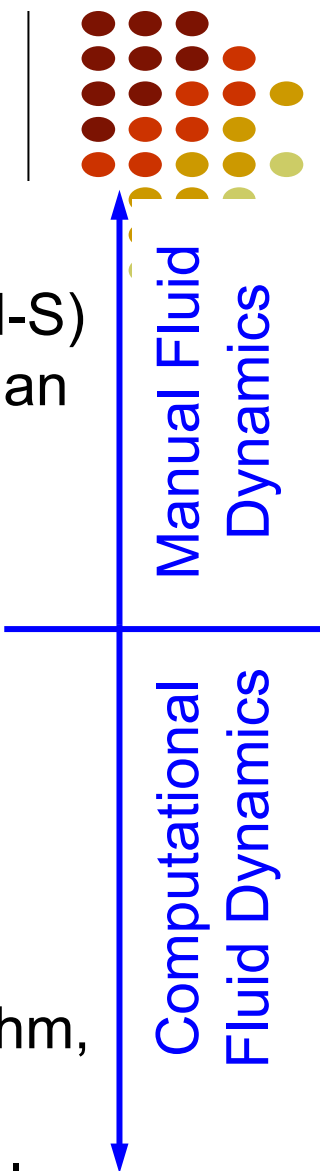
- ❖ How are pressure and density calculated in CFD codes?
- ❖ How are the partial differential equations solved? – the finite volume method (FVM)
- ❖ Strategies for coping with stability issues
- ❖ Convergence



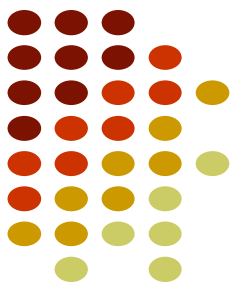
EQUATION DISCRETISATION

In Module 1

- ❖ L. Euler (1707-1783), the Euler equation
- ❖ C.L. Navier (1785-1836) and G.G. Stokes (1819-1903), the Navier-Stokes (N-S) equations – \$US 1 million prize offered by the Clay Mathematics Institute for an analytical solution
- ❖ Lewis F. Richardson (FDM, 1911), A. Thom (1933), ...
- ❖ Harlow and Fromm, 1965, “computer experiments” – **the birth of CFD**
- ❖ Los Alamos Lab, 1960's, PIC algorithm, ... **Digital Computers were used to solve the N-S equations, successfully.**
- ❖ McDonald (1971) and MacCormack and Paullay (1972), the finite volume method
- ❖ S.V. Patanka & D.B. Spalding, 1970 – 1980's, the k- ϵ model, SIMPLE algorithm, up-wind differencing, ...
- ❖ CHM Ltd. (UK), 1981, Phoenix – the world's first general-purpose commercial CFD package
- ❖ Exponential growth since 1980's: Fluent, CFX, OpenFoam, SimScale, ...



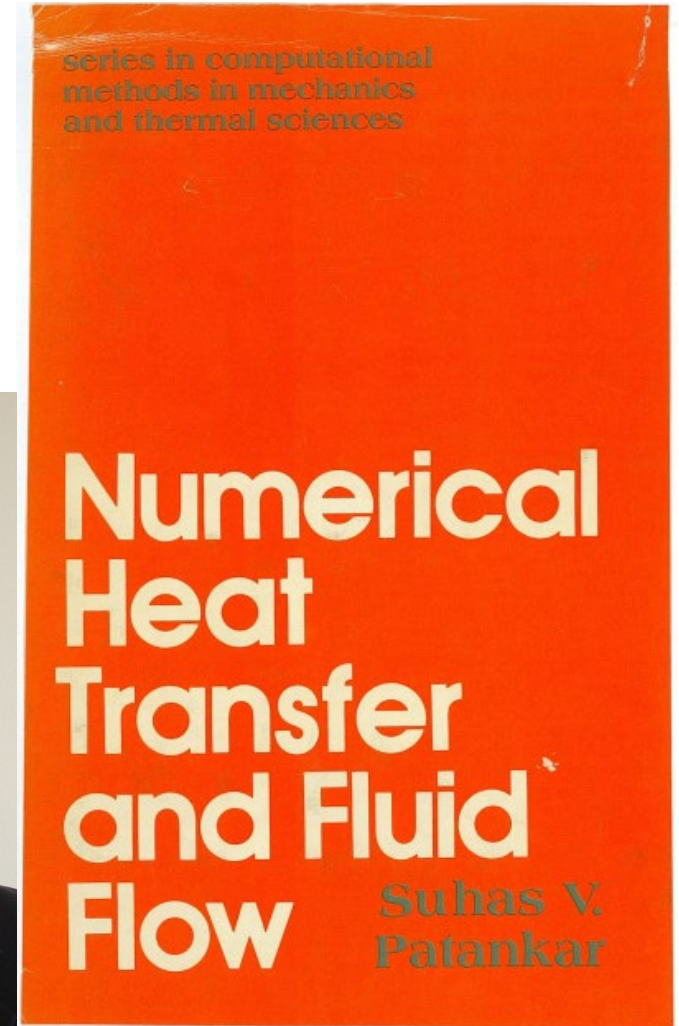
In Module 1 – Discrete numerical methods



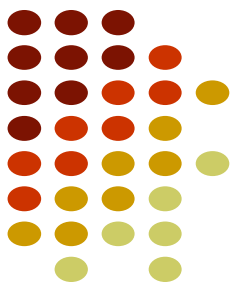
- ❖ Boundary element method
- ❖ Spectral methods
- ❖ Finite difference method
- ❖ **Finite volume method**
- ❖ Finite element method
- ❖ Vorticity based methods
- ❖ And more

S.V. Patankar, D.B. Spalding, A calculation procedure for heat, mass and momentum transfer in three-dimensional parabolic flow. Int J Heat Mass Trans, 15, 1972: 1787-1806

Published in 1980



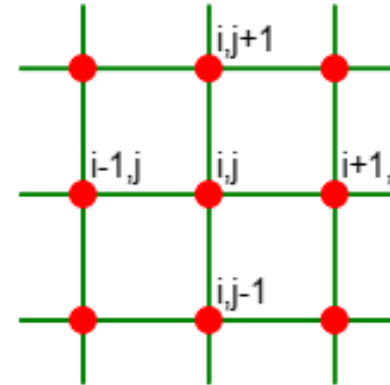
FDM vs FVM



- **Finite-difference:**

- discretise **differential** equations

$$0 = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \approx \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + \frac{v_{i,j+1} - v_{i,j-1}}{2\Delta y}$$

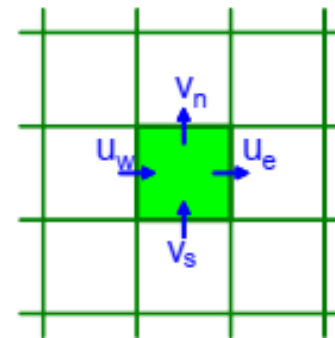


Considering the
change at a point

- **Finite-volume:**

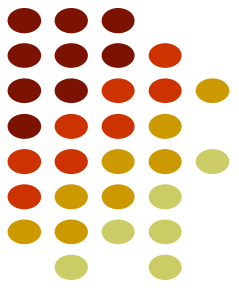
- discretise **control-volume** equations

$$0 = \text{net mass outflow} = (\rho u A)_e - (\rho u A)_w + (\rho v A)_n - (\rho v A)_s$$

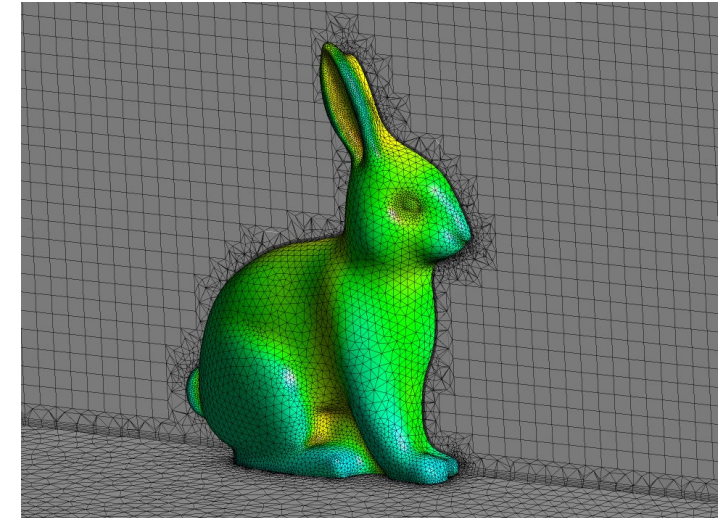


Considering the
change in a volume

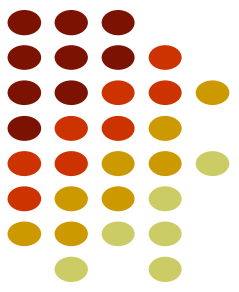
The finite volume method (FVM)



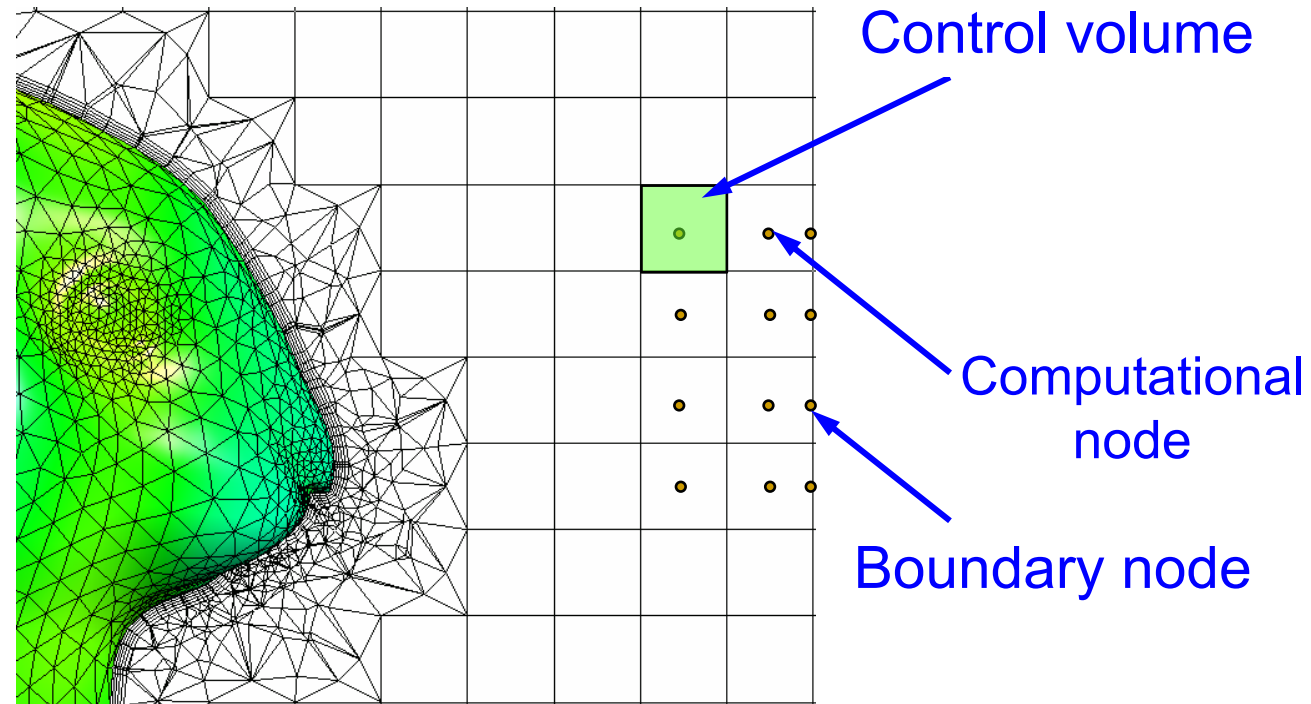
- ❖ The most common in commercial CFD packages (www.bakker.org)
 - The FVM – 80%
 - The finite element method – 15%
 - Other (including the FDM) – 5%
- ❖ First documented by Evans and Harlow (1957) at Los Alamos
- ❖ Robust when variables may not be continuously differentiable
- ❖ Advantage in memory use and speed for very large problems
- ❖ Not limited to cell shape
- ❖ False diffusion possible



The FVM



- ❖ Discretise the domain into control volumes (cells/mesh elements)
- ❖ Integrate the differential equations over the control volume and its faces
 - Cells and nodes
- ❖ Values at control volume faces are need to evaluate the derivatives – interpolation.
- ❖ Results in a set of linear algebraic equations, one for each control volume



The FVM – Equation discretisation

- ❖ For a conserved variable ϕ , the partial differential conservation equation over the control volume P can be discretised to

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\bar{U} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S_\phi$$



$$A_e u_e \phi_e - A_w u_w \phi_w + A_n v_n \phi_n - A_s v_s \phi_s =$$

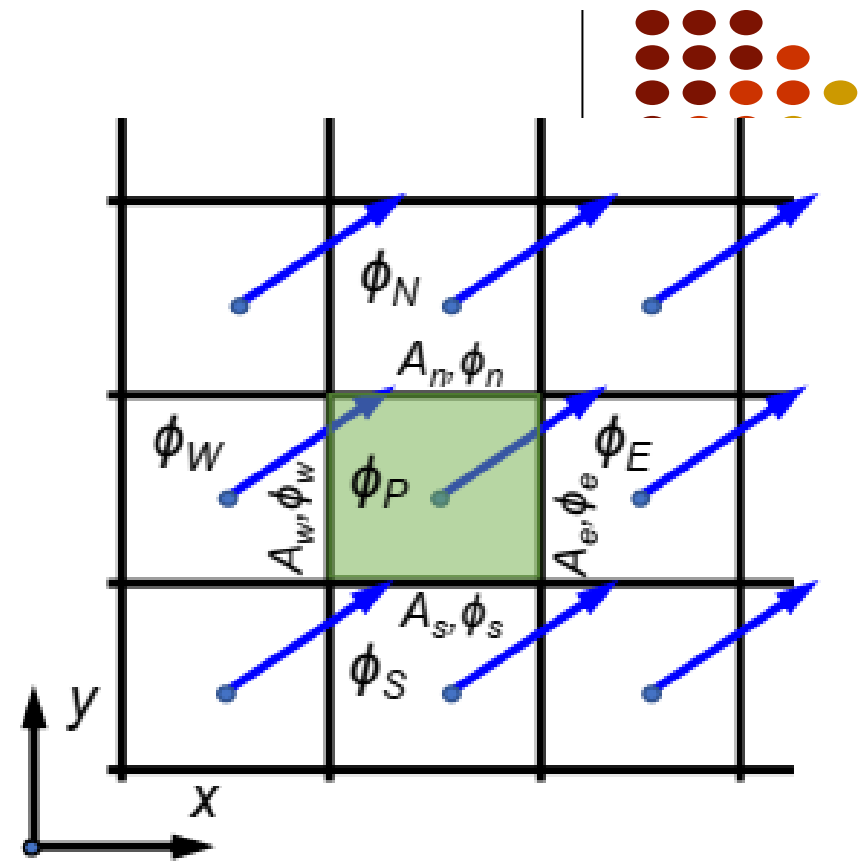
$$\Gamma A_e (\phi_E - \phi_P) / \delta x_e - \Gamma A_w (\phi_P - \phi_W) / \delta x_e$$

$$+ \Gamma A_n (\phi_N - \phi_P) / \delta y_n - \Gamma A_s (\phi_P - \phi_S) / \delta y_s + S_P$$

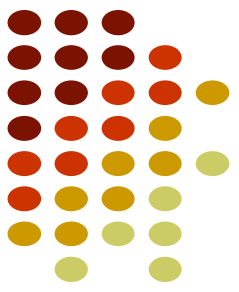


$$a_P \phi_P = \sum a_{nb} \phi_{nb} + b$$

- ❖ Then the value of ϕ at the cell faces will be found through **interpolation**.



Interpolation



- ❖ First-order upwind scheme
- ❖ Central differencing scheme
- ❖ Power-law scheme
- ❖ Second-order upwind scheme
- ❖ QUICK scheme

$$\phi_e = \phi_P + \frac{d\phi}{dx}(x_e - x_P) + \frac{d^2\phi}{dx^2} \frac{(x_e - x_P)^2}{2!} + \dots + \frac{d^n\phi}{dx^n} \frac{(x_e - x_P)^n}{n!} + \dots$$

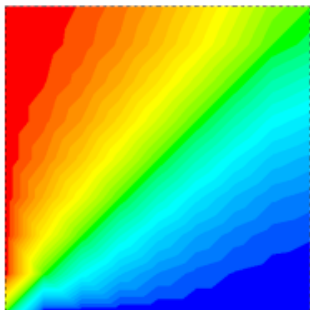
- First-order upwind: 1st term in RHS
- Central and 2nd-order: 2 first terms in RHS
- QUICK: 3 first terms in RHS

Interpolation – 1st-order upwind

❖ First-order upwind scheme

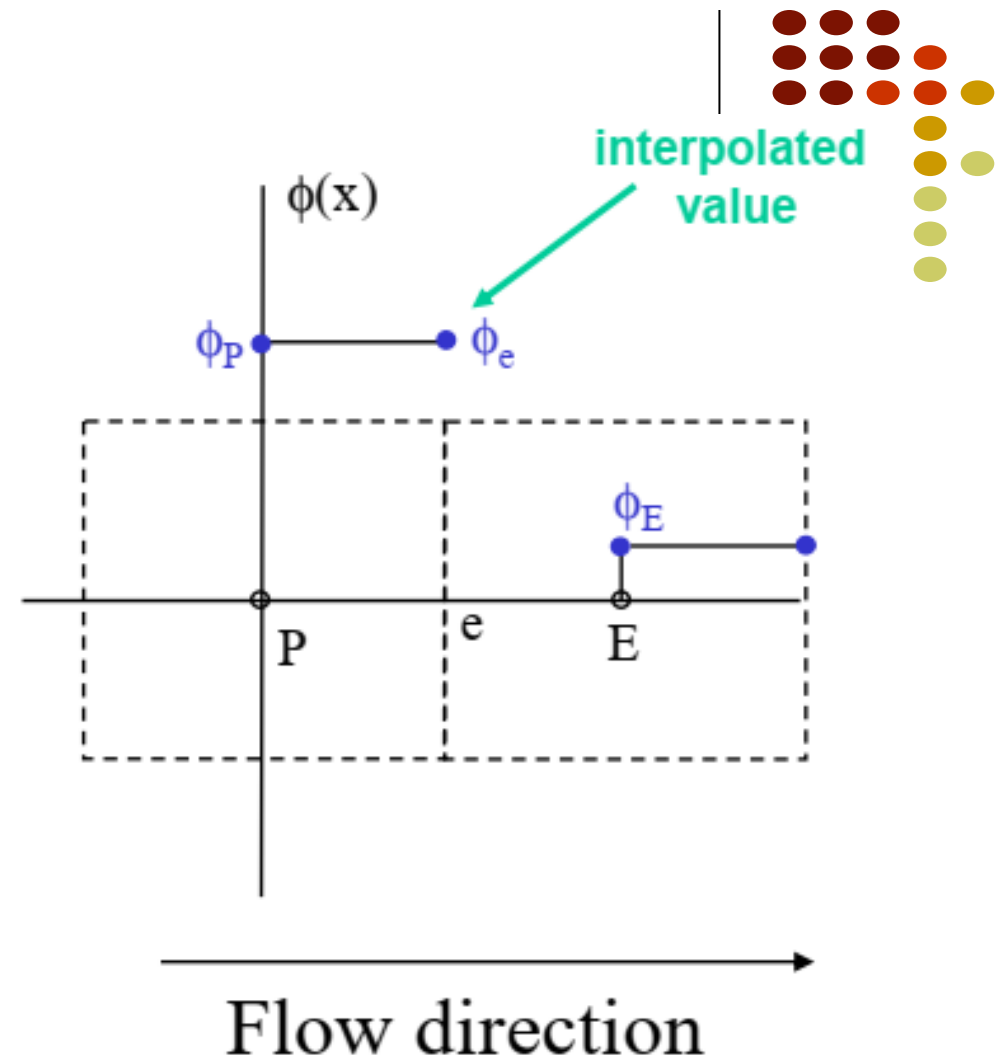
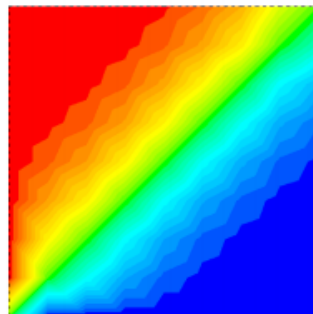
- Very stable
- Best scheme to start with
- Very diffusive: gradients can be smeared out – numerically induced diffusion, also called “**false diffusion**”

First-order Upwind

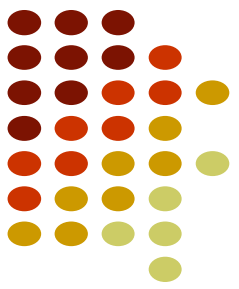


False diffusion

Second-order Upwind

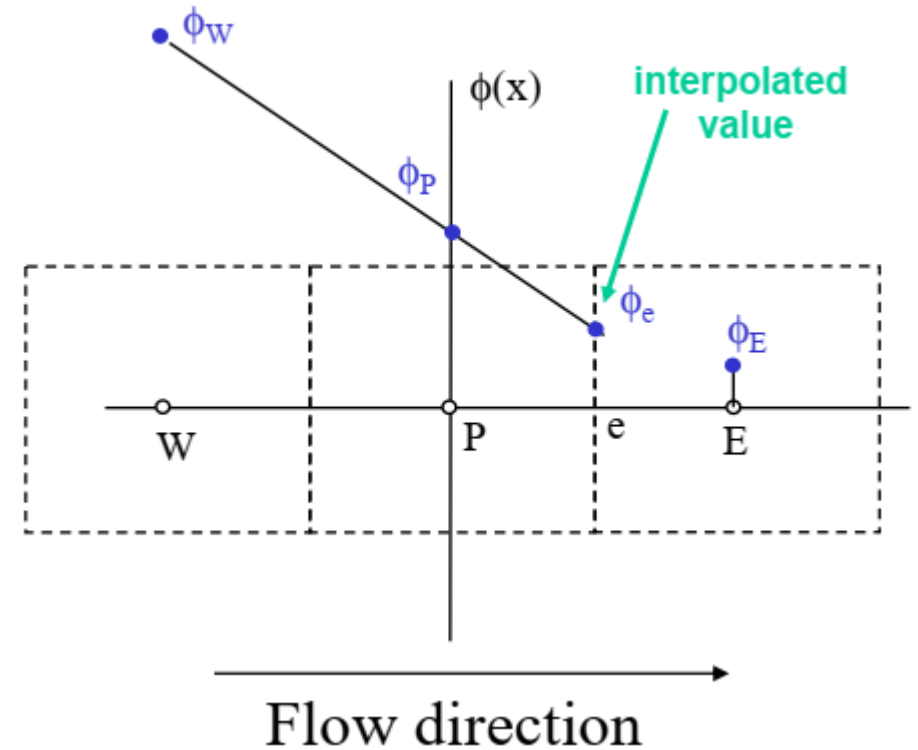


Interpolation – 2nd-order upwind

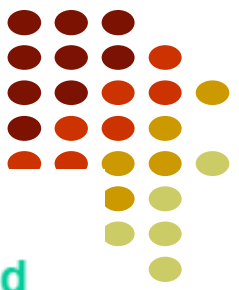


❖ Second-order upwind scheme

- Better than 1st-order upwind
- Sometimes demands limit



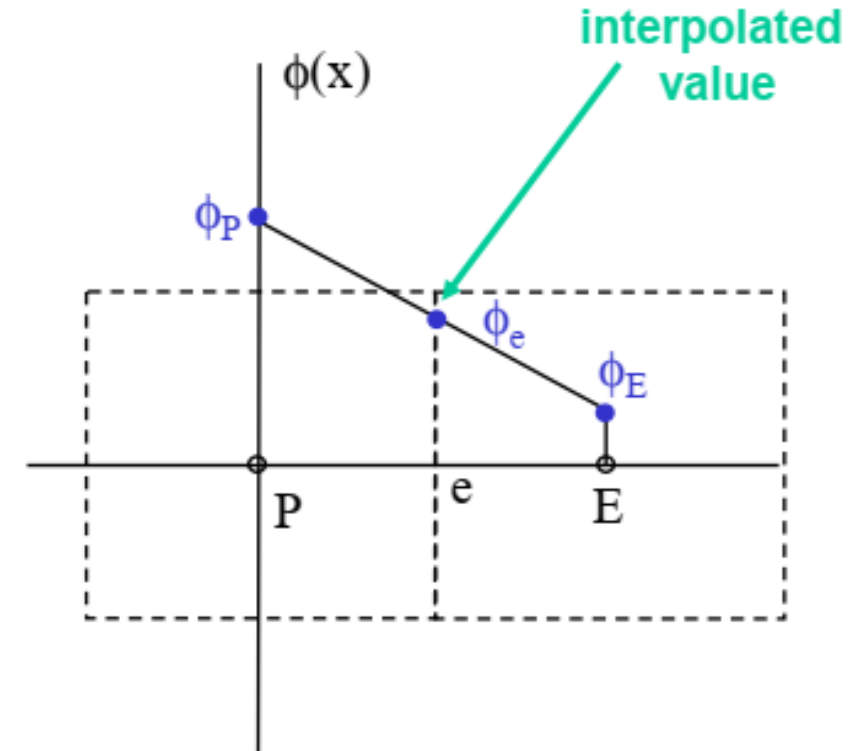
Interpolation – central differencing



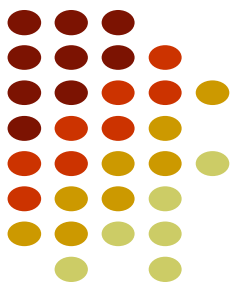
❖ Central differencing scheme

- More accurate than 1st-order upwind scheme
- Leads to oscillation when the Peclet number (Pe) is larger than 2 (often switch to 1st-order upwind scheme when $Pe > 2$)
- Pe is the ratio between convective and diffusive transport

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



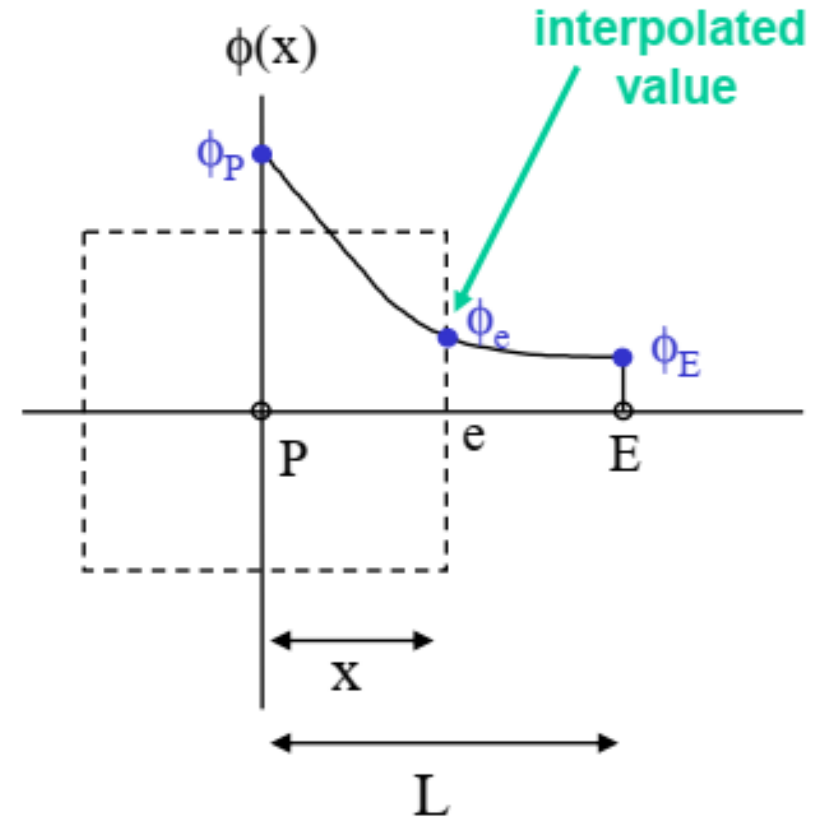
Interpolation – power law



❖ Power-law scheme

- A theoretical solution
- Switch to 1st-order upwind scheme when $Pe > 10$

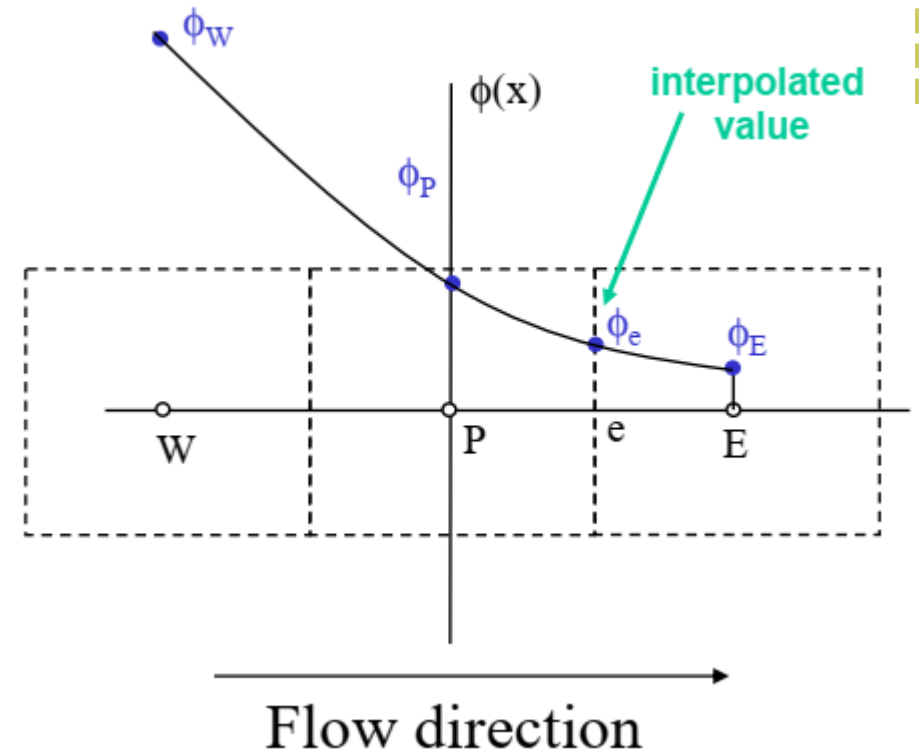
$$\phi_e = \phi_P - \frac{(1 - 0.1Pe)^5}{Pe} (\phi_E - \phi_P)$$



Interpolation – QUICK

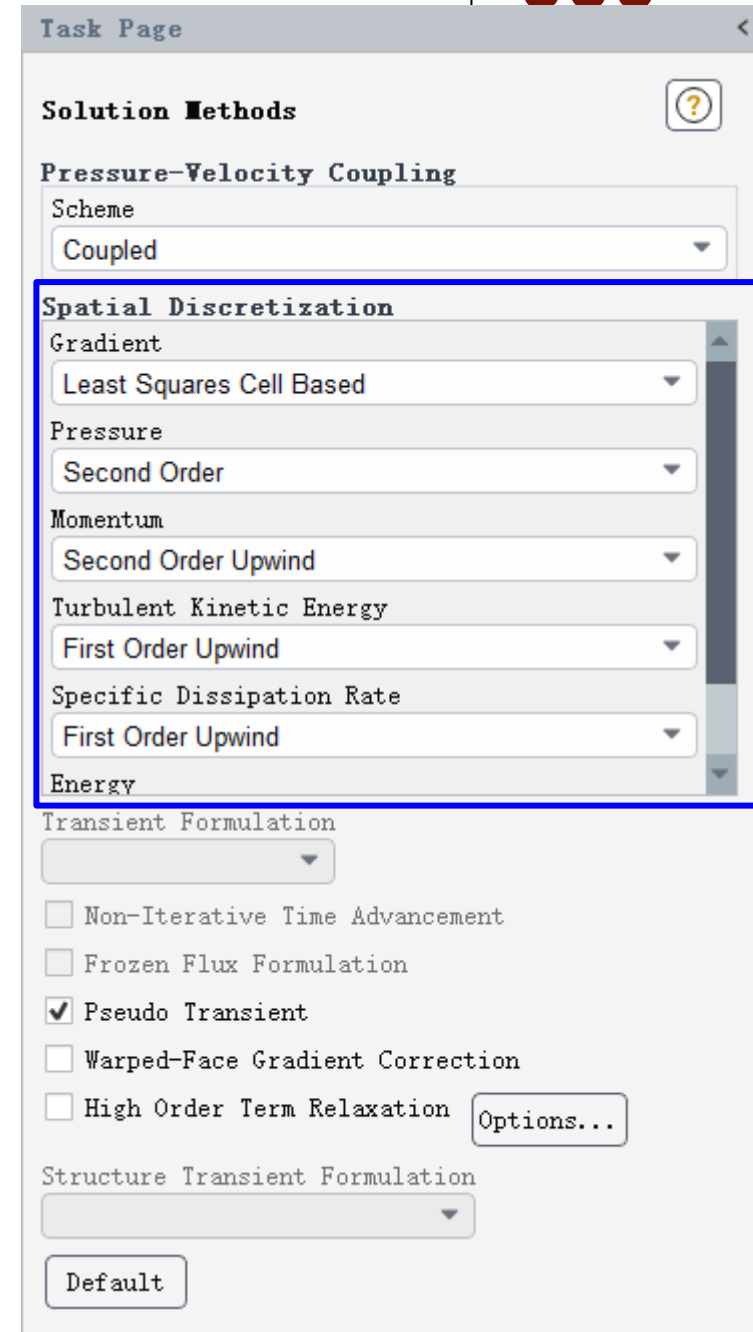
❖ QUICK scheme

- Quadratic Upwind Interpolation for Convective Kinetics
- Very accurate
- But can lead to stability problems in high-gradient regions



Interpolation - recommendations

- ❖ Higher-order schemes are more accurate, but less stable
- ❖ Start with 1st-order upwind scheme then switch over to 2nd-order upwind scheme
- ❖ Central differencing scheme should only be used for transient LES where mesh is fine enough to ensure $Pe < 1$
- ❖ Power law and QUICK schemes are only used for especially suitable problems



The screenshot shows a software interface titled "Task Page" with a "Solution Methods" section. The "Pressure-Velocity Coupling" is set to "Coupled". The "Spatial Discretization" section is highlighted with a blue border and contains the following settings:

- Gradient: Least Squares Cell Based
- Pressure: Second Order
- Momentum: Second Order Upwind
- Turbulent Kinetic Energy: First Order Upwind
- Specific Dissipation Rate: First Order Upwind
- Energy: (empty dropdown)

Below the "Spatial Discretization" section, the "Transient Formulation" is set to (empty dropdown). The following options are listed with checkboxes:

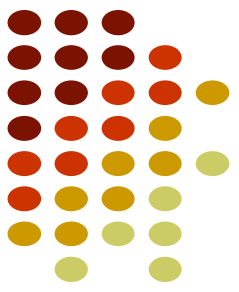
- ☐ Non-Iterative Time Advancement
- ☐ Frozen Flux Formulation
- ☒ Pseudo Transient
- ☐ Warped-Face Gradient Correction
- ☐ High Order Term Relaxation

An "Options..." button is located next to the "High Order Term Relaxation" checkbox. The "Structure Transient Formulation" is set to (empty dropdown). A "Default" button is at the bottom.



PRESSURE, VELOCITY AND DENSITY

The issue of pressure



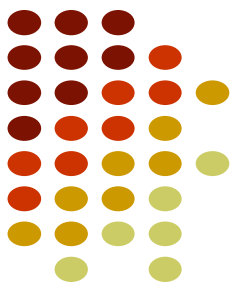
- ❖ Think about the continuity equation and momentum equation: we have the momentum equations for u , v , w , and we have the continuity equation for constraining the mass conservation; however, we don't have an equation for p .

$$\frac{\partial \rho}{\partial t} + \vec{U} \cdot \nabla \rho = 0$$

$$\frac{\partial}{\partial t}(\rho \vec{U}) + \nabla \cdot (\rho \vec{U} \vec{U}) = -\nabla p + \nabla \cdot \left(\mu \left(\nabla \vec{U} + (\nabla \vec{U})^T \right) \right) - \nabla \cdot \left(\frac{2}{3} \mu (\nabla \cdot \vec{U}) \right) I + S_M$$

- ❖ What's the solution?

Solutions in Fluent

A screenshot of the 'Task Page' window in ANSYS Fluent. The 'General' tab is active. Under the 'Mesh' section, there are buttons for 'Scale...', 'Check', 'Report Quality', 'Display...', and 'Units...'. The 'Solver' section is highlighted with a blue box; it contains a 'Type' group with 'Pressure-Based' selected (indicated by a filled radio button) and 'Density-Based' unselected (indicated by an empty radio button). To the right of the 'Solver' section is the 'Velocity Formulation' group with 'Absolute' selected and 'Relative' unselected. Below these is the 'Time' section with 'Steady' selected and 'Transient' unselected. At the bottom, there is a checked 'Gravity' checkbox and a 'Gravitational Acceleration' section with input fields for X (m/s²) set to 0, Y (m/s²) set to 0, and Z (m/s²) set to -9.8.

- ❖ Pressure-based solver (historically for low-speed incompressible flows): The pressure field is extracted by deriving and solving **a pressure (correction) equation** from the continuity and momentum equations.
- ❖ Density-based solver (historically for high-speed compressible flows): The continuity equation is used to obtain the density field while the pressure field is determined from **the equation of state**.
- ❖ ATTN: now the both solvers can be applied to most cases although the density-based solver has advantage for compressible flows.

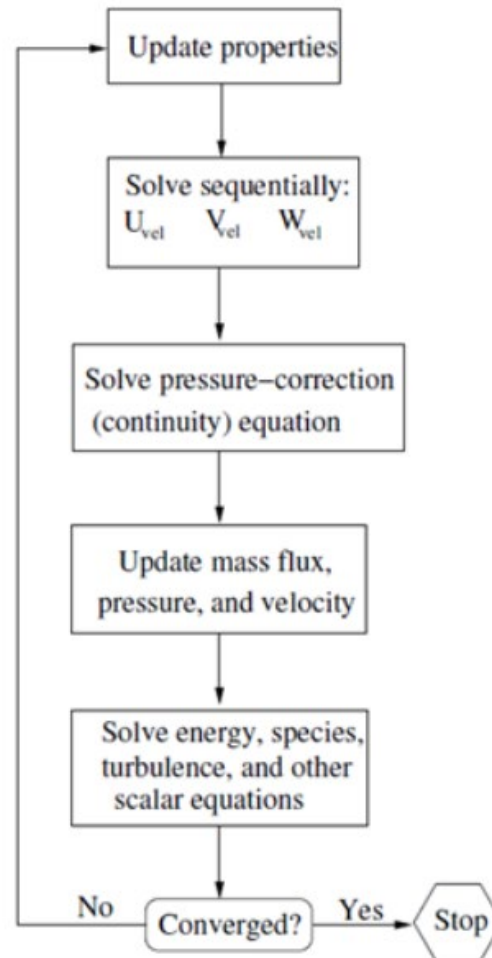
The pressure-based solver



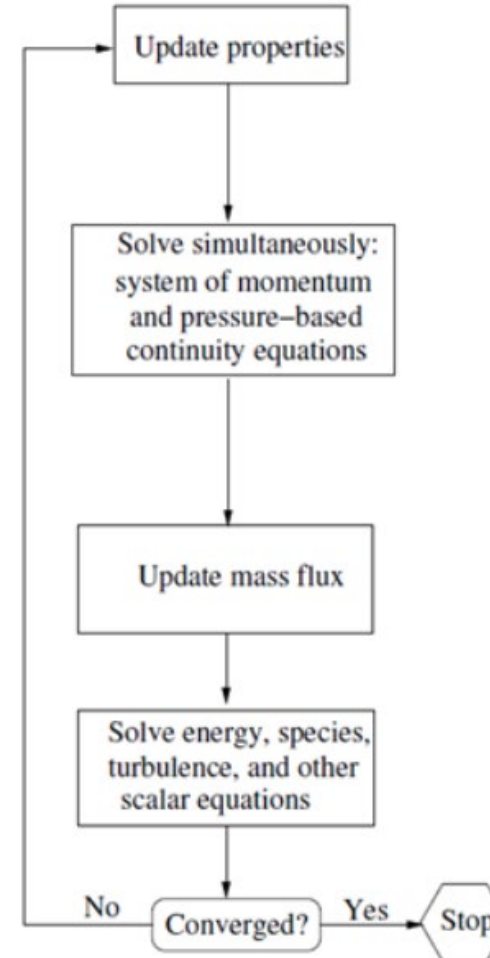
Segregated algorithm

- SIMPLE
 - SIMPLEC
 - PISO
- ❖ Memory-efficient
 - ❖ Faster per iteration
 - ❖ Slow convergence

Pressure-Based Segregated Algorithm



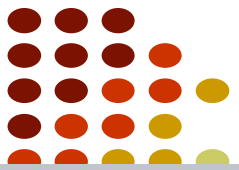
Pressure-Based Coupled Algorithm



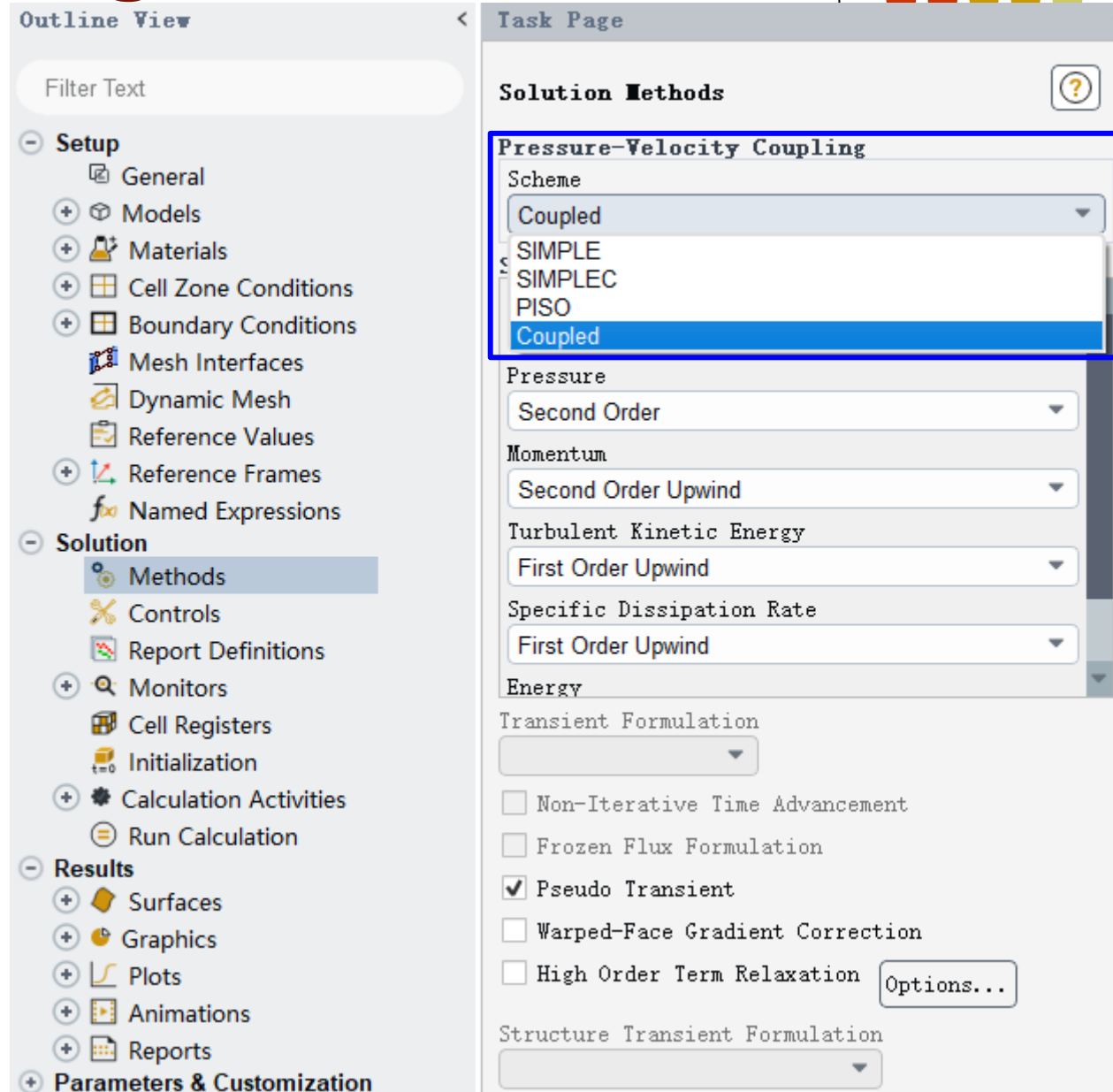
Coupled algorithm

- ❖ Memory demanding
- ❖ Fast convergence

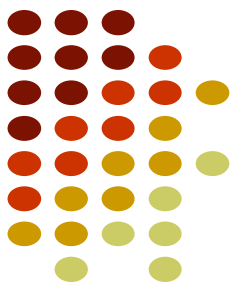
Velocity-pressure coupling in Fluent



- ❖ SIMPLE – The default scheme, robust
- ❖ SIMPLEC – Allows faster convergence than SIMPLE for simple problems, all under-relaxation
- ❖ PISO – Useful for unsteady flows or for mesh containing cells with higher than average skewness
- ❖ FSM – For unsteady flows only
- ❖ Coupled – Recommended for steady-state flows though robust for transient flows



Operating/reference pressure



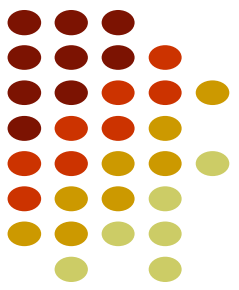
- ❖ For low speed flows, the pressure drop is small compared to the static pressure (e.g., 1 Pa / 101325 Pa) – **round-off error can affect the solution.**
- ❖ By defining an operating/reference pressure p_0 , we can only focus on the gauge pressure – **higher resolution**
- ❖ Gauge pressure ($p_g = p - p_0$) is used in the momentum equation

$$\frac{\partial}{\partial t}(\rho \vec{U}) + \nabla \cdot (\rho \vec{U} \vec{U}) = -\nabla p + \nabla \cdot \left(\mu \left(\nabla \vec{U} + (\nabla \vec{U})^T \right) \right) - \nabla \cdot \left(\frac{2}{3} \mu (\nabla \cdot \vec{U}) \right) I + S_M$$



$$\frac{\partial}{\partial t}(\rho \vec{U}) + \nabla \cdot (\rho \vec{U} \vec{U}) = -\nabla p_g + \nabla \cdot \left(\mu \left(\nabla \vec{U} + (\nabla \vec{U})^T \right) \right) - \nabla \cdot \left(\frac{2}{3} \mu (\nabla \cdot \vec{U}) \right) I + S_M$$

Density – pressure and density



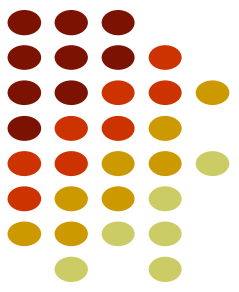
- ❖ For incompressible or mildly compressible flows, we can define a reference pressure $p_0 \gg p_g$, the density only depends on the temperature (incompressible idea gas law)

$$\rho = \frac{p_0 + p_g}{(R_U/M)T} \approx \frac{p_0}{(R_U/M)T}$$

- ❖ For compressible flows, the gauge pressure is the absolute pressure (reference pressure p_0 is 0) and the density is a function of both pressure and temperature

$$\rho = \frac{p_0 + p_g}{(R_U/M)T}$$

Density – Reference density



- ❖ At low flow speeds, if the buoyance force is large compared to others, it can make the solution unstable.

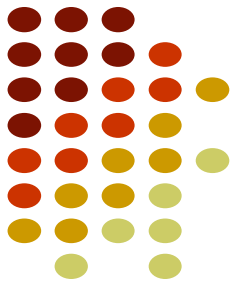
$$\frac{\partial}{\partial t}(\rho \bar{U}) + \nabla \cdot (\rho \bar{U} \bar{U}) = -\nabla p + \nabla \cdot \left(\mu \left(\nabla \bar{U} + (\nabla \bar{U})^T \right) \right) - \nabla \cdot \left(\frac{2}{3} \mu (\nabla \cdot \bar{U}) \right) I + \boxed{\rho g}$$

- ❖ A reference density is introduced to alleviate the buoyance force and improve the solution stability

$$\frac{\partial}{\partial t}(\rho \bar{U}) + \nabla \cdot (\rho \bar{U} \bar{U}) = -\nabla p + \nabla \cdot \left(\mu \left(\nabla \bar{U} + (\nabla \bar{U})^T \right) \right) - \nabla \cdot \left(\frac{2}{3} \mu (\nabla \cdot \bar{U}) \right) I + \boxed{(\rho - \rho_0) g}$$

- ❖ Reference density ρ_0 is usually set as the background density, but some CFD codes calculate it automatically as the average value of all mesh elements.

Density – the Boussinesq approx.



- ❖ Incompressible flow with small temperature variation, where the density is correlated to the thermal expansion coefficient and temperature rise relative to a reference temperature

$$\rho - \rho_0 = -\beta\rho_0(T - T_0)$$

- ❖ No reference density is needed



UNDER-RELAXATION

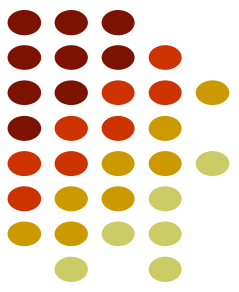
Oscillation and divergence are long-unsolved problems of CFD

Common methods for under-relaxation



- ❖ Under-relaxation factors (Explicit)
- ❖ Pseudo transient under-relaxation (Implicit)
- ❖ Courant number for transient flows

Relaxation

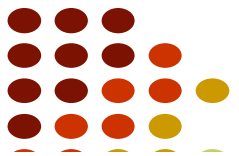


- ❖ The equations are solved iteratively: value of ϕ at cell P is recalculated from the value of last iteration.
- ❖ It is common to apply a relaxation fact U

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

- ❖ $U < 1$ is underrelaxation. This slows down convergence but increases stability.
- ❖ $U = 1$, no relaxation. The predicted value will be used.
- ❖ $U > 1$, overrelaxation. This accelerate convergence but decreases stability.

Under-relaxation factors



Task Page

Solution Methods

Pressure-Velocity Coupling

Scheme
SIMPLE

Spatial Discretization

Gradient
Least Squares Cell Based

Pressure
Second Order

Momentum
Second Order Upwind

Turbulent Kinetic Energy
First Order Upwind

Specific Dissipation Rate
First Order Upwind

Energy

Transient Formulation

☐ Non-Iterative Time Advancement

☐ Frozen Flux Formulation

☐ Warped-Face Gradient Correction

☐ High Order Term Relaxation Options...

Structure Transient Formulation

Default

Task Page

Solution Controls

Under-Relaxation Factors

Pressure
0.3

Density
1

Body Forces
1

Momentum
0.7

Turbulent Kinetic Energy
0.8

Specific Dissipation Rate
0.8

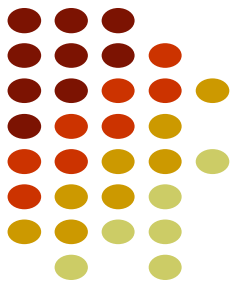
Turbulent Viscosity
1

Energy
1

Fluent-default under-relaxation factors for the segregated algorithms

- ❖ Underrelaxation factors are to suppress oscillations
- ❖ Small underrelaxation significantly slows down convergence and may cause “false convergence”.
- ❖ Always use large possible underrelaxations
- ❖ Try to stay with default underrelaxations
- ❖ Underrelax the pressure and momentum when necessary

Pseudo-transient under-relaxation



- ❖ The under-relaxation is controlled through the pseudo time step size (Δt)
- ❖ Auto pseudo time step is used in Fluent

$$\rho_p \Delta V \frac{\phi_p - \phi_p^{old}}{\Delta t} + a_p \phi_p = \sum_{nb} a_{nb} \phi_{nb} + b$$

Task Page

Solution Methods

Pressure-Velocity Coupling
Scheme: Coupled

Spatial Discretization
Gradient: Least Squares Cell Based
Pressure: Second Order
Momentum: Second Order Upwind
Turbulent Kinetic Energy: First Order Upwind
Specific Dissipation Rate: First Order Upwind
Energy: []

Transient Formulation
[] Non-Iterative Time Advancement
[] Frozen Flux Formulation
☒ Pseudo Transient
[] Warped-Face Gradient Correction
[] High Order Term Relaxation Options...
Structure Transient Formulation: []
Default

Task Page

Solution Controls

Pseudo Transient Explicit Relaxation Factors

Pressure: 0.5
Momentum: 0.5
Density: 1
Body Forces: 1
Turbulent Kinetic Energy: 0.75
Specific Dissipation Rate: 0.75
Turbulent Viscosity: 1
Energy: 0.75

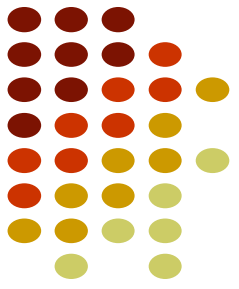
Advanced Solution Controls

Multigrid Multi-Stage Expert

Spatial Discretization Limiter
Limiter Type: Standard
[] Cell to Face Limiting
[] Cell to Cell Limiting
[] Apply Limiter Filter

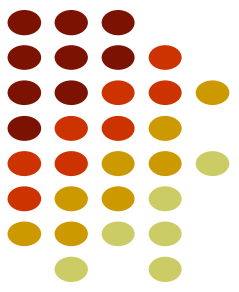
Pseudo Transient Method Usage

	On/Off	Under-Relaxation Factor	Time Scale Factor
Turbulent Kinetic Energy	<input checked="" type="checkbox"/>	0.8	1
Specific Dissipation Rate	<input checked="" type="checkbox"/>	0.8	1
Energy	<input checked="" type="checkbox"/>	1	1



CONVERGENCE CONTROL

Residuals



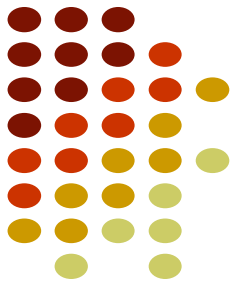
Different package use different residuals

- ❖ Absolute residual $R_P = \left| a_P \phi_P - \sum a_{nb} \phi_{nb} - b \right|$
- ❖ Scaled residual $R_{P,scaled} = \frac{\left| a_P \phi_P - \sum a_{nb} \phi_{nb} - b \right|}{\left| a_P \phi_P \right|}$
- ❖ Normalised residual $R_{P,scaled} = \frac{\left| a_P \phi_P - \sum a_{nb} \phi_{nb} - b \right|}{\left| a_{\max} \phi_{\max} \right|}$
- ❖ Overall residual of ϕ $R^\phi = \frac{\sum \left| a_P \phi_P - \sum a_{nb} \phi_{nb} - b \right|}{\sum \left| a_P \phi_P \right|}$

Convergence

- ❖ Solution does not change with additional iterations
- ❖ Targeted scaled residual $1.0\text{E-}3 \sim 1.0\text{E-}4$
- ❖ Monitor residuals

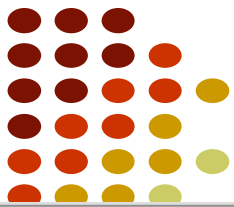
Monitor the residuals



Residuals

- ❖ More equations, higher residuals
- ❖ If the residuals have met the specified criteria but are still decreasing, the solution may not yet be converged.
- ❖ If all the residuals never meet the criteria but no longer decreasing, the solution is converged.
- ❖ Low residuals do not always mean a correct solution and high residuals do not automatically mean a wrong solution.
- ❖ High residuals are generally with higher-order discretisation – this does not mean 1st-order interpolation is better.

Monitor the fields and variables



- ❖ Monitor the flow/temperature fields during the run
- ❖ Monitor physically meaningful variables: force, etc
- ❖ **Flat and stable**

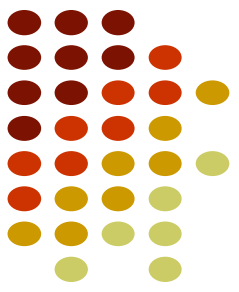
The screenshot shows the 'Force Report Definition' dialog box. It has a title bar with a blue 'F' icon and the text 'Force Report Definition'. The dialog is divided into several sections:

- Name:** A text field containing 'report-def-1'.
- Options:** A section with a checkbox 'Per Zone' (unchecked) and a dropdown 'Average Over (Iterations)' set to '1'.
- Force Vector:** A section with three input fields for X, Y, and Z, containing '1', '0', and '0' respectively.
- Report Files [0/0]:** A section with a list box and three icons (list, checkmark, delete).
- Report Plots [0/1]:** A section with a list box containing 'report-def-0-rplot' and three icons (list, checkmark, delete).
- Create:** A section with checkboxes for 'Report File' (unchecked), 'Report Plot' (unchecked), 'Print to Console' (unchecked), and 'Create Output Parameter' (unchecked).
- Frequency:** A dropdown set to '1'.
- Highlight Zones:** A checkbox (unchecked).

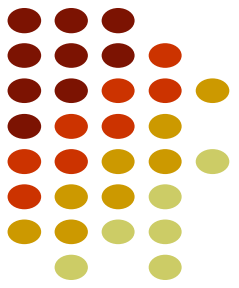
On the right side of the dialog, there is a 'Wall Zones' section with a 'Filter Text' input field and four icons (list, dropdown, checkmark, delete). Below this is a list box containing the following items: 'carbody', 'floor', 'spoiler', 'walls', and 'wheels'. The 'wheels' item is currently selected and highlighted.

At the bottom of the dialog are four buttons: 'OK', 'Compute', 'Cancel', and 'Help'.

KEY TAKEAWAYS



- ❖ Integral conservation equation applied to control volumes
- ❖ Variables at cell faces are found through interpolation
- ❖ Mesh must be refined to reduce “smearing” and false diffusion
- ❖ In incompressible flows, the density can be calculated using the equation of state or Boussinesq approximation
- ❖ SIMPLE is an iterative algorithm to couple the pressure and velocity
- ❖ Underrelaxation is good for convergence, but can cause “false convergence”
- ❖ Different ways to monitor solution: residual, variable plot, flat and stable



Q&A TIME