# 5. FVM discretization and Solution Procedure

1. The fluid domain is divided into a finite number of control volumes (cells of a computational grid).
2. Integral form of the conservation equations are discretized and applied to each of the cells.
3. The objective is to obtain a set of linear algebraic equations, where the total number of unknowns in each equation system is equal to the number of cells.
4. Solve the equation system with an solution algorithm with proper equation solvers.

# Discretization– *Solution Methods*

We want to transform the partial differential equations (PDE) to a set of algebraic equations:

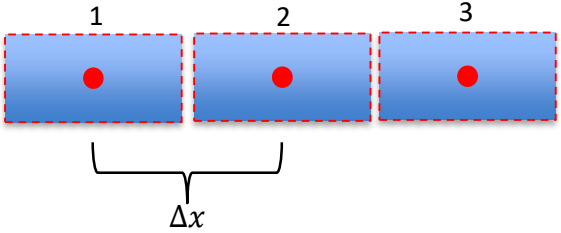
With Finite Volume Methods, the equation is first integrated. This is different from Finite Difference Method where the derivatives are approximated by truncated Taylor series expansions.

Advantage with FDM is it is easy to use, but is limited to structured grids (simpler geometry).

# Discretization– *FDM vs. FVM*

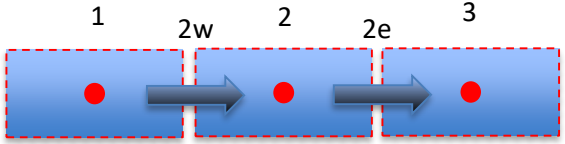
The key difference is Gauss' theorem

## FDM



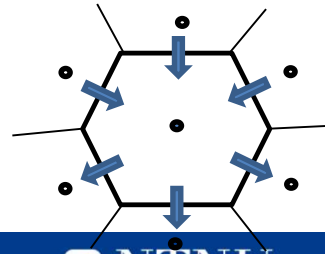

$$\left(\frac{d\phi}{dx}\right)_2 \approx \frac{\phi_2 - \phi_1}{\Delta x}$$

## FVM




$$\int_{CV_2} \frac{d\phi}{dx} dV \approx (\phi A)_{2e} - (\phi A)_{2w}$$

$$= \left(\frac{\phi_3 - \phi_2}{\Delta x}\right) - \left(\frac{\phi_2 - \phi_1}{\Delta x}\right)$$





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# Conservation Equations

We have the conservation equations:

- Mass (mass is conserved)
- Momentum (The sum of forces equals the time rate of change of momentum)
- Energy (Energy can not be created nor destroyed)

*These equations can be expressed as a single generalized transport equation*

# Discretization– *transport equation*

$$\underbrace{\frac{\partial(\rho\phi)}{\partial t}}_{\text{Transient}} + \underbrace{\frac{\partial}{\partial x_j}(\rho u_j \phi)}_{\text{Convective}} = \underbrace{\frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right)}_{\text{Diffusive}} + \underbrace{S_\phi}_{\text{Source}}$$

$\phi = 1$ gives continuity (mass)

$\phi = u$ gives momentum

$\phi$ can also be temperature or other scalars, but need to check if the equation is still satisfied.

Source terms can be external body forces, like gravity. Observe also that the pressure gradient is included in $S_\phi$ for momentum

# Solution procedure – *momentum equations*

Insertion of velocity in the transport equation gives us transport of momentum. The resulting equation requires different treatment than transport of any scalar (like temperature) because of the following reasons:

1. The convective terms are non-linear since they contain $U^2$
2. All equations are coupled because velocity component appears in all
3. Momentum equation contain a pressure gradient (inside source term) without an own explicit equation for pressure in the equation set

# Discretization– *Finite Volume Method*

The equation is first integrated.

Discretization is done in the second step.

When it's integrated, Gauss' theorem is applied and the net fluxes on cell faces must be expressed from values at the cell centers using interpolation.

Advantage is flexibility with regard to cell geometry. Advantage in less memory usage. There are also well developed solvers for this method.

FVM has the broadest applicability of all CFD methods.

# Discretization– *integration of transport equation*

Integrated over the cell volume:

$$\int_{\Delta V} \frac{\partial(\rho\phi)}{\partial t} dV + \int_{\Delta V} \frac{\partial}{\partial x_j}(\rho u_j \phi)\, dV + \int_{\Delta V} \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right) dV + \int_{\Delta V} S_\phi\, dV$$

The second and third terms can be expressed as fluxes (Gauss' theorem). That is transport across the CV boundaries.

If the time term is included, we must integrate in time as well.

# Discretization FVM– *discrete transport equation*

$$\int_{CV} \frac{\partial(\rho\phi)}{\partial t} dV \approx \frac{(\rho\phi V)^{n+1} - (\rho\phi V)^{n}}{\Delta t}$$

$$\int_{A} \frac{\partial}{\partial x_j}(\rho \boldsymbol{u}\phi)\ dA \approx \sum_{f} (\rho\phi \boldsymbol{u} \cdot \boldsymbol{n})_f$$

$$\int_{A} \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right) dA \approx \sum_{f} \left(\Gamma \frac{\partial \phi}{\partial x_j} \cdot \boldsymbol{n}\right)_f$$

# Discretization– *system of equations*

We have already mentioned that we wish to discretize the PDE's and express them as linear algebraic equations of the form:

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

Solving these set of equations (for each cell) requires an equation solver. If the algebraic equations are non-linear they may be linearized.

In addition to having an efficient solver for the algebraic equations, we need a solution algorithm solves the equations in the correct order.

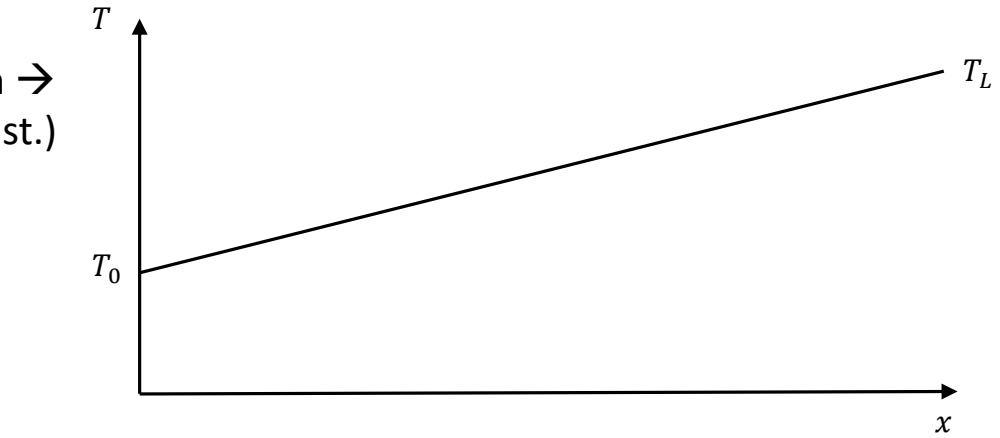
# A simple numerical example

(On blackboard)

Steady-state one-dimensional diffusion equation:

$$\frac{d}{dx}\left(\Gamma\frac{d\phi}{dx}\right)=0$$

Solution → (if $\Gamma$ const.)




$\phi$ can be temperature,
and $\Gamma$ thermal conductivity.

# A simple numerical example - *Physics*

Classification of the problem:

1. What does this equation describe if $\phi$ is temperature?
2. $k$ is a function of temperature, but can be taken as constant in many situations

Physical boundary conditions:

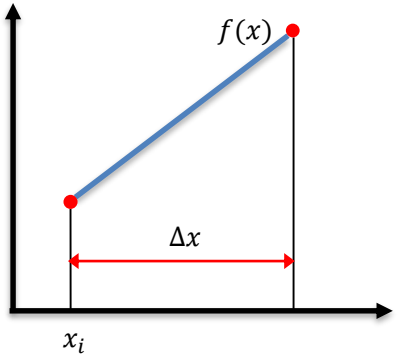
1. Dirichlet: $T = const.$ -> constant temperature

2. Neumann: $\frac{dT}{dx} = const.$ -> constant heat flux, constant normal temperature gradient

# Derivative vs. Numerical

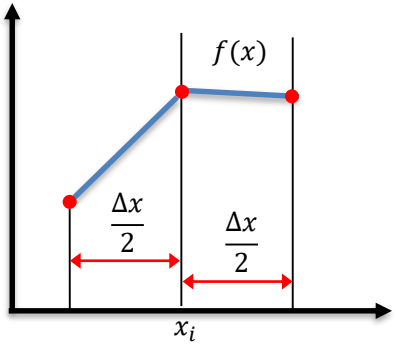
Definition derivative of function $f = f(x)$:

$$\frac{\partial f}{\partial x} = C_1 \rightarrow f(x) = C_1 \cdot x + C_2 \rightarrow \frac{\partial f}{\partial x} \approx \frac{\Delta f}{\Delta x}$$




$$\frac{\partial^2 f}{\partial x^2} = C_1 \rightarrow \frac{\partial f}{\partial x} = C_1 \cdot x + C_2 \rightarrow f(x) = C_1 \cdot \frac{x^2}{2} + C_2 \cdot x + C_3$$

$$\rightarrow \frac{\partial^2 f}{\partial x^2} \approx \frac{\Delta\left(\frac{\partial f}{\partial x}\right)}{\Delta x} = \frac{\left(\frac{\partial f}{\partial x}\right)_2 - \left(\frac{\partial f}{\partial x}\right)_1}{\Delta x} = \frac{\left(\frac{\Delta f}{\Delta x/2}\right)_2 - \left(\frac{\Delta f}{\Delta x/2}\right)_1}{\Delta x}$$



# Approximation of the first derivative, the FDM approach

Forward-differences (FD), 1st order accuracy:

$$\left(\frac{d\phi}{dx}\right)_i \approx \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} = \frac{\phi_{i+1} - \phi_i}{\Delta x}$$

Backward-differencing (BD), 1st order:

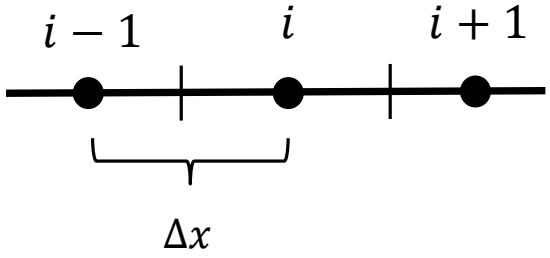
$$\left(\frac{d\phi}{dx}\right)_i \approx \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}} = \frac{\phi_i - \phi_{i-1}}{\Delta x}$$

Central-differencing (CD), 2nd order:

$$\left(\frac{d\phi}{dx}\right)_i \approx \frac{\phi_{i+1} - \phi_{i-1}}{x_{i+1} - x_{i-1}} = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$

CD with higher order is normally applied to diffusion terms

Local interior grid



# Approximation of the second derivative…

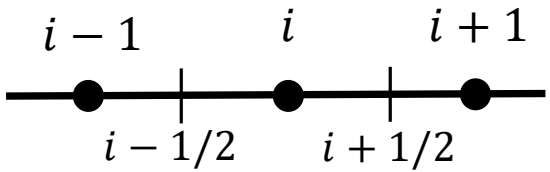
Evaluate the inner derivative at half-way between nodes, and central differences with $\Delta x$ spacing for the outer derivative:

$$\left[\frac{d}{dx}\left(\Gamma\frac{d\phi}{dx}\right)\right]_i \approx \frac{\left(\Gamma\frac{d\phi}{dx}\right)_{i+1/2} - \left(\Gamma\frac{d\phi}{dx}\right)_{i-1/2}}{\Delta x}$$

Where

$$\left(\frac{d\phi}{dx}\right)_{i+1/2} \approx \frac{\phi_{i+1}-\phi_i}{\Delta x}, \left(\frac{d\phi}{dx}\right)_{i-1/2} \approx \frac{\phi_i-\phi_{i-1}}{\Delta x}$$

Local interior grid



# Approximation of the second derivative (FDM)

Evaluate the inner derivative at half-way between nodes, and central differences with $\Delta x$ spacing for the outer derivative:

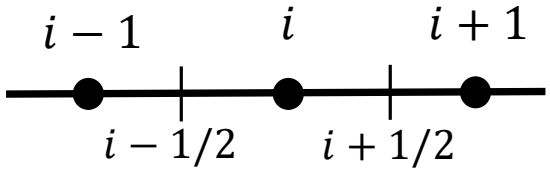
$$\left[\frac{d}{dx}\left(\Gamma\frac{d\phi}{dx}\right)\right]_i \approx \frac{\Gamma_{i+1/2}\dfrac{\phi_{i+1}-\phi_i}{\Delta x} - \Gamma_{i-1/2}\dfrac{\phi_i-\phi_{i-1}}{\Delta x}}{\Delta x}$$

$$\Gamma_{i+1/2} \approx \frac{\Gamma_i + \Gamma_{i+1}}{2}$$

If $\Gamma = const.$:

$$= \frac{-2\phi_i + \phi_{i+1} + \phi_{i-1}}{\Delta x^2}$$

Local interior grid



# Resulting equation system

We wish to express the resulting system in a form

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

With constant $\Gamma$ we get:

$$2 \cdot \phi_i - \phi_{i+1} - \phi_{i-1} = 0$$

$A_i = 2, A_{nb} = 1$ and $Q_i = 0$

# Resulting equation system

$\phi_1 = \phi_0$
$2\,\phi_2 - \phi_1 - \phi_3 = 0$
$2\,\phi_3 - \phi_2 - \phi_4 = 0$
……..
$\phi_N = \phi_L$

On a structured mesh (FDM), mesh and the equation matrix is much of the same thing.

A x = b

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} * \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \end{bmatrix} = \begin{bmatrix} \phi_0 \\ 0 \\ 0 \\ 0 \\ \phi_L \end{bmatrix}$$

# Discretization– *Finite-Volume Approach*

$$\int_{\Delta V} \frac{d}{dx}\left(\Gamma \frac{d\phi}{dx}\right) dV = \left(\Gamma A \frac{d\phi}{dx}\right)_e - \left(\Gamma A \frac{d\phi}{dx}\right)_w = 0$$

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

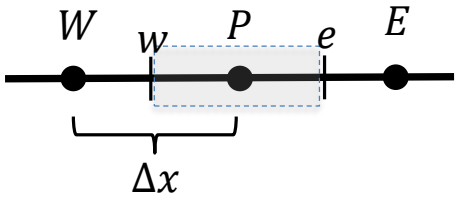
Fluxes

$$\left(\Gamma A \frac{d\phi}{dx}\right)_e = \Gamma_e A_e \left(\frac{\phi_E - \phi_P}{\Delta x_{PE}}\right)$$

$$\left(\Gamma A \frac{d\phi}{dx}\right)_w = \Gamma_w A_w \left(\frac{\phi_P - \phi_W}{\Delta x_{WP}}\right)$$

Central differences

Local interior grid



# Discretization– *Finite-Volume Approach*

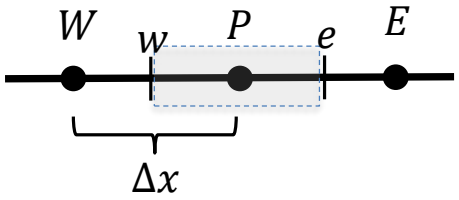
Express on this form (algebraic equation):

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

$$\frac{\Gamma_e A_e}{\Delta x_{PE}} (\phi_E - \phi_P) - \frac{\Gamma_w A_w}{\Delta x_{WP}} (\phi_P - \phi_W) = 0$$

$$\underbrace{\left( \frac{\Gamma_e A_e}{\Delta x_{PE}} + \frac{\Gamma_w A_w}{\Delta x_{WP}} \right)}_{a_P} \phi_P = \underbrace{\frac{\Gamma_e A_e}{\Delta x_{PE}}}_{a_E} \phi_E + \underbrace{\frac{\Gamma_w A_w}{\Delta x_{WP}}}_{a_W} \phi_W + \underbrace{0}_{S_P}$$

Local interior grid




Fluxes

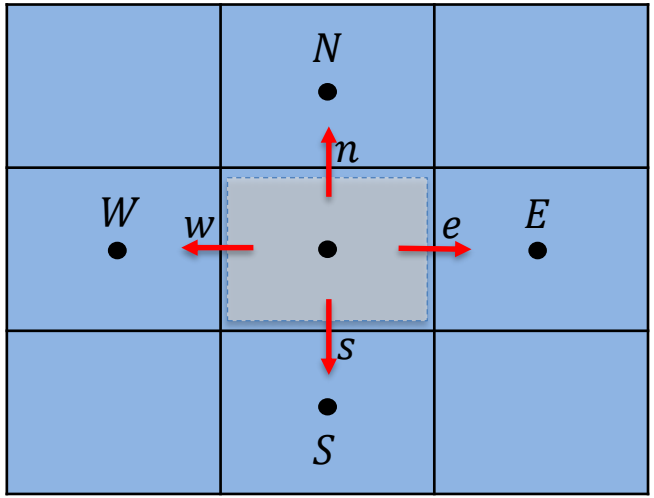
# Discretization– *2D Diffusion fluxes*

$$\int_{\Delta V} \frac{d}{dx}\left(\Gamma \frac{d\phi}{dx}\right) dV = \left[\left(\Gamma A \frac{d\phi}{dx}\right)_e - \left(\Gamma A \frac{d\phi}{dx}\right)_w\right] + \left[\left(\Gamma A \frac{d\phi}{dx}\right)_n - \left(\Gamma A \frac{d\phi}{dx}\right)_s\right]$$

Its a CV equation just like we showed earlier. Flux *in* equals *out*

Approximating face absolute values and derivatives poses similar problems as in FDM.

Need discretization of $\frac{\partial \phi}{\partial x}$



# Discretization– *1D Convection fluxes*

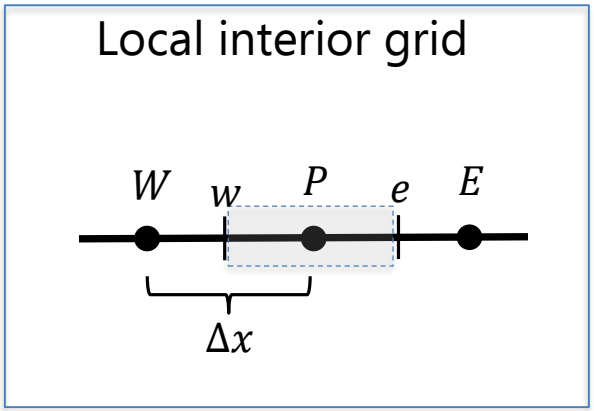
$$\int_{\Delta V} \frac{d}{dx}(\rho u \phi) dV = A_e(\rho u \phi)_e - A_w(\rho u \phi)_w$$

Dealing with these terms are not straightforward, and central differences as for the diffusion leads to unphysical results for high velocities.

Introduction of the Peclet number:

$$Pe = \frac{\rho u}{\Gamma/\Delta x}$$

Expresses ratio between *convection* and *diffusion*



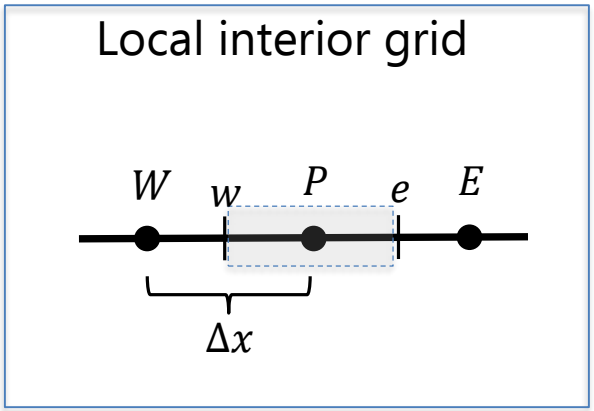
# Discretization– *1D Convection fluxes*

The right discretization scheme is important for the convective fluxes at high *Peclet* numbers.

Different alternatives:

First-order upwind scheme: $\phi_e = \phi_P$ (if $(\rho u \phi)_e > 0$)
Second-order upwind
Hybrid scheme: Combination of central- and upstream
QUICK scheme

General: Central differences only if $Pe < 2$
If large *Peclet* numbers, use the upstream value



# Solution – *Residuals*

Convergence criteria when solving:

$$\frac{\sum_{nb} a_{nb}\phi_{nb} + S_\phi - a_P\phi_P}{a_P\phi_P} < \epsilon \quad \text{(small number)}$$

# Solution – *Residuals*

Decreasing residuals means the solution may not be converged

If they flatten out and have a low value, like *1E-4* or lower we may assume that convergence have been reached. But this depends on the case. Increasing residuals is normally a bad sign.

Correct residuals only mean that our algebraic equation system have been solved, not that the solution is correct.

Other variables should be monitored as well to judge convergence (forces, moment, temperature)

# Solution procedure – *Solution algorithms*

Pressure-velocity coupling is a general problem that must be dealt with. Solution algorithm SIMPLE is an example of an algorithm that considers this issue.

SIMPLE belongs to the family of solvers called pressure-based solvers

In Star CCM+, there are two pressure-based solution algorithms available, Segregated and Coupled

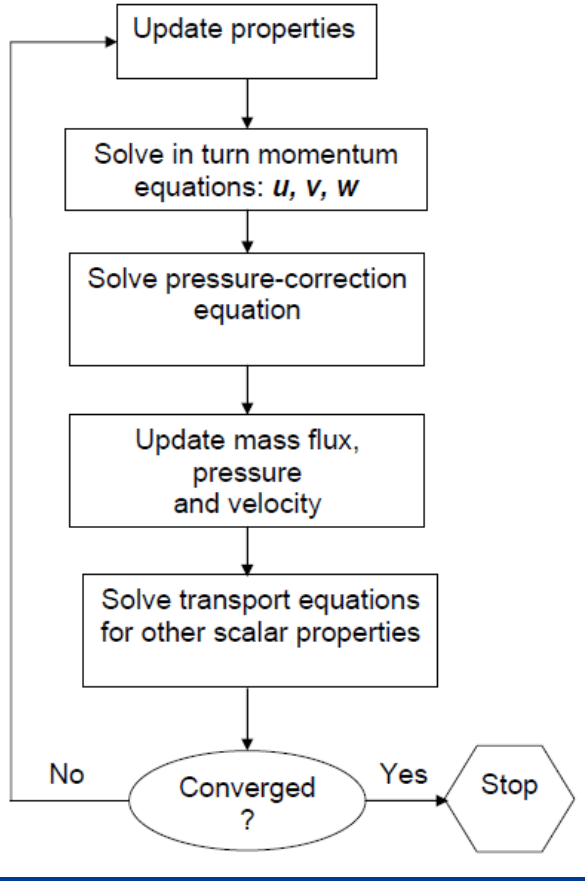
# Solution procedure – Segregated algorithm

Use less memory, but more time required for convergence

- Equations of different variables solved in a sequential manner (*u, v, w, p*)

- Uses a pressure-velocity coupling algorithm
- Two such algorithms implemented: SIMPLE & PISO

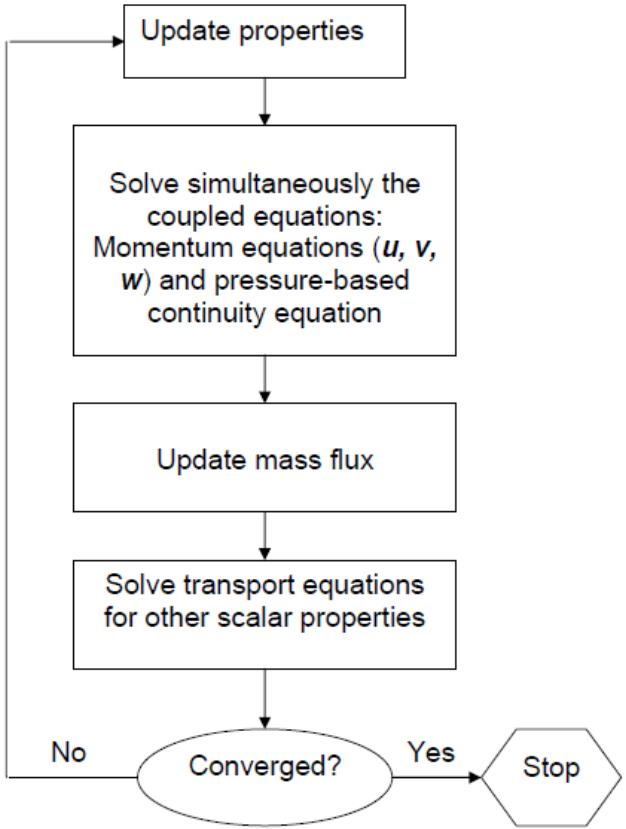
- Not suitable for flows with variable density. Suitable for incompressible flow.



# Solution procedure – Coupled algorithm

Use more memory, but less time required for convergence

- Equations solved simultaneously as a vector of equations.
- Suitable for variable density and compressible flow or natural convection problems



# Solution procedure – *Choice in Star CCM+*



## Choosing Between Coupled and Segregated

To guide the choice between the Segregated Flow model and the Coupled Flow model, consider their relative strengths and weaknesses.

- The segregated algorithm uses less memory than the coupled.
- The coupled algorithm yields more robust and accurate solutions in compressible flow, particularly in the presence of shocks.
- The coupled algorithm is more robust for high-Rayleigh number natural convection.
- The number of iterations that the coupled algorithm requires to solve a given flow problem is independent of mesh size. However, the number of iterations that the segregated algorithm requires increases with mesh size.
- In some situations the coupled algorithm can be combined with the implicit solver to permit large CFL numbers. This scenario would be analogous to an under-relaxation factor of 1 for all variables in a segregated algorithm. In contrast, the segregated algorithm needs significant under-relaxation for both velocity and pressure and, in compressible flows, energy.

With these strengths and weaknesses in mind, it is suggested that you proceed as follows to select the algorithm:

- Choose the Coupled Flow and Coupled Energy models for compressible flows, natural convection problems, and flows with large body forces or energy sources.
- If computational resources are not an issue, choose the Coupled Flow model for incompressible and/or isothermal flows.
- Choose the Segregated Flow model for incompressible or mildly compressible flows.

**See Also**

Modeling Flow and Energy Using a Coupled Approach

Modeling Flow Using a Segregated Approach

# Solution – *Residuals*

## Judging Convergence

Residual monitor plots are useful for judging the convergence (or divergence) of a solution.

Residual monitor plots are useful for judging the convergence (or divergence) of a solution, and they are created automatically within every simulation. However, it is important to understand both the significance of residuals and their limitations. While it is true that the residual quantity tends toward a small number when the solution is converged, the residual monitors cannot be relied on as the only measure of convergence. The limitations of residuals are as follows:

- The amount that a residual decreases by depends on the particulars of the simulation. Therefore, a three-order-of-magnitude drop in residuals is possibly acceptable for one simulation, but not another. The initial guess also strongly influences the amount that residuals are reduced. If the initial solution satisfies the discretized equations perfectly, the residuals do not drop at all.
- There are two types of discretization errors: dissipative errors and dispersive errors. Dissipative errors are characteristic of first-order upwind schemes; they are inherently stabilizing and produce residual plots that tend to decrease monotonically. Dispersive errors are characteristic of second-order upwind schemes which tend to "smear" solutions less than first-order schemes. While dispersive errors tend to produce residual plots that are not monotonic. This outcome is generally an acceptable price to pay for the enhanced accuracy.

  In some cases, often because of poor mesh quality, dispersive errors result in oscillating solutions (that is, changing from one iteration to the next) within a few cells. The result is that the residual plots can indicate that the solution is not "converged". You have a choice to either accept the solution, or to try to stabilize it by choosing a lower-order numerical scheme. Frequently, it is better to accept the solution.
- Residuals do not necessarily relate to quantities of engineering interest in the simulation such as integrated forces, pressure losses, or mass flow rates.

With the issues above in mind, it is advisable to monitor quantities of engineering interest, such as integrated forces, pressure changes, or mass flow rates as well as the residuals. STAR-CCM+ features such as scenes and plots can help you examine these quantities while the solution progresses. The features are described in detail in the chapter on analyzing.

The choice of the engineering quantity, as well as the convergence criterion, is your judgment call. In the example below, taken from a large external aerodynamics solution, both lift and drag coefficients are monitored as well as the residuals. It is clear that not all quantities reach an asymptotic limit at the same time. Use your judgment and decide which coefficient is the most critical.

# Suggested Reading

- User Guide Star CCM+
  - User Guide > Modeling Physics > Modeling Flow and Energy
  - User Guide > Modeling Physics > Solving Transport Equation

- Krasilnikov section 5.3 & 5.4