Numerical solution of Navier-Stokes Equations

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Contents

Objective:

Learning how to solve Navier-Stokes equations.

Hypothesis:

- Laminar flow
- Incompressible flow
- Newtonian fluid
- Boussinesq hypothesis
- Negligible viscous dissipation, compression or expansion work
- Non-participating medium in radiation
- Mono-component and mono-phase fluid

Equations to solve

Continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

Momentum equations

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \frac{\mu}{\rho}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) - \beta g_x (T - T_{ref})$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \frac{\mu}{\rho}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2}\right) - \beta g_y (T - T_{ref})$$

$$\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + w\frac{\partial w}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial z} + \frac{\mu}{\rho}\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) - \beta g_z (T - T_{ref})$$

Energy equation

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} + w\frac{\partial T}{\partial z} = \frac{\lambda}{\rho c_p}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right)$$

NS-Equations characteristics

They are partial coupled partial differential equations. The unknowns are the pressure, temperature, and velocity components. Appropriate boundary and initial conditions are required to close the problem.

Two strong coupling characterise this equations system:

- Pressure-velocity. There is no specific pressure equation. For incompressible flows, the pressure is the field that makes the velocity accomplish the mass conservation equation.
- Temperature-velocity. This coupling is only present for natural convection, mixed convection or temperature dependent physical properties.

Abbreviated notations

Cartesian tensorial notation: repeated index means summation.

Continuity equation

$$\frac{\partial u_i}{\partial x_i} = 0$$

Momentum equation

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p_i}{\partial x_i} + \frac{\mu}{\rho}\frac{\partial}{\partial x_j}\left(\frac{\partial u_i}{\partial x_j}\right) + \beta(T - T_0)g_i$$

Energy equation

$$\frac{\partial T}{\partial t} + u_j \frac{\partial T}{\partial x_j} = \frac{1}{\rho c_p}\frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right)$$

More compact:

$$M(\vec{u}) = 0$$

$$\rho\frac{\partial \vec{u}}{\partial t} + C(u)\vec{u} + D\vec{u} + Gp = 0$$

$$\underbrace{\frac{\partial(\rho\phi)}{\partial t}}_{transient} + \underbrace{\frac{\partial(\rho u_j \phi)}{\partial x_j}}_{convection} - \underbrace{\alpha \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right)}_{diffusion} = \underbrace{S_\phi}_{source}$$

Parameters to replace in convection - diffusion equation.

Equation	ϕ	α	Γ	S
Continuity	1	0	0	0
Mom. in x	u	μ	1	$-\partial p_x/\partial x + \rho g_x \beta(T - T_\infty)$
Mom. in y	v	μ	1	$-\partial p_y/\partial y + \rho g_y \beta(T - T_\infty)$
Mom. in z	w	μ	1	$-\partial p_z/\partial z + \rho g_z \beta(T - T_\infty)$
Energy	T	$1/c_p$	λ	Φ/c_p

- Analytical solution to a PDE $-->$ continuous value of ϕ as function of x, y, z, t.
- Numerical solution $-->$ values of ϕ at a **discrete** number of **grid points, nodes, cell centroids**, etc.
- Process of converting PDE into a set of algebraic equations for ϕ is called **discretization process.**
- Conversion of PDEs into algebraic equations requires the discretization of space $-->$ **mesh generation.**

Development of numerical methods focusses on both the discretization process and a method to solve the set of obtained algebraic equations.

- **Accuracy** of numerical solution $--\ >$ discretization method.
- Solution methods determines if we are successful in obtaining a solution, and how much time and effort it will cost to us.
- No matter what discretization method is employed, all well-behaved discretization methods should tend to the exact solution when a large enough number of grid points is employed $--\ >$ **consistency**.

Finite difference method:

- Truncated Taylor series expansion.
- It does not explicity exploit conservation principle in deriving discrete equations,e.g. unstructured meshes.

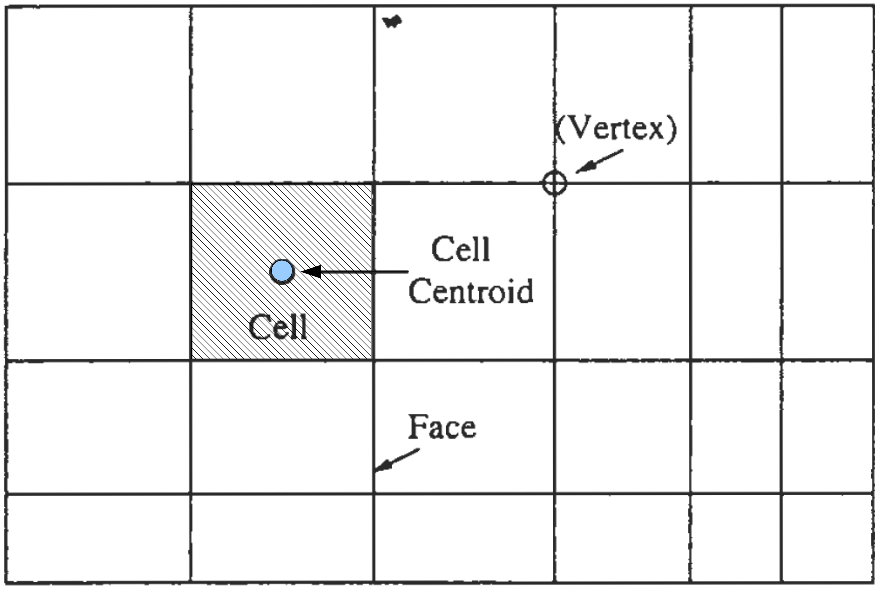
Finite element method:

- Galerkin method needs residual and weight functions.
- It does not enforce the conservation principle.

Finite(control) volume method:

- Divides the domain in to a finite number of non-overlapping cells or control volumes over which conservation of ϕ is enforce in a discrete sense.

Terminology:

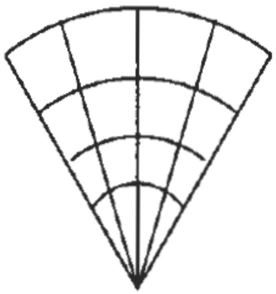


Cartesian grid

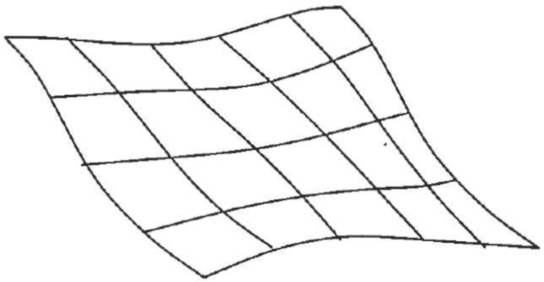
Mesh Types

Structured

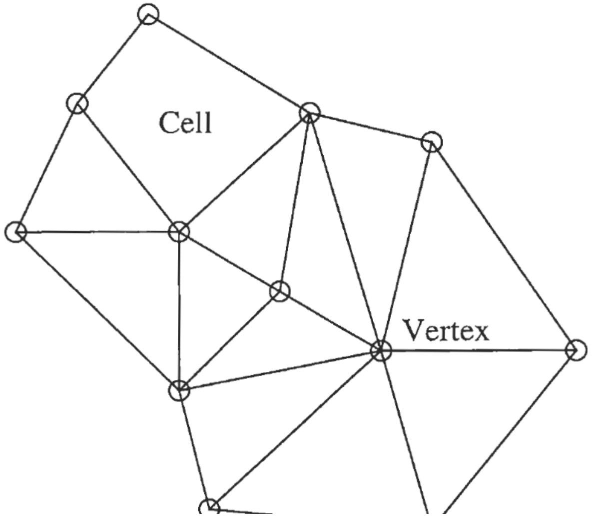
Orthogonal:
- Cartesian
- Cylindric
- Spheric



Body-fitted



Unstructured



Diffusion Equation

Diffusion Equation

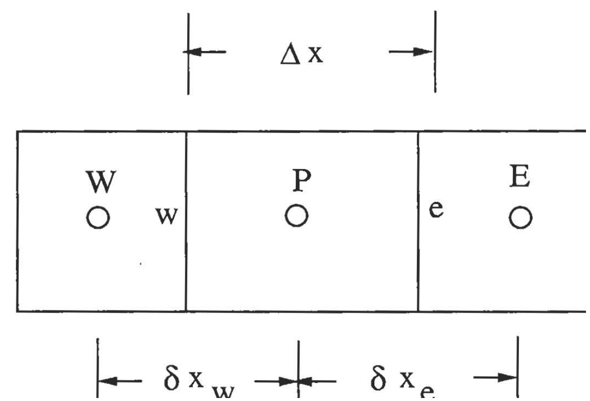
$$\underbrace{\rho\frac{\partial \phi}{\partial t}}_{transient} + \underbrace{\rho u_j \frac{\partial \phi}{\partial x_j}}_{convection} - \underbrace{\alpha \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right)}_{diffusion} = \underbrace{S_\phi}_{source}$$

Assuming steady state, one-dimensional x-direction variation and solid material (conduction):

$$\underbrace{\frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right)}_{diffusion} + \underbrace{S_\phi}_{source} = 0 \,, \qquad \Gamma = \lambda$$

Discretization

Solving fot temperature ($\phi = T$) and integrating on the cell associated to P:



$$\int_w^e \frac{d}{dx}\left(\Gamma \frac{dT}{dx}\right) dx + \int_w^e S dx = 0$$

$$\left(\Gamma \frac{dT}{dx}\right)_e - \left(\Gamma \frac{dT}{dx}\right)_w + \int_w^e S dx = 0$$

If we assume that T varies linearly between nodes, we have

$$\frac{\Gamma_e (T_E - T_P)}{\delta x_e} - \frac{\Gamma_w (T_P - T_W)}{\delta x_w} + S\Delta x = 0$$

This expression is no longer exact.

Collecting terms, we obtain

$$a_P T_P = a_E T_E + a_W T_W + b$$

where

$$\begin{aligned} a_E &= \Gamma_e / \delta x_e \\ a_W &= \Gamma_w / \delta x_w \\ a_P &= a_E + a_W \\ b &= S \Delta x \end{aligned}$$

- Conservation is guaranteed for each cell regardless of mesh size.
- Conservation does not guarantee accuracy.
- Cell balance is written in terms of face fluxes. Therefore, Γ needs to be interpolated to the faces.

Algebraic equation

The four rules

1. **Consistency at control-volume faces.** Quadratic approximation inconsistency and use of nodal properties.

2. **Positive coefficients.**

3. **Linearization of the source term.**

4. $a_p = \sum a_{nb}$

Interface Conductivity

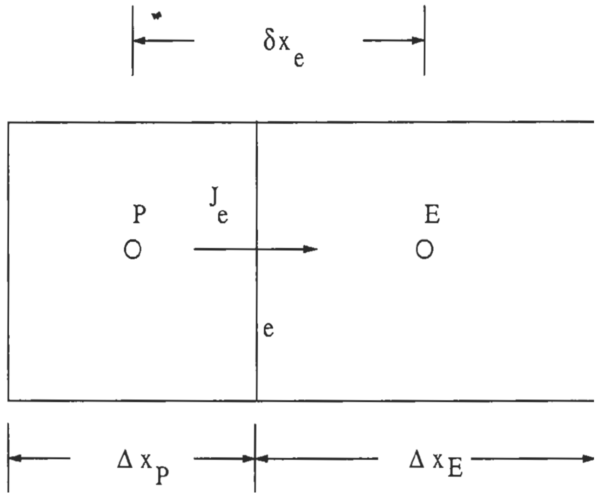
The simplest option is to interpolate Γ linearly as:

$$\Gamma_e = f_e \Gamma_P + (1 - f_e)\Gamma_E$$

where

$$f_e = \frac{0.5\Delta x_E}{\delta x_e}$$

Only valid if Γ is smoothly varying.



Harmonic interpolation Γ can be written as

$$\Gamma_e = \left(\frac{1 - f_e}{\Gamma_P} + \frac{f_e}{\Gamma_E} \right)^{-1}$$

With this interpolation, nothing special need be done to treat conjugate interfaces (solid-fluid, solid-solid,etc)

Boundary conditions

- Dirichlet

$$\begin{aligned} a_E = a_W &= 0 \\ a_B &= 1 \\ b &= \phi \end{aligned}$$

- Neumann

$$\begin{aligned} a_I &= 1 \\ a_B &= 1 \\ b &= 0 \end{aligned}$$

- Conjugate $\Gamma_B \frac{\phi_I - \phi_B}{\delta x_i} = h(\phi_B - \phi_\infty)$

$$\begin{aligned} a_I &= \Gamma_i / \delta x_i \\ a_B &= a_I + h \\ b &= h\phi_\infty \end{aligned}$$

Solvers

Solvers Types

$$A\phi = B$$

where A is the coefficient matrix, $\phi = [\phi_1, \phi_2, ...]^T$ is a vector of ϕ, and B is the vector of source terms.

Direct Methods

- Matrix inversion $\phi = A^{-1}B$.
- Large computational and storage requirements.
- A is sparse, for structured meshes is banded. For diffusion equation, the matrix is symmetric.
- Tri-Diagonal Matrix Algorithm (TDMA) takes advantage of these characteristics.
  - Matrix is upper-triangularized: entries below diagonal eliminated. The last eq. has only one unknown.
  - Back-substitution is carried out.

Iterative Methods: Gauss-Seidel

- Employ a guess-and-correct philosophy which progressively improves the guessed solution by repeated application.
- Overall solution loop:
  1. Guess ϕ at all grid points in the domain.
  2. Visit each grid point solving: $\phi_P = \frac{a_E\phi_E + a_W\phi_W + b}{a_P}$. Use last values available.
  3. Complete iteration covering all nodes.
  4. Check if appropriate convergence criterion is met. If true stop. Else, go to step 2.
- Complementary methods necessary to accelerate convergence.

Verification of the code:

- Bugs detection in the coding stage.
- Global balances, comparison with analytical solution, MMS,...

Verification and validation

Verification of the code:

- Bugs detection in the coding stage.
- Global balances, comparison with analytical solution, MMS,...

Verification of the numerical results:

- Detection of discretization errors
  due to numerical schemes and grid used.
- Two procedures:
  - Simple: Study the evolution of a global or local variable when grid is refined.
  - Detailed: Based on generalized Richardson extrapolation, and on the *Grid Convergence Index* (GCI).

Validation of the mathematical model:

- Reviewing that mathematical formulation reproduces the physical problem being investigated.
- Comparison with experimental or DNS data.

Programming Suggestions

- Underrelaxation.
- Source term linearization.
- Tanh function to concentrate the grid.

En algunos casos de interés es necesario tener mayor densidad de volumenes de control, en ciertas regiones del dominio estudiado; en un caso que será posteriormente relacionado, es importante tener más nodos hacia las orillas del dominio y con el propósito de lograr esto se define la distancia entre nodos de la siguiente manera; si tenemos una zona r de longitud L_r, localizada a una distancia x_r, del origen de coordenadas; las lineas correspondientes a Nr numero de volumenes de control estan distribuidas según las siguiente expresión:

$$xvc(i) = \delta + \frac{\Delta\delta}{2}\left[1 + \frac{\tanh\left(2k_{x(r)}\frac{\tilde{i}-1}{n} - k_{x(r)}\right)}{\tanh(k_{x(r)})}\right] \tag{1}$$

Verification and validation

where
$xvc(i)$: es la distancia a la cara del i-volumen de control en la dirección X.
i_r: es el primer nodo dentro de la zona r concentrada.
$k_{x(r)}$: es el factor de concentración en la dirección X.
Y dependiendo del tipo de concentración que se necesite tendremos:

Concentración simétrica:
$n = 2N_r,\ \delta = x_r,\ \Delta\delta = L_r,\ \tilde{i} = i - i_r + 1.$

Concentración lado derecho:
$n = 2N_r,\ \delta = x_r,\ \Delta\delta = 2L_r,\ \tilde{i} = i - i_r + 1.$

Concentración lado izquierdo:
$n = 2N_r,\ \delta = x_r - L_r,\ \Delta\delta = 2L_r,\ \tilde{i} = i + N_r - i_r + 1.$

De tal forma que podemos elegir todas las combinaciones posibles en que se deseen concentrar la malla.

$$\underbrace{\rho\frac{\partial\phi}{\partial t}}_{transient} + \underbrace{\rho u_j\frac{\partial\phi}{\partial x_j}}_{convection} - \underbrace{\alpha\frac{\partial}{\partial x_j}\left(\Gamma\frac{\partial\phi}{\partial x_j}\right)}_{diffusion} = \underbrace{S_\phi}_{source}$$

Hypothesis:

- One-dimensional unsteady conduction$-- > \phi = T$.
- $\Gamma = \lambda,\ \alpha = 1/c_p$.
- ρ and c_p constants. No source terms

$$\underbrace{\rho c_p\frac{\partial T}{\partial t}}_{transient} = \underbrace{\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)}_{diffusion}$$

Given T at $t -- >$ find T at $t + \Delta t$

Temporal Discretization

$$\rho c_p \int_w^e \int_t^{t+\Delta t} \frac{\partial T}{\partial t} dt dx = \int_t^{t+\Delta t} \int_w^e \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) dx dt$$

$$\rho c_p \int_w^e (T_P - T_P^0) dx = \int_t^{t+\Delta t} \left[\frac{\lambda_e (T_E - T_P)}{\delta x_e} - \frac{\lambda_w (T_P - T_W)}{\delta x_w}\right] dt$$

Assumption about how T_P, T_E, T_W vary in time required.
Euler (first order) approximation and weighting factor f:

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

$$\Downarrow$$

$$\rho c_p \frac{\Delta x}{\Delta t}(T_P - T_P^0) = f\left[\frac{\lambda_e (T_E - T_P)}{\delta x_e} - \frac{\lambda_w (T_P - T_W)}{\delta x_w}\right] + (1-f)\left[\frac{\lambda_e (T_E^0 - T_P^0)}{\delta x_e} - \frac{\lambda_w (T_P^0 - T_W^0)}{\delta x_w}\right]$$

$\Downarrow$ Rearranging

Temporal Discretization

$$a_P T_P = a_E[fT_E + (1-f)T_E^0] + a_W[fT_W + (1-f)T_W^0] + [a_P^0 - (1-f)a_E - (1-f)a_W]T_P^0$$

$$\Downarrow$$

$$a_E = \frac{\lambda_e}{\delta x_e}, \; a_W = \frac{\lambda_w}{\delta x_w}, \; a_P^0 = \frac{\rho c_p \Delta x}{\Delta t}, \; a_P = f a_E + f a_W + a_P^0$$

Explicit scheme $f = 0$

$$a_P T_P = a_E T_E^0 + a_W T_W^0 + [a_P^0 - a_E - a_W]T_P^0$$

$$\Uparrow$$

$$a_E = \frac{\lambda_e}{\delta x_e}, \; a_W = \frac{\lambda_w}{\delta x_w}, \; a_P^0 = \frac{\rho c_p \Delta x}{\Delta t}, \; a_P = a_P^0, \; b = S\Delta x + [a_P^0 - a_E - a_W]T_P^0$$

Notes:

- We can find T_P at time $t + \Delta t$ without solving a set of linear algebraic equations because right hand side of this equation contains values exclusively from the previous time.
- Unrealistic values when $a_P^0 \leq a_E + a_W$. This implies that a higher T_P^0 results in a lower T_P. Then for uniform conductivity and uniform mesh:

$$\Delta t < \frac{\rho c_p (\Delta x)^2}{2\lambda}$$

- Smaller time steps required as mesh is refined $\Longrightarrow$ long computational times.

Implicit scheme $f = 1$

$$a_P T_P = a_E T_E + a_W T_W + a_P^0 T_P^0$$

$$\Uparrow$$

$$a_E = \frac{\lambda_e}{\delta x_e},\ a_W = \frac{\lambda_w}{\delta x_w},\ a_P^0 = \frac{\rho c_p \Delta x}{\Delta t},\ a_P = a_E + a_W + a_P^0,\ b = S\Delta x + a_P^0 T_P^0$$

Notes:

- The solution at time $t + \Delta t$ requires the solution of a set of algebraic equations.
- There is not time step restriction. However, physical plausibility does not imply accuracy.

Closure Explicit Methods

- Euler method: $\phi^{t+\Delta t} = \phi^t + \Delta t R(t^t, \phi^t)$
- Second order Adams-Bashforth method:
  $\phi^{t+\Delta t} = \phi^t + \Delta t[3/2R(t^t, \phi^t) - 1/2R(t^{t-\Delta t}, \phi^{t-\Delta t})]$
  (homework: to obtain algebraic equation)
- Higher order methods

Two-Dimensional situations

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda \frac{\partial T}{\partial y}\right) + S$$

Discrete algebraic equation:

$$a_P T_P = a_E T_E + a_W T_W + a_N T_N + a_S T_S + b$$

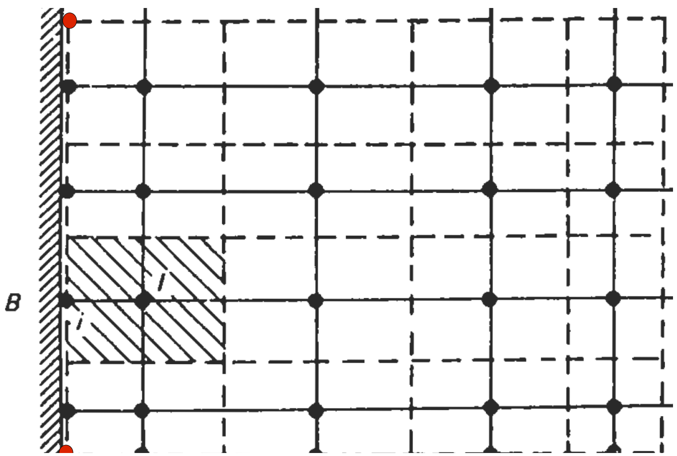
where

$$a_E = \frac{\lambda_e \Delta y}{\delta x_e}, \quad a_W = \frac{\lambda_w \Delta y}{\delta x_w},$$
$$a_N = \frac{\lambda_n \Delta x}{\delta y_n}, \quad a_S = \frac{\lambda_s \Delta x}{\delta y_s},$$
$$a_P^0 = \frac{\rho c_p \Delta x \Delta y}{\Delta t}, \quad b = S \Delta x \Delta y + a_P^0 T_P^0$$
$$a_P = a_E + a_W + a_N + a_S + a_P^0$$

$\Delta x \Delta y$ represents the volume of the control volume

Location of the Control-Volume Faces

- Grid points placed at centres of CVs
- Faces located midway between the nodes



Boundary nodes

- Boundary face passes through the boundary point
- Nodes located at the corners of the computational domain (dummy nodes)

Convection and Diffusion

Convection-Diffusion Equation

$$\underbrace{\rho \frac{\partial \phi}{\partial t}}_{transient} + \underbrace{\rho u_j \frac{\partial \phi}{\partial x_j}}_{convection} - \underbrace{\alpha \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right)}_{diffusion} = \underbrace{S_\phi}_{source}$$

Hypothesis:

- Steady one-dimensional situation.
- ρ and c_p constants. No source terms. Velocity field known
- $\Gamma = \Gamma \times \alpha$.

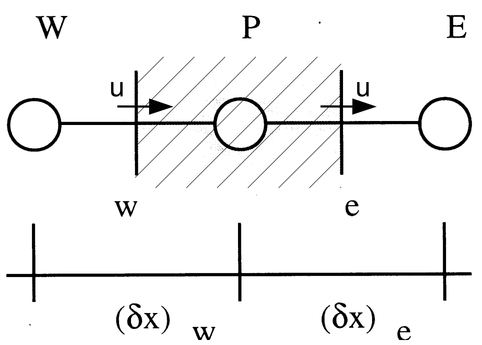
$$\underbrace{\frac{\partial (\rho u \phi)}{\partial x}}_{convection} = \underbrace{\frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right)}_{diffusion}$$

How do you evaluate convection term?

$$\int_w^e \frac{\partial(\rho u\phi)}{\partial x}dx = \int_w^e \frac{\partial}{\partial x}\left(\Gamma\frac{\partial\phi}{\partial x}\right)dx$$

$$\Downarrow$$

$$(\rho u\phi)_e - (\rho u\phi)_w = \left(\Gamma\frac{\partial\phi}{\partial x}\right)_e - \left(\Gamma\frac{\partial\phi}{\partial x}\right)_w$$



Central Differencing

If the grid is uniform and we assume a linear variation of ϕ, the result is

$$\phi_e = \frac{1}{2}(\phi_E + \phi_P) \text{ and } \phi_w = \frac{1}{2}(\phi_P + \phi_W)$$

Velocities are stored at CV faces and diffusion is expressed as before

$$\frac{1}{2}(\rho u)_e(\phi_E + \phi_P) - \frac{1}{2}(\rho u)_w(\phi_P + \phi_W) = \frac{\lambda_e(\phi_E - \phi_P)}{\delta x_e} - \frac{\lambda_w(\phi_P - \phi_W)}{\delta x_w}$$

We can define:

$$F \equiv \rho u, \;\; D \equiv \frac{\Gamma}{\delta x}$$

where F is the mass flow ($\pm$) and D is the diffusion conductance ($+$)

Central Differencing

$$a_P \phi_P = a_E \phi_E + a_W \phi_W$$

where

$$a_E = D_e - \frac{F_e}{2},\ a_W = D_w + \frac{F_w}{2}$$
$$a_P = a_E + a_W + (F_e - F_w)$$

Notes:

- Since by continuity $F_e = F_w$, we get the property $a_P = a_E + a_W$
- When $|F| > 2D$ then there is a possibility of a_E or a_W becoming negative
- For the case of zero diffusion $(\Gamma = 0) -- > a_P = 0$. Unsuitable for iterative methods
- We must seek better formulations to approximate convective terms. This is one of the CFD classic problems

Upwind Differencing

- We realize that the reason to find negative coefficients in the previous procedure is the aritmetic averaging
- In the upwind scheme, the face value of ϕ is set equal to the upwind node value

$$\begin{aligned} \phi_e &= \phi_P \text{ if } F_e \geqslant 0 \\ \phi_e &= \phi_E \text{ if } F_e < 0 \end{aligned}$$

- The value at the face is determined entirely by the mesh direction from which the flow is coming to the face
- If we define $F_e \phi_e = \phi_P MAX[F_e, 0] - \phi_E MAX[-F_e, 0]$, we obtain

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\end{aligned}
$$

- The value at the face is determined entirely by the mesh direction from which the flow is coming to the face
- If we define $F_e\phi_e = \phi_P MAX[F_e, 0] - \phi_E MAX[-F_e, 0]$, we obtain

$$
a_E = D_e + MAX[-F_e, 0], \; a_W = D_w + MAX[F_w, 0]
$$

$$
a_P = D_e + MAX[F_e, 0] + D_w + MAX[-F_w, 0] = a_E + a_w + (F_e - F_w)
$$

Notes:

- Highly diffusive: stable scheme, but generates false diffusion.
- First order scheme. It does not preserve energy.

Alternatives

- Low order schemes: they try to reproduce exact solution.
- High order schemes
- Spectrum consistent schemes

Exact solution

The one-dimensional convection diffusion equation can be solved analytically in $0 \leqslant x \leqslant L$, if Γ is constant, with the boundary conditions $\phi = \phi_0$ at $x = 0$ and $\phi = \phi_L$ at $x = L$ the solution is

$$\frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{exp(Px/L) - 1}{exp(P) - 1}$$

Where $P \equiv \frac{\rho u L}{\Gamma}$ is the Peclet number

If we replace $\phi_0 = \phi_P$, $\phi_L = \phi_E$ and $L = \delta x_e$ we will obtain the exact scheme (only in one-dimensional cases)

Low-Order Schemes

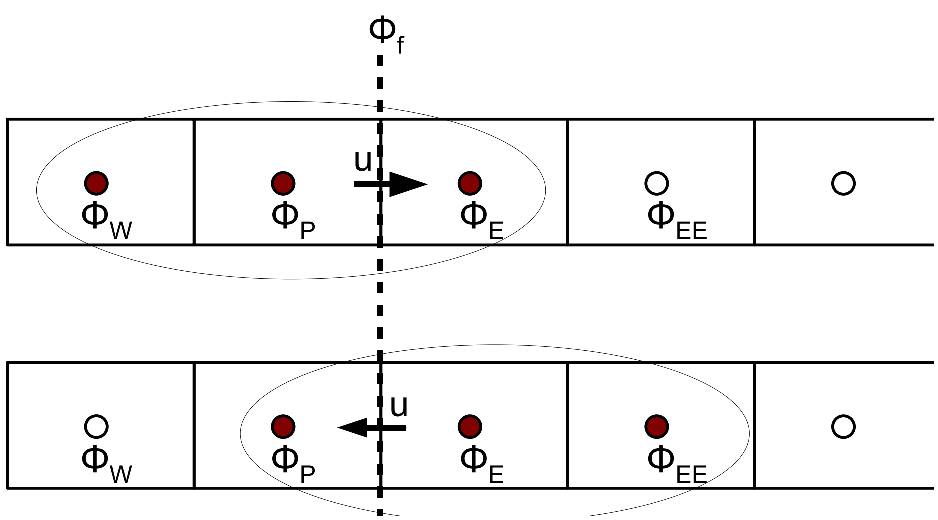
Some schemes follow the idea of reproducing exponential scheme, but using easy-to-compute functions.

- **Hybrid scheme:** Use two lines to approximate exact solution.
- **Power-Law scheme:** approximates the exact solution by means of fifth order polynomial curves.

Notes:

- There are small differences among them.
- They try to follow a solution which is exact only in one-dimensional situations.

- These schemes use two or more nodal values to evaluate variable at the cell face
- The number of CVs considered determines the order of the scheme
  - **Second order Upwind scheme:** linear extrapolatio of upstream values. Still diffusive
  - **Third order Quick scheme:** quadratic interpolation using two nodes upstream and one downstream
- Direction of the flow indicates which nodes are taken into account



High Order Schemes

- Considering uniform mesh we have

Scheme	Order	$\mathbf{u} \geq 0$	$\mathbf{u} < 0$
UDS	1	$\phi_f = \phi_P$	$\phi_f = \phi_E$
UDS2	2	$\phi_f = \frac{(3\phi_P - \phi_W)}{2}$	$\phi_f = \frac{(3\phi_E - \phi_{EE})}{2}$
QUICK	3	$\phi_f = \frac{(\phi_P + \phi_E)}{2} - \frac{\phi_E - 2\phi_P + \phi_W}{8}$	$\phi_f = \frac{(\phi_P + \phi_E)}{2} - \frac{\phi_P - 2\phi_E + \phi_{EE}}{8}$

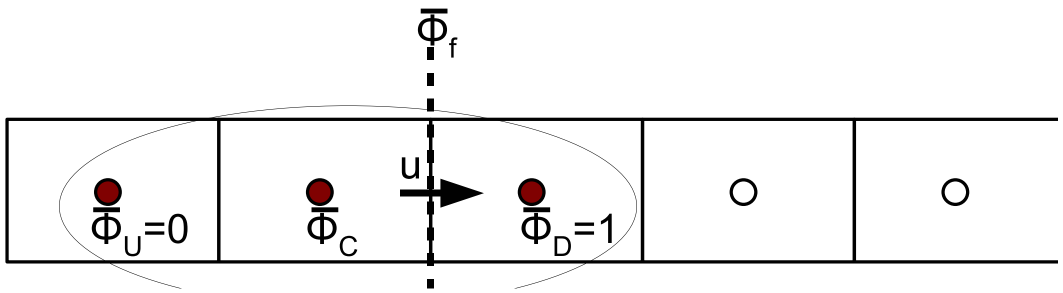
Exercise

Consider a one dimensional situation of length L, with a given velocity u. Compare exact solution with those obtained using UDS, UDS2 and QUICK schemes. Determine the mesh that gives grid independent solution for each case.

High Order Schemes

- Accurate numerical schemes suffer from instability. Then they have to be bounded or normalised by its nearest CV values

$$\bar{\phi}_f = \frac{\phi_f - \phi_U}{\phi_D - \phi_U}$$



- If the grid is non uniform, therefore, the cell face is not placed at the middle between two nodes, it is neccesary to introduce geometric variables. Then $\phi_f = \mathrm{f}(\phi_U, \phi_C, \phi_D, x_U, x_C, x_f, x_D)$
- Distances are also normalized

$$\bar{x} = \frac{x - x_U}{x_D - x_U} \qquad \Rightarrow \qquad \bar{\phi}_f = \mathrm{f}(\overline{\phi}_C, \overline{x}_C, \overline{x}_f)$$

Normalised High-Order Schemes

Scheme	Order	$\overline{\phi}_{\mathbf{f}}$	
UDS2	2	$\overline{\phi}_f = \frac{\overline{x}_f}{\overline{x}_C}\overline{\phi}_C$	
QUICK	3	$\overline{\phi}_f = \overline{x}_f + \frac{\overline{x}_f\left(\overline{x}_f - 1\right)}{\overline{x}_C\left(\overline{x}_C - 1\right)}\left(\overline{\phi}_C - \overline{x}_C\right)$	
SMART	2 - 4	$\overline{\phi}_f = \frac{\overline{x}_f(1-3\overline{x}_c+2\overline{x}_f)}{\overline{x}_c(1-\overline{x}_c)}\overline{\phi}_C$	if $0 < \overline{\phi}_C \leq \frac{\overline{x}_C}{3}$
mix of		$\overline{\phi}_f = \frac{\overline{x}_f\left(\overline{x}_f - \overline{x}_C\right)}{1-\overline{x}_C} + \frac{\overline{x}_f\left(\overline{x}_f - 1\right)}{\overline{x}_C\left(\overline{x}_C - 1\right)}\overline{\phi}_C$	if $\frac{\overline{x}_C}{3} < \overline{\phi}_C \leq \frac{(1+\overline{x}_f-\overline{x}_C)\overline{x}_C}{\overline{x}_f}$
UDS, CDS		$\overline{\phi}_f = 1$	if $\frac{(1+\overline{x}_f-\overline{x}_C)\overline{x}_C}{\overline{x}_f} < \overline{\phi}_C \leq 1$
UDS2, QUICK		$\overline{\phi}_f = \overline{\phi}_C$	otherwise

Since we want to keep our tri-diagonal structure the high order schemes are introduced into the general formulation by means of a deferred correction term.

$$F_e\phi_e^{UDS} - F_w\phi_w^{UDS} = D_e(\phi_E - \phi_P) - D_w(\phi_P - \phi_W) + \underbrace{F_e(\phi_e^{UDS} - \phi_e^{HS}) - F_w(\phi_w^{UDS} - \phi_w^{HS})}_{\text{source term}}$$

where ϕ_f^{HS} is the variable ϕ evaluated at the cell face f with high order numerical scheme

Notes:

- Term introduced explicitly
- Stability is reduced
- Easy to implement

Exercises revision

- One dimensional conduction
- One dimensional convection
- Adam-Bashforth discretization
- Meaning of Peclet number

Unsteady Two Dimensional Situations

General Convection-Diffusion

$$\underbrace{\rho\frac{\partial \phi}{\partial t}}_{\text{transient}} + \underbrace{\rho u_j \frac{\partial \phi}{\partial x_j}}_{convection} - \underbrace{\alpha\frac{\partial}{\partial x_j}\left(\Gamma\frac{\partial \phi}{\partial x_j}\right)}_{diffusion} = \underbrace{S_\phi}_{\text{source}}$$

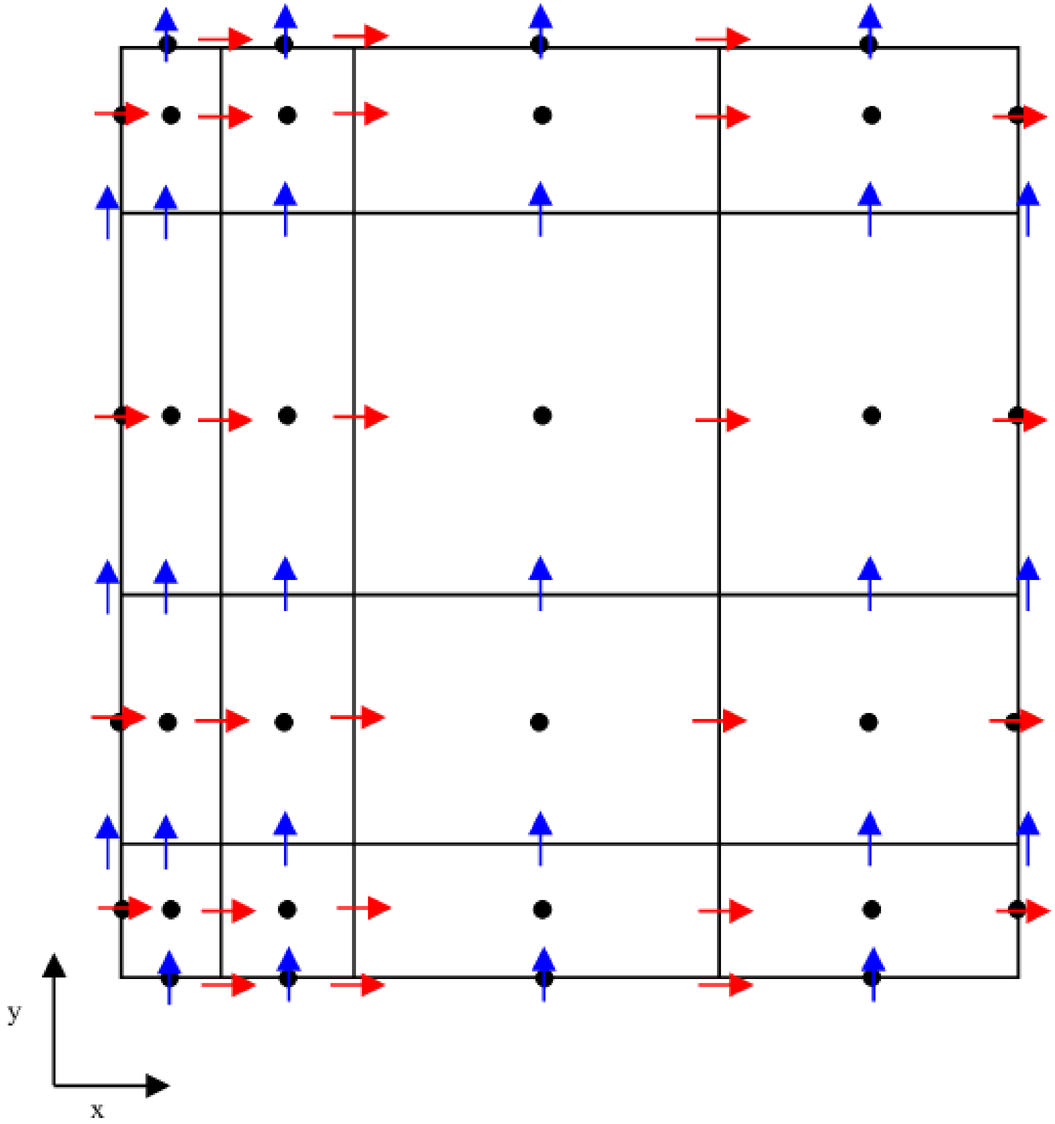
Hypothesis:

- Transient two-dimensional situation.
- ρ and c_p constants. Velocity field known
- $\Gamma = \Gamma \times \alpha$.

$$\underbrace{\rho\frac{\partial \phi}{\partial t}}_{transient} + \underbrace{\rho u\frac{\partial \phi}{\partial x} + \rho v\frac{\partial \phi}{\partial y}}_{convection} = \underbrace{\frac{\partial}{\partial x}\left(\Gamma\frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\Gamma\frac{\partial \phi}{\partial y}\right)}_{diffusion} + \underbrace{S_\phi}_{source}$$

Solve complete convection-diffusion equation

Velocity Arrangement



Discretization

The convection-diffusion equation in this situation reads:

$$\frac{\partial(\rho\phi)}{\partial t}+\frac{\partial J_x}{\partial x}+\frac{\partial J_y}{\partial y}=S$$

where $J_x=\rho u\phi-\Gamma\frac{\partial\phi}{\partial x}$ and $J_y=\rho v\phi-\Gamma\frac{\partial\phi}{\partial y}$ are the integrated total fluxes over faces $\int J_x dy$.

Integrating this equation over a control volume, assuming implicit time integration, and applying divergence theorem:

$$\int_{\Delta V}\nabla\cdot\mathbf{J}dV\approx\int_{A}\mathbf{J}\cdot dA$$

we obtain

$$\frac{(\rho\phi)_P-(\rho\phi)_P^0}{\Delta t}\Delta x\Delta y+J_e\cdot A_e-J_w\cdot A_w+J_n\cdot A_n-J_s\cdot A_s=S\Delta x\Delta y$$

where, for example:
$J_e\cdot A_e=(\rho u\phi)_e\Delta y-\Gamma_e\Delta y\left(\frac{\partial\phi}{\partial x}\right)_e\approx F_e\phi_{\mathbf{e}}-D_e(\phi_E-\phi_P)$,
being $F_e=(\rho u)_e\Delta y$ and $D_e=\Gamma_e\frac{\Delta y}{\delta x_e}$

Central Differencing

Writtin the face flux $\mathbf{J_e}$ requires two types of information:

- The face value ϕ_e $==>$ convective schemes
- The face gradient $(\partial\phi/\partial x)_e$ $==>$ known how to approximate

Central Differencing

Assuming linear variation of ϕ between nodes and uniform mesh

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- The face gradient $(\partial\phi/\partial x)_e$ ==> known how to approximate

Central Differencing

Assuming linear variation of ϕ between nodes and uniform mesh

$$\phi_e = \frac{\phi_E + \phi_P}{2} \qquad \Rightarrow \qquad F_e\frac{(\phi_E + \phi_P)}{2}$$

Resulting the algebraic equation

$$a_P\phi_P = a_E\phi_E + a_W\phi_W + a_N\phi_N + a_S\phi_S + b$$
$$a_E = D_e - F_e/2$$
$$a_W = D_w + F_w/2$$
$$a_N = D_n - F_n/2$$
$$a_S = D_s + F_s/2$$
$$a_P = a_E + a_W + a_N + a_S + \rho\frac{\Delta x\,\Delta y}{\Delta t} + (F_e - F_w + F_n - F_s)$$
$$b = \rho\frac{\Delta x\,\Delta y}{\Delta t}\phi_P^0 + S\Delta x\,\Delta y$$

If we repeat the process using Upwind scheme

Upwind Scheme

If we repeat the process using Upwind scheme

$$\begin{aligned} \phi_e &= \phi_P \text{ if } F_e \geq 0 \qquad \phi_n = \phi_P \text{ if } F_n \geq 0 \\ \phi_e &= \phi_E \text{ if } F_e < 0 \qquad \phi_n = \phi_N \text{ if } F_n < 0 \end{aligned}$$

and use $F_e\phi_e = \phi_P MAX[F_e, 0] - \phi_E MAX[-F_e, 0]$ obtain

Upwind Scheme

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and use $F_e \phi_e = \phi_P MAX[F_e, 0] - \phi_E MAX[-F_e, 0]$ obtain

$$a_P \phi_P = a_E \phi_E + a_W \phi_W + a_N \phi_N + a_S \phi_S + b$$

$$a_E = D_e + MAX[-F_e, 0]$$

$$a_W = D_w + MAX[F_w, 0]$$

$$a_N = D_n + MAX[-F_n, 0]$$

$$a_S = D_s + MAX[F_s, 0]$$

$$a_P = a_E + a_W + a_N + a_S + \rho \frac{\Delta x \, \Delta y}{\Delta t} + (F_e - F_w + F_n - F_s)$$

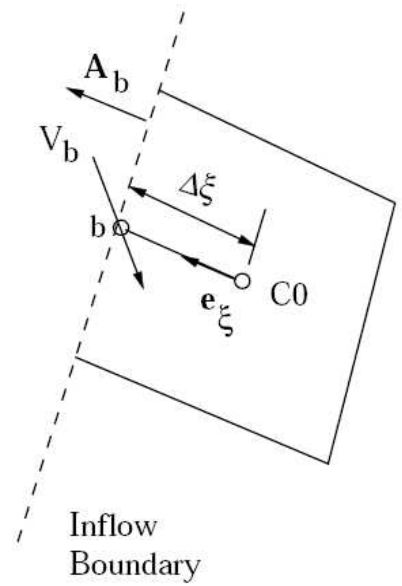
$$b = \rho \frac{\Delta x \, \Delta y}{\Delta t} \phi_P^0 + S \Delta x \, \Delta y$$

- **Geometric boundaries:** physical boundaries, e.g. walls. Dirichlet, Neumann or conjugate conditions.
- **Flow boundaries:** flow enters or leaves the computational domain. We can not include the entire universe in our computational domain. We must supply the appropriate information that represents the part we are not considering.
  - Inflow boundary.
  - Outflow boundary.

Inflow Boundaries

Should be placed at places where we have sufficient data. Inlet velocity distribution and ϕ value are known

$$\begin{aligned} V &= V_b; \quad V_b \cdot A_b \leq 0 \\ \phi &= \phi_{given} \end{aligned}$$



- Boundary node (b) Dirichlet condition
- Inner node (CO) special treatment

$$\frac{\rho(\phi_{CO}-\phi^0_{CO})}{\Delta t}\Delta V + J_b \cdot A_b + \sum_f J_f \cdot A_f = S\Delta V$$

$$J_b \cdot A_b = \rho v_b \cdot A_b \phi_b - \Gamma_b (\nabla\phi)_b \cdot A_b$$

using $\phi_b = \phi_{given}$

$$J_b \cdot A_b = \rho v_b \cdot A_b \phi_{given} - \frac{\Gamma_b}{\Delta\xi}\frac{A_b \cdot A_b}{A_b \cdot e_\xi}(\phi_{CO} - \phi_{given})$$

Outflow Boundaries

- Flow is directed out of the domain at all points on the boundary, i.e. do not cut across recirculation (BFS case)
- Using a first-order Upwind scheme no boundary-condition information is needed
- It is recommended to impose Neumann condition

$$-\Gamma_b(\nabla\phi)_b \cdot A_b = 0$$

$$J_b \cdot A_b = \rho v_b \cdot A_b \phi_b; \quad V_b \cdot A_b > 0$$

$$J_b \cdot A_b = \rho v_b \cdot A_b \phi_{CO}; \quad \phi_b = \phi_{CO}$$

Smith-Hutton Problem

Introduction to Fluid Flow Calculation

- We have considered convection and diffusion of a scalar in the presence of a **known flow field**.
- Now particular issues associated with the computation of the flow field are studied.
- The momentum equations have the same form as the general scalar equation, then we know how to discretize them.
- Primary obstacle: pressure field is unknown. For its determination continuity equation is applied.
- Flow field calculation complicated by the coupling between continuity-momentum equations.

Generalities

- Icompressible flows: pressure does not appear in the continuity equation directly==> it is necessary to find a way to introduce the pressure in the continuity equation.
- Pressure-based methods selected
  - ✦ Semi-Implicit Method for Pressure Linked Equations, SIMPLE
  - ✦ Fractional Step Method (FSM) or Projection Method
- Equations solved sequentially and iteratively.

SIMPLE Method

1. For a given initial pressure, solve momentum equations

$$\frac{\vec{v}^{*} - \vec{v}^{n}}{\Delta t} = -\vec{\nabla} \cdot (\vec{v} \otimes \vec{v})^{n} - \frac{1}{\rho}\vec{\nabla} p^{n} + \nu \Delta \vec{v}^{n} \tag{2}$$

2. Obtained velocity does not satisfy the divergence free, continuity equation and has to be corrected

$$\vec{v}^{n+1} = \vec{v}^{*} + \vec{v}' \qquad p^{n+1} = p^{n} + p' \tag{3}$$

3. Since this correction has an impact on the pressure field, a related pressure correction is obtained by imposing that the corrected velocity satisfies the continuity equation.

$$\frac{\vec{v}^{n+1} - \vec{v}^{n}}{\Delta t} = -\vec{\nabla} \cdot (\vec{v} \otimes \vec{v})^{n} - \frac{1}{\rho}\vec{\nabla} p^{n+1} + \nu \Delta \vec{v}^{n}; \quad \vec{\nabla} \cdot \vec{v}^{n+1} = 0$$

4. Replacing 3 in 4 and substracting 2, leads to a Poisson equation for pressure.

$$\Delta p' = \frac{\rho}{\Delta t} \vec{\nabla} \cdot \vec{v}^{*}$$

SIMPLE Algorithm

1. Guess pressure field
2. Solve momentum equations to obtain intermediate velocities $\vec{v}^*$
3. Solve the p' equation
4. Correct velocities and pressure
5. Treat the corrected pressure as a new guessed pressure and return to step 2
6. Solve additional scalar equations (energy equation)

Helmholtz-Hodge Theorem

A given vector $\vec{w}$, defined in a bounded domain Ω with smooth boundary $\partial\Omega$, is uniquely decomposed in a pure gradient field ϕ and a divergence-free vector $\vec{a}$ parallel to $\partial\Omega$

$$\vec{w} = \vec{a} + \nabla\phi$$

or

$$\vec{w} = \vec{a} + G\phi$$

where

$$\nabla \cdot \vec{a} = 0 \qquad \vec{a}\epsilon\Omega$$

$$\vec{a} \cdot \vec{n} = 0 \qquad \vec{a}\epsilon\partial\Omega$$

- Momentum equation

$$\frac{\partial \vec{v}}{\partial t} = R(\vec{v}) - \frac{1}{\rho}\vec{\nabla} p, \qquad R(\vec{v}) \equiv -\vec{\nabla}\cdot(\vec{v}\otimes\vec{v}) + \nu\Delta\vec{v}$$

- Fully explicit time integration. For transient term linear variation

$$\frac{\partial \vec{v}}{\partial t}\Big|^{t+1/2\Delta t} \approx \frac{\vec{v}^{t+\Delta t} - \vec{v}^{t}}{\Delta t}$$

- Adams-Bashforth scheme selected to evaluate $R(\vec{v})$

$$R^{t+1/2\Delta t}(\vec{v}) \approx \frac{3}{2}R(\vec{v}^{t}) - \frac{1}{2}R(\vec{v}^{t-\Delta t})$$

- First-order backward Euler scheme (fully implicit) applied to evaluate pressure-gradient term. Incompressibility constraint is treated implicitly

$$\frac{\vec{v}^{t+\Delta t} - \vec{v}^{t}}{\Delta t} = \frac{3}{2}R(\vec{v}^{t}) - \frac{1}{2}R(\vec{v}^{t-\Delta t}) - \frac{1}{\rho}\vec{\nabla} p^{t+\Delta t}$$

$$\vec{\nabla}\cdot\vec{v}^{t+\Delta t} = 0$$

Navier-Stokes equations

$$\frac{\partial \vec{v}}{\partial t} + \vec{\nabla} \cdot (\vec{v} \otimes \vec{v}) = -\frac{1}{\rho}\vec{\nabla} p + \nu \Delta \vec{v}$$

If the pressure term is omitted, intermediate velocity is decoupled from pressure

$$\frac{\partial \vec{v^p}}{\partial t} + \vec{\nabla} \cdot (\vec{v^p} \otimes \vec{v^p}) = \nu \Delta \vec{v^p}$$

Using Helmholtz-Hodge vector decomposition theorem

$$\vec{v}^p = \vec{v}^{t+\Delta t} + \frac{1}{\rho}\vec{\nabla} p^{t+\Delta t}$$

taking the divergence and taking into account continuity

$$\vec{\nabla} \cdot \vec{v}^p = \vec{\nabla} \cdot \vec{v}^{t+\Delta t} + \frac{1}{\rho}\vec{\nabla} \cdot \vec{\nabla} p^{t+\Delta t}$$

$$\frac{1}{\rho}\nabla^2 p^{t+\Delta t} = \frac{1}{\rho}\Delta p^{t+\Delta t} = \vec{\nabla} \cdot \vec{v}^p$$

Poisson equation

1. Evaluate $R(\vec{v}^t)$
2. Evaluate $\vec{v}^p$ from
$$\vec{v}^p = \vec{v}^t + \frac{\Delta t}{\rho\Omega}\left[\frac{3}{2}R(\vec{v}^t) - \frac{1}{2}R(\vec{v}^{t-\Delta t})\right]$$
3. Calculate $\vec{\nabla} \cdot \vec{v}^p$
4. Solve the discrete Poisson equation to obtain $p^{t+\Delta t}$
$$\triangle p^{t+\Delta t} = \frac{\rho}{\Delta t}\vec{\nabla} \cdot \vec{v}^p$$
5. Obtain the new velocity field
$$\vec{v}^{t+\Delta t} = \vec{v}^p - \frac{\Delta t}{\rho}\vec{\nabla} p^{t+\Delta t}$$
6. Solve explicitly additional scalar equations

Time Step

- Due to stability reasons explicit temporal schemes introduce restrictions on the time step
- Minimum Courant number has to be taken into account

$$\Delta t_{conv} \left(\frac{|u_i|}{\Delta x_i} \right)_{max} \leq 0.35$$

$$\Delta t_{visc} \left(\frac{\nu}{\Delta x_i^2} \right)_{max} \leq 0.2$$

$$\Delta t = MIN(\Delta t_{conv}, \Delta t_{visc})$$

- Since the viscosity and mesh remain constant during simulation, only Δt_{conv} must be calculated each time step

Numerical solution of Navier-Stokes Equations

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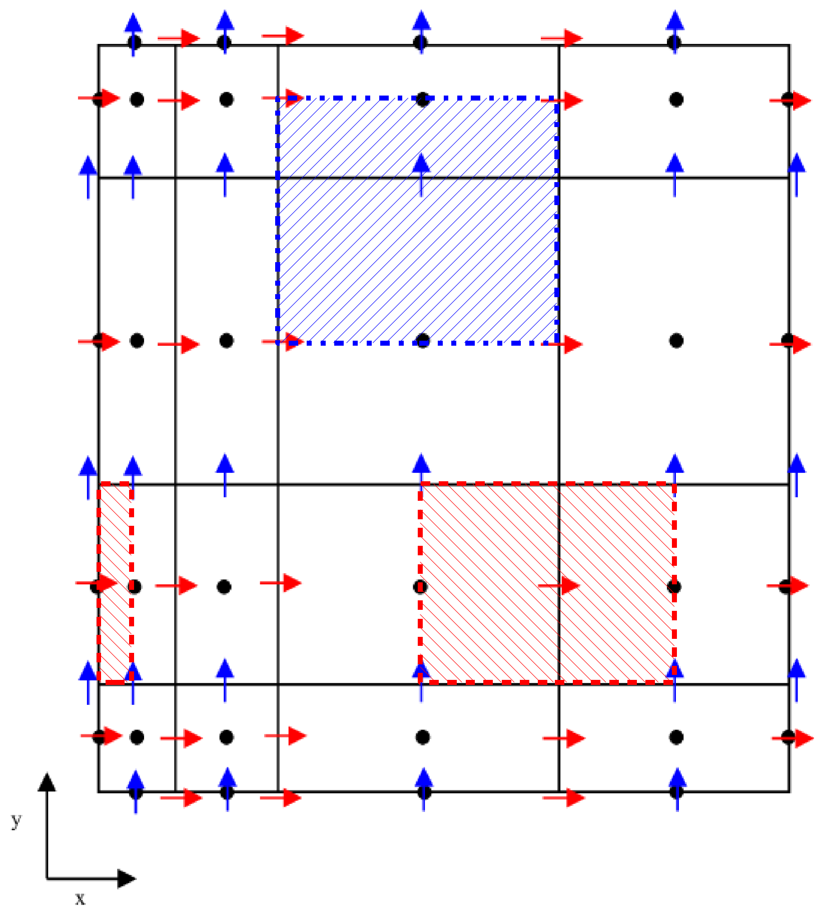
Discretization Details

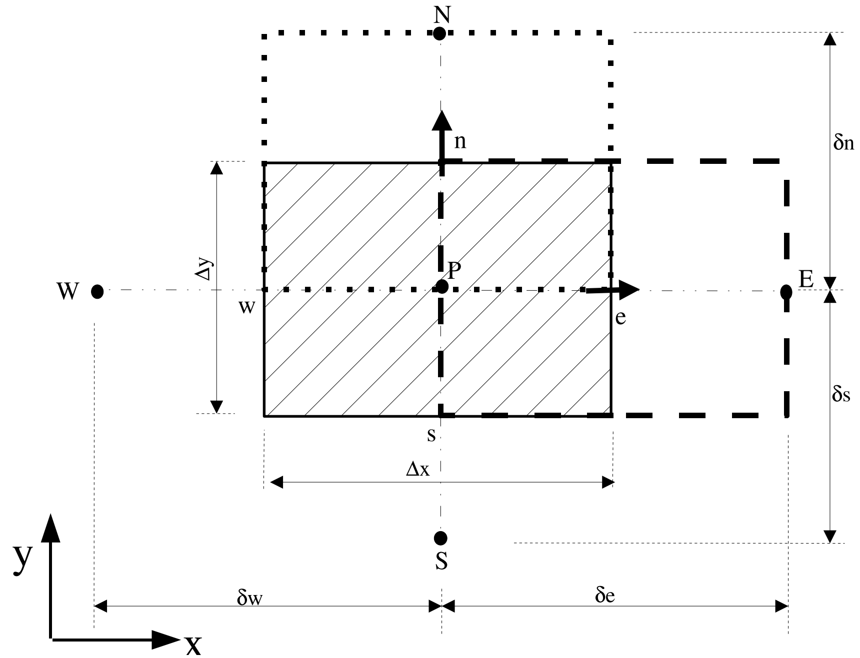
- Checkerboard problem: evaluation of the pressure-gradient term and continuity equation.

$$-\int \frac{\partial p}{\partial x} dx \approx p_w - p_e = \frac{p_W + p_P}{2} - \frac{p_P + p_E}{2}$$
$$= \frac{p_W - p_E}{2}$$

  Momentum equation will contain pressure information from two alternate grid points, and not between adjacent ones

- A remedy is the use of a staggered mesh or methods that add an artificial dissipation term, filtering small frecuencies, e.g. Rhie and Chow method.





Note that because of grid staggering, the coefficients, volume and faces size are different for the scalars, u and v equations solution

Mass Flows Evaluation

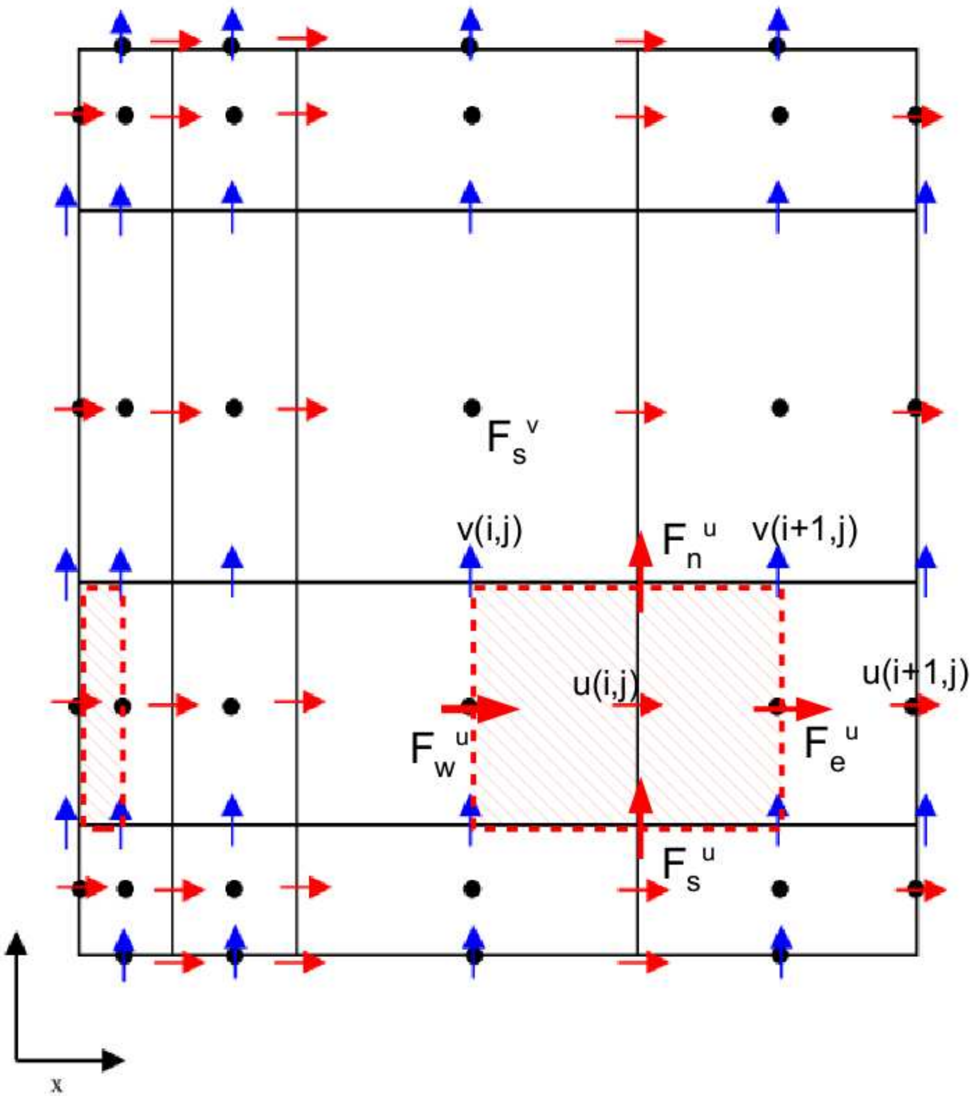
$$u_e^u \approx 0.5[u(i,j) + u(i+1,j$$

$$F_e^u = u_e^u \rho \Delta y$$

$$v_n^u \approx \frac{v(i,j)\Delta x_i + v(i+1,j)\Delta x_{i+1}}{\Delta x_i + \Delta x_{i+1}}$$

$$F_n^u = v_n^u \rho \delta x_e$$

Γ_n^u => double Harmonic inte



Mass Flows Evaluation

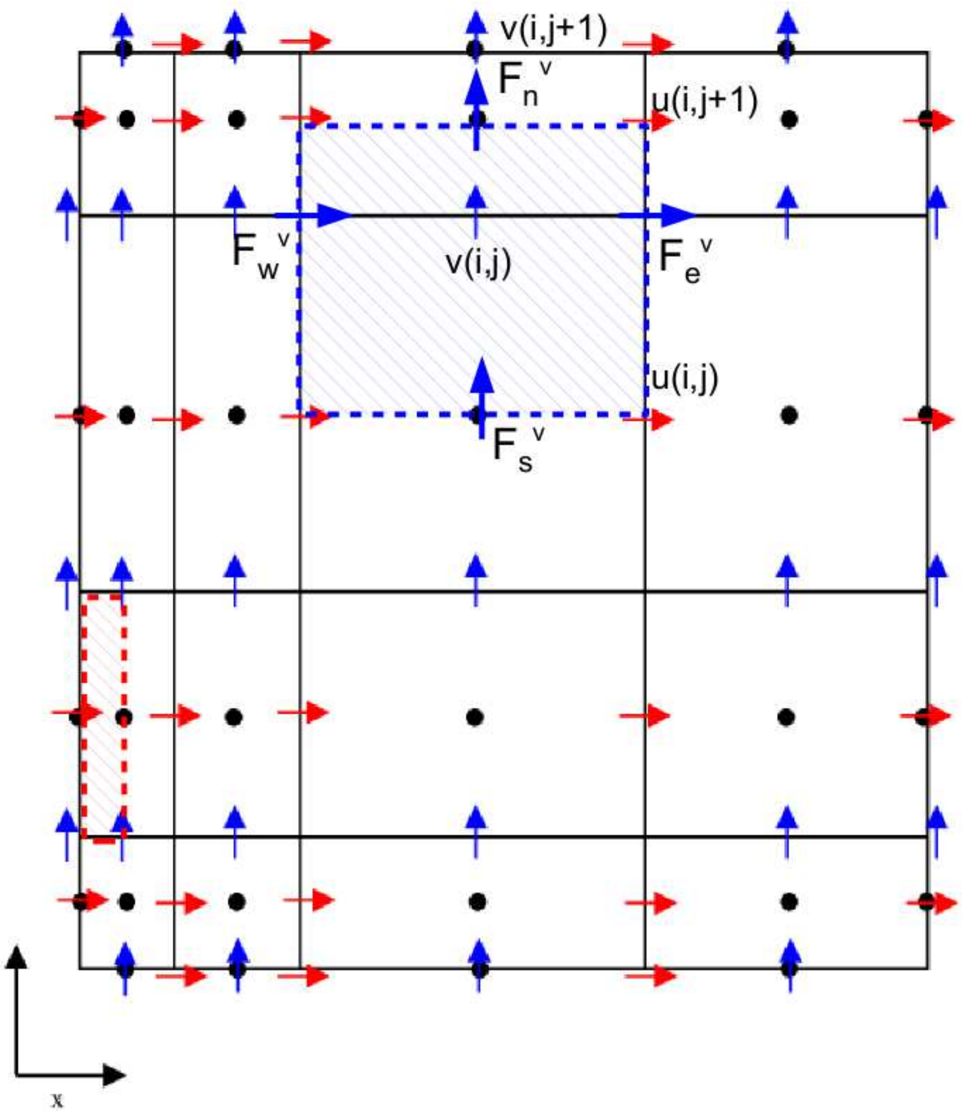
$$v_n^v \approx 0.5[v(i,j) + v(i,j+1$$

$$F_n^v = v_n^v \rho \Delta x$$

$$u_e^v \approx \frac{u(i,j)\Delta y_j + u(i,j+1)\Delta y_{j+1}}{\Delta y_j + \Delta y_{j+1}}$$

$$F_e^v = u_e^v \rho \delta y_n$$

$\Gamma_e^v =>$ double Harmonic inte



$R(\phi)$ Discretization

Position of mass flows, Γ, ϕ, areas and volumes considered vary depending on the variable which is being solved.

$$R(\phi_P) = -[F_e^\phi \phi_e - F_w^\phi \phi_w + F_n^\phi \phi_n - F_s^\phi \phi_s]$$
$$+D_e^\phi(\phi_E - \phi_P) - D_w^\phi(\phi_P - \phi_W) + D_n^\phi(\phi_N - \phi_P) - D_s^\phi(\phi_P - \phi_s)$$

where

$$F_e^\phi = \rho u_e^\phi \Delta y \quad \text{(or corresponding area)}$$
$$D_e^\phi = \frac{\Gamma_e^\phi \Delta y}{\delta x_e} \quad \text{(or corresponding area and distance)}$$
$$\phi_{(e,w,n,s)} \implies \text{evaluated directly using UDS, UDS2, QUICK...}$$

Pressure is a scalar solved in the main centred grid

$$\bigtriangledown^2 p^{t+\Delta t} = \frac{\rho}{\Delta t}\vec{\bigtriangledown}\cdot\vec{v}^p, \quad \text{dropping superscript } t+\Delta t$$

$$\bigtriangledown^2 p = \frac{\rho}{\Delta t}\vec{\bigtriangledown}\cdot\vec{v}^p \quad ==> \int_\Omega \triangle p \, d\Omega = \frac{\rho}{\Delta t}\int_\Omega \vec{\bigtriangledown}\cdot\vec{v}^p d\Omega$$

$\Downarrow$ applying Gauss theorem

$$\int_{ds} \vec{\bigtriangledown} p\cdot\vec{n}ds = \frac{\rho}{\Delta t}\int_{ds}\vec{v}^p\cdot\vec{n}ds$$

$$\left(\frac{\partial p}{\partial x}\right)_e \Delta y - \left(\frac{\partial p}{\partial x}\right)_w \Delta y + \left(\frac{\partial p}{\partial y}\right)_n \Delta x - \left(\frac{\partial p}{\partial y}\right)_s \Delta x$$
$$= \frac{1}{\Delta t}[F_e(\vec{v}^p) - F_w(\vec{v}^p) + F_n(\vec{v}^p) - F_s(\vec{v}^p)]$$

Discrete Poisson Equation

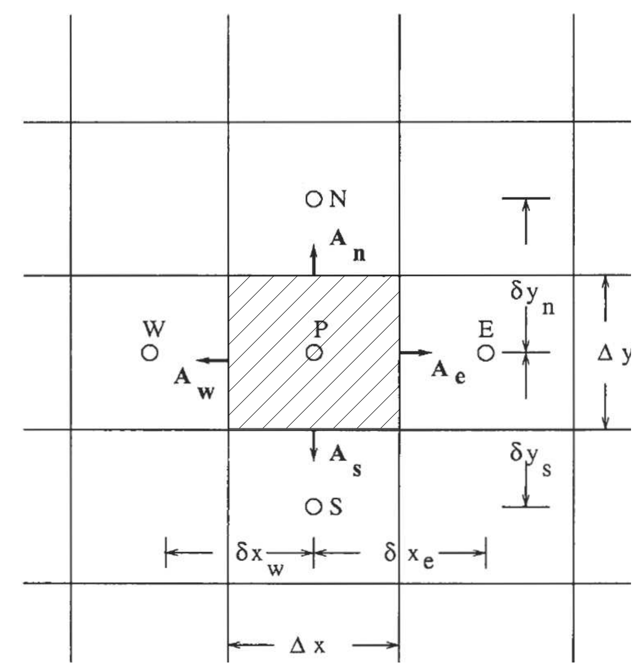
$$\frac{p_E - p_P}{\delta x_e}\Delta y - \frac{p_P - p_W}{\delta x_w}\Delta y + \frac{p_N - p_P}{\delta y_n}\Delta x - \frac{p_P - p_S}{\delta y_s}\Delta x$$
$$= \frac{1}{\Delta t}[F_e(\vec{v}^p) - F_w(\vec{v}^p) + F_n(\vec{v}^p) - F_s(\vec{v}^p)]$$

Discrete algebraic equation:

$$a_P p_P = a_E p_E + a_W p_W + a_N p_N + a_S p_S + b$$

where

$$a_E = \frac{\Delta y}{\delta x_e}, \quad a_W = \frac{\Delta y}{\delta x_w},$$
$$a_N = \frac{\Delta x}{\delta y_n}, \quad a_S = \frac{\Delta x}{\delta y_s},$$
$$b = -\frac{1}{\Delta t}[F_e(\vec{v}^p) - F_w(\vec{v}^p) + F_n(\vec{v}^p) - F_s(\vec{v}^p)]$$
$$a_P = a_E + a_W + a_N + a_S$$



Solved using GS+TDMA or any direct method, e.g. LU

Boundary Conditions:

- Velocity is given in most cases
- $\vec{v}^{t+\Delta t}$ is known
- Generally is imposed $\vec{v}^p = \vec{v}^{t+\Delta t}$
- Using $\vec{v}^{t+\Delta t} = \vec{v}^p - \frac{\Delta t}{\rho} \vec{\nabla} p^{t+\Delta t}$
- Then $\vec{\nabla} p = 0 \;\; ==>$ Neumann condition

Note:

Since the system is not determined, it is necessary to fix the pressure in one point:

$$a_E = a_W = a_N = a_S = 0$$
$$b = p_{fix} \approx 0$$
$$a_P = 1$$

Velocity Correction

$$\vec{v}^{t+\Delta t} = \vec{v}^{p} - \frac{\Delta t}{\rho} \vec{\nabla} p^{t+\Delta t}$$

Must be remembered velocities are solved over a staggered grid. Then pressure is placed in the faces of the control volume

$$u_P^{t+\Delta t} = u_P^{p} - \frac{\Delta t}{\rho} \left(\frac{p_E - p_P}{\delta x_e} \right)^{t+\Delta t}$$

$$v_P^{t+\Delta t} = v_P^{p} - \frac{\Delta t}{\rho} \left(\frac{p_N - p_P}{\delta y_n} \right)^{t+\Delta t}$$

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