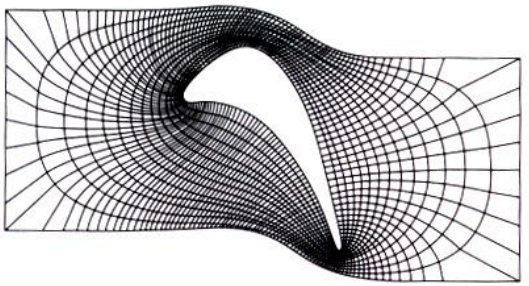

Computational Methods in Transport Phenomena

Integrated Master in Chemical Engineering 2024/2025

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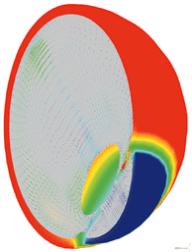
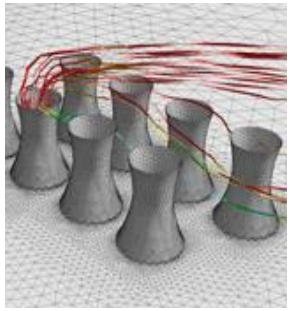




I - INTRODUCTION TO COMPUTATIONAL FLUID DYNAMICS

Literature

Patankar, S., 1980. *Numerical heat transfer and fluid flow*. CRC press. Chapters 1-6

”Although there is an extensive literature on computational thermofluid analysis, the newcomer to the field has insufficient help available. The graduate student, the researcher, and the practicing engineer must struggle through journal articles or be content with elementary presentation in books on numerical analysis. Often, it is the subtle details that determine the success or failure of a computational activity; yet, the practices that are learned through experience by successful computing groups rarely appear in print. A consequence is that many workers either give up the computational approach after many months of frustrating pursuit or struggle through to the end with inefficient computer programs.

Being aware of this situation, I have tried to present in this book a self-contained, simple, and practical treatment of the subject. “ Suhas Patankar, 1980

- Greenshields, C.J. and Weller, H.G., 2022. Notes on computational fluid dynamics: General principles. (Open source)
  - https://doc.cfd.direct/notes/cfd-general-principles/

- Jasak, Hrvoje. "Error analysis and estimation in the Finite Volume method with applications to fluid flows." PhD Thesis (1996).

WHAT IS COMPUTATIONAL FLUID DYNAMICS?

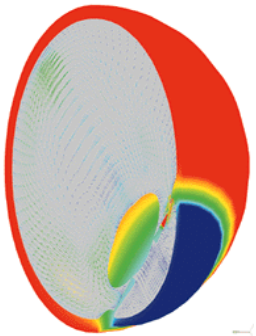
- **COMPUTATIONAL FLUID DYNAMICS (Computational Fluids Dynamics - CFD) is a method of predicting fluid flow, heat and mass transfer, chemical reaction and other related phenomena by numerically solving the equations that govern these phenomena. This methodology can be seen as a form of "virtual reality".**

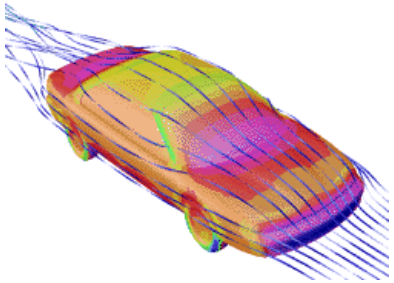
- **The results obtained by CFD are relevant to:**
  - **Process Equipment Design and Optimization**
  - **Pollution Control and Environmental Management:**
  - **Analysis of processes malfunctioning**
  - **Process revamping**

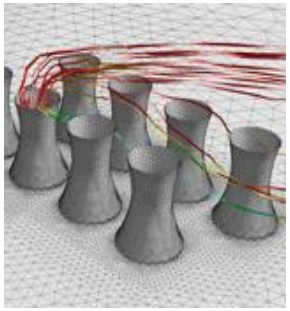
- **CFD complements the experimental analysis of the systems.**
  - **Predictive Insights and Preliminary Analysis**
  - **Optimization of Experimental Design**
  - **Validation and Calibration**

CFD: APPLICATIONS

- **Chemical Industry: mixing tanks, chemical reactors, aerators, etc.**
- **Environment: dispersion of pollutants, soil recovery, etc.**
- **Automotive Industry: combustion modeling, fuel cell analysis, areodynamics, etc.**
- **Biomedical Sciences: blood flow modeling in artificial valves, simulation of artificial organs, etc.**
- **Safety analysis: Simulation of fires.**







Experiments vs. Simulations

- **CFD gives an insight into equipment's with fluid flow that may be difficult, expensive or impossible to study using experimental techniques.**

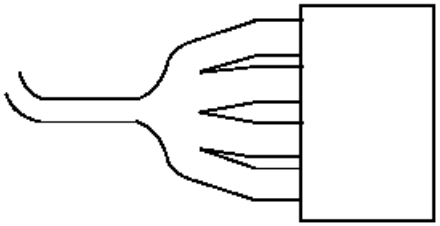
- **Optimization of a given system can be achieved by a careful combination of CFD simulation with experimental analysis.**

- **Balancing CFD and Experiments for Cost Efficiency**

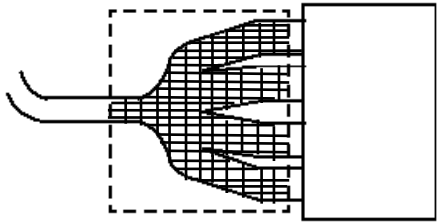
  Engineers should strategically choose between Computational Fluid Dynamics (CFD) and experimental methods based on cost-effectiveness. CFD offers in-depth simulations and can be costlier with complex models, whereas experiments provide direct measurements but can incur high setup costs. Selecting the appropriate method—or a combination of both—depends on achieving accurate results within budget constraints, ensuring economic viability in engineering projects.

CFD METHODOLOGY - I

- **Problem definition - for example excessive head loss in the system:**



- **Identification of the simulation region and mesh creation.**

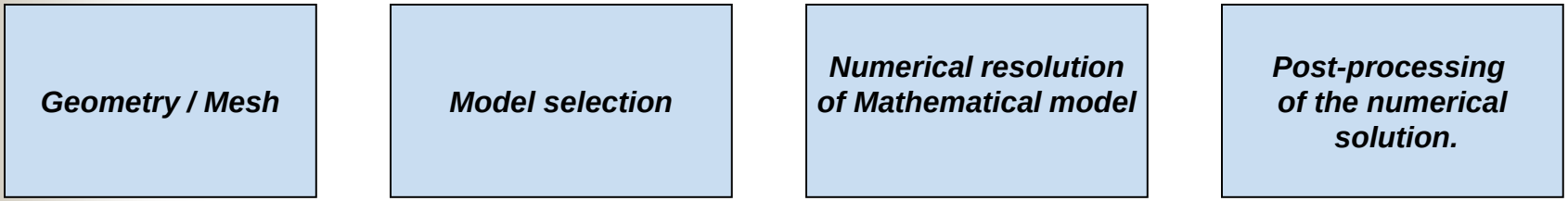


- **Selection of the appropriate mathematical model and specification of boundary conditions and fluid properties:**
  - **3D or 2D simulation? Steady or transient state? Laminar or turbulent flow? With or without chemical reaction? Etc.**

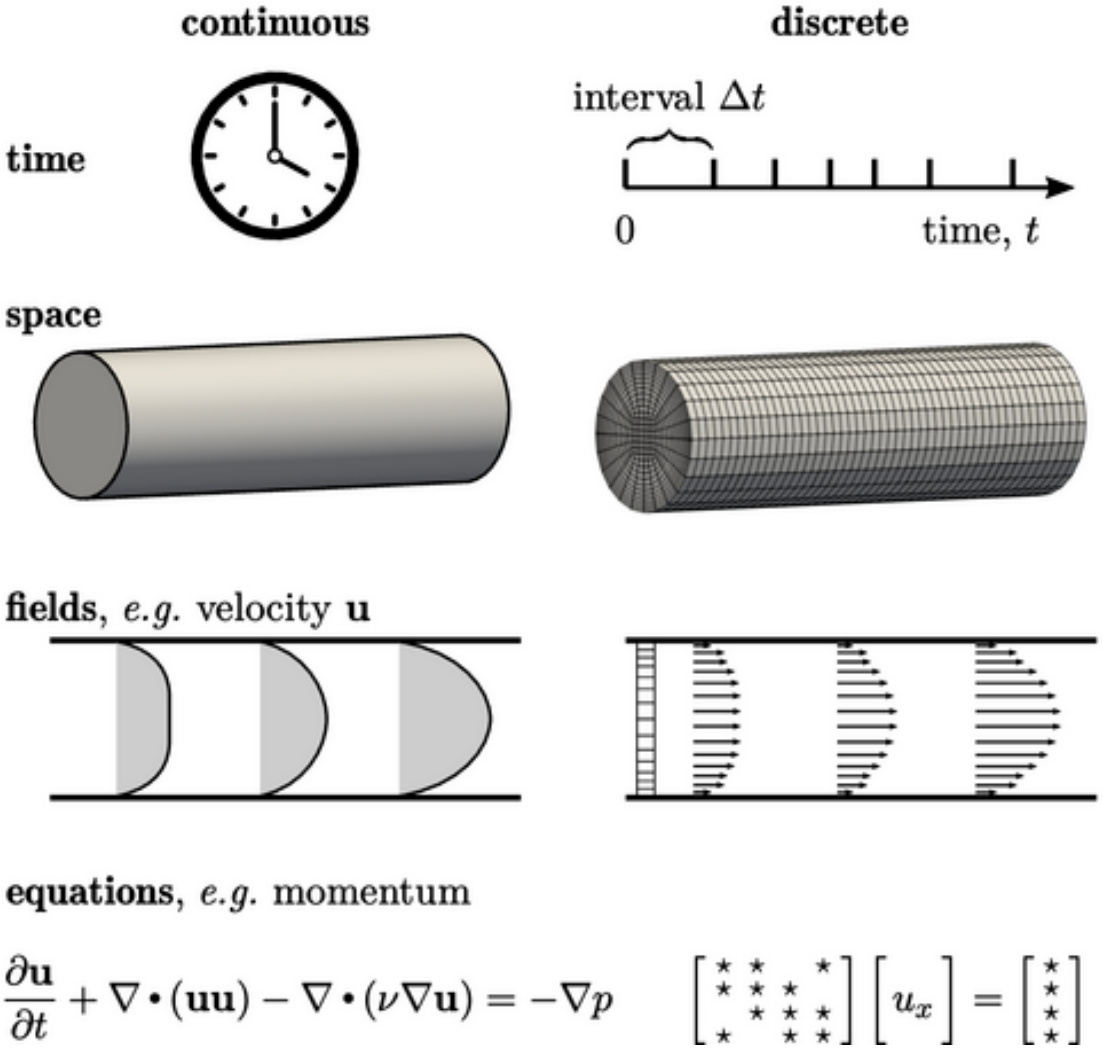
CFD METHODOLOGY - II

- **Numerical resolution of the model**
- **Post-processing and visualization of numerical results**
  - **Calculation of average inlet and outlet pressure, shear stresses, average speeds, etc.**
  - **Visualization of velocity distributions, pressure, turbulence intensity, etc.**

- **Schematically we have:**

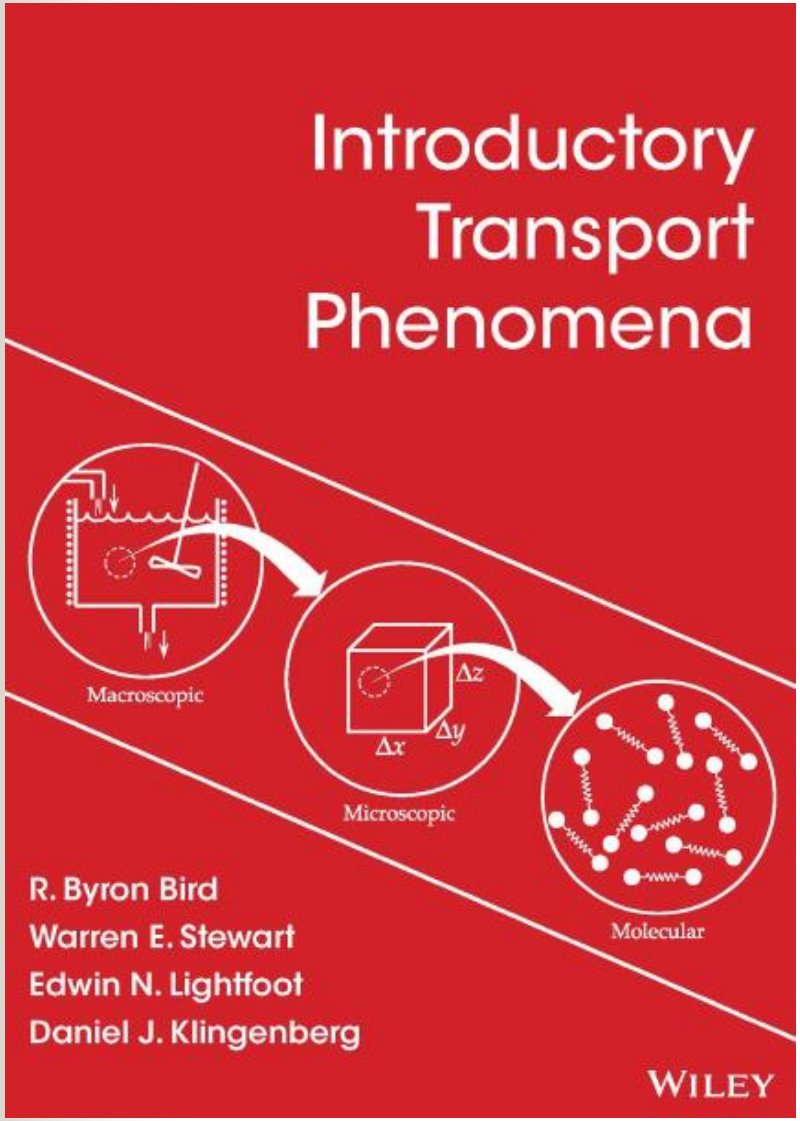


CFD METHODOLOGY- III



Source: https://doc.cfd.direct/notes/cfd-general-principles/numerical-method

TRANSPORT EQUATIONS: Classical Approach



$$\frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho v^2\right) = -\left(\nabla\cdot\tfrac{1}{2}\rho v^2\mathbf{v}\right) \quad -(\nabla\cdot p\mathbf{v}) \quad -p(-\nabla\cdot\mathbf{v})$$

rate of increase of kinetic energy per unit volume

rate of addition of kinetic energy by convection per unit volume

rate of work done by pressure of surroundings on the fluid per unit volume

rate of *reversible* conversion of kinetic energy into internal energy per unit volume

$$-(\nabla\cdot[\boldsymbol{\tau}\cdot\mathbf{v}]) \quad -(-\boldsymbol{\tau}:\nabla\mathbf{v}) \quad +\rho(\mathbf{v}\cdot\mathbf{g})$$

rate of work done by viscous force on the fluid per unit volume

rate of *irreversible* conversion from kinetic to internal energy per unit volume

rate of work done by external force on the fluid per unit volume

$$\frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho v^2+\rho\hat{\Phi}\right) = -\left(\nabla\cdot\left(\tfrac{1}{2}\rho v^2+\rho\hat{\Phi}\right)\mathbf{v}\right) - (\nabla\cdot p\mathbf{v}) - p(-\nabla\cdot\mathbf{v}) - (\nabla\cdot[\boldsymbol{\tau}\cdot\mathbf{v}]) - (-\boldsymbol{\tau}:\nabla\mathbf{v})$$

$$(-\boldsymbol{\tau}:\nabla\mathbf{v}) = \frac{1}{2}\mu\sum_i\sum_j\left[\left(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i}\right)-\frac{2}{3}(\nabla\cdot\mathbf{v})\delta_{ij}\right]^2+\kappa(\nabla\cdot\mathbf{v})^2 \equiv \mu\Phi_v+\kappa\Psi_v$$

Table 3.5-1. The Equations of Change for Isothermal Systems in the D/Dt-Form[a].
Note: At the left are given the equation numbers for the $\partial/\partial t$ forms.

(3.1-4)	$\frac{D\rho}{Dt} = -\rho(\nabla\cdot\mathbf{v})$	(A)
(3.2-9)	$\rho\frac{D\mathbf{v}}{Dt} = -\nabla p - [\nabla\cdot\boldsymbol{\tau}] + \rho\mathbf{g}$	(B)
(3.3-1)	$\rho\frac{D}{Dt}\left(\frac{1}{2}v^2\right) = -(\mathbf{v}\cdot\nabla p) - (\mathbf{v}\cdot[\nabla\cdot\boldsymbol{\tau}]) + \rho(\mathbf{v}\cdot\mathbf{g})$	(C)
(3.4-1)	$\rho\frac{D}{Dt}[\mathbf{r}\times\mathbf{v}] = -[\nabla\cdot\{\mathbf{r}\times p\boldsymbol{\delta}\}^\dagger] - [\nabla\cdot\{\mathbf{r}\times\boldsymbol{\tau}\}^\dagger] + [\mathbf{r}\times\rho\mathbf{g}]$	(D)

TRANSPORT EQUATIONS: Generic Equations

- **Continuity equation:** $\frac{\partial \rho}{\partial t} + \sum_{j=1}^{3} \frac{\partial \rho u_j}{\partial x_j} = 0$

- **Differential equation for a generic variable ϕ:**

$$\frac{\partial \rho \phi}{\partial t} + \sum_{j=1}^{3} \frac{\partial}{\partial x_j}(\rho u_j \phi) = \sum_{j=1}^{3} \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right) + S_\phi$$

  - **Mass transfer: ϕ = mass fraction (kg solute/ kg)**
  - **Heat transfer : ϕ = specific enthalpy (J / kg)**
  - **Momentum transfer : ϕ = speed (kg ms^{-1}/ kg = m / s)**
  - **s_ϕ = source term:**
    production rate per unit volume of the quantity transported
    - for solute mass : kg / s.m^3
    - for heat : J / s.m^3
    - for momentum : kg m.s^{-1}/ s.m^3

(A note of caution)

- "As every science student knows, solving differential equations is hard.“
- "Most differential equations cannot be solved at all."
- "Confronted with a nonlinear system, scientists would have to substitute linear approximations or find some other uncertain backdoor approach."
- "Textbooks showed students only the rare nonlinear systems that would give way to such techniques. They did not display sensitive dependence on initial conditions.“

Gleick, J. (1987). Chaos: Making a New Science. Penguin Books

Using Einstein Notation

(sum over an index if it appears twice (upper and lower positions) in a term.

$$\frac{\partial \rho}{\partial t} + \sum_{j=1}^{3} \frac{\partial \rho u_j}{\partial x_j} = 0 \quad \Rightarrow \quad \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0$$

$$\frac{\partial \rho \phi}{\partial t} + \sum_{j=1}^{3} \frac{\partial}{\partial x_j}(\rho u_j \phi) = \sum_{j=1}^{3} \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right) + S_\phi \quad \Rightarrow \quad \frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho u_j \phi}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right) + S_\phi$$

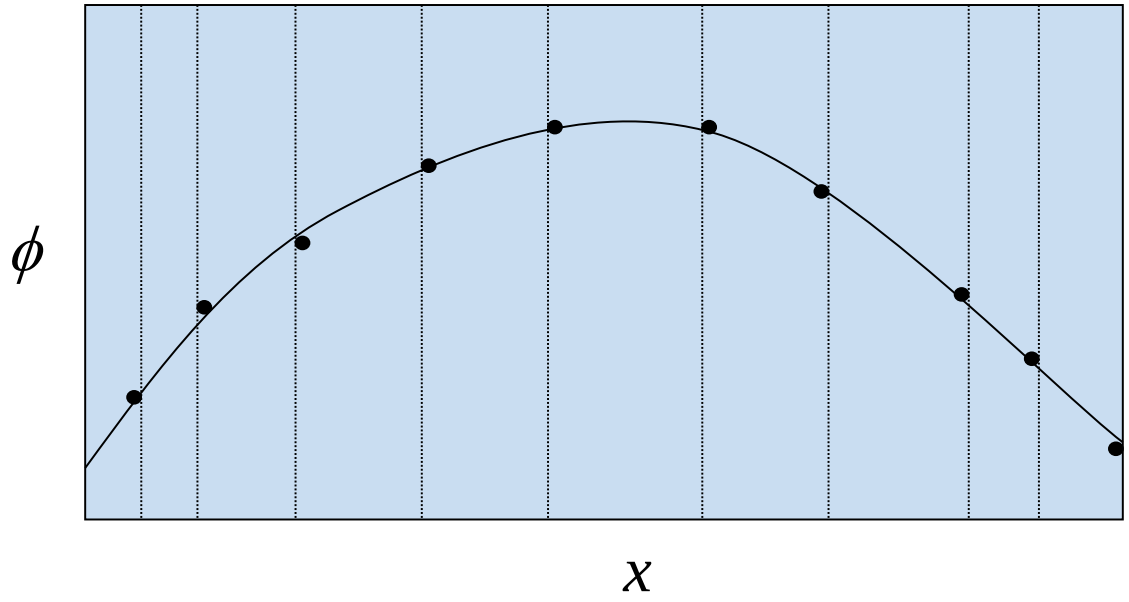
For $\phi = u_i$ ⇒

$$\frac{\partial \rho u_i}{\partial t} + \sum_{j=1}^{3} \frac{\partial \rho u_j u_i}{\partial x_j} = \sum_{j=1}^{3} \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial u_i}{\partial x_j}\right) + S_{u_i} \quad \Rightarrow \quad \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial u_i}{\partial x_j}\right) + S_{u_i}$$

SPATIAL DISCRETIZATION OF TRANSPORT EQUATIONS

- **THE EXACT SOLUTION OF TRANSPORT EQUATIONS IS A CONTINUOUS FUNCTION.**
  - **However, analytical solutions only exist for very particular simplifications of these equations.**

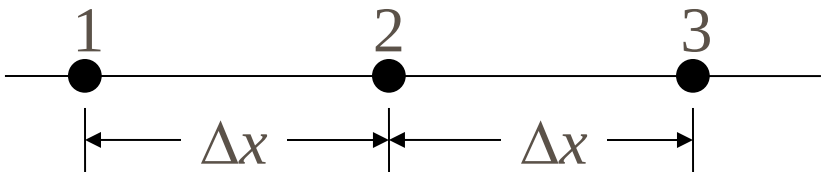
- **IN THE DISCRETIZATION PROCESS, THE EXACT SOLUTION IS APPROXIMATED BY A SET OF VALUES IN DISCRETE POINTS OF THE CALCULATION DOMAIN.**



METHODS OF SPATIAL DISCRETIZATION:

Differential equations → Algebraic equations of discretization:

- **Finite difference method.**



$$\Delta x = x_2 - x_1 = x_3 - x_2$$

$$\phi_1 = \phi_2 - \Delta x\left(\frac{d\phi}{dx}\right)_2 + \frac{1}{2}(\Delta x)^2\left(\frac{d^2\phi}{dx^2}\right)_2 - \cdots$$

$$\phi_2 = \phi_3 + \Delta x\left(\frac{d\phi}{dx}\right)_2 - \frac{1}{2}(\Delta x)^2\left(\frac{d^2\phi}{dx^2}\right)_2 + \cdots$$

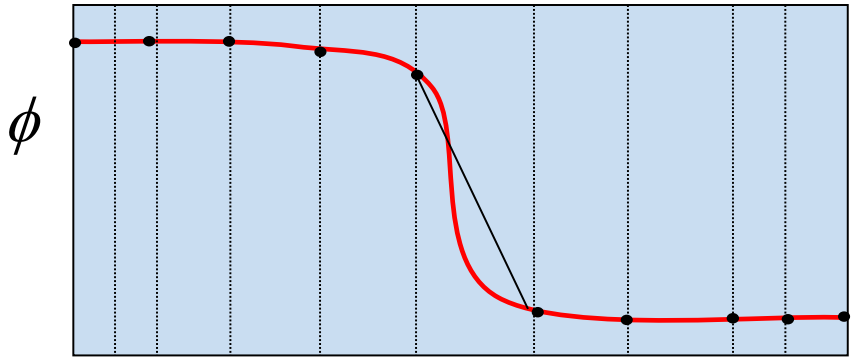
$$\left(\frac{d\phi}{dx}\right)_2 = \frac{\phi_3 - \phi_1}{2\Delta x}$$

$$\left(\frac{d^2\phi}{dx^2}\right)_2 = \frac{\phi_1 + \phi_3 - 2\phi_2}{(\Delta x)^2}$$

- **The substitution of these expressions in the transport equations leads to an equation for finite differences for each node in the mesh.**

Problems associated with the finite difference method:

- **How does a polynomial variation of ϕ between two nodes, the zeroing error becomes very high when the actual variation of ϕ it is the exponential type.**



- **For sparsely dense meshes - which lead to shorter calculation times - the finite difference equations can lead to physically unfeasible solutions.**

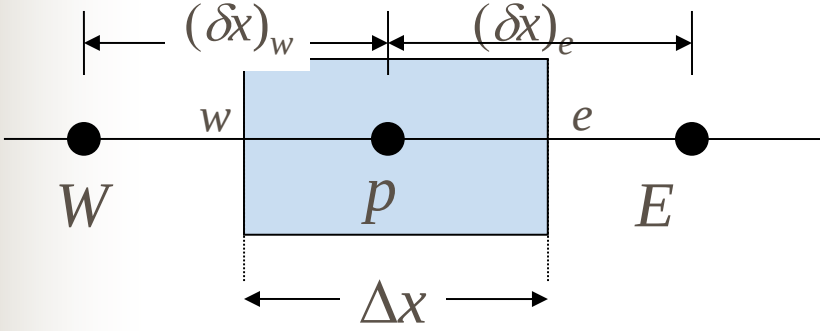
- **The system of finite difference equations can present convergence difficulties.**

Control Volume Method (Patankar, 1972)

- The calculation domain is divided into non-overlapping control volumes so that there is a control volume surrounding each node in the mesh.
- Each transport equation is integrated into each of the control volumes.
- Function segments that define how ϕ varies between two nodes are used to calculate the various integrals involved.
- The resulting finite difference equations have physical significance insofar as they express the principle of conservation of the various quantities involved in the balance at the control volume.

ILLUSTRATIVE EXAMPLE OF THE APPLICATION OF THE CONTROL VOLUME METHOD

- **One-dimensional heat conduction**

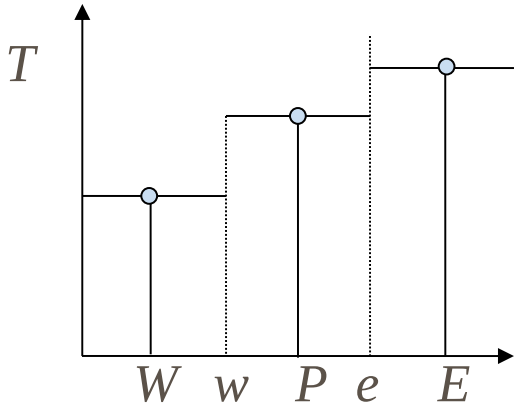


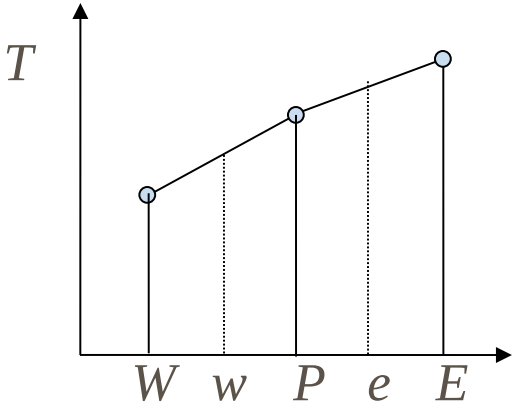
$$\frac{d}{dx}\left(k\frac{dT}{dx}\right)+S=0$$

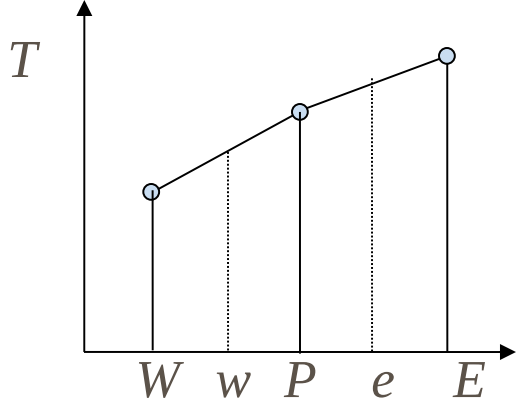
- **VC integration $\Delta x \times 1 \times 1$:**

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

Profiles assumed:





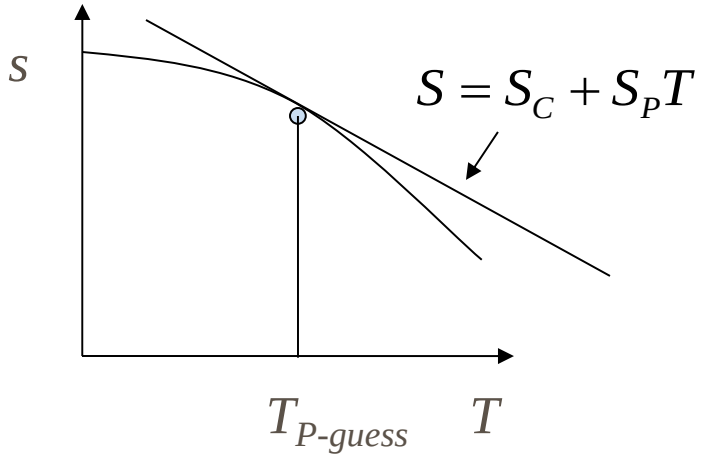


- **Discretization equation:**

$$\frac{k_e(T_E - T_P)}{(\delta x)_e} - \frac{k_w(T_P - T_W)}{(\delta x)_w} + \bar{S}\Delta x = 0$$

- **The term source is usually linearized to accelerate convergence:**

$$\bar{S} = S_C + S_P T_P$$



- **It is obtained as follows:**

$$\rightarrow \quad a_P T_P = a_E T_E + a_W T_W + b$$

$$a_E = k_e / (\delta x)_e$$

$$a_W = k_w / (\delta x)_w$$

$$a_P = a_E + a_W - S_P \Delta x$$

$$b = S_C \Delta x$$

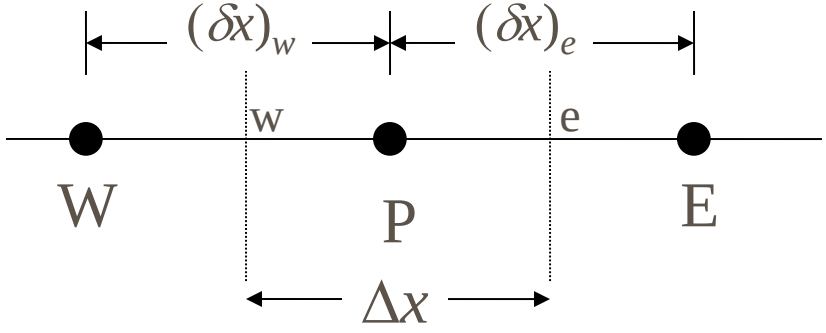
Basic rules to guarantee physically correct solutions and good numerical stability.

- **The flows on both sides of a VC face must be the same.**
- **All coefficients must be positive.**
- **S_P must always be negative. If in a given range S_P is positive, then it is assumed to be zero.**

II - HEAT CONDUCTION
(in orthogonal meshes)

1- One-dimensional stationary conduction
2- One-dimensional transient conduction
3- Two and three-dimensional conduction

1- UNIDIMENSIONAL HEAT CONDUCTION



$$\frac{d}{dx}\left(k\frac{dT}{dx}\right)+S=0$$

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

$$a_E = k_e/(\delta x)_e$$

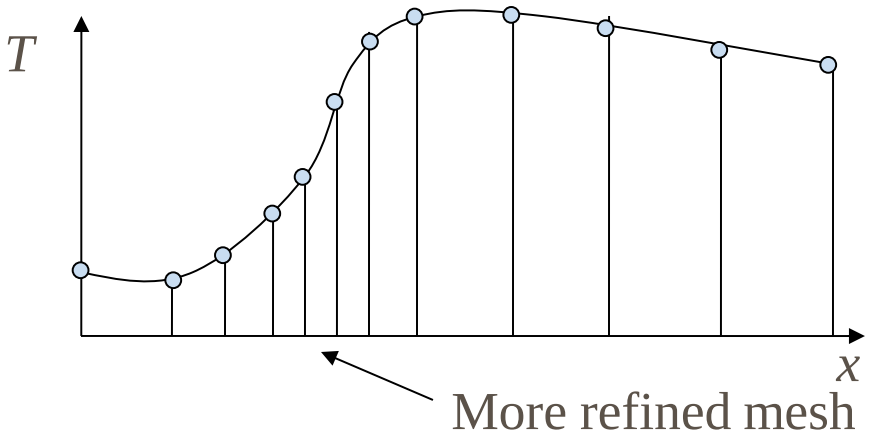
$$a_W = k_w/(\delta x)_w$$

$$a_P = a_E + a_W - S_P \Delta x$$

$$b = S_C \Delta x$$

$$\bar{S} = S_C + S_P T_P$$

Mesh refinement



- **The mesh should be more refined in regions where the gradient of *T* is higher.**
- **At an early stage, if there is no additional information, a uniform wide mesh can be used. In a second phase, the T distribution of the first mesh is used as an indicator of mesh refinement.**
- **One of the advantages of the control volumes method is that it allows to obtain physically consistent initial solutions with very large meshes.**

Nonlinearity

- **The coefficients of the discretization equation**

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

depend on temperature in non-linear systems.

- **This case of non-linearity is solved by an iterative process:**
  1. **Arbitrate an initial temperature profile.**
  2. **Estimate the value of the various coefficients based on this profile.**
  3. **Solve the pseudo-linear system of algebraic equations to obtain a new temperature profile.**
  4. **Return to point 2 until the iterative process does not lead to improvements in the solution.**

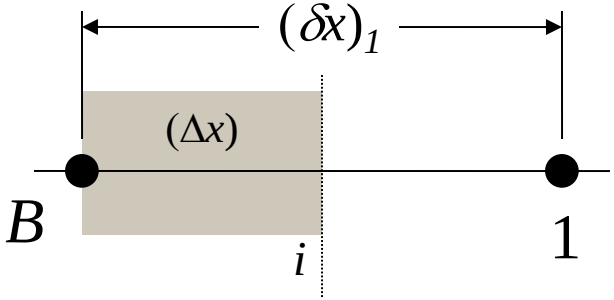
- The most appropriate convergence test is to determine the rate of violation to the balance of the quantity in question, after re-calculating the coefficients of the system of equations: the control volumes method is only conservative as long as the constant coefficients are assumed in a given iteration. .

Boundary conditions

- **Classification**
  - **Dirichlet condition:**
    Temperature value specified.
  - **Neumann's condition:**
    Gradient value specified (known heat flux)
  - **Mixed condition (or Robin condition)**

- **Discretization:**
  - **Dirichlet's condition poses no additional problems.**
  - **Neumann and mixed conditions require a new discretization equation at the boundary.**

Neumann boundary condition



- **Discretization equation for shaded control volume:**

$$q_B - q_i + (S_C + S_P T_B)\Delta x = 0$$

$$q_B - \frac{k_i (T_B - T_I)}{(\delta x)_i} + (S_C + S_P T_B)\Delta x = 0$$

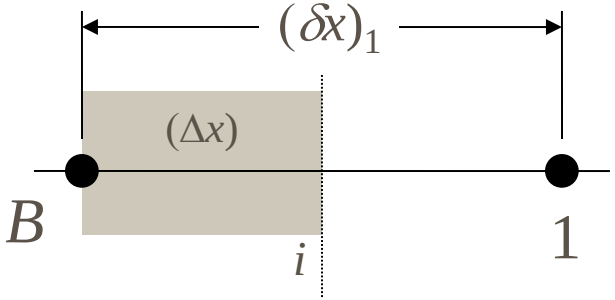
$$\Rightarrow \quad a_B T_B = a_1 T_1 + b$$

$$a_1 = k_1 / (\delta x)_1$$

$$b = S_C \Delta x + q_B$$

$$a_B = a_1 - S_P \Delta x$$

Mixed boundary condition



- **Discretization equation for shaded control volume:**

$$q_B - q_i + (S_C + S_P T_B)\Delta x = 0 \qquad \text{with} \qquad q_B = h(T_f - T_B)$$

$$h(T_f - T_B) - \frac{k_i (T_B - T_I)}{(\delta x)_i} + (S_C + S_P T_B)\Delta x = 0$$

$$\Rightarrow \qquad a_B T_B = a_1 T_1 + b$$

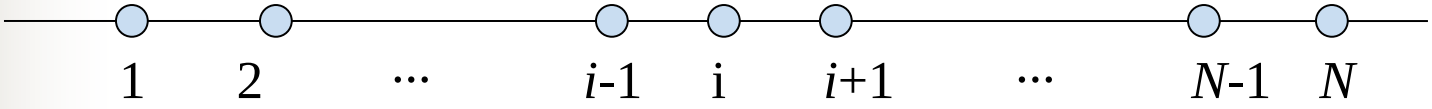
$$a_1 = k_1 / (\delta x)_1$$

$$b = S_C \Delta x + h T_f$$

$$a_B = a_1 - S_P \Delta x + h$$

Numerical solution of the system of equations

- **Algorithm of the tri-diagonal matrix (TDMA)**



$$a_i T_i = b_i T_{i+1} + c_i T_{i-1} + d_i \quad \text{with} \quad i = 1, 2, \ldots, N \quad ; \quad c_1 = 0 \quad \text{e} \quad b_N = 0$$

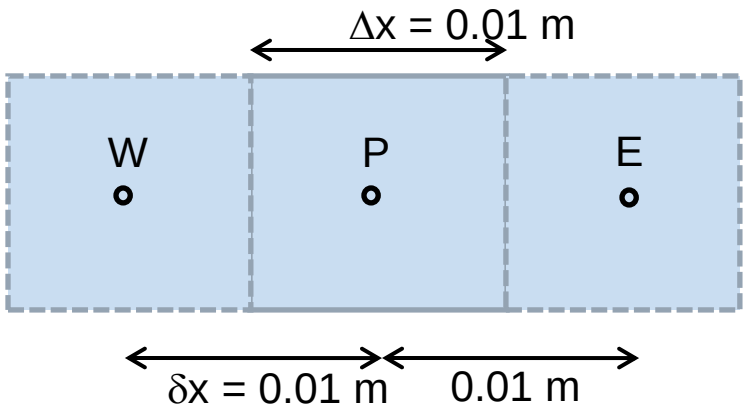
(It is a particular case of the Gaussian elimination method.)

Algorithm:

- 1- $P_1 = b_1 / a_1 \quad ; \quad Q_1 = d_1 / a_1$
- 2- $P_i = \dfrac{b_i}{a_i - c_i P_{i-1}} \quad ; \quad Q_i = \dfrac{b_i + c_i Q_{i-1}}{a_i - c_i P_{i-1}}$
- 3- $T_i = P_i T_{i+1} + Q_i \quad \text{for} \quad i = N-1, N, \cdots, 2, 1$

Exercise

Consider the control volume shown in the following figure, in which there is unidirectional heat conduction with internal generation, in steady state. Determine the canonical temperature equation at point P, using the following information:



Initial temperature distribution: T_{W0} = 400K, T_{P0} = 420K, T_{E0} = 440K

$S = A - BT^{1/2}$, A = 100 J m^{-3} s^{-1}, B = 2.5 J m^{-3} s^{-1} $K^{-1/2}$

$k = k_1 + k_2T$, k_1 = 10 W m^{-1} K^{-1}, k_2 = 0.02 W m^{-1} K^{-2}

$$a_P T_P = a_E T_E$$

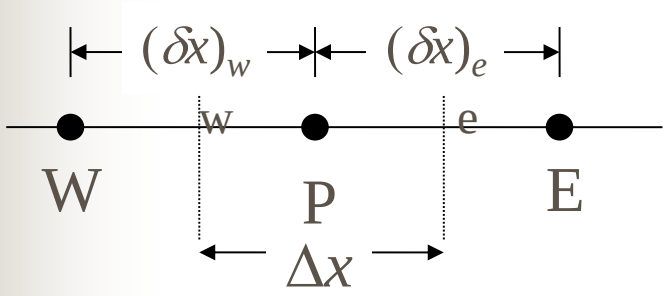
$$a_E = k_e /(\delta x)$$

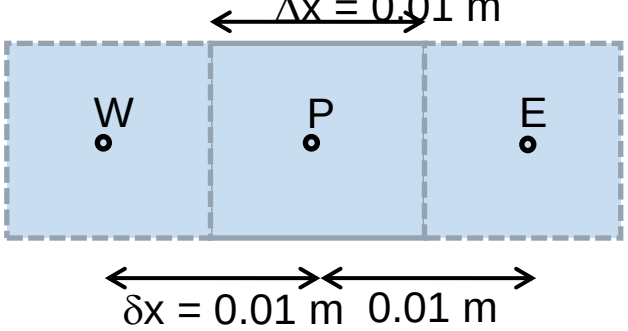
$$a_W = k_w /(\delta x$$

$$a_P = a_E + a_W$$

$$b = S_C \Delta x$$

$$\bar{S} = S_C + S_P T$$





$$\frac{d}{dx}\left(k\frac{dT}{dx}\right)+S=0$$

$S = A - B\,T^{1/2}$, $A = 100$ J m^{-3} s^{-1}, $B = 2.5$ J m^{-3} s^{-1} K$^{-1/2}$

$k = k_1 + k_2 T$, $k_1 = 10$ W m^{-1} K^{-1}, $k_2 = 0.02$ W m^{-1} K^{-2}

$T_{W0} = 400$ K
$T_{P0} = 420$ K
$T_{E0} = 440$ K

→

$T_{w0} = 410$ K
$T_{e0} = 430$ K

→

$k_{w0} = 10+0.02\times410 = 18.2$
$k_{e0} = 10+0.02\times430 = 18.6$

Taylor linearization of S:

$$S = S(T_{p0}) + \left(\frac{\partial S}{\partial T}\right)\Big|_{T_{p0}} (T_p - T_{p0})$$

→

$$S = \underbrace{S(T_{p0}) - T_{p0}\left(\frac{\partial S}{\partial T}\right)\Big|_{T_{p0}}}_{S_c} + \underbrace{\left(\frac{\partial S}{\partial T}\right)\Big|_{T_{p0}}}_{S_p} T_p$$

$$\frac{\partial S}{\partial T} = -\frac{1}{2}B.T^{-\frac{1}{2}}$$

$$\left(\frac{\partial S}{\partial T}\right)\Big|_{T_{p0}} = -\frac{1}{2}2.5\times420^{-0.5} = -0.061$$

$$S(T_{p0}) = 100 - 2.5\times420^{0.5} = 48.8$$

$$S_c = 48.8 + 420\times0.061 = 74.4$$

$S_p = -0.061 < 0$:
OK! Linearization can be done.

$a_E = k_e/(\delta x)_e$	$a_E = 18.2/0.01 = 1820$
$a_W = k_w/(\delta x)_w$	$a_W = 18.6/0.01 = 1860$
$a_P = a_E + a_W - S_P\Delta x$	$a_P = 1820 + 1860 + 0.061\times0.01$
$b = S_C\Delta x$	$b = 74.4\times0.01 = 0.744$

$$\mathbf{3680\,T_P = 1820\,T_E + 1860\,T_W + 0.744}$$

2- ONE-DIMENSIONAL TRANSIENT CONDUCTION

- **The method of discretizing the terms driving and source of the transport equation uni-directional of heat were already been presented.**

- **In the most general case, in addition to the driving and source terms, there is the accumulation term:**

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

- **Integration:**

$$\rho \hat{c}_p \int_w^e \int_t^{t+\Delta t} \frac{\partial T}{\partial t} dt dx = \int_w^e \int_t^{t+\Delta t} \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x} \right) dt dx + \int_w^e \int_t^{t+\Delta t} S dt dx$$

- **Assuming that T_P and s prevail throughout the VC:**

$$\rho\hat{c}_p\int_w^e\int_t^{t+\Delta t}\frac{\partial T}{\partial t}dtdx=\rho\hat{c}_p\Delta x(T_P^1-T_P^0)$$

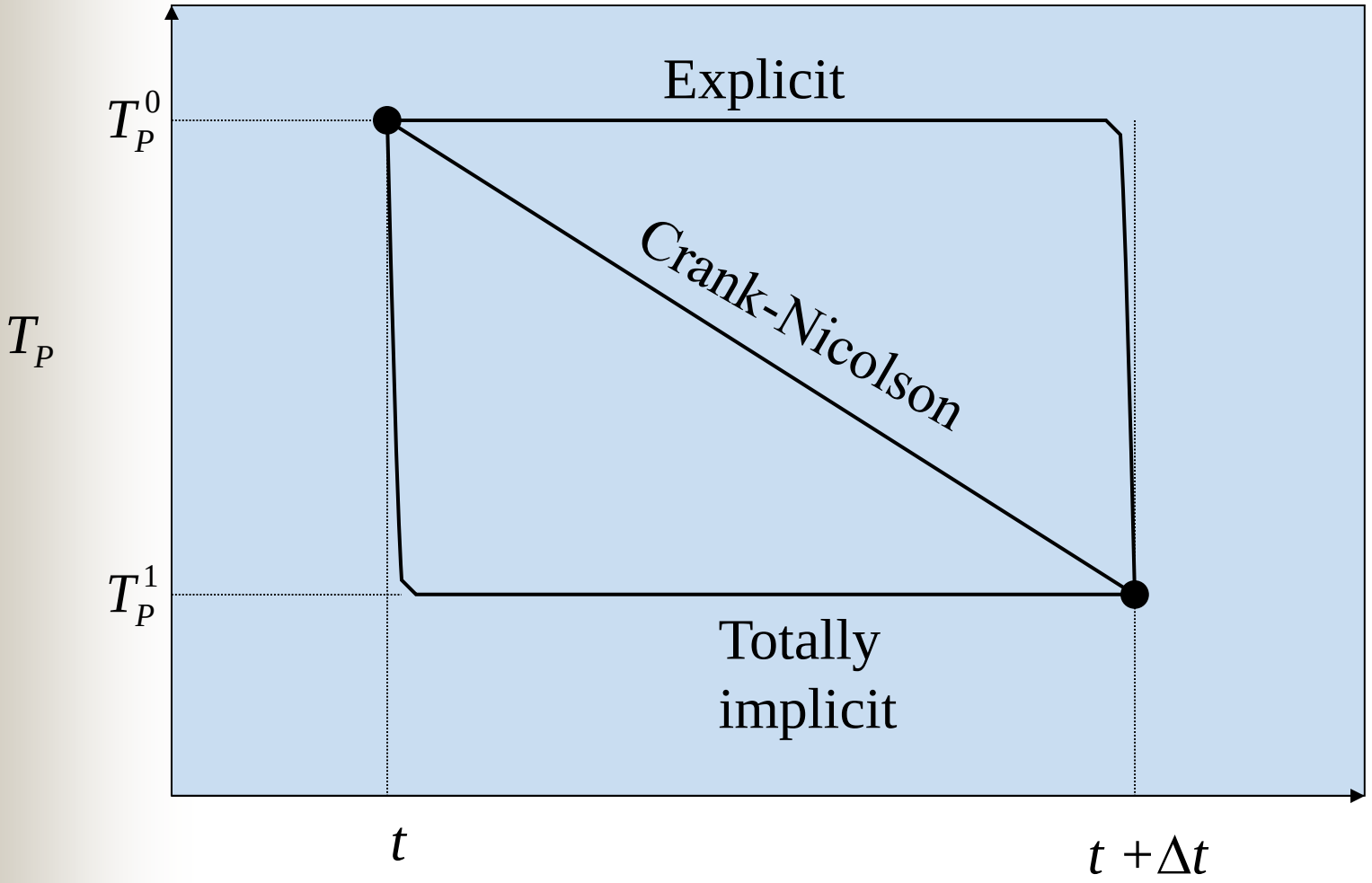
$$\int_w^e\int_t^{t+\Delta t}Sdtdx=S\Delta x\Delta t$$

- **To perform the temporal integration it is necessary to assume a profile of variation of T and S with time in each node.**

$$\int_w^e\int_t^{t+\Delta t}\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)dtdx=\int_t^{t+\Delta t}\left[\frac{k_e(T_E-T_P)}{(\delta x)_e}-\frac{k_w(T_P-T_W)}{(\delta x)_w}\right]dt$$

Temporal discretization

- **Schemes of temperature variation with time**



Integration schemes

- **The integral**

$$\int_t^{\Delta t} T_P dt$$

assuming the different integration schemes has been given by

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

  - ***f* = 0: Explicit layout**
  - ***f* = 0.5: Crank-Nicholson scheme**
  - ***f* = 1: Scheme totally implicit**

Discretization equation

- **We then have:**

$$\rho\hat{c}_p\Delta x(T_P^1 - T_P^0) = \int_t^{t+\Delta t}\left[\frac{k_e(T_E - T_P)}{(\delta x)_e} - \frac{k_w(T_P - T_W)}{(\delta x)_w}\right]dt + \Delta x\int_t^{t+\Delta t} S dt$$

$$\Rightarrow \quad \rho\hat{c}_p\Delta x(T_P^1 - T_P^0) = f\left[\frac{k_e(T_E^1 - T_P^1)}{(\delta x)_e} - \frac{k_w(T_P^1 - T_W^1)}{(\delta x)_w}\right] +$$

$$+(1-f)\left[\frac{k_e(T_E^0 - T_P^0)}{(\delta x)_e} - \frac{k_w(T_P^0 - T_W^0)}{(\delta x)_w}\right] + S\Delta x\Delta t$$

In the next notation we are going to eliminate exponent 1 and consider that, eg, T_P is the value of T in the node P at $t+\Delta t$.

Discretization equation

- **General canonical form (0 <f <1)**

$$a_p T_P = a_E \left[f T_E + (1-f) T_E^0 \right] + a_W \left[f T_W + (1-f) T_W^0 \right] + \\ + \left[a_P^0 - (1-f) a_E - (1-f) a_W \right] T_P^0 + S_C \Delta x$$

$$a_E = k_e / (\delta x)_e$$

$$a_W = k_w / (\delta x)_w$$

$$a_P^0 = \rho \hat{c}_p \Delta x / \Delta t$$

$$a_P = f a_E + f a_W + a_P^0 - S_P \Delta x$$

Discretization equation

- **Canonical form for the explicit scheme (*f* = 0):**

$$a_p T_P = a_E T_E^0 + a_W T_W^0 + (a_P^0 - a_E - a_W) T_P^0 + b$$

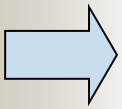
$$a_E = k_e / (\delta x)_e$$

$$a_W = k_w / (\delta x)_w$$

$$a_P^0 = \rho \hat{c}_p \Delta x / \Delta t$$

$$a_P = a_P^0 - S_P \Delta x$$

$$b = S_C \Delta x$$



The method is explicit because T_P is determined based only on the initial temperature values .

Limitations of the explicit scheme

- **The method is unstable or leads to physically invalid solutions if:**

$$a_P^0 - a_E - a_W < 0$$

  - **Assuming,** $(\delta x)_e = (\delta x)_e = \Delta x$

    this is equivalent to :

$$\Delta t < \frac{\rho C_p (\Delta x)^2}{2k}$$

  - **Therefore, when the mesh is refined, it is necessary to refine the temporal integration step too much for the scheme to be stable. This leads to excessively long calculation times.**

Discretization equation

- **Canonical form for the fully implicit scheme (*f* = 1):**

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

$$a_E = k_e / (\delta x)_e$$

$$a_W = k_w / (\delta x)_w$$

$$a_P^0 = \rho \hat{c}_p \Delta x / \Delta t$$

$$a_P = a_E + a_W + a_P^0 - S_P \Delta x$$

$$b = S_C \Delta x + a_P^0 T_P^0$$

For $\Delta t \to \infty$ **we get the canonical equation for steady-state**

The method is implicit because both T_P, T_E and T_W are unknown.

Recommended discretization scheme

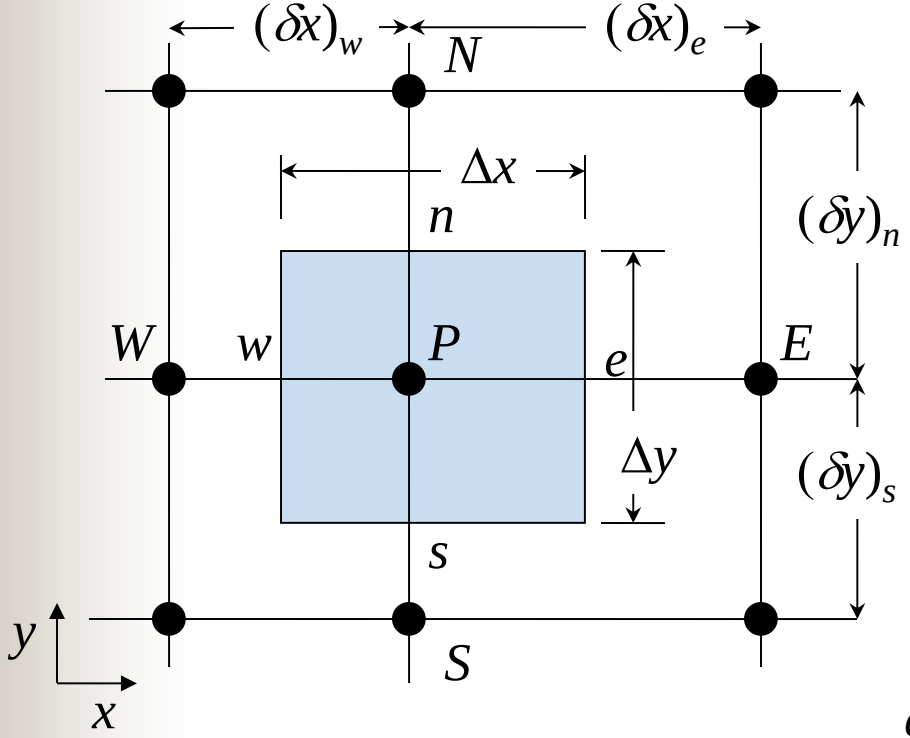
- **The totally implicit method is unconditionally stable and always leads to solutions with physical significance.**
- **The explicit method is not recommended because it is only stable for integration steps that are too small.**
- **The method of Cranck-Nicholson although it is also unconditionally stable, it can lead to solutions that fluctuate due to numerical problems.**

3- DISCRETIZATION IN TWO DIMENSIONS

(orthogonal meshes)

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

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



$$a_E = \frac{k_e \Delta y}{(\delta x)_e}$$

$$a_W = \frac{k_w \Delta y}{(\delta x)_w}$$

$$a_N = \frac{k_n \Delta x}{(\delta y)_n}$$

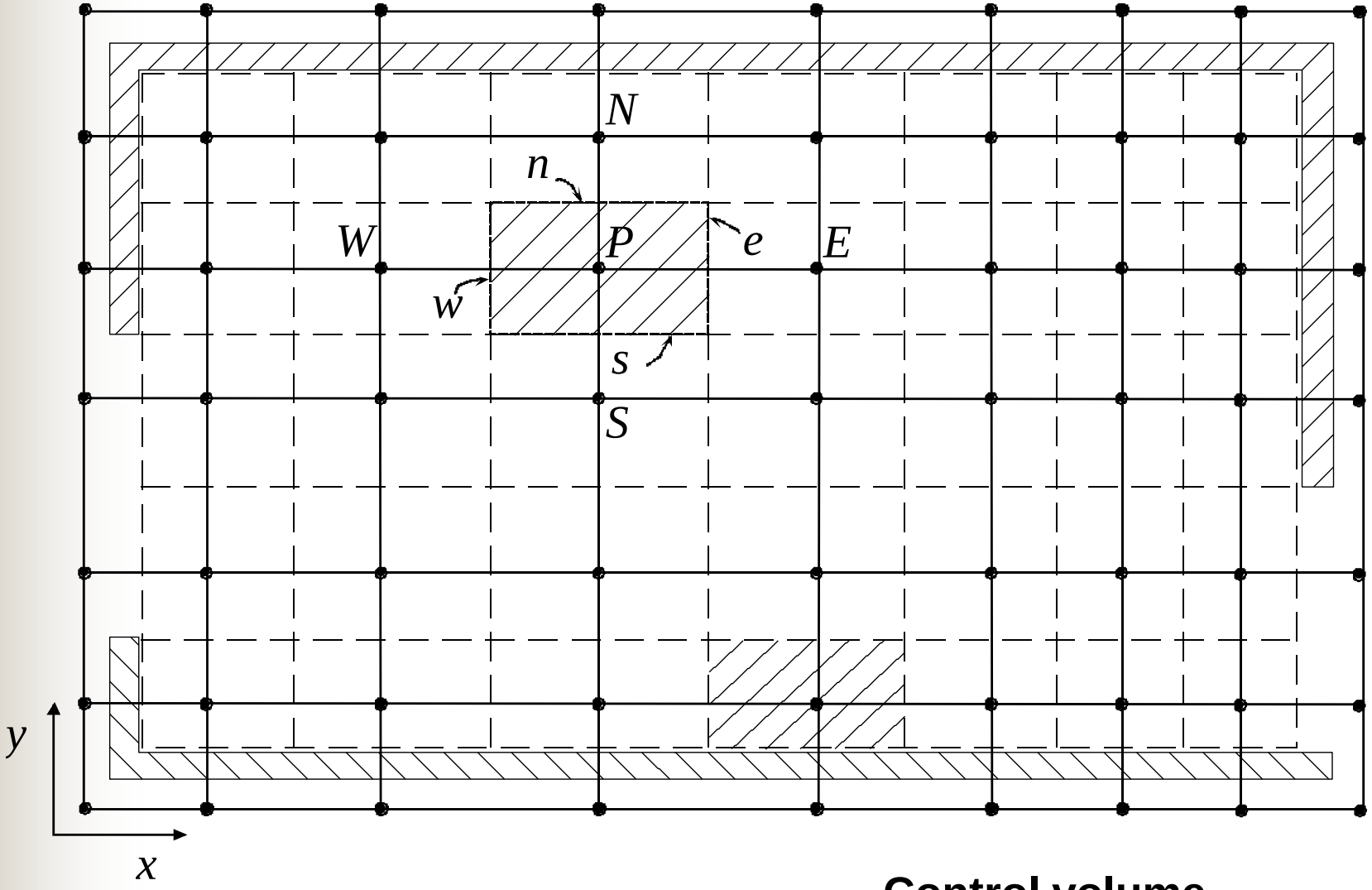
$$a_S = \frac{k_s \Delta x}{(\delta y)_s}$$

$$a_P^0 = \rho c_p \Delta x \Delta y / \Delta t$$

$$b = S_c \, \Delta x \, \Delta y + a_P^0 T_P^0$$

$$a_P = a_E + a_W + a_N + a_S + a_P^0 - S_p \, \Delta x \, \Delta y$$

Typical mesh



Control volume near the border

Solution of algebraic equations for two dimensions

- **Although the canonical discretization equation for 2 dimensions is a simple extension of that for 1 dimension, the solution of the resulting equations system is now more difficult because the TDMA algorithm cannot be applied.**

- **Solution algorithms for the system of equations:**
  - **Direct: they do not require iterations, but they do require a large amount of computer memory. If the problem is linear, it can lead to shorter calculation times than iterative methods.**

  - **Direct methods (e.g., Gaussian elimination) can cause fill-in, where zeros become non-zeros, destroying sparsity and increasing memory and computation costs.** in real CFD problems with thousands or millions of control volumes, these methods are critical.

  - **Iterative: they are much simpler than direct algorithms and require less computer memory. In non-linear problems, it is not necessary to achieve convergence in each iteration.**

Gauss-Seidel iterative method

$$a_p T_P = \sum a_{nb} T_{nb} + b$$

em que

$$a_{nb} = a_E, a_W, a_N, a_S, \ldots$$

$$T_{nb} = T_E, T_W, T_N, T_S, \ldots$$

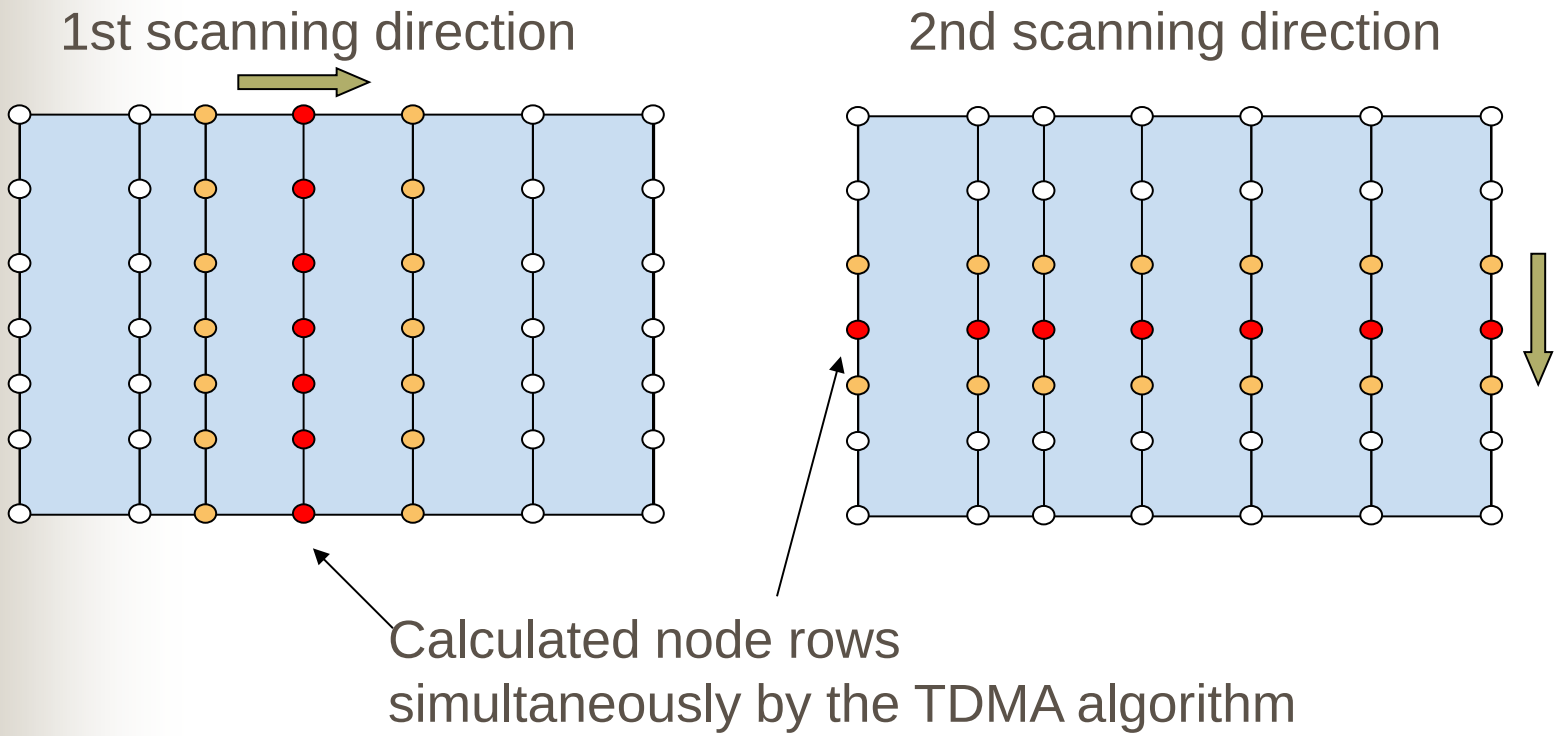
- **An initial temperature distribution is arbitrated** T_{nb}^{*}
- **In a sequential way it is calculated**

$$T_P = \frac{\sum a_{nb} T_{nb}^{*} + b}{a_p}$$

- **Scarborough convergence criterion:**

$$\frac{\sum |a_{nb}|}{|a_P|} \begin{cases} \leq 1 & \text{para todas as equações} \\ < 1 & \text{para uma equação pelo menos} \end{cases}$$

Line-by-line TDMA method



- **Starting from an initial temperature distribution, the TDMA algorithm is applied line-by-line, sweeping the entire domain in several directions in an alternating way.**
- **The Gauss-Seidel algorithm is slow because the information on the boundary conditions is only carried out after several iterations that is carried into the domain. In the TDMA line-by-line algorithm, this information is transferred only once on each line.**

Limitations of the line-by-line TDMA method

- **For simple differential equations of scalar quantities, this method gives good results.**
- **Convergence becomes more difficult as the number of nodes in the grid increases.**
- **For very dense meshes and systems with strong non-linearity there may be a need to use other, more robust methods.**

Stepest Descent Method

https://doc.cfd.direct/notes/cfd-general-principles/descent-methods

$$\mathbf{A} \cdot \boldsymbol{\Psi} = \mathbf{b}$$

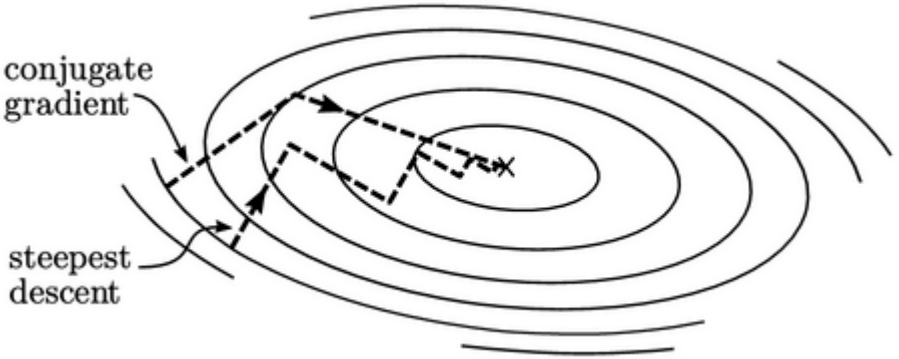
Minimize: $$f(\boldsymbol{\Psi}) = \frac{1}{2}\boldsymbol{\Psi} \cdot \mathbf{A} \cdot \boldsymbol{\Psi} - \mathbf{b} \cdot \boldsymbol{\Psi}$$

- Jonathan Richard Shewchuk An introduction to the conjugate gradient method without the agonizing pain, 1994.

$\partial f(\boldsymbol{\Psi})/\partial \boldsymbol{\Psi} = 0$ corresponds to a minimum in the quadratic function

$$\boldsymbol{\Psi} := \boldsymbol{\Psi}^c + \alpha \mathbf{p}$$

P is the direction of the line search



Example

$$\begin{bmatrix} 6 & -2 \\ -2 & 4 \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}.$$

$$f(\boldsymbol{\Psi}) = 3\Psi_1^2 + 2\Psi_2^2 - 2\Psi_1\Psi_2 - \Psi_1 - 3\Psi_2$$

$$\frac{\partial f(\boldsymbol{\Psi})}{\partial \boldsymbol{\Psi}} = \begin{bmatrix} \partial f/\partial \Psi_1 \\ \partial f/\partial \Psi_2 \end{bmatrix} = \begin{bmatrix} 6\Psi_1 - 2\Psi_2 - 1 \\ -2\Psi_1 + 4\Psi_2 - 3 \end{bmatrix}$$

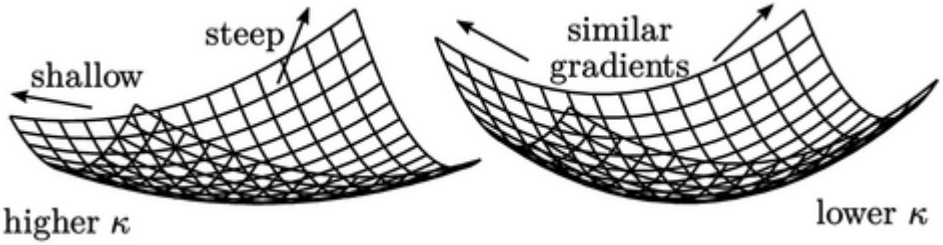
For this method to work, the quadratic form must have a minimum, which requires that eqn. is symmetric and positive-definite.

Preconditioning Methods:

CG Method Basics: Primarily used in computational fluid dynamics (CFD) as an iterative matrix solver. Designed to handle large problems that are impractical for direct solution methods.
Limitation of Direct CG: Ideally, CG solves equations in a number of steps equal to the number of variables (eqn steps). However, finite precision arithmetic leads to rounding errors, preventing an exact solution within these steps.
Iterative Approach: CG aims to reduce the solution residual to within a specified tolerance, making the convergence rate a critical aspect.
Impact of Matrix Condition Number:

- Convergence speed inversely related to the condition number of the matrix.
- Condition number derived from the ratio of the largest to the smallest eigenvalues (kappa = lambda_max / lambda_min).
- High condition numbers result in slower convergence rates.

Geometric Interpretation: In a quadratic system, the eigenvalues are linked to the gradients of the principal axes of the paraboloid. Lower condition numbers mean a "rounder" bowl, leading to better convergence.



Role of Preconditioning:

- Aims to transform the matrix A to a form closer to the identity matrix for faster convergence.
- $A.X = B \quad \rightarrow (M^{-1} A).X = M^{-1} B$
- Involves calculating a preconditioner matrix M so that $(M^{-1} A)$. is closer to the identity matrix.

Effective Preconditioning Methods:

- Diagonal-based incomplete Cholesky (DIC) for symmetric matrices.
- Diagonal-based incomplete LU (DILU) for asymmetric matrices.

Bi-Conjugate Gradient Method (BiCG)

the matrices arising from the discretization of the governing equations (like the Navier-Stokes equations) often are not symmetric

For systems where the matrix is not symmetric or not positive definite, alternative methods are typically used instead of the standard conjugate gradient method. Some common approaches include:

- Bi-Conjugate Gradient Method (BiCG): This method extends the conjugate gradient approach to non-symmetric matrices. It operates by simultaneously considering the system and its transpose, effectively managing the lack of symmetry.

- Preconditioning: Using preconditioners can significantly improve the convergence of iterative methods, even for non-symmetric or indefinite matrices. Preconditioners transform the matrix into a form that is more amenable to these iterative solvers, sometimes even making the preconditioned system symmetric and positive definite.

- For CFD applications where matrices are often large, sparse, and non-symmetric, selecting the right solver and preconditioner becomes crucial to achieve efficient and accurate simulations. These adaptations allow the use of gradient-based iterative methods even when the strict mathematical prerequisites (symmetry and positive definiteness) of the standard conjugate gradient method are not met.

Solver Selection Heuristic

Matrix Type	Recommended Solver	Notes
Symmetric (e.g. Laplacian arising in heat transfer)	PCG (Preconditioned Conjugate Gradient)	Use DIC preconditioning
Asymmetric (e.g. Advection in momentum equation)	PBiCGStab (Preconditioned BiCG Stabilised)	Use DILU preconditioning
Highly Asymmetric or Stiff	PBiCGStab	Robust and smooth convergence
Asymmetric, with convergence issues	Avoid PBiCG	Unstable; erratic residual behaviour
Symmetric but slow convergence	PCG with better preconditioner	Try GAMG or other multigrid methods

- CG – Conjugate Gradient
- PCG – Preconditioned Conjugate Gradient
- BiCG – Biconjugate Gradient
- PBiCG – Preconditioned Biconjugate Gradient
- PBiCGStab – Preconditioned Biconjugate Gradient Stabilised
- DIC – Diagonal Incomplete Cholesky (Preconditioner)
- DILU – Diagonal Incomplete LU factorisation (Preconditioner)
- GAMG – Geometric-Algebraic Multigrid (Solver)

Sub-Relaxation

- In non-linear systems, the coefficients of the discretization equation depend on the temperature. It is therefore necessary to have an iterative global scheme in which the coefficients of the discretization equation are recalculated after obtaining a more accurate estimate of the temperature distribution.
- In these cases, although the systems of equations generated are unconditionally stable, the overall iterative process may differ.
- In this situation, it is customary to sub-relax the temperature variation from one iteration to the next.

Sub-Relaxation

- **If is the initial temperature and is the temperature at the end of the iteration, the sub-relaxation leads to a value of less than :**

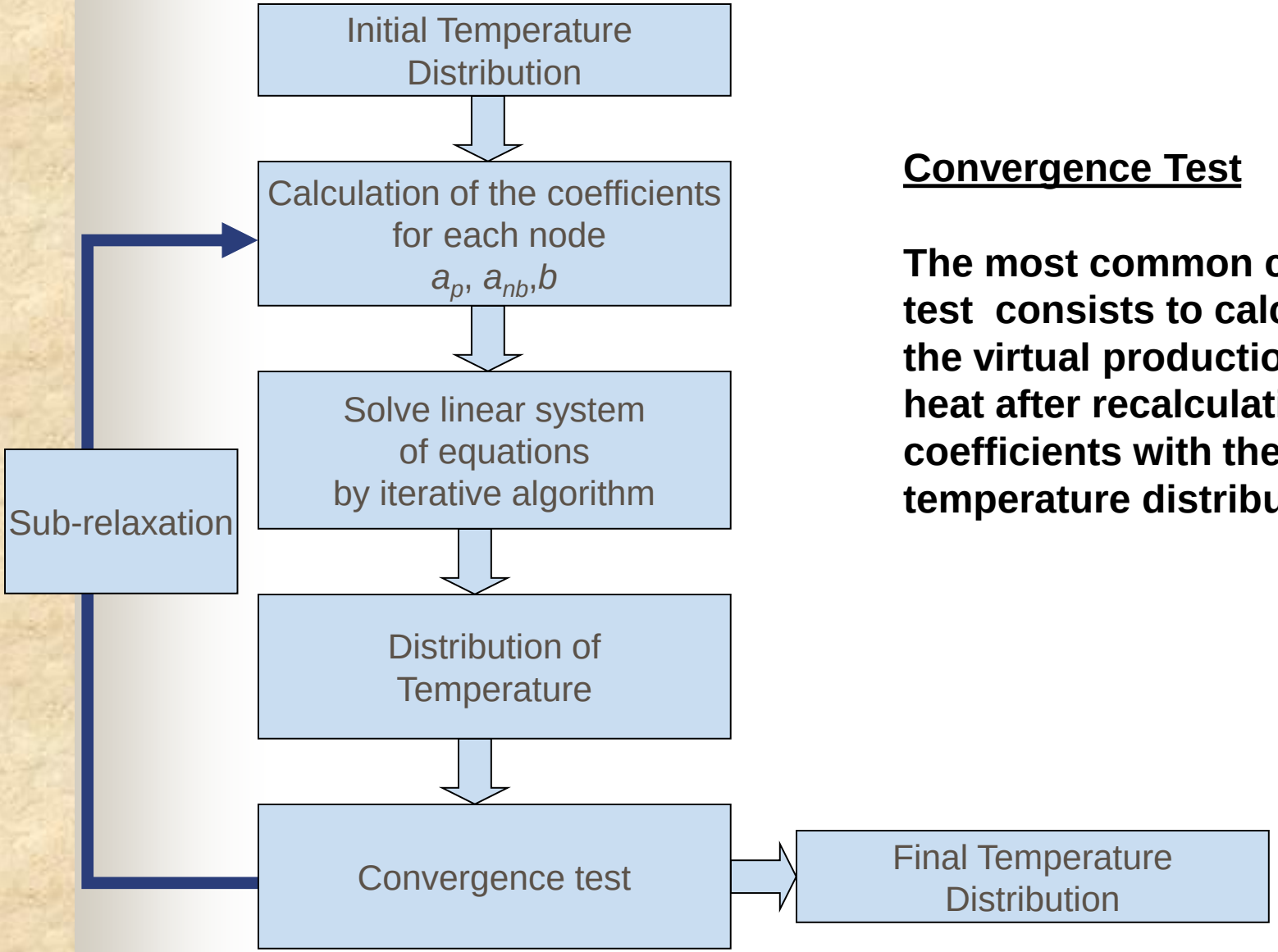
$$T_{Psub} = T_P^0 + \alpha(T_P^1 - T_P^0) \qquad \textbf{where } 0 < \alpha < 1.$$

- **The discretization equation can be modified to incorporate the sub-relaxation coefficient directly.**

$$T_P^1 = \frac{\sum a_{nb} T_{nb} + b}{a_p} \quad \Rightarrow \quad T_{Psub} = T_P^0 + \alpha\left(\frac{\sum a_{nb} T_{nb} + b}{a_p} - T_P^0\right)$$

$$\Rightarrow \quad \frac{a_p}{\alpha} T_{Psub} = \sum a_{nb} T_{nb} + b + (1-\alpha)\frac{a_p}{\alpha} T_P^0$$

Global iterative method



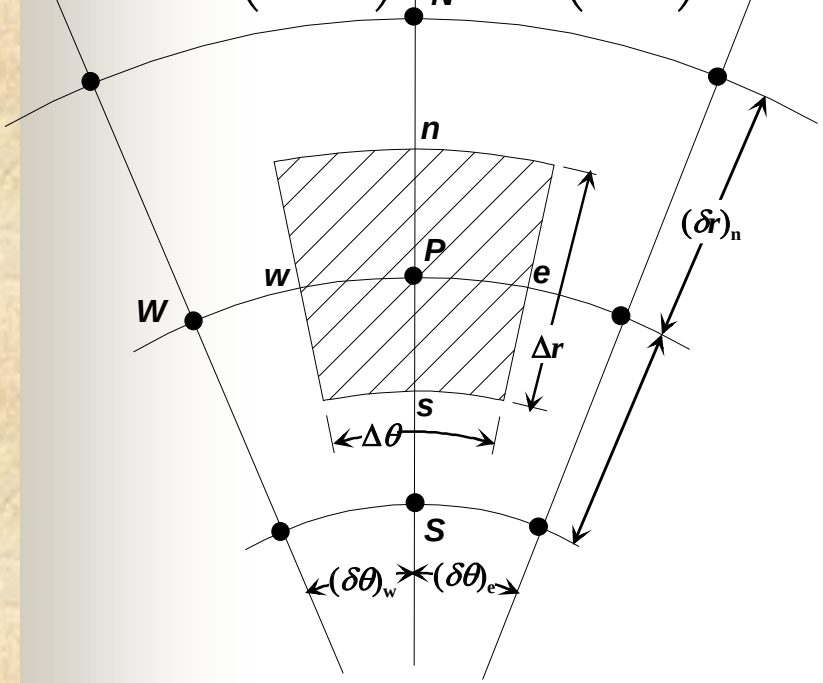
Convergence Test

The most common convergence test consists to calculate the virtual production rate of heat after recalculating the coefficients with the new temperature distribution.

Other orthogonal coordinate systems

- **Polar coordinates in two dimensions**

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(kr\frac{\partial T}{\partial r}\right) + \frac{1}{r}\frac{\partial}{\partial \theta}\left(k\frac{\partial T}{\partial \theta}\right) + S$$



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

$$a_E = \frac{k_e \Delta r}{r_e (\delta\theta)_e}$$

$$a_W = \frac{k_w \Delta r}{r_w (\delta\theta)_w}$$

$$a_N = \frac{k_n r_n \Delta\theta}{(\delta r)_n}$$

$$a_S = \frac{k_s r_s \Delta\theta}{(\delta r)_s}$$

$$a_P = a_E + a_W + a_N + a_S + a_P^0 - S_P \Delta V$$

$$a_P^0 = (\rho \hat{c}_p \Delta V)/\Delta t$$

$$b = S_C \Delta V + a_P^0 T_P^0$$

$$\Delta V = 0.5(r_n + r_s)\Delta\theta\Delta r$$

- **For orthogonal coordinate systems, the canonical equations remain unchanged: it is only necessary to introduce the new geometric characteristics.**

III - CONVECTION AND DIFUSION

1- Upwind Scheme
2- Exponential Scheme
3- Hybrid Scheme
4- General discretization equation

Transport equation with convective term:

- **Generic transport equation with the convective term:**

$$\frac{\partial \rho\phi}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j \phi) = \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right) + S$$

- **Continuity equation:**

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0$$

- **Combination of the two equations:**

$$\rho \frac{\partial \phi}{\partial t} + \rho u_j \frac{\partial \phi}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right) + S$$

INTERPOLATION SCHEMES FOR CONVECTIVE TERM - One-dimensional case

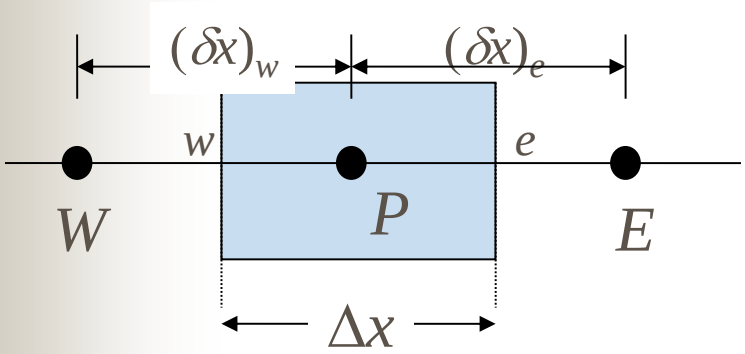
- **Scheme of central differences.**
  - **It is assumed for now that the velocity distribution is known and satisfies the continuity equation:**

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

  - **In the case of one-dimensional stationary and without source term:**

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

  - **The integration of this equation in the marked VC gives:**



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

Scheme of central differences

- **To calculate** $\left(\Gamma\frac{d\phi}{dx}\right)_e$, $\left(\Gamma\frac{d\phi}{dx}\right)_w$, $(\rho u\phi)_e$ e $(\rho u\phi)_w$

  it is necessary to use an interpolation scheme.
- **Assuming that each interface is in the middle of two nodes and assuming linear profiles between two points, we have:**

$$\phi_e = \tfrac{1}{2}(\phi_E + \phi_P), \quad \phi_w = \tfrac{1}{2}(\phi_P + \phi_W)$$

- **The discretization equation then takes the form:**

$$\tfrac{1}{2}(\rho u)_e(\phi_E + \phi_P) - \tfrac{1}{2}(\rho u)_w(\phi_P + \phi_W) = \frac{\Gamma_e(\phi_E + \phi_P)}{(\delta x)_e} - \frac{\Gamma_w(\phi_P + \phi_W)}{(\delta x)_w}$$

Scheme of central differences

- **In canonical form the discretization equation is:**

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

$$a_E = D_e - \frac{F_e}{2}$$

$$a_W = D_w + \frac{F_w}{2}$$

$$a_P = D_e + \frac{F_e}{2} + D_w - \frac{F_w}{2}$$

$$= a_E + a_W + (F_e - F_w)$$

$$= a_E + a_W$$

where

$$F \equiv \rho u$$

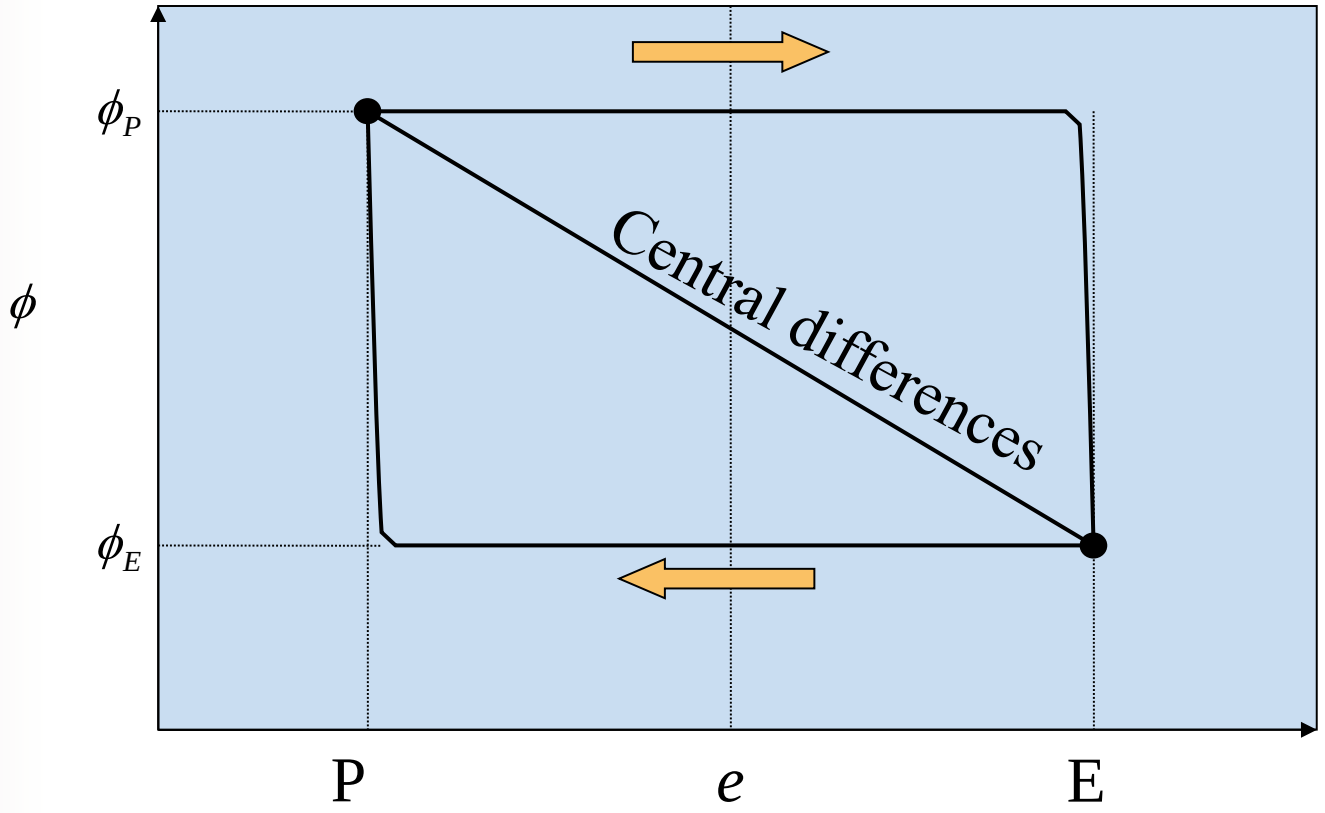
$$D \equiv \frac{\Gamma}{\delta x}$$

- **The biggest problem with this interpolation scheme is that it leads to discretization equations that may violate the Scarborough criterion (a_E and a_W can assume negative values).**

- **When the convection is dominant, the interpolation function deviates a lot from linearity.**

Upwind scheme

- **The central difference method leads to poor results for poorly refined meshes because when convection is dominant at a value of ϕ tends to be equal to the value of the upstream node:**



- **The "Up-wind" interpolation scheme discretizes the convective term assuming that ϕ is equal to the value of the upstream node and uses the central difference scheme to calculate the diffusive term.**

Upwind scheme

- **The Upwind scheme additionally assumes that the diffusive component continues to lead to:**

$$\phi_e = \begin{cases} \phi_P & \text{se} \quad F_e > 0 \\ \phi_E & \text{se} \quad F_e < 0 \end{cases} \Rightarrow F_e\phi_e = \phi_P \|F_e, 0\| - \phi_E \|-F_e, 0\|$$

$$\phi_w = \begin{cases} \phi_W & \text{se} \quad F_w > 0 \\ \phi_P & \text{se} \quad F_w < 0 \end{cases} \Rightarrow F_w\phi_w = \phi_W \|F_w, 0\| - \phi_W \|-F_w, 0\|$$

where $\|A, B\| = max(A, B)$

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

$$a_E = D_e + \|-F_e, 0\|$$

$$a_W = D_w + \|F_w, 0\|$$

$$a_P = a_E + a_W + (F_e - F_w)$$

Exponential Scheme

- **The Upwind scheme has the disadvantage of assuming linear profiles in the interpolation of ϕ for the diffusive terms. For strong convective flows, this represents a less rigorous approach.**

- **The exponential scheme addresses this problem through the use of a profile of ϕ which corresponds to the exact transport solution with convection and uni-directional diffusion between two consecutive nodes:**

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

$$\begin{cases} \phi = \phi_0 & \text{em} \quad x = 0 \\ \phi = \phi_L & \text{em} \quad x = L \end{cases}$$

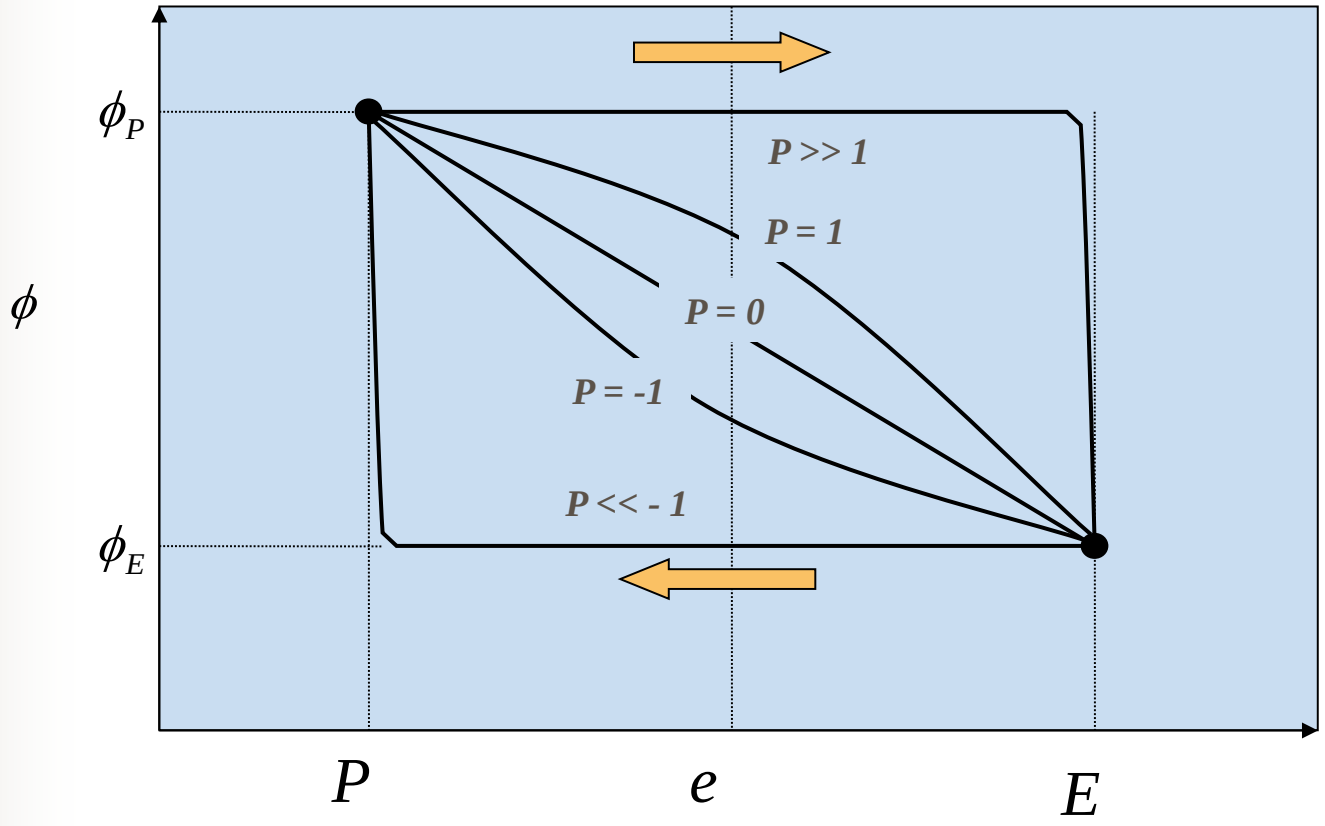
$$\frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{\exp(Px/L) - 1}{\exp(P) - 1}$$

$$P \equiv \frac{\rho u}{\Gamma / L} = \frac{F}{D}$$

Exponential scheme

- **Influence of Peclet number (P) on the profile of ϕ between two nodes.**

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



Exponential scheme

- **In this scheme, the exponential profile is used to interpolate the convective and diffusive terms, obtaining:**

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

$$a_E = \frac{F_e}{\exp(F_e / D_e) - 1}$$

$$a_W = \frac{F_w \exp(F_w / D_w)}{\exp(F_w / D_w) - 1}$$

$$a_P = a_E + a_W + (F_e - F_w)$$

- **The main problem with the exponential scheme lies in the high cost of calculating the exponential terms.**

Hybrid Scheme

- **It assumes the central difference scheme for –2 < Pe <2 and outside this range it assumes the Upwind scheme with diffusion cancellation.**

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

$$a_E = \left\| -F_e, D_e - F_e/2, 0 \right\|$$

$$a_W = \left\| F_w, D_w + F_w/2, 0 \right\|$$

$$a_P = a_W + a_E + (F_e - F_w)$$

Generic transport equation: Discretization by hybrid and implicit schemes.

- **Generic transport equation in 3 dimensions:**

$$\frac{\partial \rho\phi}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j \phi) = \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right) + S$$

- **Discretization equation:**

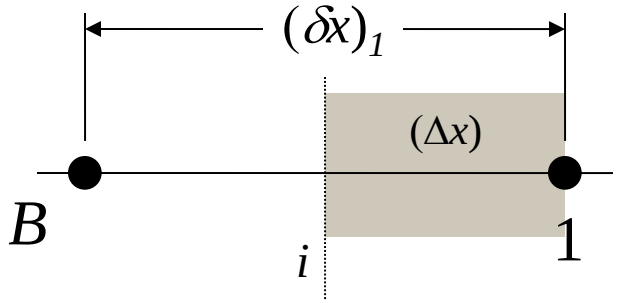
$$a_P\phi_P = a_E\phi_E + a_W\phi_W + a_N\phi_N + a_S\phi_S + b$$

$$a_E = \|-F_e, D_e - F_e/2, 0\|$$
$$a_W = \|F_w, D_w + F_w/2, 0\|$$
$$a_N = \|F_n, D_n + F_n/2, 0\|$$
$$a_S = \|F_s, D_s + F_s/2, 0\|$$
$$a_T = \|F_t, D_t + F_t/2, 0\|$$
$$a_B = \|F_b, D_b + F_b/2, 0\|$$
$$a_P^0 = \frac{\rho_P^0 \Delta x\Delta y\Delta z}{\Delta t}$$
$$b = S_C\Delta x\Delta y\Delta z + a_P^0\phi_P^0$$
$$a_P = a_E + a_W + a_N + a_S + a_T + a_B - S_p\Delta x\Delta y\Delta z$$

$$F_e = (\rho u)_e \Delta y\Delta z \qquad D_e = \frac{\Gamma_e}{(\delta x)_e}\Delta y\Delta z$$
$$F_w = (\rho u)_w \Delta y\Delta z \qquad D_w = \frac{\Gamma_w}{(\delta x)_w}\Delta y\Delta z$$
$$F_n = (\rho v)_n \Delta z\Delta x \qquad D_n = \frac{\Gamma_n}{(\delta y)_n}\Delta z\Delta x$$
$$F_s = (\rho v)_s \Delta z\Delta x \qquad D_s = \frac{\Gamma_s}{(\delta y)_s}\Delta z\Delta x$$
$$F_t = (\rho w)_t \Delta x\Delta y \qquad D_t = \frac{\Gamma_t}{(\delta z)_t}\Delta x\Delta y$$
$$F_b = (\rho w)_b \Delta x\Delta y \qquad D_b = \frac{\Gamma_b}{(\delta z)_b}\Delta x\Delta y$$

Boundary conditions

- **Dirichlet**
  - **Direct implementation.**
- **Neumann / mixed**
  - **Integration into the control volume with incorporation of the flow / transfer coefficient known in the interface.**



- **Border condition at discharge**
  - **On the discharge surface of the system, the number of local Peclet is usually very high. In this situation, the value of ϕ the downstream is equal to its upstream value and, therefore, no boundary condition is necessary. Just break the connection between the upstream node and the downstream node: e.g. $a_w = 0$.**

DISCRETIZATION OF THE MOMENTUM EQUATIONS

1- Equations of transport of momentum
2- Staggered grid
3- Pressure correction equation

Momentum Equation

- **In Cartesian coordinates and using Einstein's notation:**

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_j u_i)}{\partial x_j} = \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} + \rho b_i$$

force by unit of mass in the direction
= shear stress tensor

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_x u_i)}{\partial x_1} + \frac{\partial (\rho u_y u_i)}{\partial x_2} + \frac{\partial (\rho u_z u_i)}{\partial x_3} = \frac{\partial \tau_{ix}}{\partial x_1} + \frac{\partial \tau_{iy}}{\partial x_2} + \frac{\partial \tau_{iz}}{\partial x_3} - \frac{\partial p}{\partial x_i} + \rho b_i$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_x u_i)}{\partial x} + \frac{\partial (\rho u_y u_i)}{\partial y} + \frac{\partial (\rho u_z u_i)}{\partial z} = \frac{\partial \tau_{ix}}{\partial x} + \frac{\partial \tau_{iy}}{\partial y} + \frac{\partial \tau_{iz}}{\partial z} - \frac{\partial p}{\partial x_i} + \rho b_i$$

Equation of the amount of motion for a Newtonian fluid

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_j u_i)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) - \frac{\partial p}{\partial x_i} + \rho b_i$$

In the direction *i* =1 or *x* this equation gives:

$$\frac{\partial \rho u_x}{\partial t} + \frac{\partial (\rho u_x u_x)}{\partial x_1} + \frac{\partial (\rho u_y u_x)}{\partial x_2} + \frac{\partial (\rho u_z u_x)}{\partial x_3} =$$

$$\frac{\partial}{\partial x_1}\left(\mu \left(\frac{\partial u_x}{\partial x_1} + \frac{\partial u_x}{\partial x_1} \right) - \frac{2}{3}\left(\frac{\partial u_x}{\partial x_1} + \frac{\partial u_y}{\partial x_2} + \frac{\partial u_z}{\partial x_3} \right) \right) + \frac{\partial}{\partial x_2}\left(\mu \left(\frac{\partial u_x}{\partial x_2} + \frac{\partial u_y}{\partial x_1} \right) \right) + \frac{\partial}{\partial x_3}\left(\mu \left(\frac{\partial u_x}{\partial x_3} + \frac{\partial u_z}{\partial x_1} \right) \right)$$

$$- \frac{\partial p}{\partial x_1} + \rho b_x$$

This equation can be rewritten in the generic form:

$$\frac{\partial \rho \phi}{\partial t} + \frac{\partial (\rho u_x \phi)}{\partial x_1} + \frac{\partial (\rho u_y \phi)}{\partial x_2} + \frac{\partial (\rho u_z \phi)}{\partial x_3} = \frac{\partial}{\partial x_1}\left(\mu \frac{\partial \phi}{\partial x_1} \right) + \frac{\partial}{\partial x_2}\left(\mu \frac{\partial \phi}{\partial x_2} \right) + \frac{\partial}{\partial x_3}\left(\mu \frac{\partial \phi}{\partial x_3} \right) - \frac{\partial p}{\partial x_1} + S_{u_x}$$

on what:

$$\phi = u_x$$

$$S_{u_x} = \rho b_x + \frac{\partial}{\partial x_1}\left[\mu \frac{\partial u_x}{\partial x_1} - \frac{2}{3}\left(\frac{\partial u_x}{\partial x_1} + \frac{\partial u_y}{\partial x_2} + \frac{\partial u_z}{\partial x_3} \right) \right] + \frac{\partial}{\partial x_2}\left(\mu \frac{\partial u_y}{\partial x_1} \right) + \frac{\partial}{\partial x_3}\left(\mu \frac{\partial u_z}{\partial x_1} \right)$$

In two dimensions we have:

$$\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j u) = \frac{\partial}{\partial x_j}\left(\mu \frac{\partial u}{\partial x_j}\right) - \frac{\partial p}{\partial x} + S_u$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j v) = \frac{\partial}{\partial x_j}\left(\mu \frac{\partial v}{\partial x_j}\right) - \frac{\partial p}{\partial y} + S_v$$

where:

$$u = u_x$$

$$v = u_y$$

$$S_u = \rho b_x + \frac{\partial}{\partial x}\left[\mu \frac{\partial u}{\partial x} - \frac{2}{3}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)\right] + \frac{\partial}{\partial y}\left(\mu \frac{\partial v}{\partial x}\right)$$

$$S_v = \rho b_y + \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial y}\left[\mu \frac{\partial v}{\partial y} - \frac{2}{3}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)\right]$$

Particularities of the Navier-Stokes equation

- **In the momentum equations, the terms** x **and** y **have no equivalent in the generic equation for a scalar variable.**

- **The pressure has no scalar equation of its own being specified indirectly through the continuity equation:**

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0$$

- **When the correct pressure distribution is introduced into the momentum equations, the resulting velocity field satisfies the continuity equation.**

Particularities of the Navier-Stokes equations

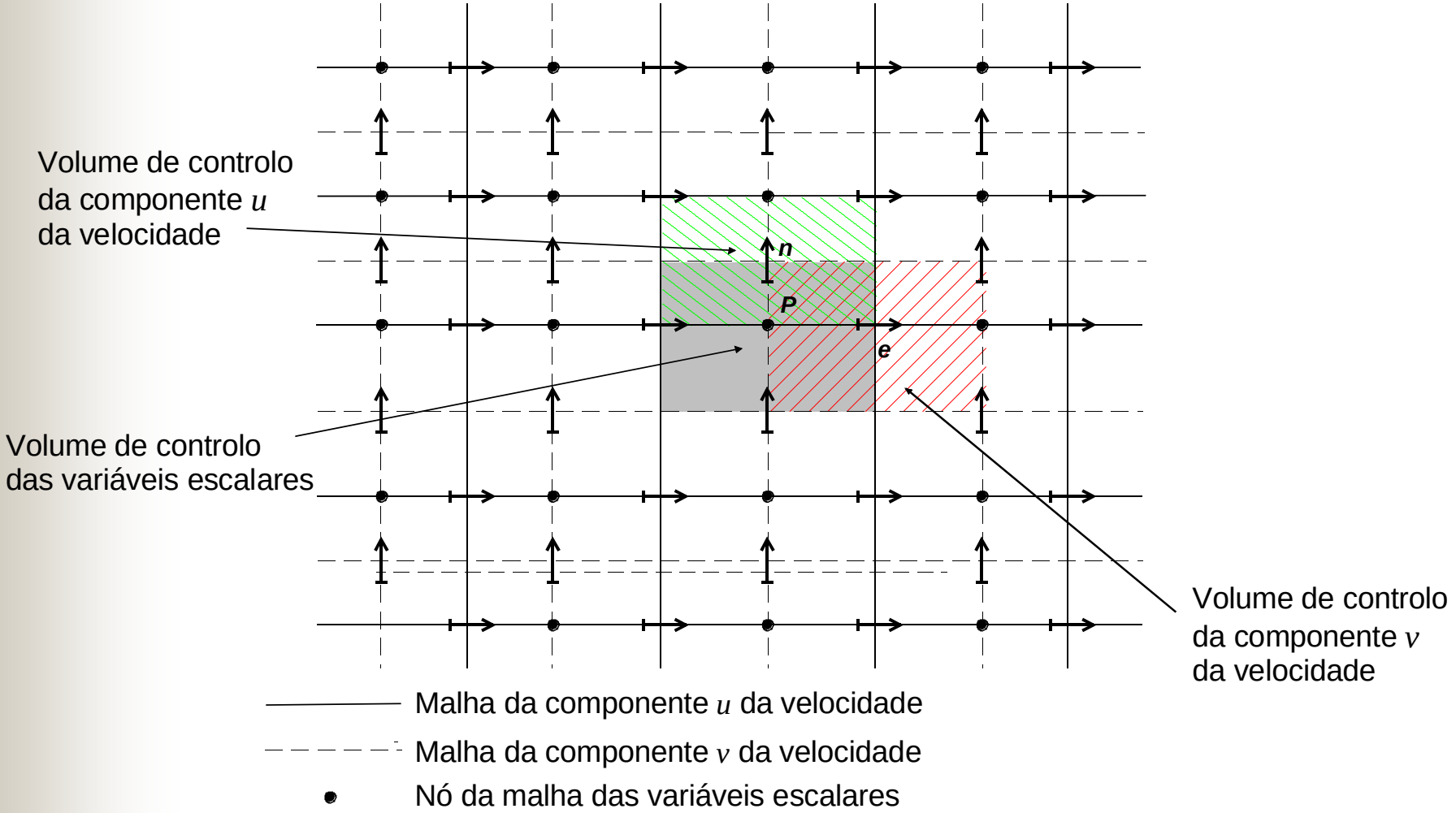
- **The 1st order derivatives x and y in the momentum equation and the first order velocity derivatives in the continuity equation it can lead to unrealistically oscillatory pressure and velocity fields, if the velocity and pressure fields are computed in a single grid.**

- **This problem of numerical instability is associated with the presence of the first derivatives and requires special care in the discretization of these differential equations.**

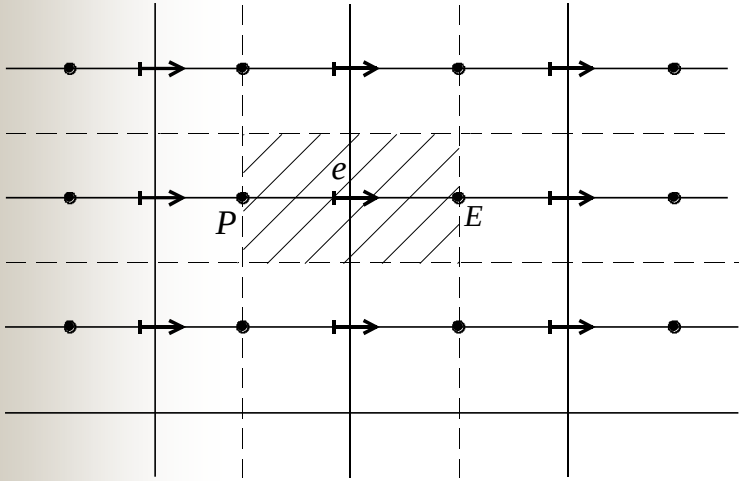
- **On practical algorithm found to solve this problem is to calculate the components *u* and *v* of the velocity in grids displaced relative to the grid of scalar variables**

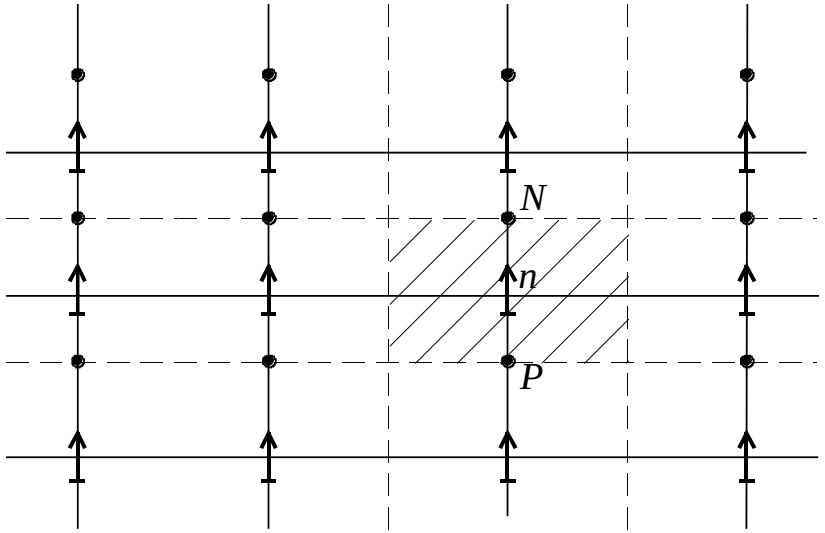
Displaced grid method

- **For reasons of numerical stability, the grids of the velocity components must be displaced in relation to the grid of scalar quantities.**



Discretization equations for velocity components





$$\frac{\partial \rho u}{\partial t}+\frac{\partial}{\partial x_j}(\rho u_j u)=\frac{\partial}{\partial x_j}\left(\mu\frac{\partial u}{\partial x_j}\right)-\frac{\partial p}{\partial x}+S_u$$

$$\frac{\partial \rho v}{\partial t}+\frac{\partial}{\partial x_j}(\rho u_j v)=\frac{\partial}{\partial x_j}\left(\mu\frac{\partial v}{\partial x_j}\right)-\frac{\partial p}{\partial y}+S_v$$

$$a_e u_e=\sum a_{nb}u_{nb}+b+A_e(p_P-p_E)$$

$$a_n v_n=\sum a_{nb}v_{nb}+b+A_n(p_P-p_N)$$

$$A_e=\Delta y\times 1$$

$$A_n=\Delta x\times 1$$

Additional pressure terms

Velocity and pressure correction

- **Momentum equations can only be solved by an iterative process if the pressure field is specified.**
- **If this pressure field is not the correct one, the resulting velocity distribution does not satisfy the continuity equation.**
- **If P^* is an initial arbitrary pressure field we have an imperfect velocity field given by the solution of:**

$$a_e u_e^* = \sum a_{nb} u_{nb}^* + b + A_e (p_P^* - p_E^*)$$

$$a_e v_e^* = \sum a_{nb} v_{nb}^* + b + A_n (p_P^* - p_N^*)$$

Speed and pressure correction

- **Since there is no equation to calculate P in an explicit way, let's look for another way to iteratively improve the pressure field P^* arbitrated:**

$$p = p^* + p' \qquad \text{where = pressure correction}$$

- **The velocity variation caused by will be and :**

$$u = u^* + u' \qquad v = v^* + v'$$

- **Subtracting the following two equations:**

$$a_e u_e = \sum a_{nb} u_{nb} + b + A_e (p_P - p_E)$$

$$a_e u_e^* = \sum a_{nb} u_{nb}^* + b + A_e (p_P^* - p_E^*)$$

- **We get** $a_e u_e' = \sum a_{nb} u_{nb}' + A_e (p_P' - p_E')$

Velocity and pressure correction

- **Considering at this stage that**

$$a_e u'_e = \sum a_{nb} u'_{nb} + A_e (p'_P - p'_E) \approx A_e (p'_P - p'_E)$$

- **We then have the following velocity correction equation:**

where

- **That is, in both directions:**

$$u_e = u^*_e + d_e (p'_P - p'_E)$$

$$v_n = v^*_v + d_n (p'_P - p'_N)$$

Pressure correction equation

- **Having the equations that relate small variations in speed with small variations in pressure, it becomes possible to obtain an explicit equation for *P′*:**

- **Integration of the continuity equation:**

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = 0$$

$$\frac{(\rho_P - \rho_P^0)}{\Delta t}\Delta x \Delta y + \left[(\rho u)_e - (\rho u)_w\right]\Delta y + \left[(\rho v)_n - (\rho v)_s\right]\Delta x = 0$$

- **The speed correction equations are now introduced in this equation.**

$$u_e = u_e^* + d_e(p'_P - p'_E) \qquad v_n = v_v^* + d_n(p'_P - p'_N)$$

Pressure correction equation

- **Finally, we get:**

$$a_P p'_P = a_E p'_E + a_W p'_W + a_N p'_N + a_S p'_S + b$$

$$a_E = \rho_e d_e \Delta y$$
$$a_W = \rho_w d_w \Delta y$$
$$a_N = \rho_n d_n \Delta x$$
$$a_S = \rho_s d_s \Delta x$$
$$b = \frac{(\rho_P^0 - \rho_P)\Delta x \Delta y}{\Delta t} + [(\rho u^*)_w - (\rho u^*)_e]\Delta y + [(\rho v^*)_s - (\rho v^*)_n]\Delta x$$

SIMPLE algorithm

- Arbitrate the initial pressure field p *.
- Solve the equations of the amount of movement to obtain u * and v *.
- Solve the pressure correction equation.
- Calculate the new corrected pressure field
  $p = p^* + p'$
- Calculate the corrected velocity field
  $u = u^* + u'$ $v = v^* + v'$
  the speed field now satisfies the continuity equation.
- Solve the equations for the remaining scalar quantities.
- Repeat the process as the new pressure field until convergence is achieved.