# THE FINITE VOLUME METHOD: A CRASH COURSE

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- Navier-Stokes for steady, incompressible, laminar flow (on *conservative form*)

$$\frac{\partial u_j}{\partial x_j} = 0 \tag{1}$$

$$\frac{\partial u_j u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu\frac{\partial^2 u_i}{\partial x_j \partial x_j} \tag{2}$$

- The Poisson equation (the diffusion equation)

$$\nu\frac{\partial^2 u}{\partial x_j \partial x_j} = S \tag{3}$$

- **pyCALC-RANS** solves 2D Navier-Stokes equation. The grid may be curvi-linear. It is fully vectorized (no `for` loops). 1300 lines.
- **pyPoisson** solves the 2D Poisson equation. The grid may be curvi-linear. It is a stripped version of **pyCALC-RANS** . 450 lines.
- pyPoisson-3D is a simplified 3D Poisson solver on equidistant (i.e. constant $\Delta x$, $\Delta y$ and $\Delta z$) Cartesian grids. It is fully vectorized (no `for` loops). 175 lines.

# NOMENCLATURE FOR A 2D GRID

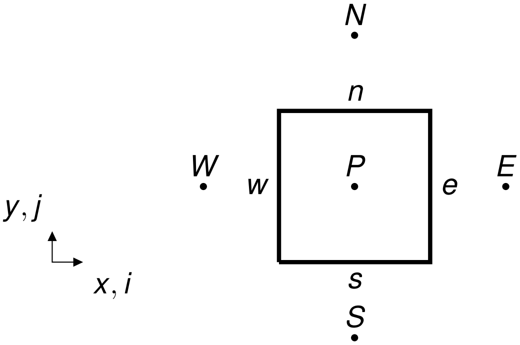



FIGURE: Control volume.

- A schematic 2D control volume grid is shown above
- Capital letters define nodes E(ast), W(est), N(orth) and S(outh), and small letters define faces of the control volumes.

# 1D Poisson Equation

$$\nu \frac{\partial^2 u}{\partial x^2} = S \tag{4}$$

# 1D GRID

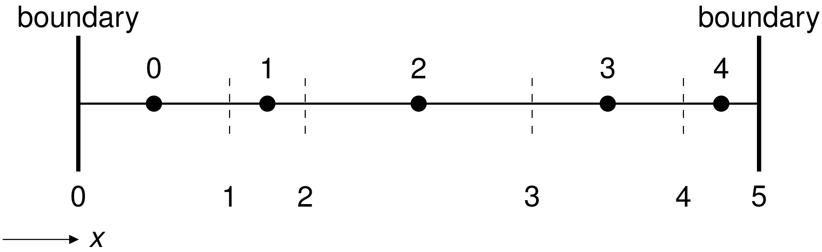



FIGURE: `ni=5`. The bullets denote cell centers of the control volumes where the solution vector, $u$, is stored. They are labeled 0–4. Dashed lines denote control volume faces labeled 0–5.

- The size of the full coefficient matrix will be $5 \times 5$
- If I want to solve the matrix system with a Python sparse-matrix solver, the size of the solution vector must be $5 \times 1$
- That's the reason why the boundary values of $u$ cannot be stored in the $u$ array.
- The b.c. are implemented as source terms, see Slide 10.

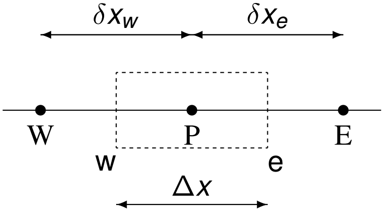



FIGURE: 1D control volume. Node $P$ located in the middle of the control volume.

$$\int_w^e \left[\frac{d}{dx}\left(\Gamma\frac{du}{dx}\right) + S\right] dx = \left(\Gamma\frac{du}{dx}\right)_e - \left(\Gamma\frac{du}{dx}\right)_w + \bar{S}\Delta x = 0 \tag{5}$$

$$\left(\frac{du}{dx}\right)_e \simeq \frac{u_E - u_P}{\delta x_e}, \quad \left(\frac{du}{dx}\right)_w \simeq \frac{u_P - u_W}{\delta x_w} \tag{6}$$

$$\Gamma_w = f_x \Gamma_P + (1 - f_x)\Gamma_W, \quad \Gamma_w = f_x \Gamma_P + (1 - f_x)\Gamma_W \tag{7}$$

-

$$f_x = \frac{|\overrightarrow{Ww}|}{|\overrightarrow{Pw}| + |\overrightarrow{Ww}|} \tag{8}$$

- $|\overrightarrow{Pw}|$ is the distance from P (the node) to $w$ (the west face).
- In **pyCALC-RANS** and **pyPoisson** the interpolation factors ($f_x$, $f_y$) are stored in the Python arrays `fx` and `fy`.

# The Discretized Equation

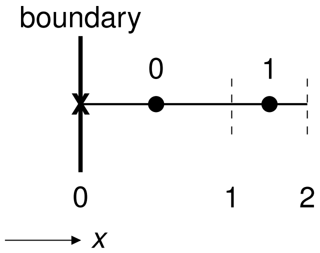
- Insertion of Eq. 6 into Eq. 5 gives

$$
\begin{aligned}
&a_P u_P = a_E u_E + a_W u_W + S_U \\
&a_E = \frac{\Gamma_e}{\delta x_e},\, a_W = \frac{\Gamma_w}{\delta x_w},\, S_U = \bar{S}\Delta x,\, a_P = a_E + a_W - S_P,\, S = S_U + S_P u_P
\end{aligned}
\tag{9}
$$

- The resulting sparse-matrix reads

$$
\begin{array}{r}
\\ L0: \\ L1: \\ L2: \\ L3: \\ L4:
\end{array}
\begin{array}{c}
\begin{array}{ccccc} \quad C0 & \quad C1 & \quad C2 & \quad C3 & \quad C4 \end{array} \\
\begin{bmatrix}
\color{red}{a_{P,0}} & -a_{E,0} & 0 & 00 & \\
-a_{W,1} & \color{red}{a_{P,1}} & -a_{E,1} & 0 & 0 \\
0 & -a_{W,2} & \color{red}{a_{P,2}} & -a_{E,2} & 0 \\
0 & 0 & -a_{W,3} & \color{red}{a_{P,3}} & -a_{E,3} \\
0 & 0 & 0 & a_{W,4} & \color{red}{a_{P,4}}
\end{bmatrix}
\end{array}
$$

# Boundary Conditions at $x = 0$




- For the $u$ equation at cell $i = 0$ the discretized equation reads
$$a_{P,0}u_P = a^X_{W,0}u_W + a_{E,0}u_E + S_{U,0}, \quad a_{P,0} = a^X_{W,0} + a_{E,0} - S_{P,0}$$
- $u_W = u_{bc}$ is the b.c. (**X** above)
- But $a^X_{w,0}$ does not exist in the coefficient matrix (see previous slide)
- I set b.c. via $S_{U,0}$ and $S_{P,0}$ as $S_{U,0} = a^X_{W,0}u_{bc}$ and $S_{P,0} = -a^X_{W,0}$
- Note that if I don't set $S_{U,0}$ and $S_{P,0}$ then the b.c. is $du/dx = 0$ (hom. Neumann)

# 2D Poisson (Diffusion) Equation

$$\nu\frac{\partial^2 u}{\partial x^2}+\nu\frac{\partial^2 u}{\partial y^2}=S \qquad (10)$$

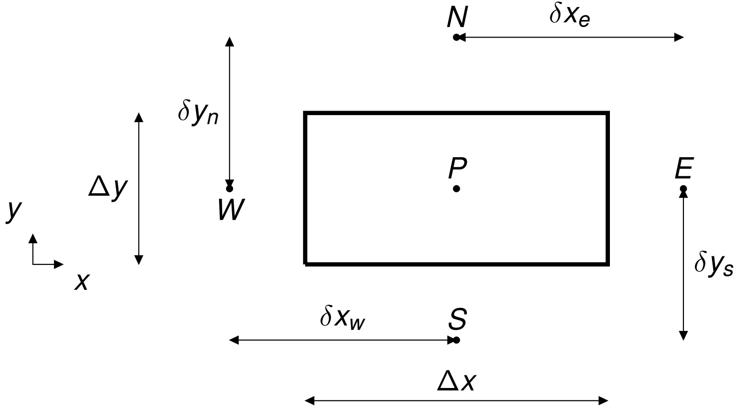



FIGURE: 2D control volume.

$$\int_w^e \int_s^n \left[\frac{\partial}{\partial x}\left(\Gamma \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\Gamma \frac{\partial u}{\partial y}\right) + S\right] dxdy = 0.$$

- I start by the first term. The integration in $x$ direction is carried out in exactly the same way as in 1D, i.e.

$$\int_w^e \int_s^n \left[\frac{\partial}{\partial x}\left(\Gamma \frac{\partial u}{\partial x}\right)\right] dxdy = \int_s^n \left[\left(\Gamma \frac{\partial u}{\partial x}\right)_e - \left(\Gamma \frac{\partial u}{\partial x}\right)_w\right] dy$$

$$= \int_s^n \left(\Gamma_e \frac{u_E - u_P}{\delta x_e} - \Gamma_w \frac{u_P - u_W}{\delta x_w}\right) dy$$

- Now integrate in the $y$ direction. I do this by estimating the integral

$$\int_s^n f(y)dy = f_P \Delta y + \mathcal{O}\left((\Delta y)^2\right)$$

(i.e. $f$ is taken at the mid-point $P$) which is second order accurate, since it is exact if $f$ is a linear function. For our equation I get

$$\int_s^n \left(\Gamma_e \frac{u_E - u_P}{\delta x_e} - \Gamma_w \frac{u_P - u_W}{\delta x_w}\right) dy$$
$$= \left(\Gamma_e \frac{u_E - u_P}{\delta x_e} - \Gamma_w \frac{u_P - u_W}{\delta x_w}\right) \Delta y$$

- Rewriting it as an algebraic (i.e. the discretized) equation for $u_P$, I get

$$
\begin{aligned}
a_P u_P &= a_E u_E + a_W u_W + a_N u_N + a_S u_S + S_U \\
a_E &= \frac{\Gamma_e \Delta y}{\delta x_e},\ a_W = \frac{\Gamma_w \Delta y}{\delta x_w},\ a_N = \frac{\Gamma_n \Delta x}{\delta y_n},\ a_S = \frac{\Gamma_s \Delta x}{\delta y_s} \\
S_U &= \bar{S} \Delta x \Delta y,\ a_P = a_E + a_W + a_N + a_S - S_P.
\end{aligned}
\tag{11}
$$

# Matrix for 2D flow. $ni \times nj = (3,2)$.

$\longrightarrow$ j and N

| | |
|---|---|
| 0 | 1 |
| 2 | 3 |
| 4 | 5 |

$\downarrow$ i and E

$$
\begin{array}{c}
 \\ L0: \\ L1: \\ L2: \\ L3: \\ L4: \\ L5:
\end{array}
\begin{array}{c}
\begin{array}{cccccc} C0 & C1 & C2 & C3 & C4 & C5 \end{array} \\
\left[\begin{array}{cccccc}
a_{P,0} & -a_{N,0} & -a_{E,0} & 0 & 0 & 0 \\
-a_{S,1} & a_{P,1} & 0 & -a_{E,1} & 0 & 0 \\
-a_{W,2} & -a_{S,2} & a_{P,2} & -a_{N,2} & -a_{E,2} & 0 \\
0 & -a_{W,3} & -a_{S,3} & a_{P,3} & 0 & a_{E,3} \\
0 & 0 & -a_{W,4} & 0 & a_{P,4} & -a_{N,4} \\
0 & 0 & 0 & -a_{W,5} & 0 & a_{P,5}
\end{array}\right]
\end{array}
$$

# Matrix for 2D flow. $ni \times nj = (3,4)$.

$\longrightarrow$ y,j and N

$\downarrow$ x,i and E

| | | | |
|---|---|---|---|
| 0 | 1 | 2 | 3 |
| 4 | 5 | 6 | 7 |
| 8 | 9 | 10 | 11 |

$$\begin{array}{rl}
 & \begin{array}{cccccccccccc} C0 & C1 & C2 & C3 & C4 & C5 & C6 & C7 & C8 & C9 & C10 & C11 \end{array} \\
\begin{array}{r} L0: \\ L1: \\ L2: \\ L3: \\ L4: \\ L5: \\ L6: \\ L7: \\ L8: \\ L9: \\ L10: \\ L11: \end{array} &
\left[\begin{array}{cccccccccccc}
\color{red}{a_{P,0}} & -a_{N,0} & 0 & 0 & -a_{E,0} & 0 & 0 & 0 & \color{blue}{-a_{W,0}} & 0 & 0 & 0 \\
-a_{S,1} & \color{red}{a_{P,1}} & -a_{N,1} & 0 & 0 & -a_{E,1} & 0 & 0 & 0 & \color{blue}{-a_{W,1}} & 0 & 0 \\
0 & -a_{S,2} & \color{red}{a_{P,2}} & -a_{N,2} & 0 & 0 & -a_{E,2} & 0 & 0 & 0 & \color{blue}{-a_{W,2}} & 0 \\
0 & 0 & -a_{S,3} & \color{red}{a_{P,3}} & 0 & 0 & 0 & -a_{E,3} & 0 & 0 & 0 & \color{blue}{-a_{W,3}} \\
-a_{W,4} & 0 & 0 & 0 & \color{red}{a_{P,4}} & -a_{N,4} & 0 & 0 & -a_{E,4} & 0 & 0 & 0 \\
0 & -a_{W,5} & 0 & 0 & -a_{S,5} & \color{red}{a_{P,5}} & -a_{N,5} & 0 & 0 & -a_{E,5} & 0 & 0 \\
0 & 0 & -a_{W,6} & 0 & & -a_{S,6} & \color{red}{-a_{P,6}} & -a_{N,6} & 0 & 0 & -a_{E,6} & 0 \\
0 & 0 & 0 & -a_{W,7} & 0 & 0 & -a_{S,7} & \color{red}{-a_{P,7}} & 0 & 0 & 0 & -a_{E,7} \\
\color{blue}{-a_{E,8}} & 0 & 0 & 0 & -a_{W,8} & 0 & 0 & 0 & \color{red}{a_{P,8}} & -a_{N,8} & 0 & 0 \\
0 & \color{blue}{-a_{W,9}} & 0 & 0 & 0 & -a_{W,9} & 0 & 0 & -a_{S,9} & \color{red}{a_{P,9}} & -a_{N,9} & 0 \\
0 & 0 & \color{blue}{-a_{W,10}} & 0 & 0 & 0 & -a_{W,10} & 0 & 0 & -a_{S,10} & \color{red}{a_{P,10}} & -a_{N,10} \\
0 & 0 & 0 & \color{blue}{-a_{W,11}} & 0 & 0 & 0 & -a_{W,11} & 0 & 0 & -a_{S,11} & \color{red}{a_{P,11}}
\end{array}\right]
\end{array}$$

Figure: Cyclic in $x, i$. The coefficients due to cyclic boundary conditions are blue.

- The 1D convection-diffusion equation reads ($\phi$ is, e.g., $u$, $v$, $T$, …)

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

- I discretize this equation in the same way as the diffusion equation.

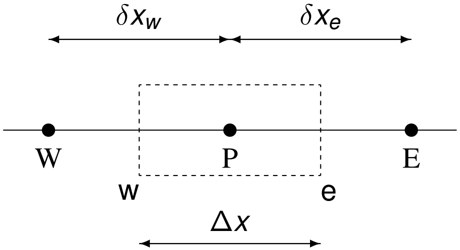



FIGURE: 1D control volume. Node $P$ located in the middle of the control volume.

- I start by integrating over the control volume

$$\int_w^e \frac{d}{dx}(u\phi)\,dx = \int_w^e \left[\frac{d}{dx}\left(\Gamma\frac{d\phi}{dx}\right) + S\right] dx. \tag{12}$$

- The convective term (the left-hand side)

$$\int_w^e \frac{d}{dx}(u\phi)\,dx = (u\phi)_e - (u\phi)_w = u_e\phi_e - u_w\phi_w$$

- I assume the velocity $u$ to be known, or, rather, I take $u$ from the previous iteration
- How to estimate $\phi_e$ and $\phi_w$? Linear interpolation (central differencing) gives

$$\phi_w = f_x\phi_P + (1-f_x)\phi_W, \quad u_w = f_x u_P + (1-f_x)u_W$$

where $f_x$ is the interpolation function (see Eq. 7, p. 8). Assuming $f_x = 0.5$, inserting the discretized diffusion and the convection terms into Eq. 12 I obtain

$$(u)_e\frac{\phi_E+\phi_P}{2} - (u)_w\frac{\phi_P+\phi_W}{2} = \frac{\Gamma_e(\phi_E-\phi_P)}{\delta x_e} - \frac{\Gamma_w(\phi_P-\phi_W)}{\delta x_w} + \bar{S}\Delta x$$

which can be rearranged as

$$\begin{aligned} &a_P\phi_P = a_E\phi_E + a_W\phi_W + S_U, \quad a_E = \frac{\Gamma_e}{\delta x_e} - \frac{1}{2}(u)_e, \quad a_W = \frac{\Gamma_w}{\delta x_w} + \frac{1}{2}(u)_w \\ &S_U = \bar{S}\Delta x, \quad a_P = \frac{\Gamma_e}{\delta x_e} + \frac{1}{2}(u)_e + \frac{\Gamma_w}{\delta x_w} - \frac{1}{2}(u)_w \end{aligned} \tag{13}$$

- $a_P \geq a_E + a_W$ is the requirement to make sure that the iterative solver converges. Hence, I add the continity equation

$$(u)_w - (u)_e = 0$$

to $a_P$ so that (see Eq. 13)

$$a_P = a_E + a_W.$$

- Now you have learnt how to solve the Poission (diffusion) equation and the convection-diffussion equation. Next step is the Navier-Stokes equation, see Eq. 2.
- Navier-Stokes includes the pressure and hence we must find an equation for it.
- The pressure is obtained from the pressure-correction equation, $p'$

- The $p'$ equation is obtained by applying the SIMPLEC algorithm [2]
- The mass flux $\dot{m}$ is divided into an old value, $\dot{m}^*$, and a correction value, $\dot{m}'$ as (in 1D)

$$\dot{m}_e = \dot{m}_e^* + \dot{m}_e', \quad \dot{m}_e' = \left(\vec{A} \cdot \vec{u}'\right)_e = A_e u_e' \tag{14}$$

where $u'$ is the correction velocity.

- The relation between $u'$ and $p'$ is obtained from the discretized Navier-Stokes

$$u' = -\frac{\Delta V_P}{a_P^u} \frac{\partial p'}{\partial x} \tag{15}$$

where $\Delta V_P =$ volume of the control volume. By introducing Eq. 14 into Eq. 15 we obtain

$$\dot{m}'_e = -\left[\frac{\Delta V_P}{a^u_P}\vec{A}\cdot\nabla p'\right]_e = -\frac{\Delta V_P}{a^u_P}A_e\left(\frac{\partial p'}{\partial x}\right)_e \tag{16}$$

# The Pressure-Correction ($p'$) Equation

- Consider, for simplicity, the continuity equation in one dimension

$$\dot{m}_e - \dot{m}_w = 0 \tag{17}$$

- If $\dot{m} = \dot{m}^* + \dot{m}'$ and Eq. 16 are substituted into eq. 17 we obtain

$$\left[\frac{\Delta V_P A_x}{a_P^u}\frac{\partial p'}{\partial x}\right]_w - \left[\frac{\Delta V_P A_x}{a_P^u}\frac{\partial p'}{\partial x}\right]_e + \dot{m}_e^* - \dot{m}_w^* = 0 \tag{18}$$

- This is a Poisson (diffusion) equation for the pressure correction $p'$ which is discretized as Eq. (11) by replacing $u$ by $p^{'}$ and setting $\Gamma = \Delta V_P / a_P$.
- The boundary conditions at all boundaries is homogeneous Neumann, i.e. $\partial p'/\partial x = 0$ at west and east boundaries and $\partial p'/\partial y = 0$ at south and north boundaries.

1. Assign initial values (usually $10^{-10}$) to the variable fields $u^*$, $v^*$ and $p^*$
2. Solve the $u$-Navier-Stokes equation by first calculating the coefficients and sources, then setting b.c. followed by application of the Python solver.
3. Point 2 is repeated for $v$
4. Solve the $p'$ equation by calculating the coefficients and sources, then setting b.c. followed by application of the Python solver.
5. Correct the velocity fields $u^*$, $v^*$ and mass fluxes (see Eq. 14) $\dot{m}_e^*$ and $\dot{m}_n^*$ with $u'$, $v'$.
6. Correct the pressure field $p^*$ with $p'$ to give the correct pressure field $p$.
7. Go to step 2 and repeat step 2 to 7 until convergence.

You can find more details about discretization and the pressure correction method in `lecture notes` (Chapter 2-9).

# pyCALC-RANS

**There are four main case-specific routines in each subdirectory**

- `generate*.py` (`generate-channel-grid.py`, `generate-bound-layer-grid.py`,...)
- `setup_case.py`
- `modify_case.py`
- `pl*.py` (`pl_uvw.py`, `plot_inlet.py`,...)

**The main program**

- `pyCALC-RANS.py`

- Generate simple Cartesian meshes

- SECTION 1 choice of differencing scheme
- SECTION 2 turbulence models
- SECTION 3 restart/save
- SECTION 4 fluid properties
- SECTION 5 relaxation factors
- SECTION 6 number of iteration and convergence criteria
- SECTION 7 all variables are printed during the iteration at node
- SECTION 8 save data for post-processing
- SECTION 9 residual scaling parameters
- SECTION 10 boundary conditions

```
def modify_init(u3d,v3d,w3d,k3d,om3d,eps3d,vis3d,dist3d):
def modify_inlet():
def modify_conv(convw,convs,convl):
def modify_u(su3d,sp3d):
def modify_v(su3d,sp3d):
def modify_k(su3d,sp3d,gen):
def modify_om(su3d,sp3d,comm_term):
def modify_outlet(convw):
def modify_vis(vis3d):
def def fix_omega():
```

# Global Declarations

They are made in the file `global` which reads

global c_omega_1, c_omega_2, cmu, ...
x2d, xp2d, y2d, yp2d

## CREATE EXECUTABLE

The bash script `run-python` is used which reads

```
#!/bin/bash # delete forst line sed '/setup_case()/d'
setup_case.py > temp_file # add new first line plus global
declarations cat ../global temp_file modify_case.py
../pyCALC-RANS.py > exec-pyCALC-RANS.py; python -u
exec-pyCALC-RANS.py > out
```

- To run **pyCALC-RANS** (and **pyPoisson** ), look at Section 10.3 in [1].

# References

[1] L. Davidson. pyCALC-RANS: a 2D Python code for RANS. Division of Fluid Dynamics, Dept. of Mechanics and Maritime Sciences, Chalmers University of Technology, Gothenburg
Download the code here, 2021.

[2] S. V. Patankar. *Numerical Heat Transfer and Fluid Flow*. McGraw-Hill, New York, 1980.