

# CFD Code Development Frameworks

Python, C, OpenFOAM, Fenics

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# Governing Equations

Incompressible Navier-Stokes Equations (INSE) in Eulerian form:

$$\partial_t \rho + \rho \nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g} \quad (2)$$

Eqn. 1: Density can be omitted, but let's keep it for now.

Eqn. 2:

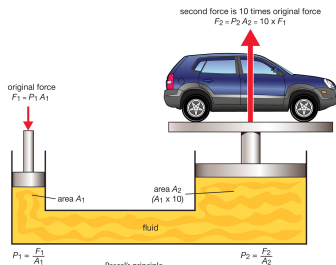
- LHS is acceleration which is intrinsically Lagrangian and when it is translated to Eulerian coordinates it becomes non-linear
- RHS describes influence of pressure gradient, viscosity and body forces.

# Governing Equations

## Complexities

Difficulties for numerical solution:

- Nonlocality of pressure gradient (Solution: None)
- Nonlinearity of acceleration term (Solution: e.g. Picard's Method)
- Pressure and velocity are coupled and there is no separate equation for pressure (Solution: e.g. SIMPLE, PISO and ACM)



# Governing Equations

## Artificial Compressibility Method

ACM first developed by A.J. Chorin in 1967 assumes a small compressibility for the fluid and isothermal condition for the flow:

$$\rho = \rho(p) \therefore \partial_t \rho = \frac{\partial \rho}{\partial p} \frac{\partial p}{\partial t} = \frac{1}{c^2} \frac{\partial p}{\partial t}$$

where  $c$  is artificial sound speed. So INSE becomes:

$$\begin{aligned}\partial_t P + c^2 \nabla \cdot \mathbf{u} &= 0 \\ \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla P + \nu \nabla^2 \mathbf{u} + \mathbf{g}\end{aligned}$$

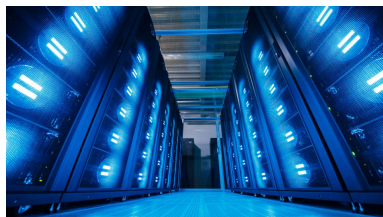
where  $P = \frac{p}{\rho}$ .

# Governing Equations

## Remarks on ACM

- Limited scope of applicability: incompressible steady state problems.
- Small time step:  $t$  is pseudo-time step and depends on  $c$ . Therefore, if an explicit discretization method is used time step should have a small value.
- Efficient parallelization: no elliptic PDE

Although applicability of the method is very limited, ACM provides a simple yet informative framework for pedagogical purposes



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# Solution algorithm

## Pseudo Code

- 1 Initialization of the domain and the variables ( $u$ ,  $v$ ,  $p$ )
- 2 While convergence is reached do:
  - 1 Solve momentum equation in  $x$ -direction to get  $u$
  - 2 Solve momentum equation in  $y$ -direction to get  $v$
  - 3 Update the boundary conditions for  $u$  and  $v$
  - 4 Solve continuity equation to get  $P$
  - 5 Check convergence criteria
- 3 Output the fields data



# Solution algorithm

## Discretization

Spatial: central difference, second order

$$\partial_x \phi = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$

Temporal: backward difference, first order

$$\partial_t \phi = \frac{\phi^{n+1} - \phi^n}{\Delta t}$$

Note: for brevity we use the superscript  $n$  to denote the variable in the current time step and no superscript for the previous time step.

# Solution algorithm

## Momentum Equation in x-direction

$$\partial_t u + \partial_x(uu) + \partial_y(uv) = -\partial_x P + \nu (\partial_{xx} u + \partial_{yy} u)$$

$$\begin{aligned} & \frac{u_{i,j}^n - u_{i,j}}{\Delta t} + \frac{\left(\frac{u_{i+1,j} + u_{i,j}}{2}\right)^2 - \left(\frac{u_{i,j} + u_{i-1,j}}{2}\right)^2}{\Delta x} \\ & + \frac{\left(\frac{u_{i,j+1} + u_{i,j}}{2}\right) \left(\frac{v_{i+1,j} + v_{i,j}}{2}\right) - \left(\frac{u_{i,j} + u_{i,j-1}}{2}\right) \left(\frac{v_{i+1,j-1} + v_{i,j-1}}{2}\right)}{\Delta y} \\ & = \\ & - \frac{P_{i+1,j} - P_{i,j}}{\Delta x} \\ & + \nu \left( \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} \right) \end{aligned}$$

# Solution algorithm

## Momentum Equation in y-direction

$$\begin{aligned}
 \partial_t v + \partial_x(uv) + \partial_y(vv) &= -\partial_y P + \nu (\partial_{xx} v + \partial_{yy} v) \\
 \frac{v_{i,j}^n - v_{i,j}}{\Delta t} + \frac{\left(\frac{u_{i,j+1} + u_{i,j}}{2}\right) \left(\frac{v_{i+1,j} + v_{i,j}}{2}\right) - \left(\frac{u_{i-1,j+1} + u_{i-1,j}}{2}\right) \left(\frac{v_{i,j} + v_{i-1,j}}{2}\right)}{\Delta x} \\
 + \frac{\left(\frac{v_{i,j+1} + v_{i,j}}{2}\right)^2 - \left(\frac{v_{i,j} + v_{i,j-1}}{2}\right)^2}{\Delta y} \\
 &= \\
 - \frac{P_{i,j+1} - P_{i,j}}{\Delta y} \\
 + \nu \left( \frac{v_{i+1,j} - 2v_{i,j} + v_{i-1,j}}{\Delta x^2} + \frac{v_{i,j+1} - 2v_{i,j} + v_{i,j-1}}{\Delta y^2} \right)
 \end{aligned}$$

# Solution algorithm

## Continuity Equation

$$\partial_t P + c^2 (\partial_x u + \partial_y v) = 0$$

$$\frac{P_{i,j}^n - P_{i,j}}{\Delta t} + c^2 \left( \frac{u_{i,j}^n - u_{i-1,j}^n}{\Delta x} + \frac{v_{i,j}^n - v_{i,j-1}^n}{\Delta y} \right) = 0$$

# Solution algorithm

## Boundary Conditions

The two common boundary conditions can be formulated as follows:

- Dirichlet:  $\phi_g = 2\phi_b - \phi_i$
- Neumann:  $\phi_g = \phi_i - \left( \Delta n \frac{\partial \phi}{\partial n} \right)_b$

Indices:  $g$ ,  $b$  and  $i$  denote a ghost, boundary and inner node, respectively

Variables:  $\phi$  is a quantity of interest ( $u$ ,  $v$  or  $P$ ) and  $n$  represents a direction normal to the boundary cell face

# Solution algorithm

## Convergence Criteria

$$1 \quad E_u = \sqrt{(\Delta t \Delta x \Delta y) \sum_{i,j} (u_{i,j}^{n+1} - u_{i,j}^n)^2}$$

$$2 \quad E_v = \sqrt{(\Delta t \Delta x \Delta y) \sum_{i,j} (v_{i,j}^{n+1} - v_{i,j}^n)^2}$$

$$3 \quad E_p = \sqrt{\frac{\Delta t \Delta x \Delta y}{c^2} \sum_{i,j} (P_{i,j}^{n+1} - P_{i,j}^n)^2}$$

$$4 \quad E_{\nabla} = (\Delta t \Delta x \Delta y) \nabla \cdot \mathbf{u}$$

$$5 \quad E_{tot} = \max\{E_u, E_v, E_p, E_{\nabla}\} < \varepsilon$$

where  $\varepsilon$  is the desired tolerance.

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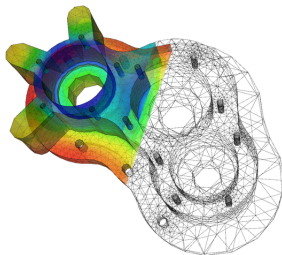
3 Grid

4 Problem Statement

# Grid

There are two types of grids from variable placement point of view:

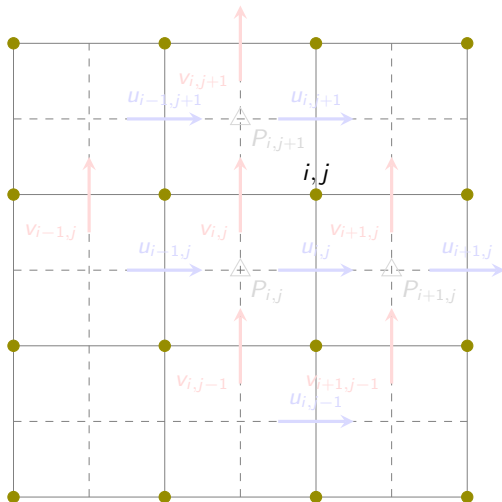
- Collocated: all the variables at the node centers; easier to implement and extend while issues such as checkerboard problem arise
- Staggered: scalar variables at the node centers and vector variables at the face centers; more accurate though more difficult to implement





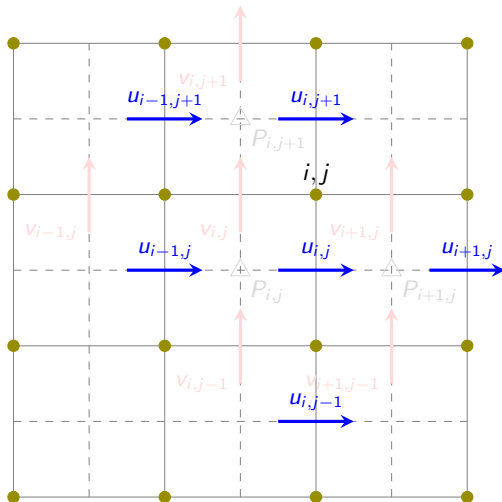
# Grid

## Staggered Grid



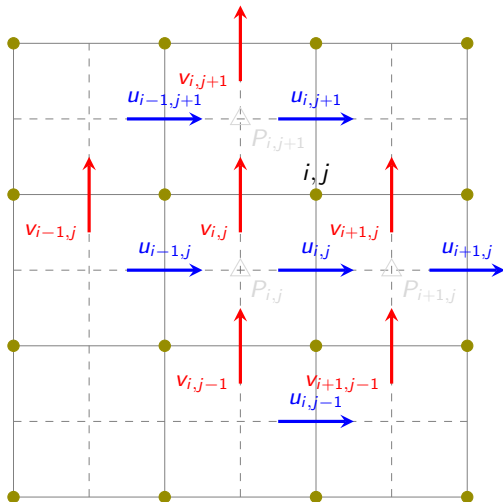
# Grid

## Staggered Grid



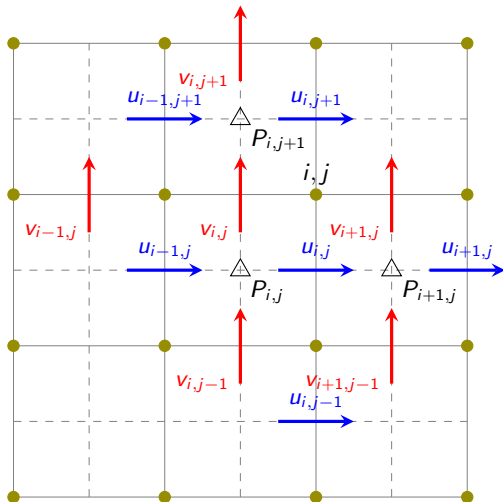
# Grid

## Staggered Grid



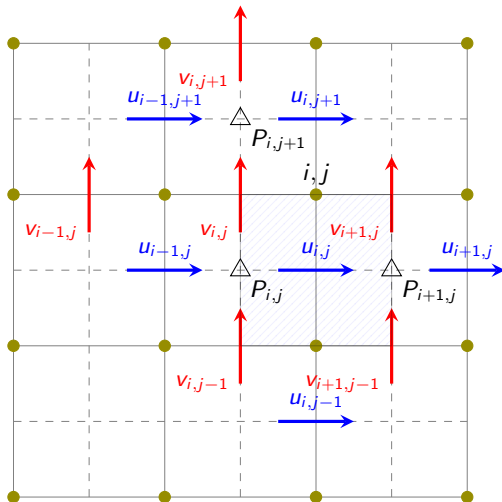
# Grid

## Staggered Grid



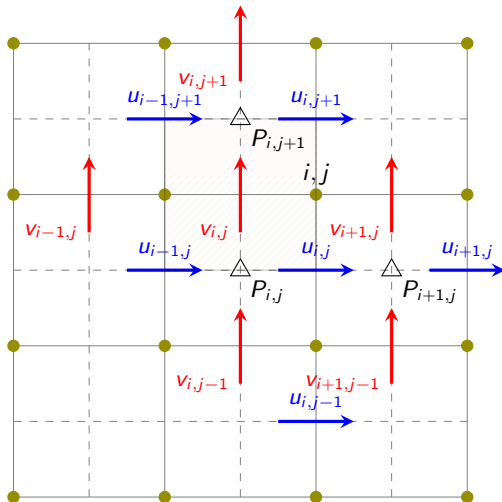
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## Staggered Grid



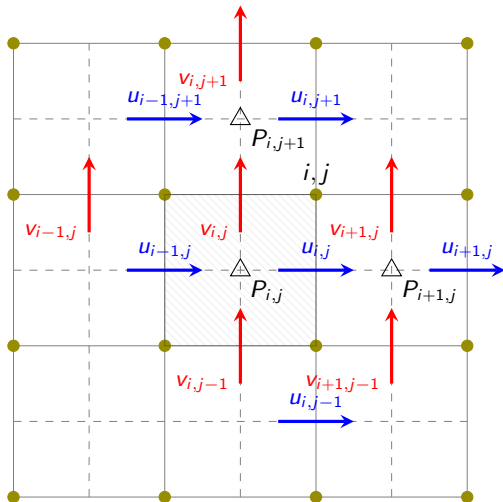
# Grid

## Staggered Grid



# Grid

## Staggered Grid



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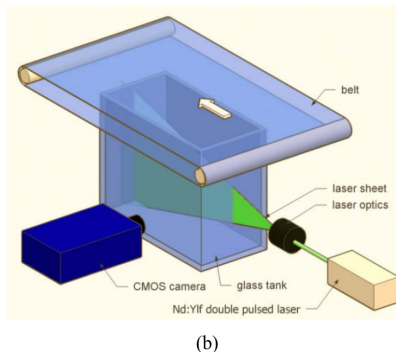
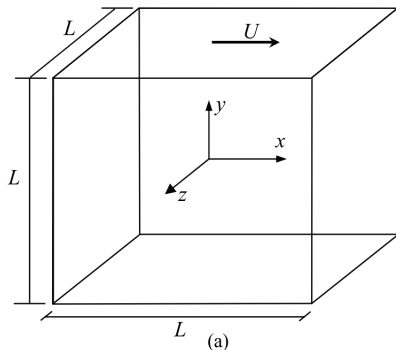


# Problem Statement

## Lid-Driven Cavity

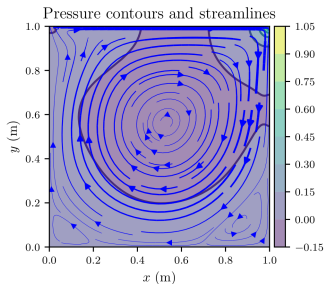
Characteristics: steady-state, incompressible

BC: walls everywhere (top wall is moving)

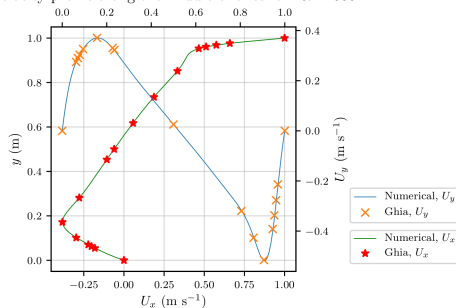


# Problem Statement

## Outputs



Velocity profile along the middle of axes for  $Re=1000$



# Problem Statement

## Workshop

A numerical solution to this benchmark problem will be presented based on:

- (Finite Difference) Coding from scratch: Python, C
- (Finite Volume) Modifying one of the solvers in OpenFOAM
- (Finite Element) Using libraries provided by FEniCS



# Final Remarks

Some other interesting open source CFD projects to look into:

- **Basilisk**: solution of partial differential equations on adaptive Cartesian meshes. (C)

<http://basilisk.fr>

- **FluidDyn**: some Python packages specialized for different tasks, in particular for 2D and 3D Fast Fourier Transforms, numerical simulations, laboratory experiments and processing of images of fluid.

<https://fluiddyn.readthedocs.io/en/latest>

- **Firedrake**: an automated system for the solution of partial differential equations using the finite element method. (Python)

<https://firedrakeproject.org>

# Let's Get Started!

A stylized illustration of a computer monitor with a grey frame and a light grey stand. The screen is dark grey and displays four lines of white text representing terminal commands. The commands are: '\$ mkdir UHWS', '\$ cd UHWS', '\$ git clone https://github.com/taataam/UHOFWorkshop.git', and '\$ cd UHOFWorkshop/workshop3'. The URL is underlined in blue.

```
$ mkdir UHWS  
  
$ cd UHWS  
  
$ git clone https://github.com/taataam/UHOFWorkshop.git  
  
$ cd UHOFWorkshop/workshop3
```