CFD Code Development Frameworks

Python, C, OpenFOAM, Fenics

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Governing Equations

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

$$\partial_t \rho + \rho \nabla . \mathbf{u} = 0 \tag{1}$$

$$\partial_t \mathbf{u} + \mathbf{u} . \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g} \tag{2}$$

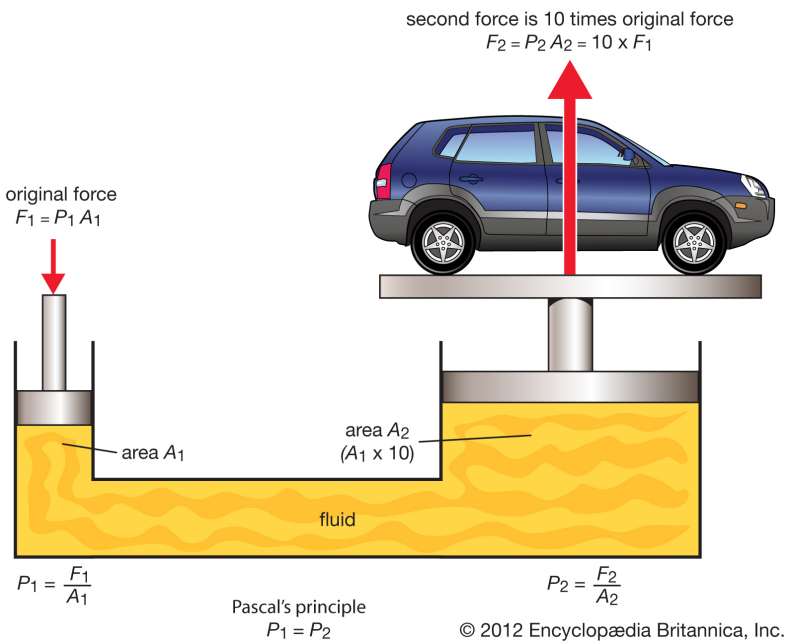
Eqn. 1: Density can be omitted, but let's keep it for now.
Eqn. 2:

- 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.

Complexities

Difficulties for numerical solution:

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



From INSE to ACM

ACM first was developed by A.J. Chorin in 1967 and 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:

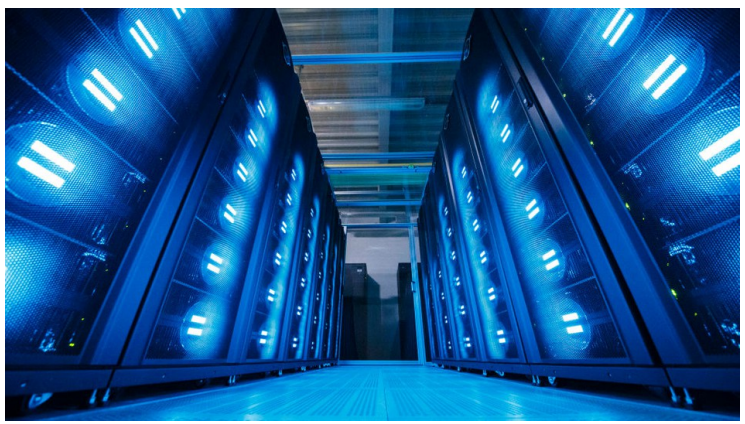
$$\partial_t P + c^2 \nabla . \mathbf{u} = 0$$
$$\partial_t \mathbf{u} + \mathbf{u}.\nabla \mathbf{u} = -\nabla P + \nu \nabla^2 \mathbf{u} + \mathbf{g}$$

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

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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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

Note: a flowchart is provided in the repository (`UHWorkshop/workshop3/flowchart.pdf`).

Boundary Conditions

The two common boundary conditions can be formulated as follows:

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

Indicies: g, b and i denote a ghost, boundary and inner node, respectively
Variables: ϕ is a quantity of interest (u, v or P) and n represents a direction normal to the boundary cell face

Convergence Criteria

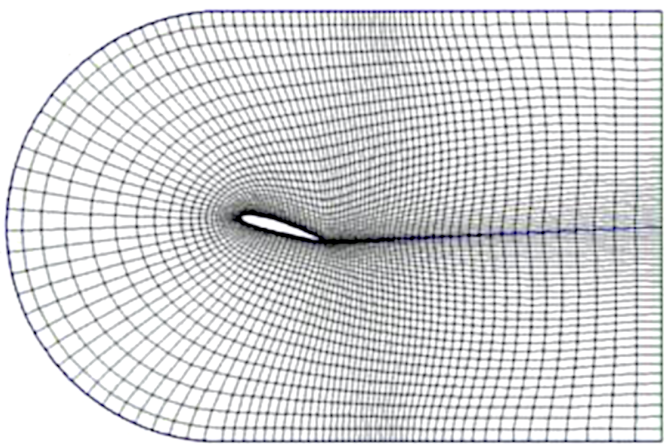
1. $E_u = \sqrt{(\Delta t \Delta x \Delta y) \sum_{i,j} (u_{i,j}^{n+1} - u_{i,j}^{n})^2}$
2. $E_v = \sqrt{(\Delta t \Delta x \Delta y) \sum_{i,j} (v_{i,j}^{n+1} - v_{i,j}^{n})^2}$
3. $E_p = \sqrt{\frac{\Delta t \Delta x \Delta y}{c^2} \sum_{i,j} (P_{i,j}^{n+1} - P_{i,j}^{n})^2}$
4. $E_\nabla = (\Delta t \Delta x \Delta y) \nabla . \mathbf{u}$
5. $E_{total} = \max\{E_u, E_v, E_p, E_\nabla\} < \varepsilon$

where ε is the desired tolerance.

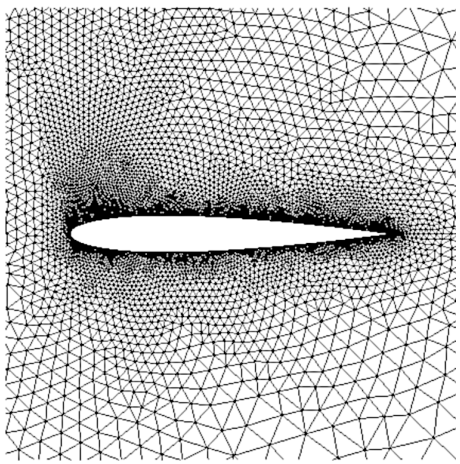
Structured Mesh (SM) vs. Unstructured Mesh (UM)

- Node connection: SM has regular connectivities while UM has irregular ones
- Quality: SM gives better results if applicable
- Memory usage: SM requires less memory and converge faster while UM requires storage of cell–to–cell pointers so take up more memory and is slower

Structured

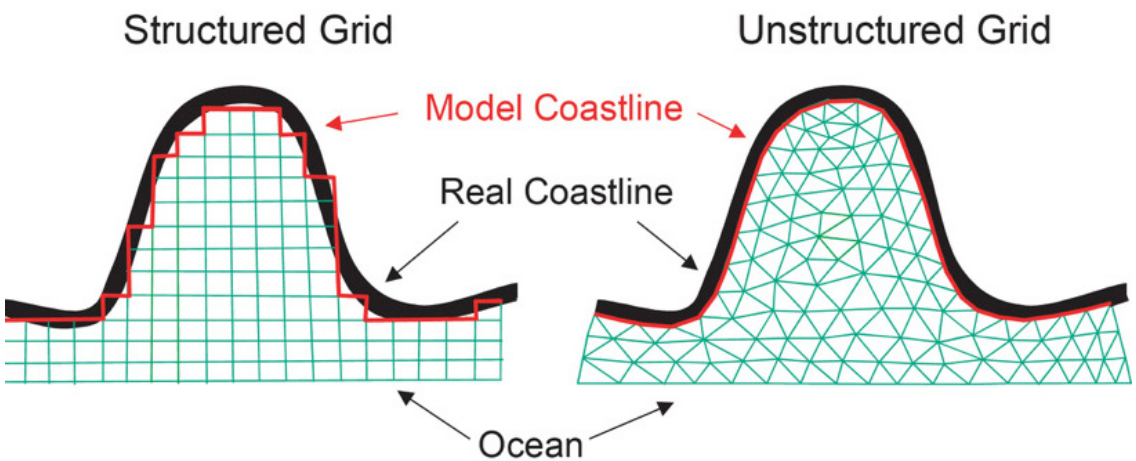


Unstructured



Structured Mesh (SM) vs. Unstructured Mesh (UM)

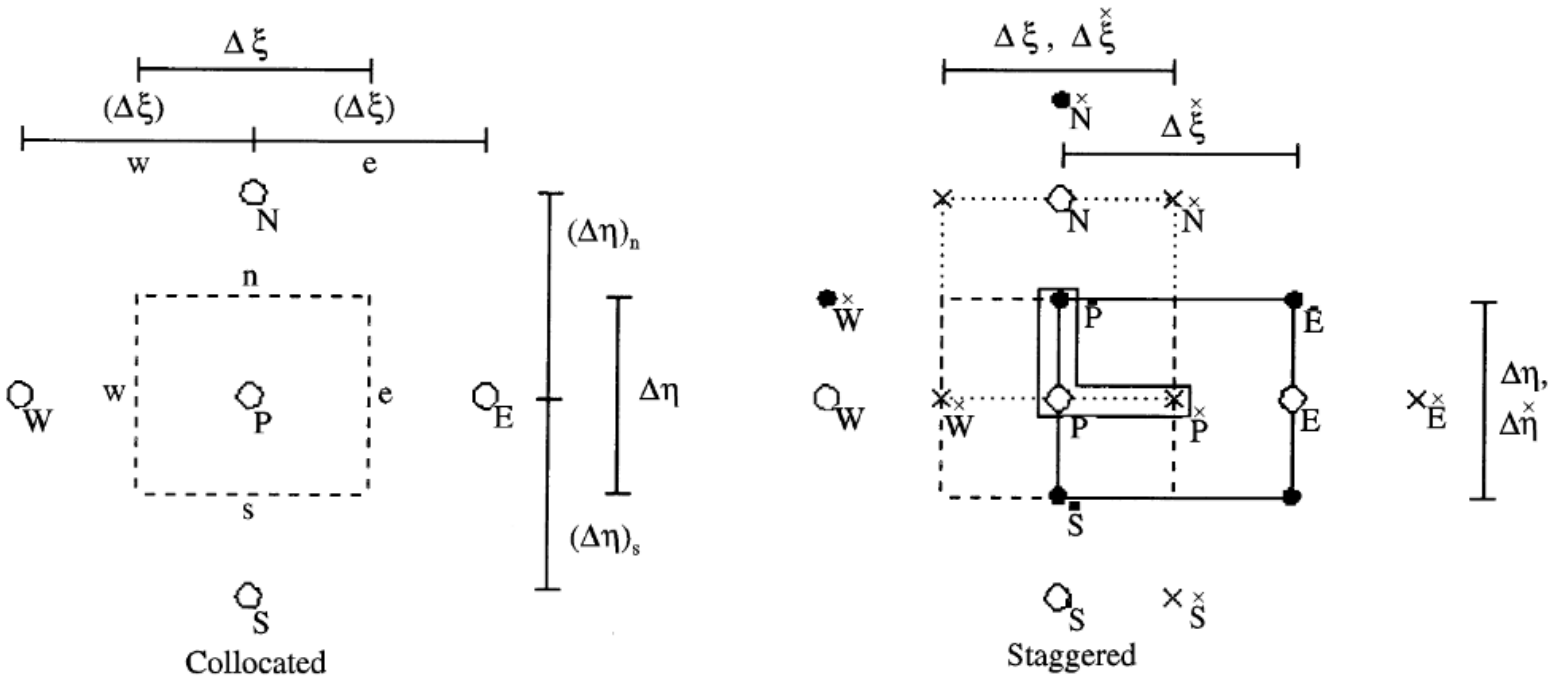
- Generation: UMs are usually highly automated and take less time to generate while generating SMs could be cumbersome
- Complex geometry: UM can fit complex geometries much better



Chen, C., R.C. Beardsley, and G. Cowles. 2006. An unstructured grid, finite-volume coastal ocean model (FVCOM) system. Oceanography 19(1):78–89, https://doi.org/10.5670/oceanog.2006.92.

Staggered (SG) vs. Collocated (CG)

- Variables: for CG, all at node centers while for SG scalars at node centers and vectors at face centers



Meier, H. F., Alves, J. J. N., & Mori, M. (1999). Comparison between staggered and collocated grids in the finite-volume method performance for single and multi-phase flows. Computers & Chemical Engineering

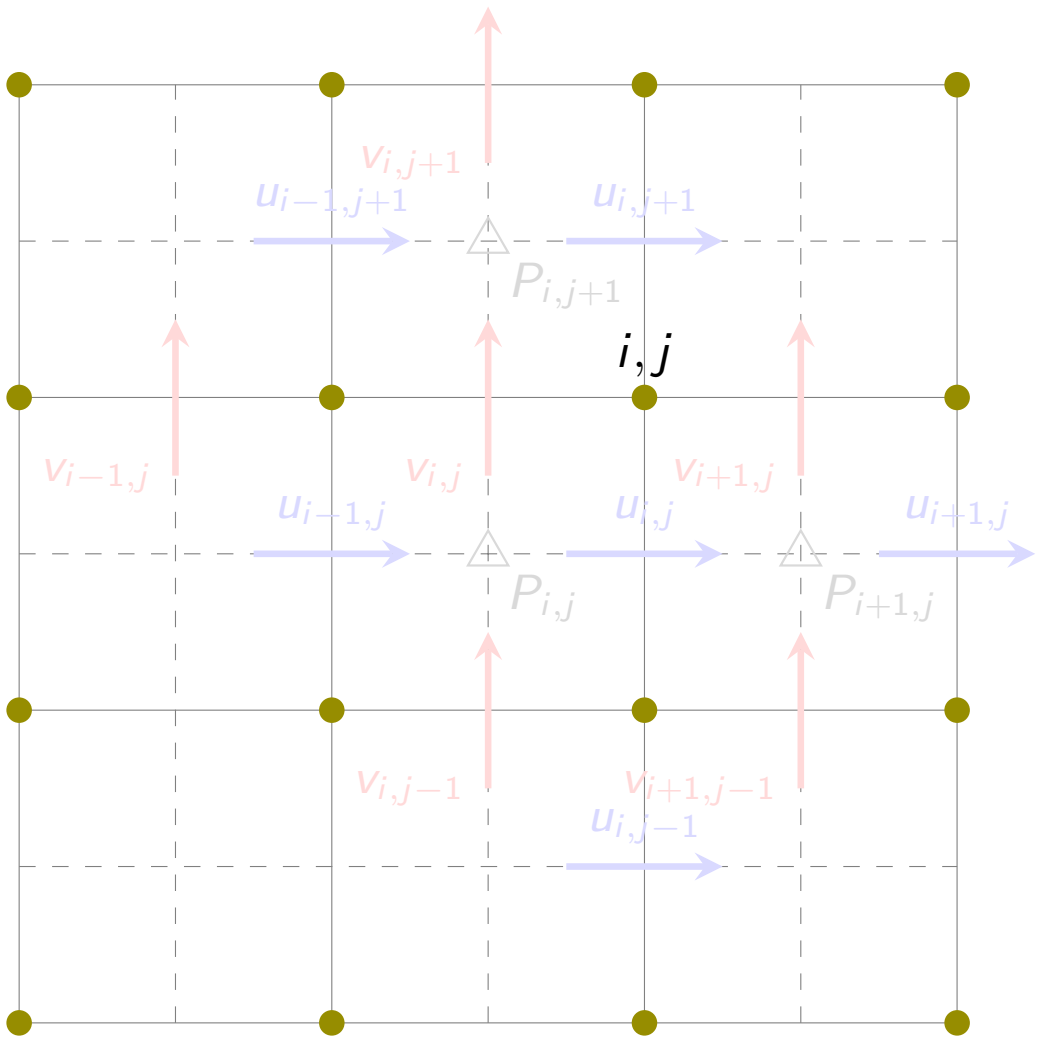
Staggered (SG) vs. Collocated (CG)

- Accuracy: SG is more accurate while CG has issues such as checkerboard (Rhie–Chow interpolation is one of the remedies)
- Implementation: CG is easier to implement and extend

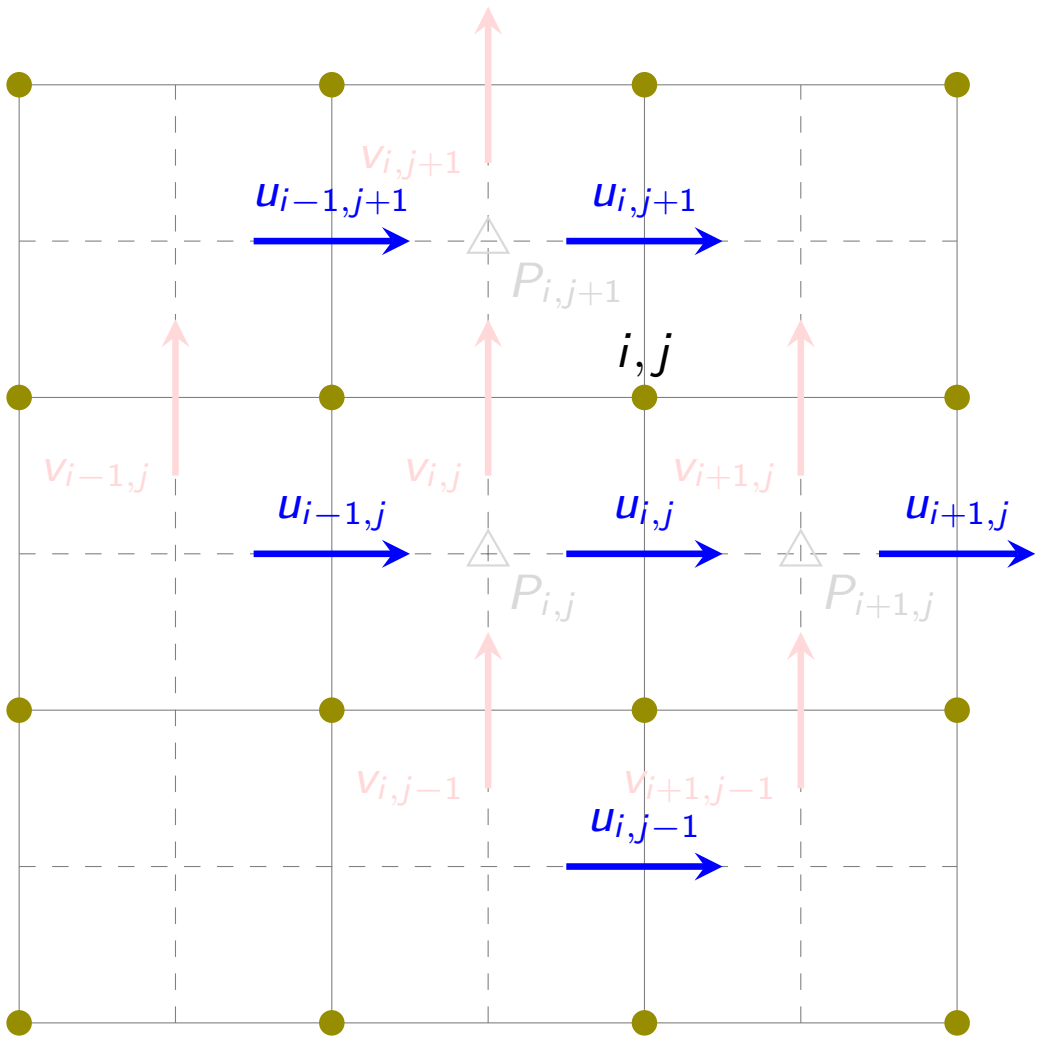
We use SG for this project:

- Simple geometry
- No additional remedy is required for implementing the numerical schemes
- Get more accurate results

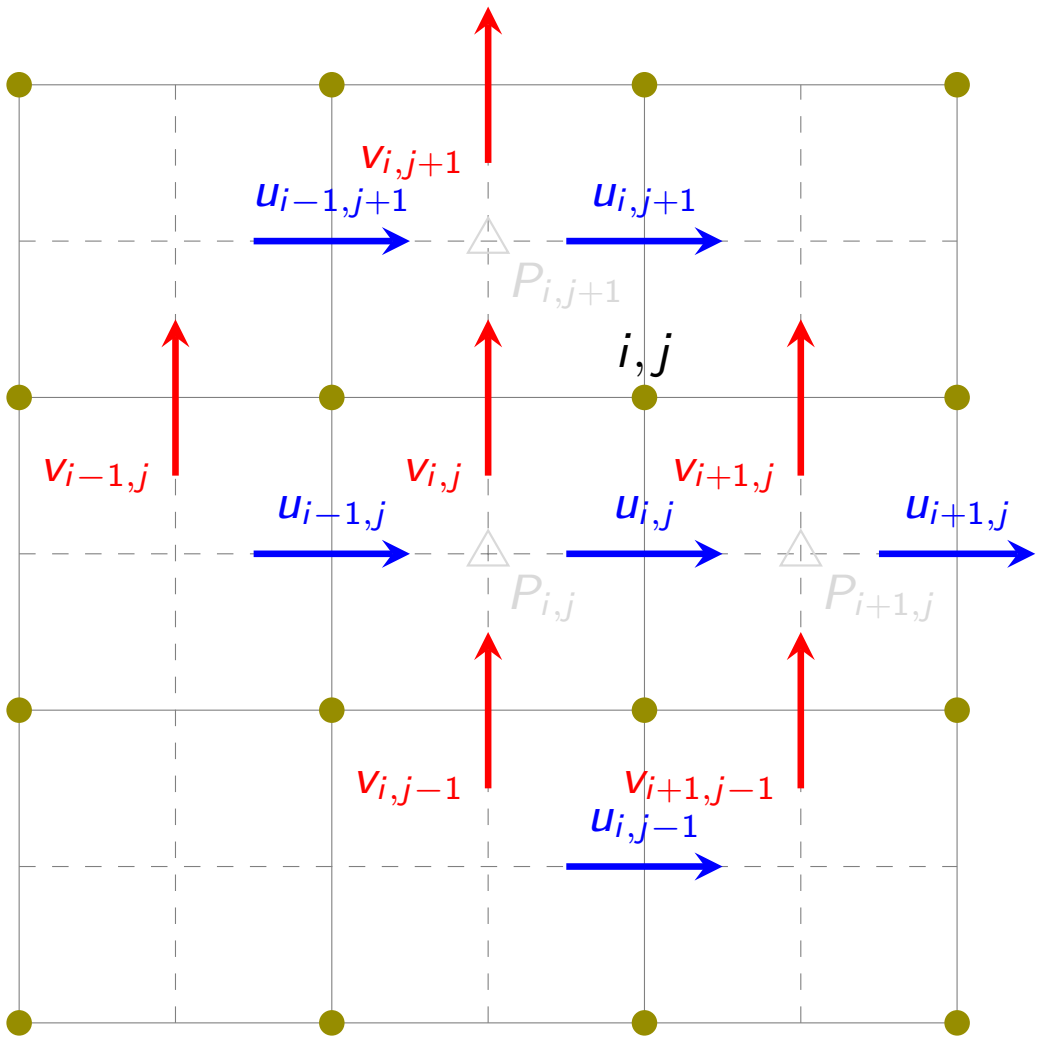
More On Staggered Grid



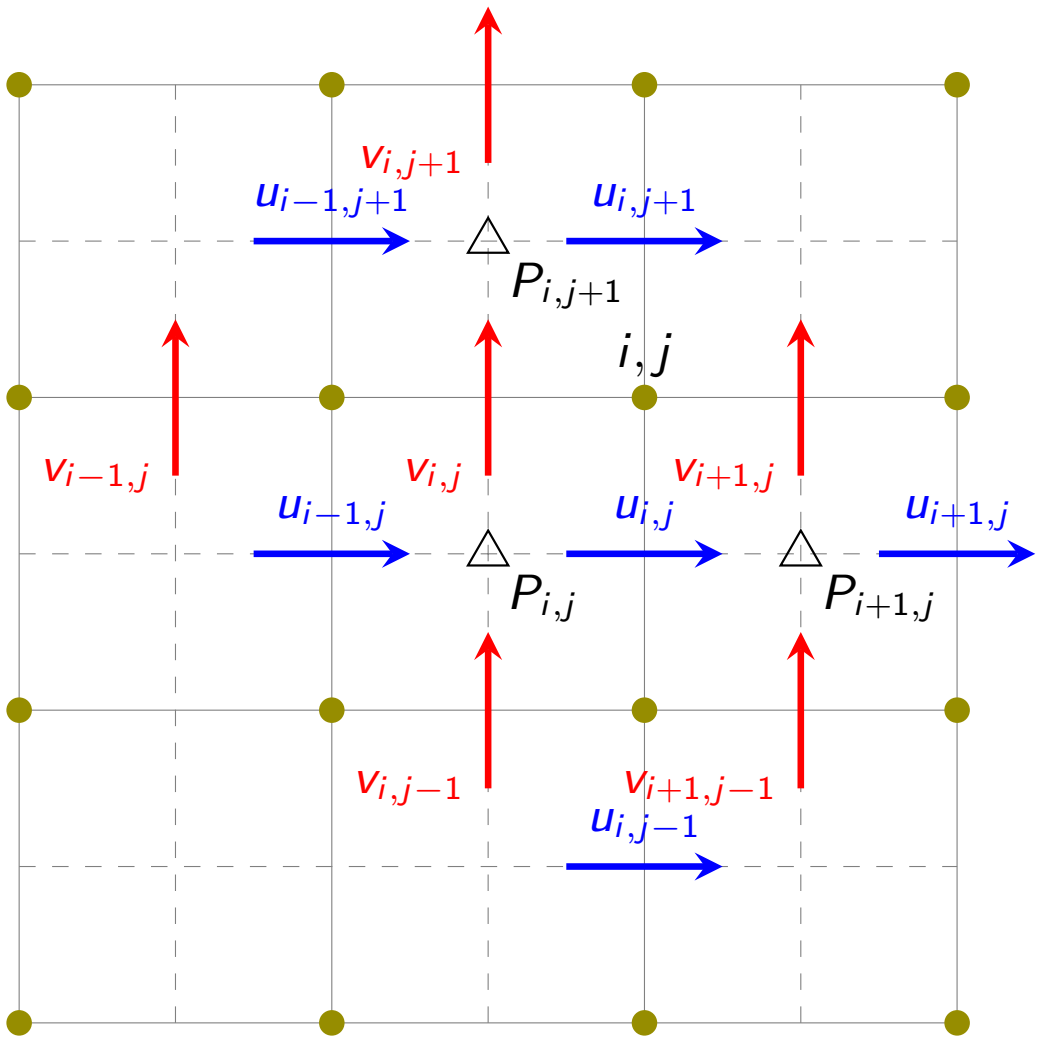
More On Staggered Grid



More On Staggered Grid



More On Staggered Grid



Formulation of discretized form

Spatial: central difference, second order

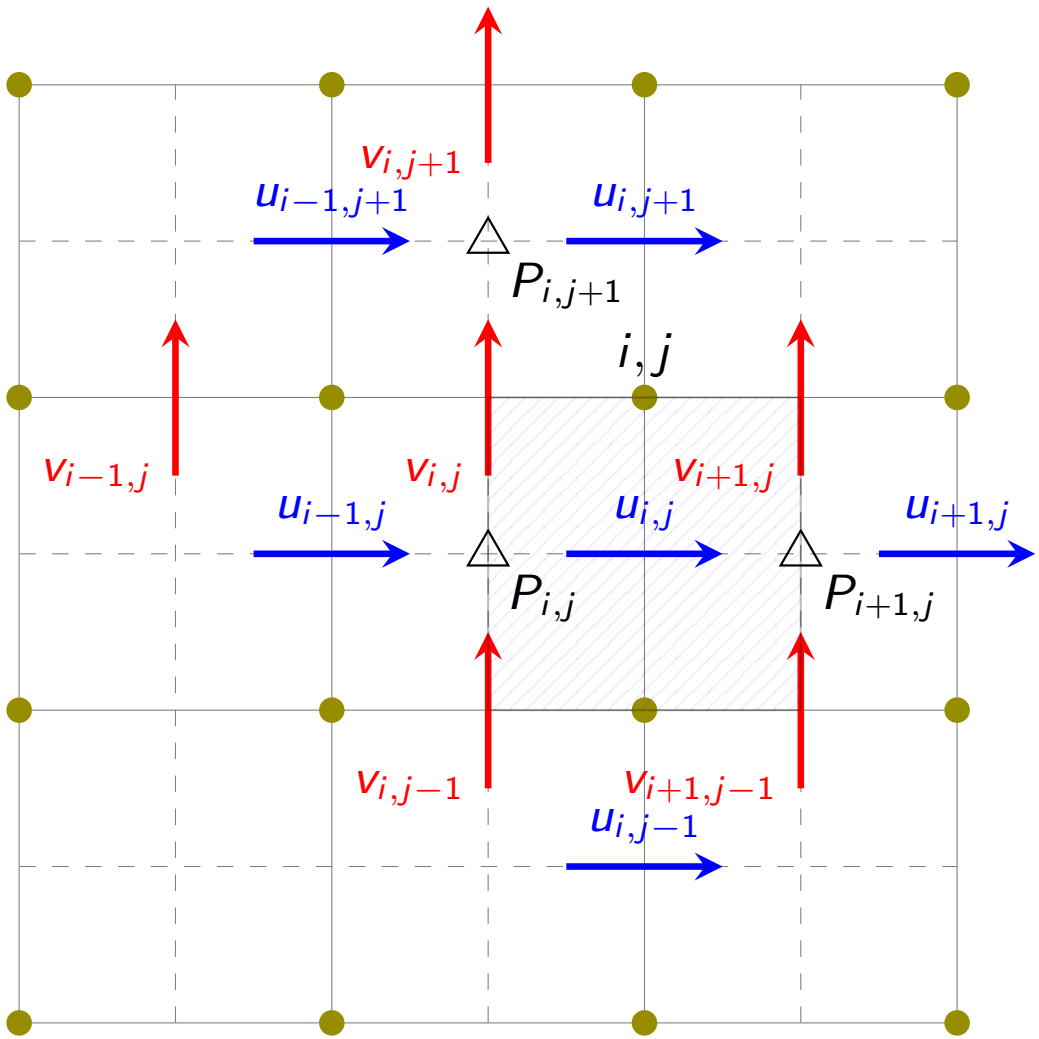
$$\partial_x \phi = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$

Temporal: backward difference, first order

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

Note: for brevity we use the superscript $n+1$ to denote the variable in the current time step and no superscript for the previous time step.
Let's discretize the equations based on a staggered grid node numbering.

Control Volume for Momentum Equation in x-direction

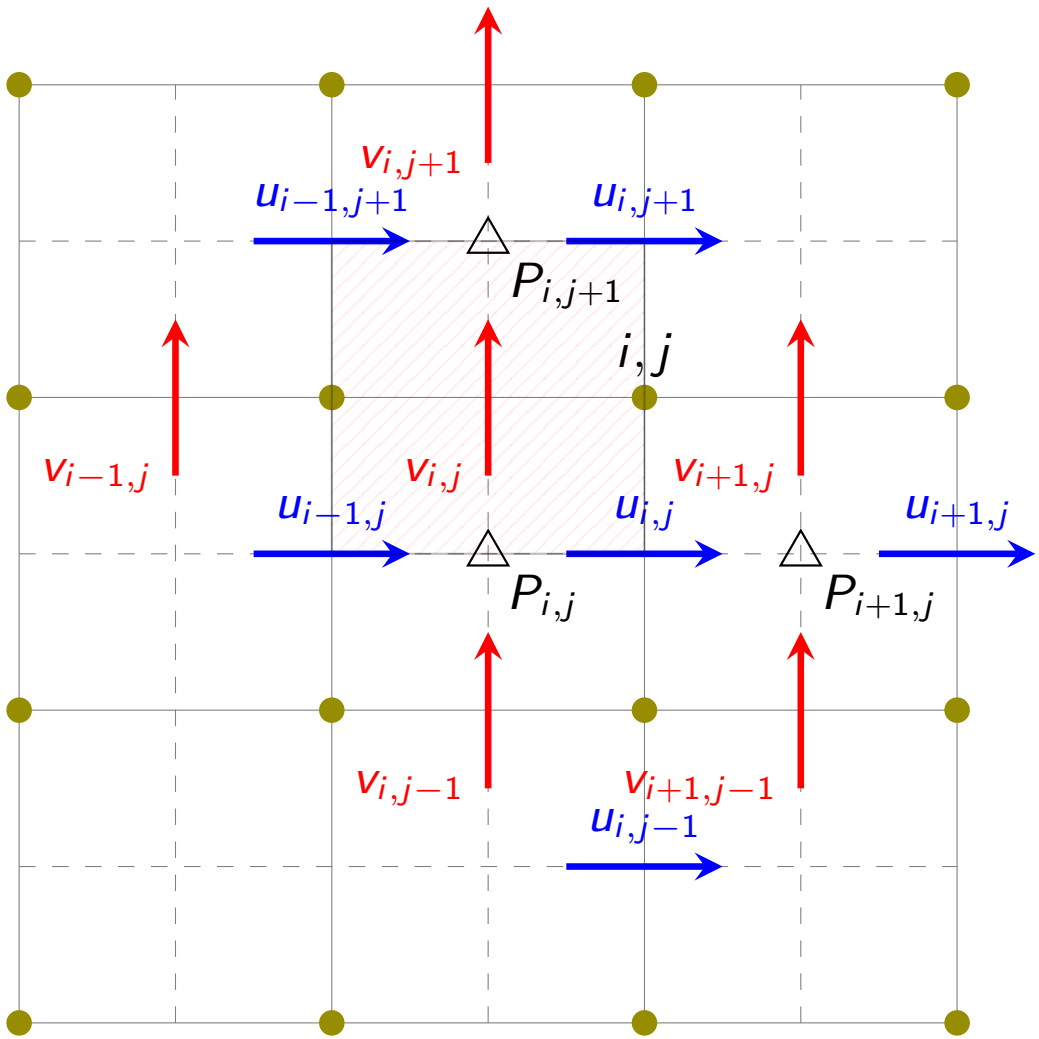


Momentum Equation in x-direction

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

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

Control Volume for Momentum Equation in y-direction



Momentum Equation in y-direction

$$\partial_t v + \partial_x(uv) + \partial_y(vv) = -\partial_y P + \nu\left(\partial_{xx} v + \partial_{yy} v\right)$$

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

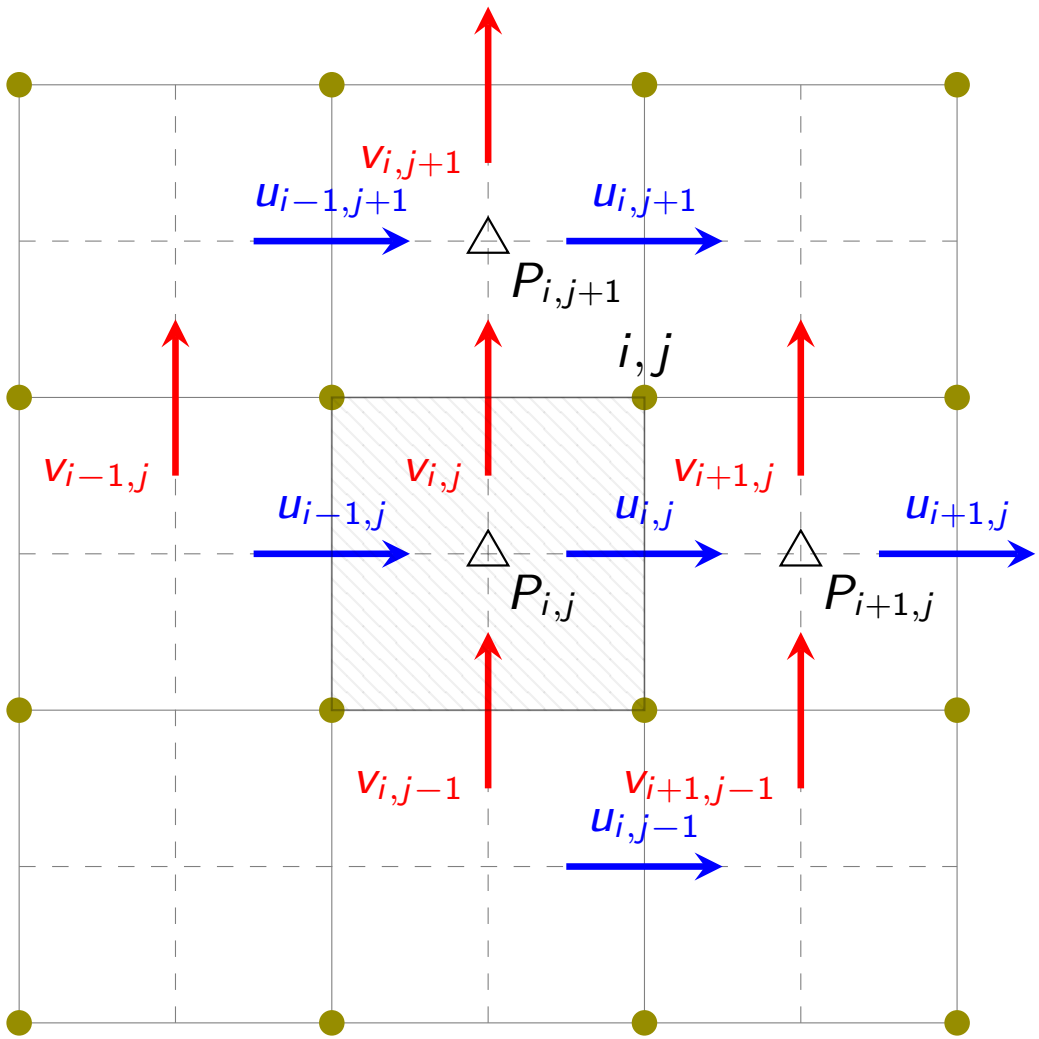
$$+ \frac{\left(\frac{v_{i,j+1}+v_{i,j}}{2}\right)^2 - \left(\frac{v_{i,j}+v_{i,j-1}}{2}\right)^2}{\Delta y}$$

$$=$$

$$- \frac{P_{i,j+1} - P_{i,j}}{\Delta y}$$

$$+ \nu\left(\frac{v_{i+1,j} - 2v_{i,j} + v_{i-1,j}}{\Delta x^2} + \frac{v_{i,j+1} - 2v_{i,j} + v_{i,j-1}}{\Delta y^2}\right)$$

Control Volume for Continuity Equation



Continuity Equation

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

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

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OpenFOAM

OpenFOAM offers a framework that can be used in three levels:

- User: use it as a blackbox to perform simulations
- Dev: manipulate solvers in high–level (modifying equations etc.)
- Hacker: manipulate the underlying engine (modifying formation of matrices etc.)

Momentum Equation

$$\partial_t \mathbf{u} + \mathbf{u}.\nabla\mathbf{u} = -\nabla P + \nu\nabla^2\mathbf{u}$$

```
fvVectorMatrix UEqn
(
        fvm::ddt(U)
    +   fvm::div(phi, U)
    +   turbulence->divDevReff(U)
    ==
        -fvc::grad(p)
);
```

Continuity Equation

$$\partial_t P + c^2 \nabla . \mathbf{u} = 0$$

```
fvScalarMatrix pEqn
(
    fvm::ddt(p)
  ==
    -c2*fvc::div(phi)
);
```

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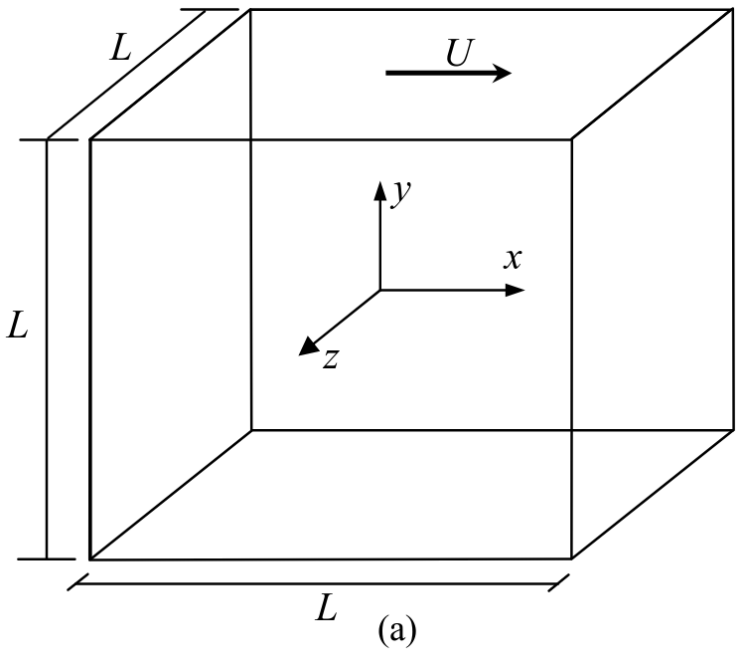
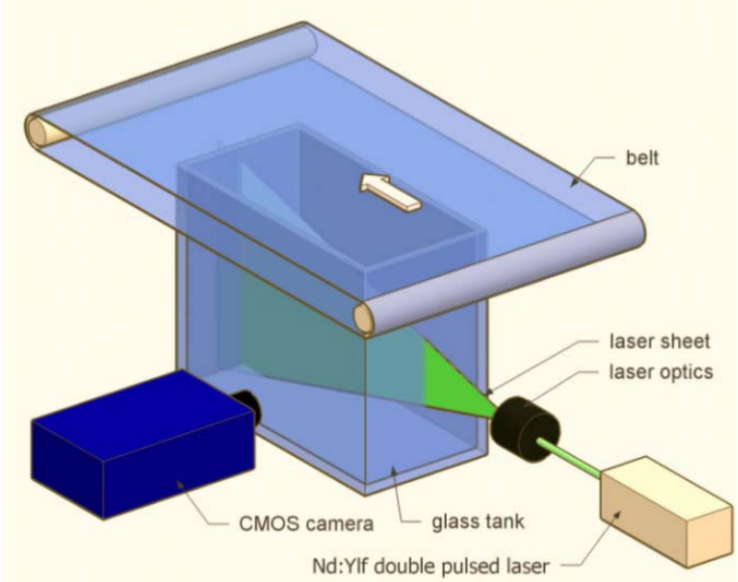
Lid-Driven Cavity

- Characteristics: steady-state, incompressible
- Boundary Conditions: walls everywhere (top wall is moving)
  - Velocity: Dirichlet ($\mathbf{U} = 0$ except for the top wall where $\mathbf{U}_x = 1$ and $\mathbf{U}_y = 0$)
  - Pressure: Neumann ($\nabla p = 0$)

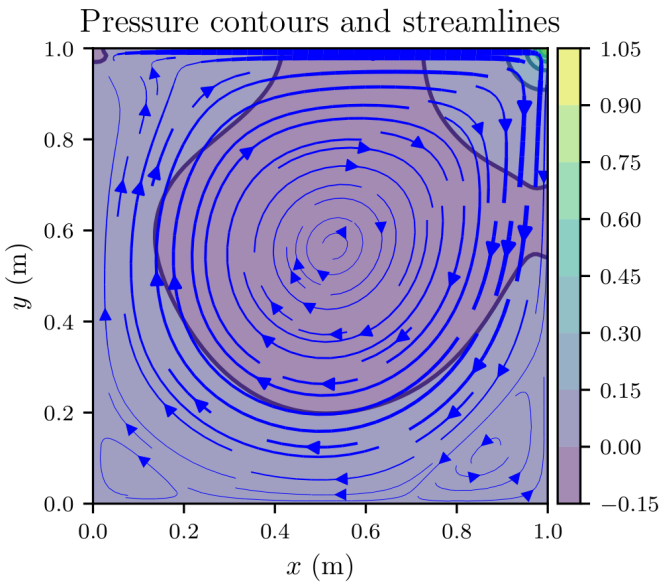


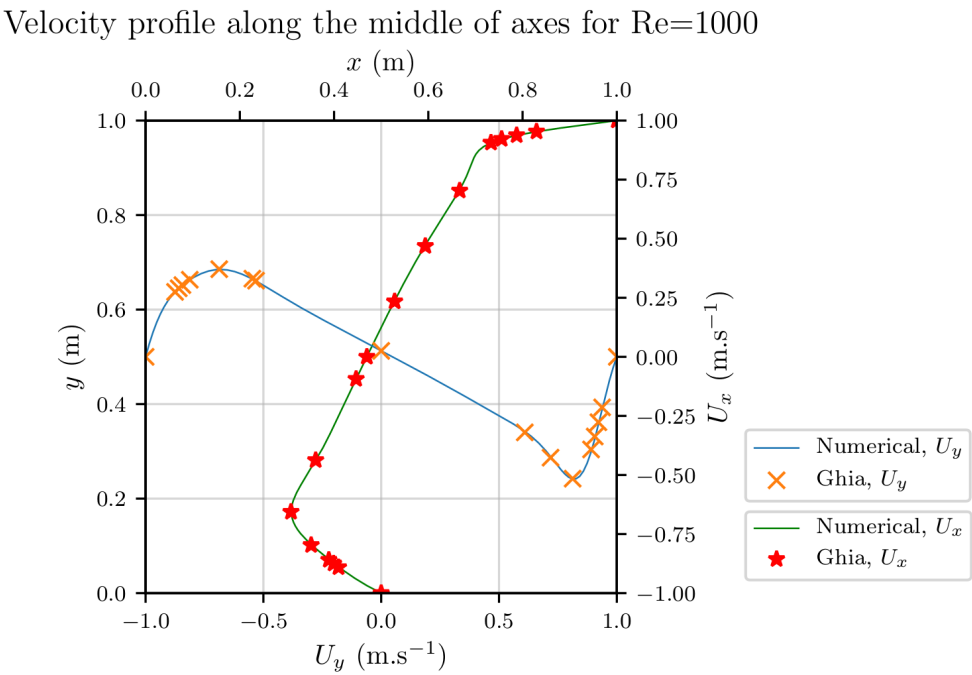
(a)



(b)

Outputs


Pressure contours and streamlines
y (m)
x (m)
0.0
0.2
0.4
0.6
0.8
1.0
1.05
0.90
0.75
0.60
0.45
0.30
0.15
0.00
−0.15


Velocity profile along the middle of axes for Re=1000
x (m)
y (m)
U_y (m.s^{-1})
U_x (m.s^{-1})
Numerical, U_y
Ghia, U_y
Numerical, U_x
Ghia, U_x

Road map

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

Exercise: Taylor–Green Vortex

A numerical solution to Taylor–Green Vortex benchmark problem:

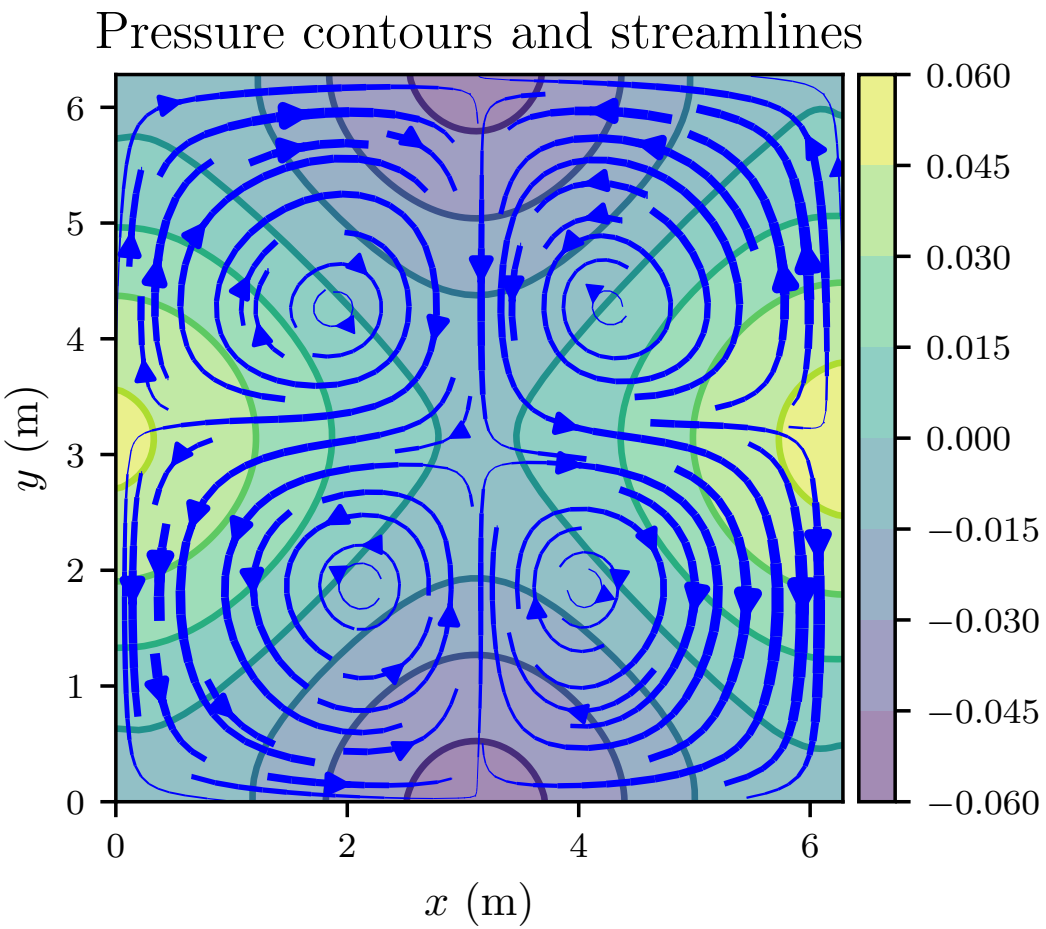
- Initial Condition:

$$u(x, y) = \sin(x)\cos(y)$$
$$v(x, y) = -\cos(x)\sin(y)$$

- Boundary condition: walls all around
- Parameters: $L = 2\pi$, $\nu = 0.2$, $\Delta t = 10^{-4}$ and $Re = 1000$.
- Analytical Solution:

$$u(x, y) = \sin(x)\cos(y)e^{-2\nu t}$$
$$v(x, y) = \cos(x)\sin(y)e^{-2\nu t}$$
$$p(x, y) = \frac{\rho}{4}(\cos(2x) + \cos(2y))e^{-4\nu t}$$

Exercise: Output



Tools

The following tools are required:

- Python 3.0+: Python 2 is deprecated
- Numpy: array operation and manipulation
- Numba: code speed–up
- Matplotlib: post–processing
- Flake8: PEP8 style guide enforcement
- CMake: managing the build process

Folders Content

```
C
├── bin
│   ├── CMakeFiles
│   └── lidCavity
├── build
│   ├── CMakeCache.txt
│   ├── CMakeFiles
│   ├── cmake_install.cmake
│   └── Makefile
├── CMakeLists.txt
├── data
│   ├── Central_U
│   ├── Central_V
│   ├── residual
│   └── xyuvp
├── output
│   ├── pressure_stream.pdf
│   └── velocity.pdf
├── run
└── src
    ├── functions.h
    ├── lidCavity.c
    └── log.plt
```

```
python
├── data
│   ├── Central_U
│   ├── Central_V
│   ├── residual
│   └── xyuvp
├── output
│   ├── pressure_stream.pdf
│   └── velocity.pdf
├── run
└── src
    ├── functions.py
    ├── functions.pyc
    ├── lidCavity.py
    ├── __pycache__
    └── setup.pyc
```

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!