CFD Code Development Frameworks

Python, C, OpenFOAM, Fenics

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Governing Equations

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

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

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

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

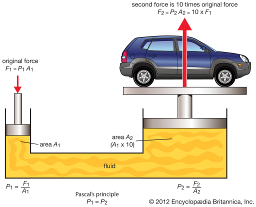
- LHS is acceleration which is intrinsically Lagrangian and when it is translated to Eulerian coordinates it becomes non-linear
- RHS describes influence of pressure gradient, viscosity and body forces.

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 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:

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

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

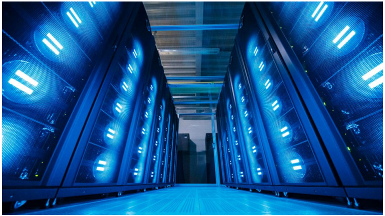
where $P = \dfrac{p}{\rho}$.

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

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

Solution algorithm

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.

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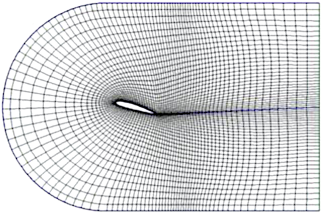
Grid

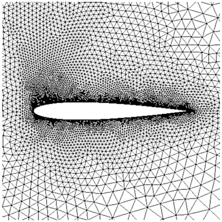
Structured Mesh (SM) vs. Unstructured Mesh (UM)

- 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



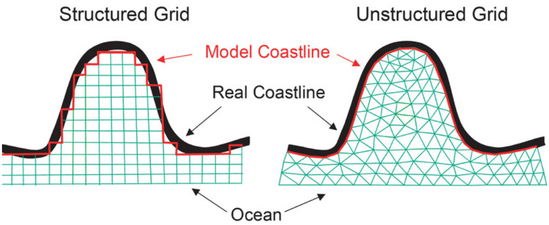
Unstructured



Grid

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

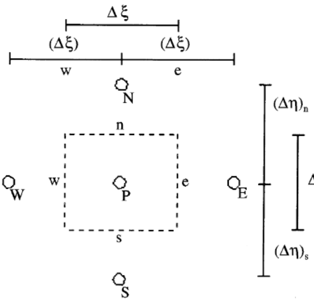


Chen, C., R.C. Beardsley, and G. Cowles. 2006. An unstructured grid, finite-volume coastal ocean model (FVCOM) system. Oceanography 19(1):78–89, https://doi.org/10.5670/oceanog.2006.92.

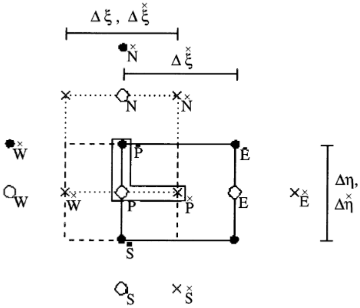
Grid

Staggered (SG) vs. Collocated (CG)

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



Collocated



Staggered

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

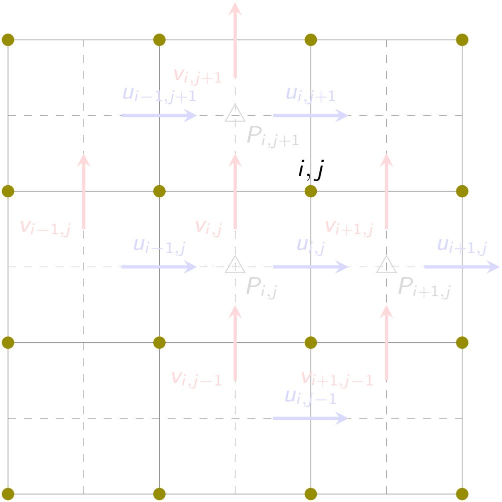
Grid

Staggered (SG) vs. Collocated (CG)

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

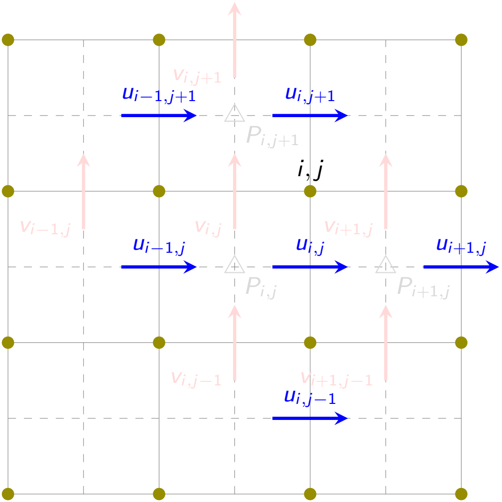
Grid

Staggered Grid



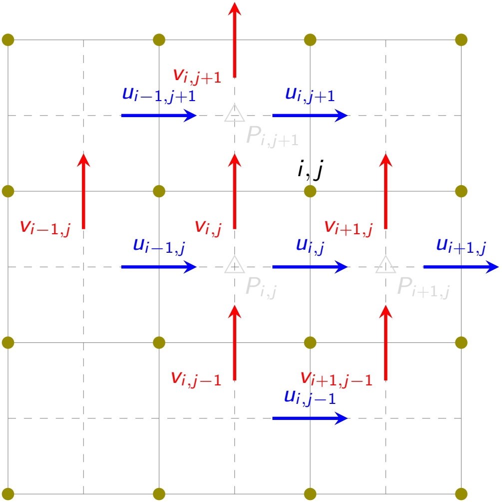
Grid

Staggered Grid



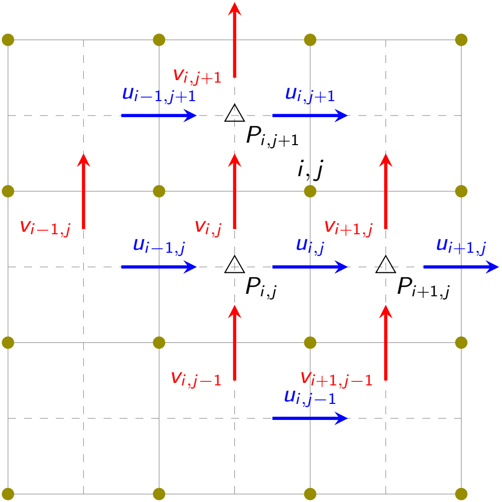
Grid

Staggered Grid



Grid

Staggered Grid



Solution algorithm

Discretization

Spatial: central difference, second order

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

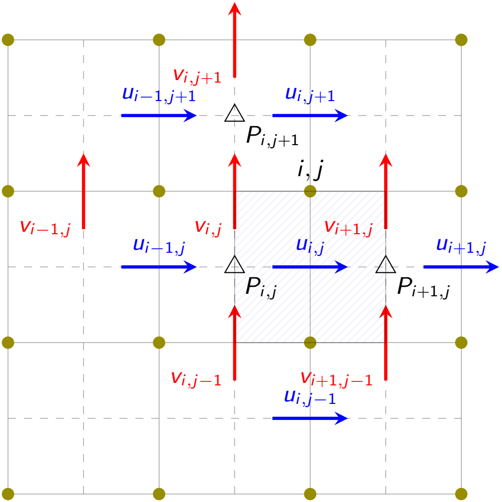
Temporal: backward difference, first order

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

Note: for brevity we use the superscript $n+1$ 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.

Discretization

Control Volume for Momentum Equation in x-direction



Discretization

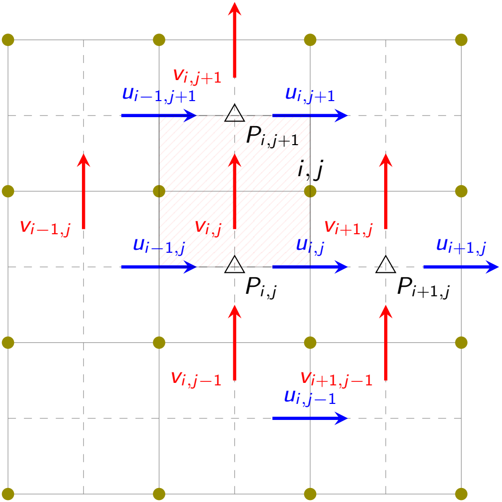
Momentum Equation in x-direction

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

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

Discretization

Control Volume for Momentum Equation in y-direction



Discretization

Momentum Equation in y-direction

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

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

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

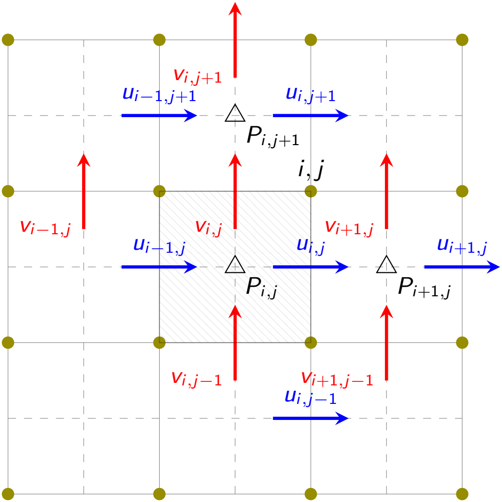
$$=$$

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

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

Discretization

Control Volume for Continuity Equation



Discretization

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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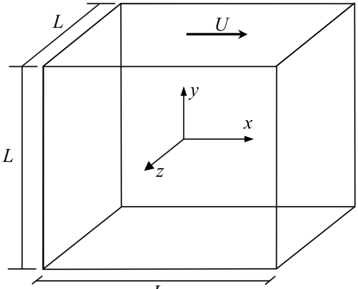
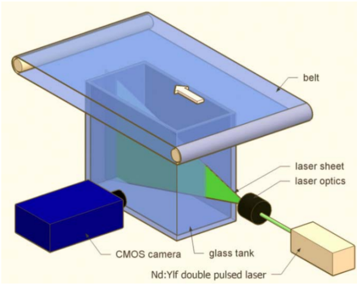
Problem Statement

Lid-Driven Cavity

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



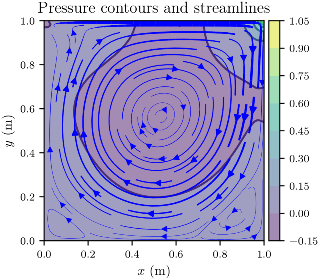
(a)

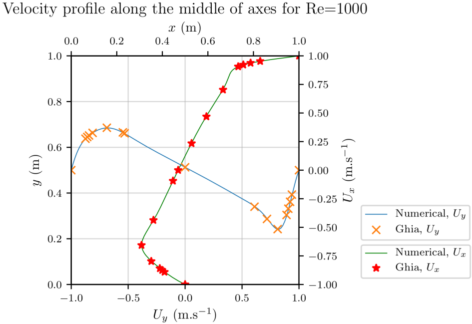


(b)

Problem Statement

Outputs





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

Problem Statement

Exercise: Taylor–Green Vortex

A numerical solution to Taylor–Green Vortex benchmark problem:

- Initial Condition:

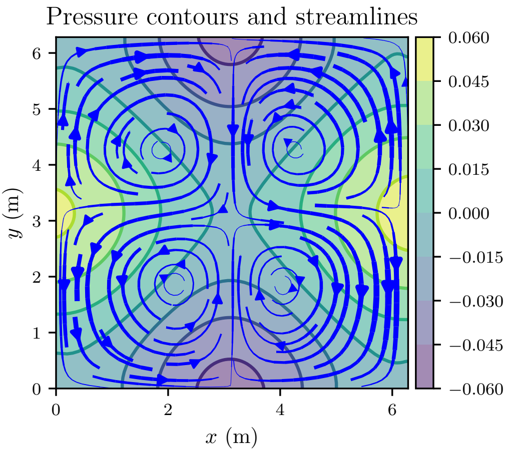
$$u(x,y) = \sin(x)\cos(y)$$
$$v(x,y) = -\cos(x)\sin(y)$$

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

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

Problem Statement

Solution



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!

```
$ mkdir UHWS

$ cd UHWS

$ git clone https://github.com/taataam/UHWorkshop.git

$ cd UHWorkshop/workshop3
```