Computation of Incompressible Flows: Fractional-Step Methods

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Navier-Stokes Equations – I

- Mass and momentum conservation equations – integral form:

$$\frac{\partial}{\partial t}\int_V \rho \, \mathrm{d}V + \int_S \rho \mathbf{v}\cdot\mathbf{n} \, \mathrm{d}S = 0$$

$$\frac{\partial}{\partial t}\int_V \rho u_i \, \mathrm{d}V + \int_S \rho u_i \mathbf{v}\cdot\mathbf{n} \, \mathrm{d}S = \int_S \mathbf{t}_i\cdot\mathbf{n} \, \mathrm{d}S + \int_V \rho b_i \, \mathrm{d}V$$

- Vector form:

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}) = 0$$

$$\frac{\partial(\rho u_i)}{\partial t} + \boldsymbol{\nabla}\cdot(\rho u_i \mathbf{v}) = \boldsymbol{\nabla}\cdot\mathbf{t}_i + \rho b_i$$

$$\mathbf{t}_i = \mu\,\boldsymbol{\nabla} u_i + \mu\,(\boldsymbol{\nabla}\mathbf{v})^{\mathrm{T}}\cdot\mathbf{i}_i - \left(p + \frac{2}{3}\mu\,\boldsymbol{\nabla}\cdot\mathbf{v}\right)\mathbf{i}_i = \tau_{ij}\mathbf{i}_j - p\mathbf{i}_i$$

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu\delta_{ij}\,\boldsymbol{\nabla}\cdot\mathbf{v}$$

Properties of Navier-Stokes Equations – I

- For computational convenience several terms are lumped together into the "pressure"-variable:

$$p - \rho_0 \mathbf{g} \cdot \mathbf{r} + \mu \tfrac{2}{3} \boldsymbol{\nabla} \cdot \mathbf{v}$$

- In the integral form of momentum equations (i.e. FV-methods), pressure can be represented in two ways:

Surface force (conservative): $-\int_S p \, \mathbf{i}_i \cdot \mathbf{n} \, \mathrm{d}S$

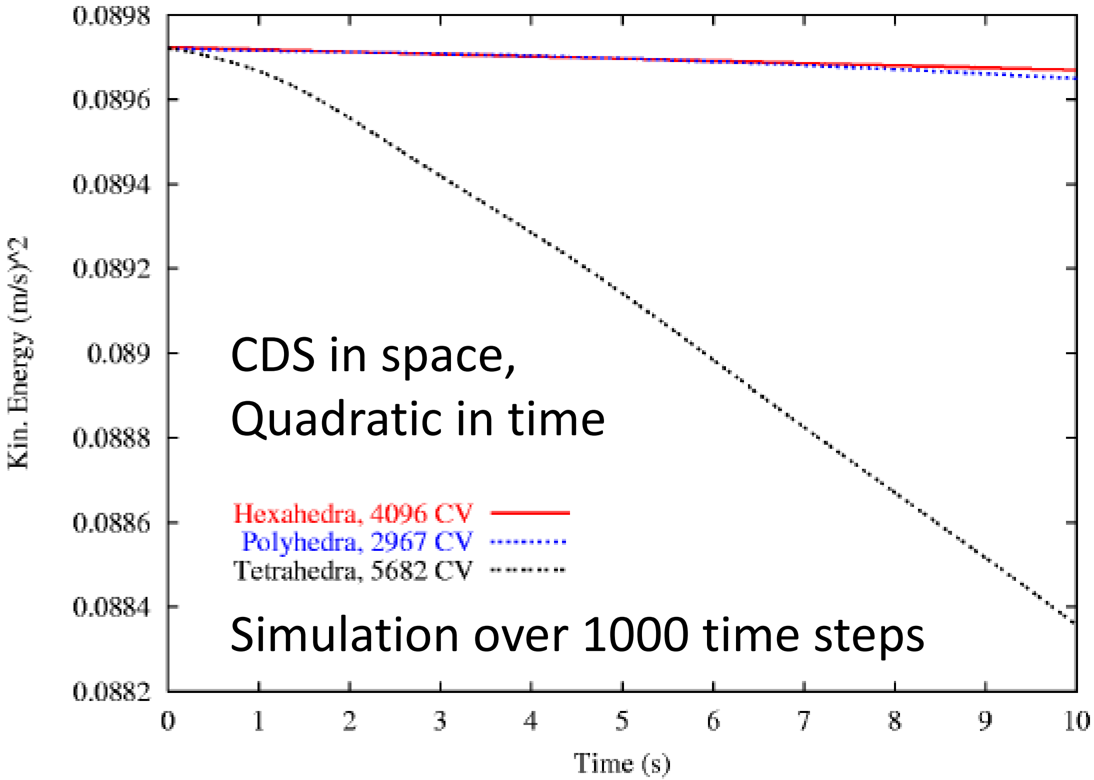
Volume force (non-conservative): $-\int_V \boldsymbol{\nabla} p \cdot \mathbf{i}_i \, \mathrm{d}V$

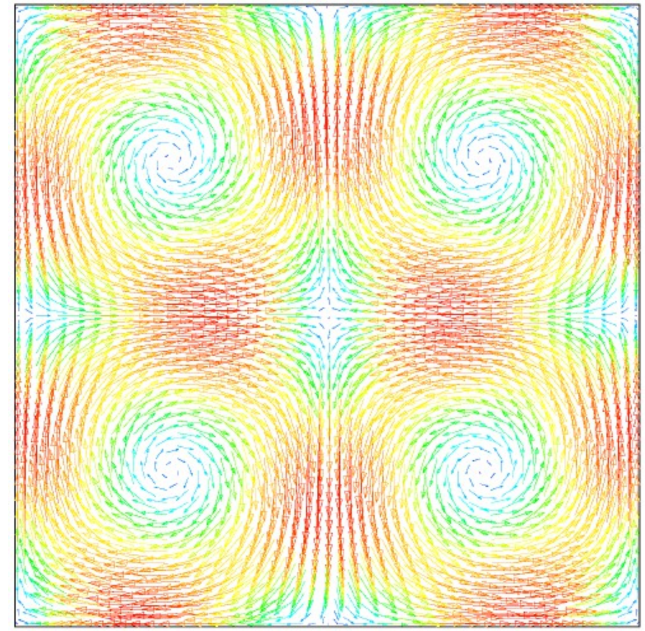
- Other body forces are evaluated at computational nodes (CV-centroids).

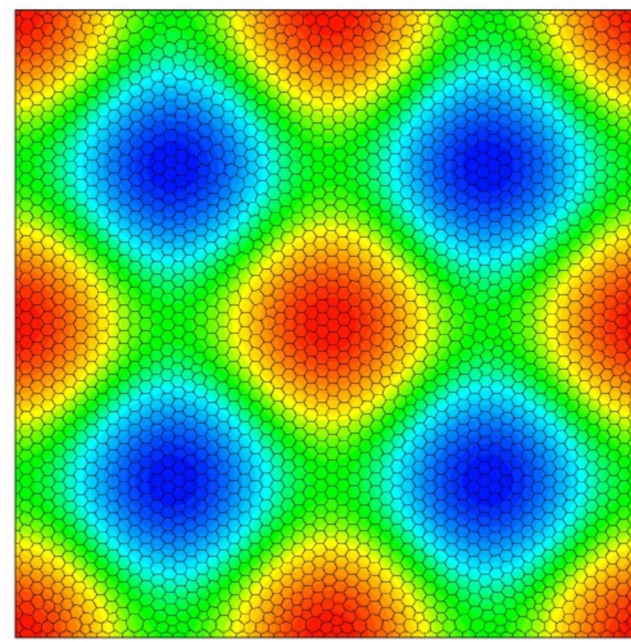
Properties of Navier-Stokes Equations – II

- FV-method guaranties conservation of mass and momentum (when properly implemented)…
- In FD-methods, the use of the conservative form of the diffe-rential momentum equation is the pre-requisite for conservativeness…
- … but depending on approximations used, the result may or may not be conservative.
- Energy conservation is more tricky: thermal energy is conserved by FV-methods, but kinetic energy cannot be separately enforced (as well as angular momentum)…
- For transient flows (like DNS, LES of turbulent flows), it is important to check whether the method conserves kinetic energy (it must not grow with time without reason).

Test of Kinetic Energy Conservation





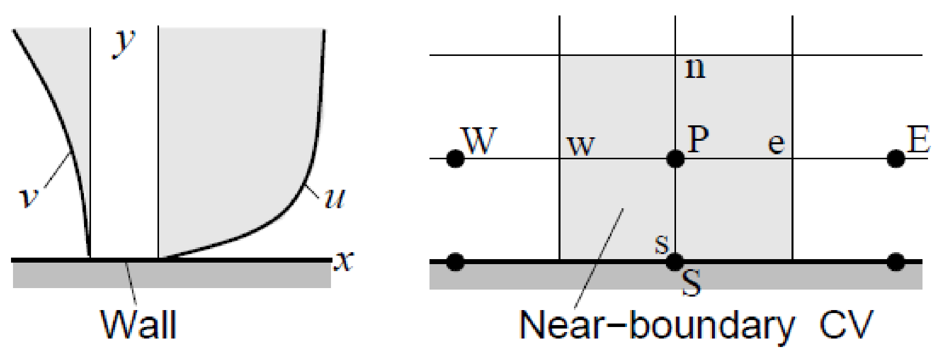


Testing of kinetic energy conservation is often done by simulating transient inviscid flow, e.g. four counter-rotating vortices: kinetic energy in the solution domain should stay constant (may reduce by numerical diffusion, but not grow!).

Boundary Conditions for Momentum Equations – I

- In FD-methods, one either specifies velocity at the boundary (Dirichlet-condition), or its derivative (Neumann-condition).
- In FV-methods, surface integrals over boundary faces need to be defined, so there are some differences…
- No-slip condition at a wall does not mean just velocity = wall velocity: viscous forces must be set properly…
- For a wall at $y = 0$ (due to continuity equation):

$$\left(\frac{\partial u}{\partial x}\right)_{\text{wall}} = 0 \;\Rightarrow\; \left(\frac{\partial v}{\partial y}\right)_{\text{wall}} = 0 \;\Rightarrow\; \tau_{yy} = 2\mu\left(\frac{\partial v}{\partial y}\right)_{\text{wall}} = 0$$



Boundary Conditions for Momentum Equations – II

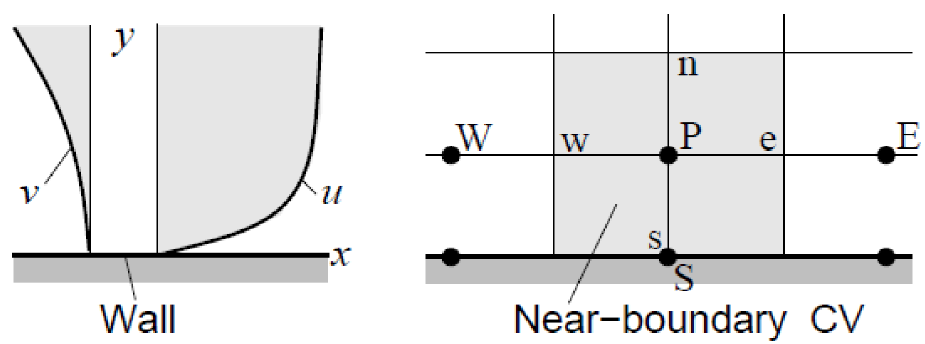
- This means that normal viscous force = 0 at wall, so in equation for v-velocity:

$$F_{\mathrm{s}}^{\mathrm{d}} = \int_{S_{\mathrm{s}}} \tau_{yy} \, \mathrm{d}S = 0$$

- Setting just $v = 0$ at wall might lead to a non-zero discretized derivative and non-zero normal viscous force.

- The shear stress at wall requires approximation of wall-normal derivative of the wall-parallel velocity component, e.g.:

$$F_{\mathrm{s}}^{\mathrm{d}} = \int_{S_{\mathrm{s}}} \tau_{xy} \, \mathrm{d}S = \int_{S_{\mathrm{s}}} \mu \frac{\partial u}{\partial y} \, \mathrm{d}S \approx \mu_{\mathrm{s}} S_{\mathrm{s}} \frac{u_{\mathrm{P}} - u_{\mathrm{S}}}{y_{\mathrm{P}} - y_{\mathrm{S}}}$$

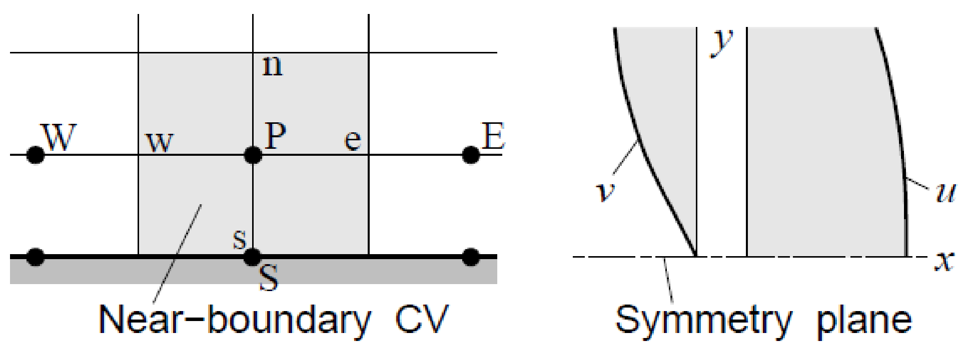


Boundary Conditions for Momentum Equations – III

- The one-sided approximation of velocity derivative in wall-normal direction over half cell is formally 1st-order accurate; however, tests show that results still converge with 2nd-order…
- A better approximation is obtained from the assumption of a quadratic variation (especially for laminar flows):

$$\left(\frac{\partial \phi}{\partial y}\right)_{\mathrm{S}} \approx \frac{-\phi_{\mathrm{N}} + 9\phi_{\mathrm{P}} - 8\phi_{\mathrm{S}}}{3\,\Delta y}$$

- At a symmetry boundary, the situation is opposite: the shear force is zero, but the normal viscous force is non-zero…



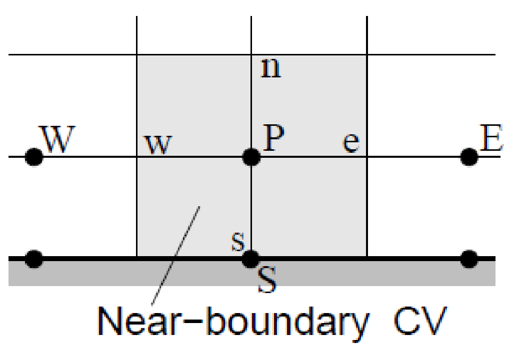
Boundary Conditions for Momentum Equations – IV

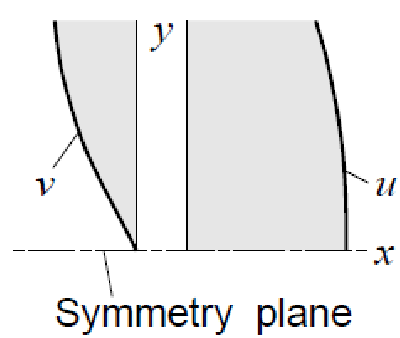
- At a symmetry boundary we have:

$$\left(\frac{\partial u}{\partial y}\right)_{\text{sym}} = 0\,; \quad \left(\frac{\partial v}{\partial y}\right)_{\text{sym}} \neq 0$$

- Thus, diffusive fluxes for the boundary-parallel velocity and all scalar variables are zero, but for the boundary-normal velocity:

$$F_{\text{s}}^{\text{d}} = \int_{S_{\text{s}}} \tau_{yy}\,\mathrm{d}S = \int_{S_{\text{s}}} 2\mu\frac{\partial v}{\partial y}\,\mathrm{d}S \approx \mu_{\text{s}}S_{\text{s}}\frac{v_{\text{P}} - v_{\text{S}}}{y_{\text{P}} - y_{\text{S}}}$$





Boundary Conditions for Momentum Equations – V

- With a *staggered* variable arrangement on Cartesian grids, pressure is not needed at boundaries where velocity is given.
- With a *colocated* variable arrangement, pressure is required at all boundaries in order to compute pressure forces…
- Linear or quadratic extrapolation from interior is usually used.
- When large body forces are present, extrapolation of pressure to boundary becomes important (otherwise, unrealistic velocities near boundary can result…).
- At Inlet, velocities are usually prescribed; this sets convective fluxes – for diffusive fluxes, approximate gradients at boundary are used.
- At outlet, velocities are usually extrapolated…

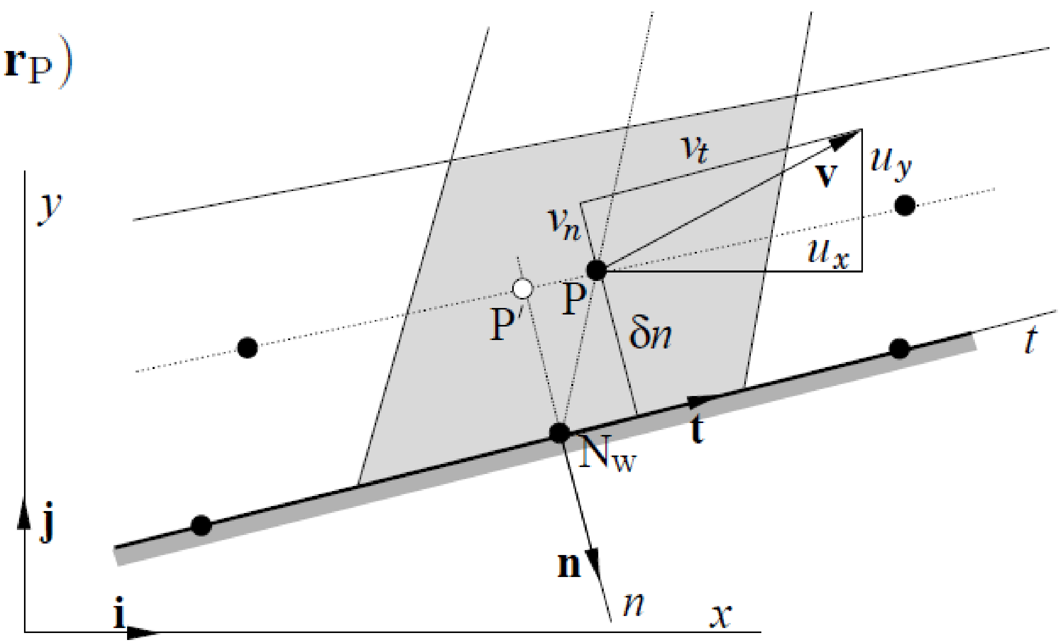
Boundary Conditions for Momentum Equations – VI

- Non-orthogonal grids require special attention when computing derivatives in boundary-normal direction; main options are:
  - Define a local non-orthogonal coordinate system aligned with grid lines and apply coordinate transformation;
  - Define a local Cartesian coordinate system aligned with wall and use auxiliary nodes along normal coordinate, e.g.:

$$\phi_{P'} = \phi_P + (\nabla\phi)_P \cdot (\mathbf{r}_{P'} - \mathbf{r}_P)$$

$$\left(\frac{\partial \phi}{\partial n}\right)_{N_w} \approx \frac{\phi_{P'} - \phi_{N_w}}{\delta n}$$

$$\delta n = (\mathbf{r}_{N_w} - \mathbf{r}_{P'}) \cdot \mathbf{n}$$



Pressure-Equation – I

- An equation in which pressure is the dominant variable can be derived by taking the divergence of the momentum equation (mimicking the continuity equation…):

$$\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}\, p) = -\boldsymbol{\nabla} \cdot \left[\boldsymbol{\nabla} \cdot (\rho \mathbf{v}\mathbf{v} - \tau_{ij}\mathbf{i}_i\mathbf{i}_j) - \rho \mathbf{b} + \frac{\partial(\rho \mathbf{v})}{\partial t} \right]$$

- Differential form in Cartesian coordinates:

$$\frac{\partial}{\partial x_i}\left(\frac{\partial p}{\partial x_i}\right) = -\frac{\partial}{\partial x_i}\left[\frac{\partial}{\partial x_j}\left(\rho u_i u_j - \tau_{ij}\right)\right] + \frac{\partial(\rho b_i)}{\partial x_i} + \frac{\partial^2 \rho}{\partial t^2}$$

- For constant density and viscosity:

$$\frac{\partial}{\partial x_i}\left(\frac{\partial p}{\partial x_i}\right) = -\frac{\partial}{\partial x_i}\left[\frac{\partial(\rho u_i u_j)}{\partial x_j}\right]$$

Pressure-Equation – II

- A possible solution procedure:
  - Discretize and solve momentum equations, using pressure from previous iteration;
  - Discretize and solve pressure equation, using velocities from previous step to compute the source term;
  - Repeat until convergence.
- Continuity equation does not have to be enforced separately – it has been used in the process implicitly…
- This approach is seldom used – mainly because boundary conditions for the pressure equation are tricky...
- The pressure equation can be used to compute the pressure when the velocity field is known (e.g. obtained in an experiment (PIV) or by solving equations for streamfunction and vorticity)...

Pressure-Equation – III

- When discretizing the pressure-equation, one has to pay attention to consistency with momentum and continuity equations...
- One can use different approximations for outer and inner derivatives – they only have to be the same as in the „parent“ equation...

Exactly as in momentum equations!

$$\frac{\partial}{\partial x_i}\left(\frac{\partial p}{\partial x_i}\right) = -\frac{\partial}{\partial x_i}\left[\frac{\partial(\rho u_i u_j)}{\partial x_j}\right]$$

Must be the same approximation, symbolizing continuity equation!

Solution Method for Compressible Flows

- If density variation is appreciable in the whole solution domain, the following approach can be used:
  - Discretize and solve continuity equation for density, using velocity field from previous iteration;
  - Discretize and solve momentum equations for velocities, using density just computed and pressure from previous iteration;
  - Discretize and solve energy equation to obtain temperature, using available values of other variables;
  - Compute new pressure from equation of state, using latest update of density and temperature;
  - Repeat until converged solution is obtained.
- Alternatively, all variables (density, velocities and tempera-ture) could be considered as a single vector of unknowns and solved as single equation (coupled solver).

Explicit Solution Method for Incompressible Flows – I

- Momentum equations in symbolic difference form:

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

- For simplicity, assume explicit-Euler method is used to solve:

$$(\rho u_i)^{n+1} - (\rho u_i)^n = \Delta t \left(H_i^n - \frac{\delta p^n}{\delta x_i} \right)$$

- Velocities obtained from this equation would not satisfy the continuity equation (which we also want to enforce):

$$\frac{\delta(\rho u_i)^{n+1}}{\delta x_i} = 0$$

Apply this numerical divergence approx. to the above eq.:

$$\underbrace{\frac{\delta(\rho u_i)^{n+1}}{\delta x_i}}_{\text{This should be } = 0} - \underbrace{\frac{\delta(\rho u_i)^n}{\delta x_i}}_{\text{This is } = 0} = \Delta t \left[\frac{\delta}{\delta x_i} \left(H_i^n - \frac{\delta p^n}{\delta x_i} \right) \right]$$

Explicit Solution Method for Incompressible Flows – II

- One obtains thus an equation for pressure (discretized):

Exactly as in momentum equations!

$$\frac{\delta}{\delta x_i}\left(\frac{\delta p^n}{\delta x_i}\right) = \frac{\delta H_i^n}{\delta x_i}$$

Must be the same approximation, continuity equation!

- When this equation is solved, new velocities can be computed; they satisfy discretized continuity equation.
- Note that, for incompressible flows, it is irrelevant to which time level the pressure is assigned (there is no pressure-derivative in equations; only pressure-differences matter).
- Similar expressions would be obtained for an explicit time-integration method of higher order.

Explicit Solution Method for Incompressible Flows – III

- An explicit solution method can be summarized as follows:
  - Start with an initial velocity field u_i^n which satisfies all equations;
  - Compute the convective, diffusive and source terms using appropriate spatial and temporal (explicit) discretization, to obtain H_i^n.
  - Apply discretized divergence operator to H_i^n and set this to the source term of the discretized Poisson-equation for pressure.
  - Solve the pressure-equation and compute discretized pressure gradient terms for the momentum equation.
  - Compute the velocity field explicitly using the new pressure gradient and H_i^n . It satisfies both discretized continuity and momentum equations.
  - Advance to the next time step.
- The problem with this approach is the stability constraint…

Fractional-Step Methods – I

- There are many variants of fractional-step method; here two versions will be presented.
- The first is based on Crank-Nicolson time-integration method for the whole equation; it involves three steps.
- In the first step, momentum equations are solved using pressure from previous time step:

$$\frac{(\rho u_i)^* - (\rho u_i)^n}{\Delta t} = \frac{1}{2}\left[H(u_i^n) + H(u_i^*)\right] - \frac{\delta p^n}{\delta x_i}$$

- In $H(u_i)$ convective, diffusive and source terms are included; their spatial discretization is not important for the time being.
- Since the time-integration method is implicit, equation system is solved and outer iterations are applied to update non-linear terms.

Fractional-Step Methods – II

- The momentum equation just presented is solved for u_i^*, which is an approximation for the solution at new time level t_{n+1}.
- The velocity just computed needs to be corrected to enforce mass conservation; the corrected velocity should also satisfy momentum equation that includes new pressure:

$$\frac{(\rho u_i)^{n+1} - (\rho u_i)^n}{\Delta t} = \frac{1}{2}\left[H(u_i^n) + H(u_i^*)\right] - \frac{1}{2}\left(\frac{\delta p^n}{\delta x_i} + \frac{\delta p^{n+1}}{\delta x_i}\right)$$

- By subtracting from this equation the one solved earlier, we obtain:

$$\frac{(\rho u_i)^{n+1} - (\rho u_i)^*}{\Delta t} = -\frac{1}{2}\left(\frac{\delta p'}{\delta x_i}\right) \qquad p' = p^{n+1} - p^n$$

- Enforce continuity: $$\frac{\delta(\rho u_i)^{n+1}}{\delta x_i} = 0$$

Fractional-Step Methods – III

- There follows an equation for pressure-correction:

$$\frac{\delta}{\delta x_i}\left(\frac{\delta p'}{\delta x_i}\right) = \frac{2}{\Delta t}\frac{\delta(\rho u_i)^*}{\delta x_i}$$

- An error is introduced by not replacing in the momentum equation $H(u_i^*)$ by $H(u_i^{n+1})$. The error is 2nd-order in time:

$$u_i^{n+1} - u_i^* = -\frac{\Delta t}{2\rho}\frac{\delta}{\delta x_i}\left(p^{n+1} - p^n\right) \approx \frac{(\Delta t)^2}{2\rho}\frac{\delta}{\delta x_i}\left(\frac{\delta p}{\delta t}\right)$$

- The error can be eliminated by including the pressure-correction equation into the outer-iteration loop for non-linearity.

- In that case, pressure-correction equation does not have to be solved to a tight tolerance in each outer iteration – the overhead is thus not as large as one might think…

Fractional-Step Methods – IV

- An alternative method uses also Crank-Nicolson scheme, except for convective fluxes, which are advanced using an explicit method of second or higher order:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \mathrm{C}_i(u^n) = -\frac{1}{2}\left[\mathrm{G}_i(p^n) + \mathrm{G}_i(p^{n+1})\right] + \frac{1}{2}\left[\mathrm{L}(u_i^n) + \mathrm{L}(u_i^{n+1})\right]$$

- Here C, G and L denote discretized convection, gradient and diffusion terms from momentum equation. For constant fluid properties, G and L are linear.
- In the first (predictor) step, velocity estimate is computed using pressure from previous time step:

$$\frac{u_i^* - u_i^n}{\Delta t} + \mathrm{C}_i(u^n) = -\mathrm{G}_i(p^n) + \frac{1}{2}\left[\mathrm{L}(u_i^n) + \mathrm{L}(u_i^*)\right]$$

Fractional-Step Methods – V

- One needs to solve a linear equation system to obtain $u*$:

$$\mathrm{A}\mathbf{u}_i^* = \mathbf{Q}_{u_i}$$

- The next step corrects velocity by updating pressure:

$$\frac{u_i^{**} - u_i^n}{\Delta t} + \mathrm{C}_i(u^n) = -\frac{1}{2}\left[\mathrm{G}_i(p^n) + \mathrm{G}_i(p^*)\right] + \frac{1}{2}\left[\mathrm{L}(u_i^n) + \mathrm{L}(u_i^*)\right]$$

- Subtract equation from previous step to obtain:

$$\frac{u_i^{**} - u_i^*}{\Delta t} = -\frac{1}{2}\mathrm{G}_i(p') \qquad \text{where} \qquad p' = p^* - p^n$$

- Enforce continuity: $\mathrm{D}(u^{**}) = 0 \quad \Rightarrow \quad \mathrm{D}\left[\mathrm{G}(p')\right] = \frac{2}{\Delta t}\mathrm{D}(u^*)$

Divergence operator

Known!

Fractional-Step Methods – VI

- Since velocities in L-operator lag one step behind, another correction should be done:

$$\frac{u_i^{***} - u_i^n}{\Delta t} + \mathrm{C}_i(u^n) = -\frac{1}{2}\left[\mathrm{G}_i(p^n) + \mathrm{G}_i(p^{**})\right] + \frac{1}{2}\left[\mathrm{L}(u_i^n) + \mathrm{L}(u_i^{**})\right]$$

- Subtract equation solved in the previous step to obtain:

$$\frac{u_i^{***} - u_i^{**}}{\Delta t} = -\frac{1}{2}\left[\mathrm{G}_i(p'') - \mathrm{L}(u_i'')\right]$$

where

$$p'' = p^{**} - p^*$$
$$u_i'' = u_i^{**} - u_i^*$$

- Corrected velocity can now be expressed as:

$$u_i^{***} = u_i^{**} - \frac{\Delta t}{2}\mathrm{G}(p'') + \tilde{u}_i'' \quad \text{where} \quad \tilde{u}_i'' = \frac{\Delta t}{2}\mathrm{L}(u_i'')$$

Known from previous step!

Fractional-Step Methods – VII

- Enforce continuity again:

$$\mathrm{D}(u^{***}) = 0 \quad \Rightarrow \quad \mathrm{D}\left[\mathrm{G}(p'')\right] = \frac{2}{\Delta t}\mathrm{D}(u^{**} + \tilde{u}'')$$

- The divergence of would already be zero if the first pressure-correction equation was solved exactly...
- Since that is not the case, the non-zero divergence is included here...
- The second pressure-correction equation has the same coefficient matrix, only different source term...
- This process can be repeated by adding * and '...
- The „splitting error“ from the first version is here eliminated...
- One has to solve pressure-correction equation multiple times – but not to a tight tolerance (computing effort similar)...

Fractional-Step Methods – VIII

- Yet another method uses also Crank-Nicolson scheme, except for convective fluxes, which are advanced using an explicit method of second or higher order:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \mathrm{C}_i(u^{\mathrm{old}}) = -\frac{1}{2}\left[\mathrm{G}_i(p^n) + \mathrm{G}_i(p^{n+1})\right] + \frac{1}{2}\left[\mathrm{L}_i(u^n) + \mathrm{L}_i(u^{n+1})\right]$$

- Here C, G and L denote discretized convection, gradient and diffusion terms from momentum equation. For constant fluid properties, G and L are linear.

- In the first (predictor) step, velocity estimate is computed using only values from previous time step (explicitly):

$$\frac{u_i^* - u_i^n}{\Delta t} + \mathrm{C}_i(u^{\mathrm{old}}) = -\mathrm{G}_i(p^n) + \mathrm{L}_i(u^n)$$

$$u_i^* = u_i^n - \Delta t\left[\mathrm{C}_i(u^{\mathrm{old}}) + \mathrm{G}_i(p^n) - \mathrm{L}_i(u^n)\right]$$

Fractional-Step Methods – IX

- In the next step, velocity is corrected to satisfy continuity equation; it should satisfy also corrected momentum equation:

$$\frac{u_i^{**} - u_i^n}{\Delta t} + \mathrm{C}_i(u^{\mathrm{old}}) = -\frac{1}{2}\left[\mathrm{G}_i(p^n) + \mathrm{G}_i(p^*)\right] + \frac{1}{2}\left[\mathrm{L}_i(u^n) + \mathrm{L}_i(u^*)\right]$$

- By subtracting the equation solved in the predictor step, we obtain:

$$\frac{u_i^{**} - u_i^*}{\Delta t} = -\frac{1}{2}\left[\mathrm{G}_i(p') - \mathrm{L}_i(u')\right]$$

$$p' = p^* - p^n$$
$$u_i' = u_i^* - u_i^n$$

- The corrected velocity can be expressed as:

$$u_i^{**} = u_i^* - \frac{\Delta t}{2}\mathrm{G}_i(p') + \tilde{u}_i' \quad \text{where} \quad \tilde{u}_i' = \frac{\Delta t}{2}\mathrm{L}_i(u')$$

- Enforce continuity: $\mathrm{D}(u^{**}) = 0 \quad \Rightarrow \quad \mathrm{D}\left[\mathrm{G}(p')\right] = \frac{2}{\Delta t}\mathrm{D}(u^* + \tilde{u}')$

Divergence operator

Known!

Fractional-Step Methods – X

- Since velocities in L-operator lag one step behind, another correction should be done:

$$\frac{u_i^{***} - u_i^n}{\Delta t} + \mathrm{C}_i(u^{\mathrm{old}}) = -\frac{1}{2}\left[\mathrm{G}_i(p^n) + \mathrm{G}_i(p^{**})\right] + \frac{1}{2}\left[\mathrm{L}_i(u^n) + \mathrm{L}_i(u^{**})\right]$$

- Subtract equation solved in the previous step to obtain:

$$\frac{u_i^{***} - u_i^{**}}{\Delta t} = -\frac{1}{2}\left[\mathrm{G}_i(p'') - \mathrm{L}_i(u'')\right] \qquad \begin{aligned} p'' &= p^{**} - p^* \\ u_i'' &= u_i^{**} - u_i^* \end{aligned}$$

$$u_i^{***} = u_i^{**} - \frac{\Delta t}{2}\mathrm{G}_i(p'') + \tilde{u}_i'' \quad \text{where} \quad \tilde{u}_i'' = \frac{\Delta t}{2}\mathrm{L}_i(u'')$$

Known!

- Enforce continuity: $\mathrm{D}(u^{***}) = 0 \quad \Rightarrow \quad \mathrm{D}\left[\mathrm{G}(p'')\right] = \dfrac{2}{\Delta t}\mathrm{D}(u^{**} + \tilde{u}'')$

- This can be continued by adding one * and ‘, until changes become negligible.

Other Methods for Solving Navier-Stokes Equations

- Streamfunction-vorticity methods are used sometimes in 2D, because one solves 2 instead of 4 equations…
- In 3D, one has to solve 6 equations, so no advantage compared to primitive variables (4 equations).
- Artificial-compressibility methods are also used: a time-derivative is added to continuity equation, so mass conservation is not satisfied until steady-state is reached.
- For transient problems, one uses false time within one time step (like outer iterations).
- Most widely used are methods based on the so-called SIMPLE-algorithm and variants of it…
- All methods are similar, if described in a similar way…