Direct Numerical Simulation : Local Discretisation Approach

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Direct Numerical Simulation

* Numerical simulation of turbulence without any turbulence models
* Capture the basic physics of fluids in simple flows
* Numerical experiments - (unphysical ones can be conceived)
* A tool for fundamental research - Most accurate results
* Computationally intensive
* Able to resolve both large and small scales

Direct Numerical Simulation (Contd.)

* Identification and study the alteration of coherent structures with buoyancy using DNS.
* 80% of TKE in wall bounded turbulence is contained in near walls coherent structures
* Reduction of turbulent (friction) drag
* Enhancement of turbulent mixing
* Enhancement/reduction of heat exchange
* Strong applicative interest - high potential benefit

Governing Equations

- Newtonian Fluid, Incompressible, constant properties , Boussinesq approximation and negligible viscous dissipation
- Governing equations in dimensional form are 3D Navier-Stokes equations expressed in vector form.
- Conservation of Mass :$\nabla.\mathbf{u} = 0$
- Conservation of Momentum :$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}.\nabla \mathbf{u} = \frac{-\nabla p}{\rho_0} + \nu \nabla^2 \mathbf{u} - \frac{1}{\rho_0}\frac{dP}{dx}\hat{\mathbf{i}} + \frac{\Delta \rho}{\rho_0} g \hat{\mathbf{k}}$
- Conservation of Energy: $\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u}.\nabla T\right) = k \nabla^2 T$

Scaling

- Scales employed for non-dimensionalisation
- Length : δ - Channel half height
- Velocity $u\tau$- friction velocity
- Pressure $\rho_o u_\tau^2$
- Time : $\frac{\delta}{u_\tau}$
- $\theta = \frac{T - T_c}{T_h - T_c}$

  Here $u_r = \sqrt{\frac{\tau_w}{\delta}}$, where τ_w is wall-shear stress.

Non-Dimensionalised Governing Equations

- Conservation of Mass $\nabla.\mathbf{u} = 0$
- Conservation of Momentum
  $\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re_\tau} \nabla^2 \mathbf{u} + F\hat{\mathbf{i}} + Ri\theta\hat{\mathbf{k}}$
- Conservation of Energy $\frac{\partial \theta}{\partial t} + \mathbf{u}.\nabla\theta = \frac{1}{Re_\tau Pr} \nabla^2 \theta$

Non-Dimensional Numbers

- Reynolds number, $Re = \frac{u_\tau \delta}{\nu}$ which is the ratio of the inertial forces to viscous forces
- Richardson number, $Ri = \frac{g\beta\delta(T_h - T_c)}{u_\tau^2}$ which represents the importance of natural relative to the forced convection
- Prandtl Number $Pr = \frac{\nu}{\alpha}$ which is the ratio of viscous diffusion rate to the thermal diffusion rate.

Geometry of Computational Domain

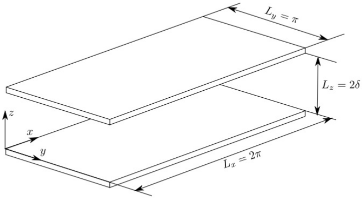


Figure: Geometry of physical domain.

Stretching Transformation

- $z(\xi_k) = 1 - cos\left(\frac{\pi}{2}\xi_k\right)$
- $\frac{\partial z}{\partial \xi} = \frac{\pi}{2} sin(\frac{\pi}{2}\xi_k)$
- $\frac{\partial^2 z}{\partial \xi^2} = \frac{\pi^2}{4} cos(\frac{\pi}{2}\xi_k)$
- Wall- normal first-order derivatives in physical space of any quantity Φ can be determined as: $\frac{\partial \Phi}{\partial z} = \frac{1}{(\frac{\partial z}{\partial \xi})}\frac{\partial \Phi}{\partial \xi}$
- The Second-order derivative can be determined using chain rule as: $\frac{\partial^2 \Phi}{\partial z^2} = \frac{1}{(\frac{\partial z}{\partial \xi})^2}\frac{\partial^2 \Phi}{\partial \xi^2} - \frac{\frac{\partial^2 z}{\partial \xi^2}}{(\frac{\partial z}{\partial \xi})^3}$

Stretching Transformation (Contd.)

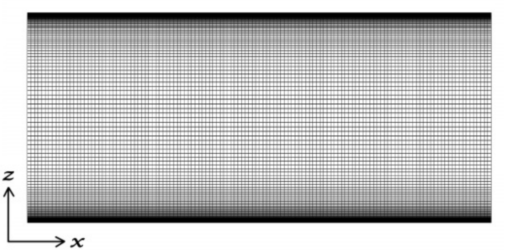
- 

Figure: Stretching mesh in wall normal direction

Initial and Boundary Conditions

- The initial condition is provided from a previous simulation of fully developed turbulent channel flow at $R_e\tau = 180$
- The presence of a solid boundary in turbulent shear flows, the velocity of the fluid is zero for a stationary solid surface (no-slip) , and is mathematically represented as :

Initial and Boundary Conditions (Contd.)

* No-Slip Condition
  The presence of a solid boundary in turbulent shear flows, the velocity of the fluid is zero for a stationary solid surface (no-slip) , and is mathematically represented as :
  $u = v = 0$

* No-Penetration
  The wall is considered impermiable, so the normal velocity at the solid surface must be zero and written as:
  $w = 0$

* Periodic Boundary Conditions :

- $\phi(x, y, z, t) = \phi(x + L_x, y, z, t)$ and
- $\phi(x, y, z, t) = \phi(x, y + L_y, z, t)$
  Where L_x and L_y are periodic lengths

Numerical Scheme

* The SMAC algorithm described by Amsden and Harlow (1970), modified by later the work of Cheng and Armfield (1995,IJNMF) is a two-step predictor corrector algorithm with implicit handling of diffusion terms and explicit discretisation of convective terms.

* Predictor Step:

- $\widetilde{u} - \frac{\delta t}{Re_\tau}\nabla^2\widetilde{u} = u^n - \delta t(\nabla p^n + (u^n.\nabla)u^n)$

* Corrector Step

- $u^{n+1} - \frac{\delta t}{Re_\tau}\nabla^2\widetilde{u} = u^n - \delta t(\nabla p^{n+1} + (u^n.\nabla)u^n)$

  Subtracting the two, we get

- $u^{n+1} - \widetilde{u} = -\delta t\{\nabla(p^{n+1} - p^n)\} = -\delta t\{\nabla(p^*)\}$

Numerical Scheme (Contd.)

- $p^{n+1} = p^n + p^*$
- $u^{n+1} = \widetilde{u} - \delta t\{\nabla p^*\}$
- Taking divergence, assuming $\nabla . u^{n+1} = 0$
- We get Pressure-Poisson Equation (PPE) for correction pressure as:
- $\nabla^2 p^* = \frac{\nabla . \widetilde{u}}{\delta t}$
- At solid walls and at inflow $\frac{\partial p^*}{\partial n} = 0$
- At outflow $p_n^* = 0$, where n is the direction of the local normal

Discretisation of Convective Terms

* Treatment of Convective Terms

- 2^{nd}- order central differencing scheme is given as:

$$\bar{U}\frac{\partial u}{\partial z}\mid_{i,j,k}=\bar{U}\frac{u_{i,j,k+1}-u_{i,j,k-1}}{2dz}$$

- The 6^{th} order central-difference scheme is expressed as:

$$\bar{U}\frac{\partial u}{\partial x}\mid_{i,j,k}= \bar{U}_{i,j,k}\frac{-u_{i-3,j,k}+9u_{i-2,j,k}-45u_{i-1,j,k}+45u_{i+1,j,k}-9u_{i+2,j,k}+u_{i+3,j,k}}{60dx}$$

Discretisation of Convective Terms (Contd.)

- The 3^{rd} order upwind scheme as proposed by Kuwahara(1999) can be expressed as:
  $\bar{U}\frac{\partial u}{\partial x}\mid_{i,j,k}= A_{i,j,k} + B_{i,j,k}$
- $A_{i,j,k} = \bar{U}_{i,j,k}(\frac{-u_{i+2,j,k}+8(u_{i+1,j,k}-u_{i-1,j,k})+u_{i-2,j,k}}{12dx})$
- $B_{i,j,k} =\mid \bar{U}_{i,j,k} \mid \frac{u_{i+2,j,k}-4u_{i+1,j,k}+6u_{i,j,k}-4u_{i-1,j,k}+u_{i-2,j,k}}{4dx}$
- $P_e = \frac{Re_\tau * \bar{U}_{i,j,k} * d\xi}{Jac(k)}$
- Peclet based hybrid scheme with 6^{th} order CDS for $Pe \leq 2$
- Kuwahara third-order upwinding for $Pe > 2$

Discretisation of Diffusion terms and Pressure terms

- Along Homogenous directions
- $\frac{\partial^2 u}{\partial x^2} |_{i,j,k} = \frac{-u_{i+2,j,k}+16u_{i+1,j,k}-30u_{i,j,k}+16u_{i-1,j,k}-u_{i+2,j,k}+u_{i-2,j,k}}{12(dx)^2}$
- Along Inhomogenous direction
- $\frac{\partial^2 u}{\partial z^2} |_{i,j,k} = C_{i,j,k} + D_{i,j,k}$
- $C_{i,j,k} = \frac{1}{Jac(k)} \frac{-u_{i,j,k+2}+16u_{i,j,k+1}-30u_{i,j,k}+16u_{i,j,k-1}-u_{i,j,k-2}}{12(d\xi)^2}$
- $D_{i,j,k} = \frac{Jac2(k)}{(Jac(k))^3} \frac{-u_{i,j,k}+8u_{i,j,k+1}-8u_{i,j,k-1}+u_{i,j,k-2}}{12d\xi}$

Discretisation of Diffusion terms and Pressure terms (Contd.)

- $\frac{\partial p}{\partial z} \mid i,j,k = \frac{p_{i,j,k+1} - p_{i,j,k-1}}{2(Jac(k)) * d\xi}$
- Here $Jac(k) = \frac{\partial z}{\partial \xi}$ and $Jac2(k) = \frac{\partial^2 z}{\partial \xi^2}$
- One sided forward differencing (Non Uniform Mesh)
  $(\frac{\partial u}{\partial x})_i = (\frac{\Delta x_{i+1} + \Delta x_{i+2}}{\Delta x_{i+2}} \frac{u_{i+1} - u_i}{\Delta x_{i+1}} - \frac{\Delta x_{i+1}}{\Delta x_{i+2}} \frac{u_{i+2} - u_i}{\Delta x_{i+1} + \Delta x_{i+2}})$
- Central differencing (Non Uniform Mesh)
  $(\frac{\partial u}{\partial x})_i = \frac{1}{\Delta x_i + \Delta x_{i+1}} [\frac{\Delta x_i}{\Delta x_{i+1}} (u_{i+1} - u_i) + \frac{\Delta x_{i+1}}{\Delta x_i} (u_i - u_{i+1})]$

Treatment of Pressure- Poisson equation

- $\nabla^2 p^* = \frac{\nabla.\widetilde{u}}{\partial t}$
- The divergence operator $\frac{\partial}{\partial x}$ is discretised on cell faces.
- $\frac{\partial}{\partial x}\{\frac{\partial p'}{\partial x}\}_{i,j,k} = \{\frac{2}{dx_1+dx_2}\}[(\frac{\partial p'}{\partial x})_{i+\frac{1}{2},j,k} - \frac{\partial p'}{\partial x})_{i-\frac{1}{2},j,k}]$
- Similarly the divergence terms are discretised using the same operator:
- $(\frac{\partial u^*}{\partial x}) = \{\frac{2}{dx_1+dx_2}\}[u^*_{i+\frac{1}{2},j,k} - u^*_{i-\frac{1}{2},j,k}]$ where $dx_1 = x_{i+1} - x_i$ and $dx_2 = x_i - x_{i-1}$

Treatment of Pressure- Poisson equation (Contd.)

- The correction Pressure-gradient terms are discretised as :

$$\frac{\partial p'}{\partial x}\Big|_{i+\frac{1}{2},j,k} = \frac{p'_{i+1,j,k} - p'_{i,j,k}}{dx_1}$$

$$\frac{\partial p'}{\partial x}\Big|_{i-\frac{1}{2},j,k} = \frac{p'_{i,j,k} - p'_{i-1,j,k}}{dx_2}$$

- This method of discretisation avoids decoupling between pressure and velocity which leads to spurious pressure oscillations

- Momentum interpolation proposed by Rhie and Chow (1983,AIAA Journal) states :

$$u^*_{i+\frac{1}{2},j,k} = \left(\frac{u^p_{i+1,j,k} + u^p_{i,j,k}}{2}\right) - \delta t\left(\frac{p^n_{i+1,j,k} - p^n_{i,j,k}}{x_{i+1} - x_i}\right)$$

$$u^*_{i-\frac{1}{2},j,k} = \left(\frac{u^p_{i,j,k} + u^p_{i-1,j,k}}{2}\right) - \delta t\left(\frac{p^n_{i,j,k} - p^n_{i,j,k}}{x_i - x_{i-1}}\right)$$

Treatment of Pressure- Poisson equation (Contd.)

- Here u^p is obtained without using the pressure gradient term as shown below

$$u^p - \frac{\delta t}{Re_\tau}(\nabla^2 u^p) = u^n - \delta t\{(u^n.\nabla)u^n\}$$

- The PPE can be solved using any iterative solver such as SOR, SIP, CGSTAB, SSOR preconditioned GMRES, multigrid, etc.

Solution of Transport Equations

- $u^* - \frac{\delta t}{Re_\tau}\nabla^2 u^* = u^n - \delta t(\nabla p^n + (u^n.\nabla)u^n + \widetilde{f}^n)$
- $A_P \phi_P + \sum_l A_l \phi_l = Q_p$
- $\phi_P^{n+1} = \frac{Q_P - A_S\phi_S^{n+1} - A_W\phi_W^{n+1} - A_N\phi_N^n - A_E\phi_E^n - A_T\phi_T^n}{A_P}$, where n is iterative counter
- Here residual $\rho^n = Q - A\phi^n$
- Iteration error $\epsilon^n = \phi - \phi^n$
- Hence $A\epsilon^n = \rho^n$
- Convergence criteria $\| \rho^n \|_2 = \sqrt{\frac{\sum_{i=1}^N (\rho^n)_i^2}{N}}$

Temporal Integration of Navier-Stokes equations

- $\frac{\partial \phi(r,t)}{\partial t} = f(\phi, r, t)$,With $f(t_0) = f_0$ as an initial-condition. On integrating the above equation between time t_n and $t_n + 1 (= t_n + \triangle t)$
- Euler (First-order) $\phi^{n+1} - \phi^n = \int_{t_n}^{t_n+1} f(\phi, r, t) dt$
- Adam Bashforth (Second-order) $\phi^{n+1} - \phi^n = \int_{t_n}^{t_n+1} (\frac{3}{2} f^n(\phi, r, t) - \frac{1}{2} f^{n-1}(\phi, r, t)) dt$

THANK YOU