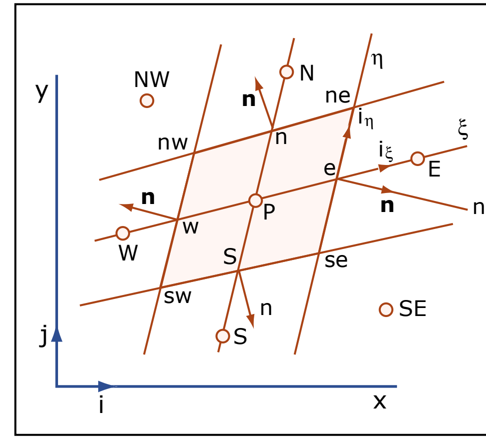
2.29 Numerical Fluid Mechanics
Spring 2015 – **Lecture 25**



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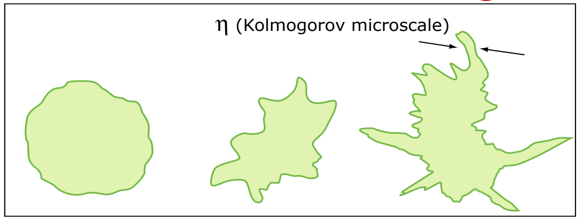
REVIEW Lecture 24:

- Finite Volume on Complex geometries
  - Computation of convective fluxes:
    - For mid-point rule: $F_e = \int_{S_e} \rho\phi\,(\vec{v}.\vec{n})\,dS \approx f_e S_e = (\rho\phi\vec{v}.\vec{n})_e S_e = \phi_e \dot{m}_e = \phi_e\,\rho_e\,(S_e^x\,u_e + S_e^y\,v_e)$
  - Computation of diffusive fluxes: mid-point rule for complex geometries often used
    - Either use shape function $\phi\,(x,y)$, with mid-point rule: $F_e^d \approx (k\nabla\phi.\vec{n})_e S_e = k_e\left(S_e^x \left.\frac{\partial\phi}{\partial x}\right|_e + S_e^y \left.\frac{\partial\phi}{\partial y}\right|_e\right)$
    - Or compute derivatives at CV centers first, then interpolate to cell faces. Option include either:
      - Gauss Theorem: $\left.\frac{\partial\phi}{\partial x_i}\right|_P \approx \left.\overline{\frac{\partial\phi}{\partial x_i}}\right|_P = \int_{CV} \frac{\partial\phi}{\partial x_i}\,dV \Big/ dV = \sum_{4\,c\ \text{faces}} \phi_c S_c^{x_i} \Big/ dV$
      - Deferred-correction approach: $F_e^d \approx k_e S_e \frac{\phi_E - \phi_P}{|\mathbf{r}_E - \mathbf{r}_P|} + k_e S_e \left[\overline{\nabla\phi}\big|_e\right]^{\text{old}} (\mathbf{n} - \mathbf{i}_\xi)$

        where $\left[\overline{\nabla\phi}\big|_e\right]^{\text{old}}$ is interpolated from $\left[\overline{\nabla\phi}\big|_P\right]^{\text{old}}$, e.g. $\left.\overline{\frac{\partial\phi}{\partial x_i}}\right|_P = \sum_{4\,c\ \text{faces}} \phi_c S_c^{x_i} \Big/ dV$
  - Comments on 3D

REVIEW Lecture 24, Cont'd:

- Turbulent Flows and their Numerical Modeling
  - Properties of Turbulent Flows
    - Stirring and Mixing
    - Energy Cascade and Scales
    - Turbulent Wavenumber Spectrum and Scales



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$$L / \eta \sim O(\mathrm{Re}_L^{3/4})$$

$$\mathrm{Re}_L = UL/\nu$$

$$S = S(K, \varepsilon) = A\, \varepsilon^{2/3} K^{-5/3} \quad L^{-1} = \ell^{-1} \ll K \ll \eta^{-1}$$

ε = turbulent energy dissipation

  - Numerical Methods for Turbulent Flows: Classification
    - Direct Numerical Simulations (DNS) for Turbulent Flows
    - Reynolds-averaged Navier-Stokes (RANS)
      - Mean and fluctuations
      - Reynolds Stresses
      - Turbulence closures: Eddy viscosity and diffusivity, Mixing-length Models, k-ε Models
      - Reynolds-Stress Equation Models
    - Large-Eddy Simulations (LES)
      - Spatial filtering
      - LES subgrid-scale stresses
    - Examples

References and Reading Assignments

- Chapter 9 on “Turbulent Flows” of “J. H. Ferziger and M. Peric, Computational Methods for Fluid Dynamics. Springer, NY, 3rd ed., 2002”
- Chapter 3 on “Turbulence and its Modelling” of H. Versteeg, W. Malalasekra, An Introduction to Computational Fluid Dynamics: The Finite Volume Method. Prentice Hall, Second Edition.
- Chapter 4 of “I. M. Cohen and P. K. Kundu. Fluid Mechanics. Academic Press, Fourth Edition, 2008”
- Chapter 3 on “Turbulence Models” of T. Cebeci, J. P. Shao, F. Kafyeke and E. Laurendeau, Computational Fluid Dynamics for Engineers. Springer, 2005
- Durbin, Paul A., and Gorazd Medic. Fluid dynamics with a computational perspective. Cambridge University Press, 2007.

Direct Numerical Simulations (DNS) for Turbulent Flows

- Most accurate approach
  - Solve NS with no averaging or approximation other than numerical discretizations whose errors can be estimated/controlled
- Simplest conceptually, all is resolved:
  - Size of domain must be at least a few times the distance L over which fluctuations are correlated (L= largest eddy scale)
  - Resolution must capture all kinetic energy dissipation, i.e. grid size must be smaller than viscous scale, the Kolmogorov scale, η
  - For homogenous isotropic turbulence, uniform grid is adequate, hence number of grid points (DOFs) in each direction is (Tennekes and Lumley, 1976):

$$L/\eta \sim O(\mathrm{Re}_L^{3/4}) \quad \mathrm{Re}_L = UL/\nu$$

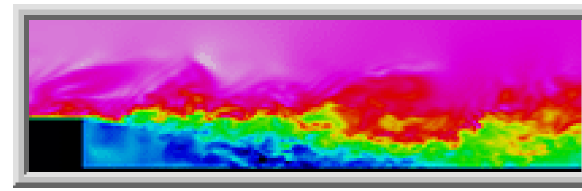
  - In 3D, total cost (if time-step scales as grid size, for stability and/or accuracy):

$$\sim O\left(\mathrm{Re}_L^{3/4}\left(\mathrm{Re}_L^{3/4}\right)^3\right) = O(\mathrm{Re}_L^3)$$

- CPU and RAM limit the size of the problem:
  - 10 Peta-Flops/s for 1 hour: $\mathrm{Re}_L \sim 3.310^6$ (extremely optimistic)
  - Largest DNS ever performed up to 2013: 15360 x 1536 x 11520 mesh, $\mathrm{Re}_L = 5200$
    - https://www.alcf.anl.gov/articles/first-mira-runs-break-new-ground-turbulence-simulations

Direct Numerical Simulations (DNS) for Turbulent Flows: **Numerics**

- DNS likely gives more information that many engineers need (closer to experimental data)
- But, it can be used for turbulence studies, e.g. coherent structures dynamics and other fundamental research
  - Allow to construct better RANS models or even correlation models



DNS, Backward facing step
Le and Moin (2008)

- Numerical Methods for DNS

– All NS solvers we have seen are useful

– Small time-steps required for bounded errors:
  - Explicit methods are fine in simple geometries (stability satisfied due to small time-step needed for accuracy)
  - Implicit methods near boundaries or complex geometries (large derivatives in viscous terms normal to the walls can lead to numerical instabilities ⇒ treated implicitly)

Direct Numerical Simulations (DNS) for Turbulent Flows: **Numerics, Cont'd**

- Time-marching methods commonly used
  - Explicit 2nd to 4th order accurate (Runge-Kutta, Adams-Bashforth, Leapfrog): R-K's often more accurate for same cost
    - For same order of accuracy, R-K's allow larger time-steps
  - Crank-Nicolson often used for implicit schemes
- Must be conservative, including kinetic energy
- Spatial discretization schemes should have low dissipation
  - Upwind schemes often too diffusive: error larger than molecular diffusion!
  - High-order finite difference
  - Spectral methods (use Fourier series to estimate derivatives)
    - Mainly useful for simple (periodic) geometries (FFT)
    - Use spectral elements instead (Patera, Karnadiakis, etc)
  - (Hybridizable)-(Discontinuous)-Galerkin (FE Methods): Cockburn et al.

Direct Numerical Simulations (DNS) for Turbulent Flows: **Numerics, Cont'd**

- Challenges:
  - Storage for states at intermediate time steps ($\Rightarrow$ R-K's of low storage)
  - Total discretization error and turbulence spectrum
    - Total error: both order of discretization and values of derivatives (spectrum)

      $\Rightarrow$ Measure of total error: integrate over whole turbulent spectrum
  - Difficult to measure accuracy due to (unstable) nature of turbulent flow
    - Due to predictability limit of turbulence
    - Hence, statistical properties of two solutions are often compared
      - Simplest measure: turbulent spectrum
  - Generating initial conditions: as much art as science
    - Initial conditions remembered over significant "eddy-turnover" time
    - Data assimilation, smoothing schemes to obtain ICs
  - Generating boundary conditions
    - Periodic for simple problems, Radiating/Sponge conditions for realistic cases

Example: Spatial Decay of Turbulence Created by an Oscillating Boundary

Briggs et al (1996)

- Oscillating grid on top of quiescent fluid creates turbulence
- Decays in intensity away from grid by “turbulent diffusion”: stirring + mixing
- Used spectral method, periodic, 3rd order R-K
- DNS results agree with data
  - Used to test turbulence “closure” models
  - Did not work well because not derived for that “type” of turbulence

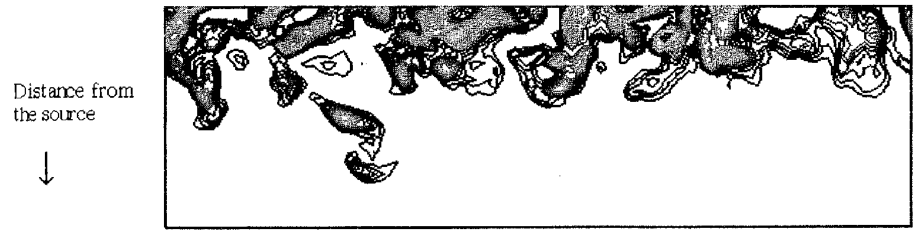


Fig. 9.1. Contours of the kinetic energy on a plane in the flow created by an oscillating grid in a quiescent fluid; the grid is located at the top of the figure. Energetic packets of fluid transfer energy away from the grid region. From Briggs et al. (1996)

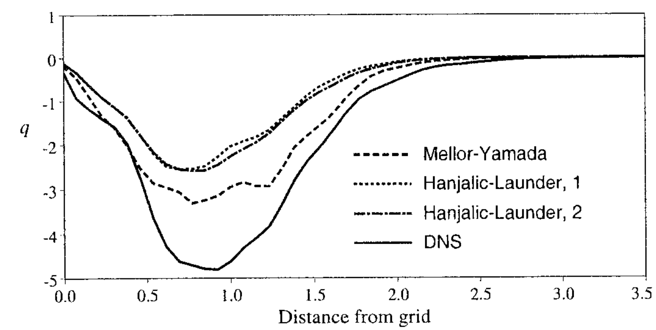


Fig. 9.2. The profile of the flux of turbulent kinetic energy, q, compared with the predictions of some commonly used turbulence models (Mellor and Yamada, 1982; Hanjalić and Launder, 1976 and 1980); from Briggs et al. (1996)

Note: DNS have at times found out when laboratory set-up was not proper

Reynolds-averaged Navier-Stokes (RANS)

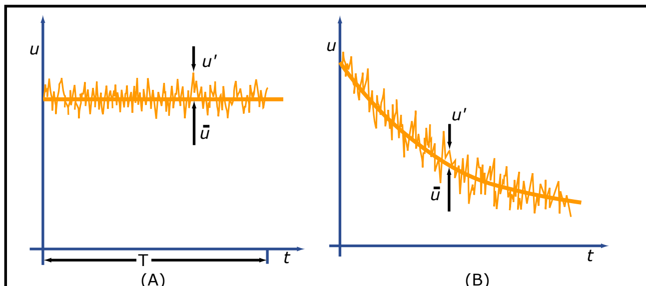
- Many science and engineering applications focus on averages
- RANS models: based on ideas of Osborne Reynolds
  - All “unsteadiness” regarded as part of turbulence and averaged out
  - By averaging, nonlinear terms in NS eqns. lead to new product terms that must be modeled
- Separation into mean and fluctuations $(\tau \ll T_0 \ll T)$
  - Moving time-average: $u = \bar{u} + u'$; $\phi(x_i,t) = \bar{\phi}(x_i,t) + \phi'(x_i,t)$

$$\text{where } \bar{\phi}(x_i,t) = \frac{1}{T_0} \int_{t-T_0/2}^{t+T_0/2} \phi(x_i,t)dt \;\; ; \quad \text{i.e.} \quad \overline{\phi'}(x_i,t) = 0$$

  - Ensemble average:

$$< \phi(x_i,t) > = \frac{1}{N} \sum_{r=1}^{N} \phi^r(x_i,t)$$

  - Reynolds-averaging: either of the above two averages



Graphs showing (A) the time average for a statistically steady flow and (B) the ensemble average for an unsteady flow.

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Reynolds-averaged Navier-Stokes (RANS)

- Variance, r.m.s. and higher-moments:

$$\overline{\phi'^{2}}(x_i,t) = \frac{1}{T_0}\int_{t-T_0/2}^{t+T_0/2} \phi'^{2}(x_i,t)\,dt \qquad \overline{u_i\phi} = \overline{(\overline{u_i}+u')(\overline{\phi}+\phi')} = \overline{u_i}\;\overline{\phi} + \overline{u_i'\phi'}$$

$$\phi_{\text{rms}} = \sqrt{\overline{\phi'^{2}}}$$

$$\overline{\phi'^{p}}(x_i,t) = \frac{1}{T_0}\int_{t-T_0/2}^{t+T_0/2} \phi'^{p}(x_i,t)\,dt \quad \text{with } p = 3,4, \quad \text{etc}$$

- Correlations:
  - In time: $R(t_1,t_2;x) = \overline{u'(x,t_1)\,u'(x,t_2)}$ for a stationary process : $R(\tau;x) = \overline{u'(x,t)\,u'(x,t+\tau)}$
  - In space:

$$R(x_1,x_2;t) = \overline{u'(x_1,t)\,u'(x_2,t)} \quad \text{for a homogeneous process} : R(\ell;t) = \overline{u'(x,t)\,u'(x+\ell,t)}$$

- Turbulent kinetic energy: $k = \frac{1}{2}\overline{u'^{2} + v'^{2} + w'^{2}}$
  - Note: some arbitrariness in the decomposition $u = \overline{u} + u'\,;\quad \phi = \overline{\phi} + \phi'$

    and in the definition that “fluctuations = turbulence”

Reynolds-averaged Navier-Stokes (RANS)

- Continuity and Momentum Equations, incompressible:

$$\frac{\partial \rho u_i}{\partial x_i} = 0$$

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

  - Applying either the ensemble or time-averages to these equations leads to the RANS eqns.
  - In both cases, averaging any linear term in conservation equation gives the identical term, but for the average quantity

- Average the equations, inserting the decomposition: $u_i = \overline{u_i} + u_i'$
  - the time and space derivatives commute with the averaging operator

$$\overline{\frac{\partial u_i}{\partial x_i}} = \frac{\partial \overline{u_i}}{\partial x_i}$$

$$\overline{\frac{\partial u_i}{\partial t}} = \frac{\partial \overline{u_i}}{\partial t}$$

Reynolds-averaged Navier-Stokes (RANS)

- Averaged continuity and momentum equations:

$$\frac{\partial \rho \overline{u_i}}{\partial x_i} = 0$$

$$\frac{\partial \rho \overline{u_i}}{\partial t} + \frac{\partial (\rho \overline{u_i}\,\overline{u_j} + \rho \overline{u_i' u_j'})}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial \overline{\tau_{ij}}}{\partial x_j}$$

where $\overline{\tau_{ij}} = \mu \left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right)$

(incompressible, no body forces)

- For a scalar conservation equation

$$\frac{\partial \rho \overline{\phi}}{\partial t} + \frac{\partial (\rho \overline{\phi}\,\overline{u_j} + \rho \overline{\phi' u_j'})}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\Gamma \frac{\partial \overline{\phi}}{\partial x_j} \right)$$

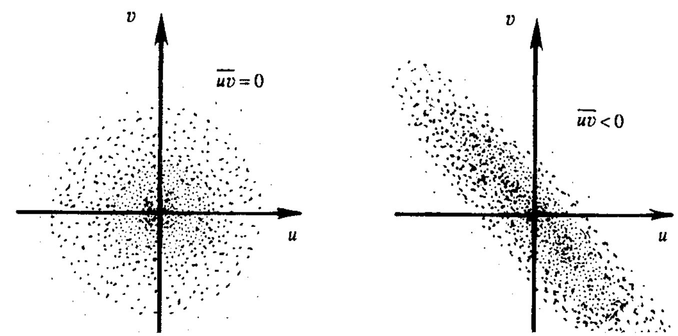
  – e.g. for $\overline{\phi} = c_p \overline{T} \Rightarrow$ mean internal energy
  – Terms that are products of fluctuations remain:
    - Reynolds stresses: $-\rho \overline{u_i' u_j'}$
    - Turbulent scalar flux: $-\rho \overline{u_i' \phi'}$
  – Equations are thus not closed (more unknown variables than equations)
    - Closure requires specifying $\rho \overline{u_i' u_j'}$ and $\rho \overline{u_i' \phi'}$ in terms of the mean quantities and/or their derivatives (any Taylor series decomposition of mean quantities)

Reynolds Stresses: $\tau_{ij}^{\mathrm{Re}} = -\rho\,\overline{u_i' u_j'}$

- Total stress acting on mean flow: $\tau_{ij} = \overline{\tau_{ij}} - \rho\,\overline{u_i' u_j'} = \overline{\tau_{ij}} + \tau_{ij}^{\mathrm{Re}}$

$$\overline{\tau_{ij}} = \mu\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right) \quad \text{and} \quad \tau^{\mathrm{Re}} = -\rho \begin{bmatrix} \overline{u'^2} & \overline{u'\,v'} & \overline{u'\,w'} \\ & \overline{v'^2} & \overline{v'\,w'} \\ & & \overline{w'^2} \end{bmatrix}$$

  – If turbulent fluctuations are isotropic:
    - Off diagonal elements of τ^{Re} cancel
    - Diagonal elements equal: $\overline{u'^2} = \overline{v'^2} = \overline{w'^2}$



  – Average of product of fluctuations not zero
    - Consider mean shear flow: $\frac{\partial \overline{u}}{\partial y} > 0$
    - If parcel is going up ($v' > 0$), it slows down neighbors, hence $u' < 0$ (opposite for $v' < 0$)
    - Hence: $\overline{u'\,v'} < 0 \quad \text{for} \quad \frac{\partial \overline{u}}{\partial y} > 0$ (acts as turb. "diffus.")

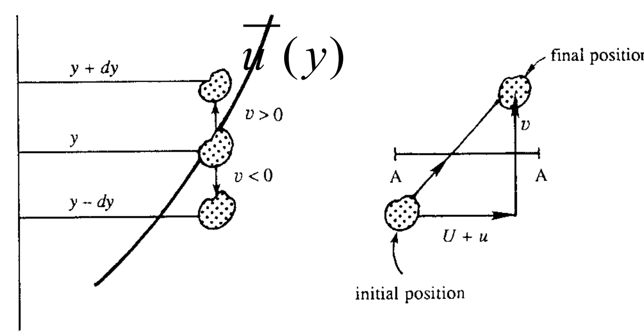


Figure 13.7 Movement of a particle in a turbulent shear flow.

  – Other meanings of Reynolds stress:
    - Rate of mean momentum transfer by turb. fluctations
    - Average flux of j-momentum along i-direction

Simplest Turbulence Closure Model

- Eddy Viscosity and Eddy Diffusivity Models
  - Effect of turbulence is to increase stirring/mixing on the mean-fields, hence increase effective viscosity or effective diffusivity
  - Hence, "Eddy-viscosity" Model and "Eddy-diffusivity" Model

$$\tau_{ij}^{\text{Re}} = -\rho\,\overline{u_i' u_j'} \cong \mu_t \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right) - \frac{2}{3}\rho k\, \delta_{ij}$$

$$-\rho\,\overline{u_i' \phi_j'} \cong \Gamma_t \frac{\partial \overline{\phi}}{\partial x_j}$$

- Last term in Reynolds stress is required to ensure correct results for the sum of normal stresses:

$$\tau_{ii}^{\text{Re}} = -\rho\,\overline{u_i' u_i'} = \mu_t 2 \frac{\partial \overline{u}_i}{\partial x_i} - \frac{2}{3}\rho k\, 3 = 0 - 2\rho \frac{1}{2}\overline{u'^2 + v'^2 + w'^2} = -\rho\left(\overline{u'^2} + \overline{v'^2} + \overline{w'^2}\right)$$

$$\equiv -2\rho k$$

- The use of scalar $\mu_t\,, \Gamma_t \Rightarrow$ assumption of isotropic turbulence, which is often inaccurate
- Since turbulent transports (momentum or scalars, e.g. internal energy) are due to "average stirring" or "eddy mixing", we expect similar values for μ_t and Γ_t . This is the so-called Reynolds analogy, i.e. Turbulent Prandtl number ~ 1:

$$\sigma_t = \frac{\mu_t}{\Gamma_t} \cong 1$$

Turbulence Closures: Mixing-Length Models

– Mixing length models attempt to vary unknown μ_t as a function of position

– Main parameters available: turbulent kinetic energy k $[\mathrm{m}^2/\mathrm{s}^2]$ or velocity u^*, large eddy length scale L

=> Dimensional analysis:

$$k = \left(u^*\right)^2 / 2$$
$$\mu_t = C_\mu \, \rho \, u^* \, L$$

C_μ dimensionless constant

– Observations and assumptions:

- Most k is contained in largest eddies of mixing-length L
- Largest eddies interact most with mean flow

$$\Rightarrow u^* = f(\bar{u}_i, \frac{\partial \bar{u}_i}{\partial x_j}, \frac{\partial^2 \bar{u}_i}{\partial x_j^2}, \cdots)$$

$$\Rightarrow \text{in} \sim \text{2D, mostly} \quad \tau_{xy}^{\mathrm{Re}} = -\rho \overline{u' v'} \quad \Rightarrow \quad u^* \cong f(\frac{\partial \bar{u}}{\partial y}) = c\, L \left|\frac{\partial \bar{u}}{\partial y}\right|$$

– Hence, $\mu_t \cong \rho\, L^2 \left|\frac{\partial \bar{u}}{\partial y}\right|$. This is Prandtl's "mixing length" model.

- Similar to mean-free path in thermodyn: distance before parcel "mixes" with others
- For a plate flow, Prandtl assumed: $L \approx \kappa y \quad \Rightarrow \quad u^* \cong \kappa y \frac{\partial \bar{u}}{\partial y} \quad \Rightarrow \quad \frac{\bar{u}}{u^*} = \frac{1}{\kappa} \ln y + \text{const.}$

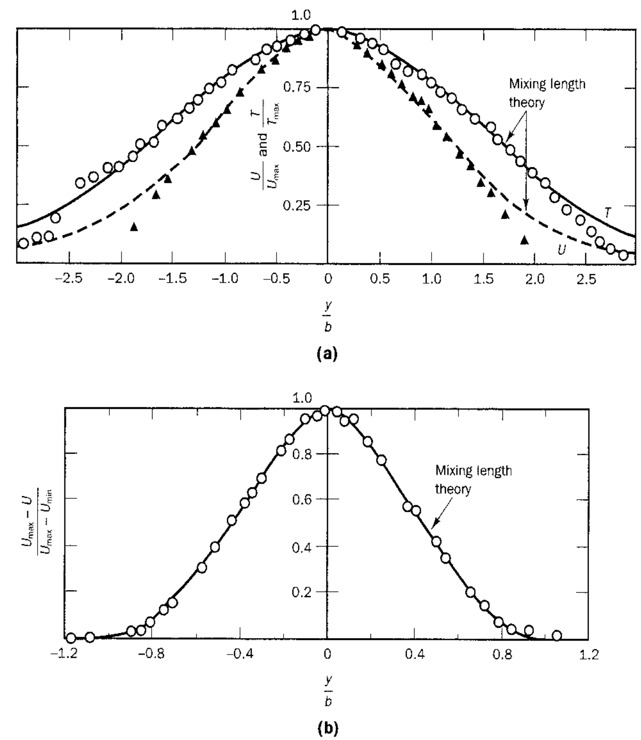
– Mixing-length turbulent Reynolds stress: $\tau_{xy}^{\mathrm{Re}} = -\rho \overline{u' v'} \cong \rho L^2 \left|\frac{\partial \bar{u}}{\partial y}\right| \frac{\partial \bar{u}}{\partial y}$

– Mixing length model can also be used for scalars: $-\rho \overline{u' \phi'} \cong \frac{\mu_t}{\sigma_t} \frac{\partial \bar{\phi}}{\partial x_j} \cong \rho \frac{L^2}{\sigma_t} \left|\frac{\partial \bar{u}}{\partial y}\right| \frac{\partial \bar{\phi}}{\partial y}$

Mixing Length Models: What is L (ℓ_m)?

- In simple 2D flows, mixing-length models agree well with data
- In these flows, mixing length L proportional to physical size (D, etc)
- Here are some examples:

Figure 3.14 Results of calculations using mixing length model for (a) planar jet and (b) wake behind a long, slender, circular cylinder
Source: Schlichting, H. (1979) *Boundary Layer Theory*, 7th edn, reproduced with permission of The McGraw-Hill Companies



Source: Schlichting, H. *Boundary Layer Theory.* 7th ed. The McGraw-Hill Companies, 1979.

- But, in general turbulence, more than one space and time scale!

Turbulence Closures: k - ε Models

- Mixing-length = "zero-equation" Model
- One might find a PDE to compute $\tau_{ij}^{\text{Re}} = -\rho \overline{u_i' u_j'}$ and $-\rho \overline{u_i' \phi'}$ as a function of k and other turbulent quantities
  - Turbulence model requires at least a length scale and a velocity scale, hence two PDEs?
- Kinetic energy equations (incompressible flows)
  - Define $\text{Total KE} = \frac{1}{2}\left(\overline{u_i}\right)^2 + \frac{1}{2}\overline{\left(u_i'\right)^2}$, $\text{K} = \frac{1}{2}\left(\overline{u_i}\right)^2$ and $\overline{\tau_{ij}} = \mu\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right) = 2\mu\,\overline{e_{ij}}$
  - Mean KE: Take mean mom. eqn., multiply by $\overline{u_i}$ to obtain:

$$\frac{\partial \rho K}{\partial t} + \frac{\partial(\rho K\,\overline{u_j})}{\partial x_j} = \frac{\partial\left(-\overline{p}\;\overline{u_j}\right)}{\partial x_j} + \frac{\partial\left(2\mu\,\overline{e_{ij}}\;\overline{u_i} - \rho\,\overline{u_i' u_j'}\;\overline{u_i}\right)}{\partial x_j} - 2\mu\,\overline{e_{ij}}\;\overline{e_{ij}} + \rho\,\overline{u_i' u_j'}\,\frac{\partial \overline{u_i}}{\partial x_j}$$

Rate of change of K	+	Advection of K	=	"Transport of K by pressure" ($\overline{p}$ work)	+	Transport of K by mean viscous stresses	+	Transport of K by Reynolds stresses	-	Rate of viscous dissipation of K	-	Rate of decay of K due turbulence production

Turbulence Closures: k - ε Models, Cont'd

- Turbulent kinetic energy equation
  – Obtain momentum eq. for the turbulent velocity u_i' (total eq. - mean eq.)
  – Define the fluctuating strain rate: $e_{ij}' \equiv \frac{1}{2}\left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right)$
  – Multiply by u_i' (sum over i) and average to obtain the eqn. for $k = \frac{1}{2}\overline{u_i' u_i'}$

$$\frac{\partial \rho k}{\partial t} + \frac{\partial(\rho k\, \overline{u}_j)}{\partial x_j} = \frac{\partial\left(-\overline{p' u_j'}\right)}{\partial x_j} + \frac{\partial\left(2\mu \overline{e_{ij}' u_i'} - \rho \frac{1}{2}\overline{u_i' u_j' . u_i'}\right)}{\partial x_j} - 2\mu \overline{e_{ij}' . e_{ij}'} - \rho \overline{u_i' u_j'} \frac{\partial \overline{u}_i}{\partial x_j}$$

Rate of change of k	+	Advection of k	=	"Transport of k by turbulent pressure"	+	Transport of k by viscous stresses (diffusion of k)	+	Transport of k by Reynolds stresses	-	Rate of viscous dissipation of k	+	Rate of production of k

  - This equation is similar than that of K, but with prime quantities
  - Last term is now opposite in sign: is the rate of shear production of k : $P_k = -\rho \overline{u_i' u_j'} \frac{\partial \overline{u}_i}{\partial x_j}$
  - Next to last term = rate of viscous dissipation of k : $\varepsilon = 2\nu \overline{e_{ij}' . e_{ij}'}$ $(= 2\mu \overline{e_{ij}' \; e_{ij}'} \; p.u.m)$
  - These two terms often of the same order (this is how Kolmogorov microscale is defined)
    – e.g. consider steady state turbulence (steady k)
  – If Boussinesq fluid, the 2 KE eqs. also contain buoyant loss/production terms

Turbulence Closures: k - ε Models, Cont'd

- Parameterizations for the standard k equation:
  - For incompressible flows, the viscous transport term is: $\frac{\partial\left(2\mu\overline{e'_{ij}u'_i}\right)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\mu\frac{\partial k}{\partial x_j}\right)$
  - The other two turbulent energy transport terms are thus modeled using:

$$-\overline{p'u'_j} + (-\rho\frac{1}{2}\overline{u'_i u'_j . u'_i}) \approx \frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x_j} \qquad (\sigma_t = \frac{\mu_t}{\Gamma_t} \cong 1)$$

    - This is analogous to an "eddy-diffusion of a scalar" model, recall: $-\rho\overline{u'_i\phi'_j} \cong \Gamma_t\frac{\partial\overline{\phi}}{\partial x_j}$
    - In some models, eddy-diffusions are tensors
  - The production term: using again the eddy viscosity model for the Rey. Stresses

$$P_k = -\rho\overline{u'_i u'_j}\frac{\partial\overline{u}_i}{\partial x_j} \approx \left(\mu_t\left(\frac{\partial\overline{u}_i}{\partial x_j}+\frac{\partial\overline{u}_j}{\partial x_i}\right)-\frac{2}{3}\rho k\,\delta_{ij}\right)\frac{\partial\overline{u}_i}{\partial x_j} = \mu_t\left(\frac{\partial\overline{u}_i}{\partial x_j}+\frac{\partial\overline{u}_j}{\partial x_i}\right)\frac{\partial\overline{u}_i}{\partial x_j}$$

  - All together, we have all "unknown" terms for the k equation parameterized, as long as $\varepsilon = 2\nu\overline{e'_{ij}.e'_{ij}}$ the rate of viscous dissipation of k is known:

$$\frac{\partial\rho k}{\partial t} + \frac{\partial(\rho k\,\overline{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_k}\left(\frac{\mu_t}{\sigma_t}\frac{\partial k}{\partial x_j}\right) + \frac{\partial}{\partial x_j}\left(\mu\frac{\partial k}{\partial x_j}\right) - \rho\,\varepsilon + \mu_t\left(\frac{\partial\overline{u}_i}{\partial x_j}+\frac{\partial\overline{u}_j}{\partial x_i}\right)\frac{\partial\overline{u}_i}{\partial x_j}$$

Turbulence Closures: k - ε Models, Cont'd

- The standard k - ε model equations (Launder and Spalding, 1974)
  - There are several choices for $\varepsilon = 2\nu \overline{e'_{ij} . e'_{ij}}$ $\left([\varepsilon] = m^2 / s^3 \right)$. The standard popular one is based on the "equilibrium turbulent flows" hypothesis:
    - In "equilibrium turbulent flows", ε the rate of viscous dissipation of k is in balance with P_k the rate of production of k (i.e. the energy cascade):

$$P_k = -\rho \overline{u'_i u'_j} \frac{\partial \overline{u_i}}{\partial x_j} \approx \mu_t \left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) \frac{\partial \overline{u_i}}{\partial x_j} = O\left(\mu_t \left(u^* \right)^2 / L^2 \right) \approx -2\mu \overline{e'_{ij} . e'_{ij}} = \rho\, \varepsilon$$

    - Recall the scalings: $k = \left(u^* \right)^2 / 2 \qquad \mu_t = C_\mu \, \rho \, u^* \, L$
    - This gives the length scale and the turbulent viscosity scalings:

$$L \approx \frac{k^{3/2}}{\varepsilon} \qquad \mu_t = C_\mu \, \rho \frac{k^2}{\varepsilon}$$

  - As a result, one can obtain an equation for ε (with a lot of assumptions):

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial (\rho\, \varepsilon\, \overline{u_j})}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) + C_{\varepsilon 1} P_k \frac{\varepsilon}{k} - C_{\varepsilon 2}\, \rho \frac{\varepsilon^2}{k}$$

where $\mu_t = C_\mu \, \rho \frac{k^2}{\varepsilon}$ and $\sigma_\varepsilon, C_{\varepsilon 1}, C_{\varepsilon 2}$ are constants. The production and destruction terms of ε are assumed proportional to those of k (the ratios ε / k is for dimensions)

Turbulence Closures: k - ε Models, Cont'd

- The standard k - ε model (RANS) equations are thus:

$$\frac{\partial \rho k}{\partial t}+\frac{\partial(\rho k\,\overline{u_j})}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x_j}\right)+\frac{\partial}{\partial x_j}\left(\mu\frac{\partial k}{\partial x_j}\right)+2\mu_t\,\overline{e_{ij}}\,.\,\overline{e_{ij}}-\rho\,\varepsilon$$

$$\frac{\partial \rho \varepsilon}{\partial t}+\frac{\partial(\rho\,\varepsilon\,\overline{u_j})}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}\right)+C_{\varepsilon 1}P_k\frac{\varepsilon}{k}-C_{\varepsilon 2}\,\rho\,\frac{\varepsilon^2}{k}$$

$$\text{with } \mu_t=C_\mu\,\rho\,\frac{k^2}{\varepsilon}$$

Rate of change of k or ε	+	Advection of k or ε	=	Transport of k or ε by "eddy-diffusion" stresses	+	Rate of production of k or ε	-	Rate of viscous dissipation of k or ε

- The Reynolds stresses are obtained from: $\tau_{ij}^{\mathrm{Re}}=-\rho\,\overline{u_i'u_j'}\cong\mu_t\left(\frac{\partial\overline{u_i}}{\partial x_j}+\frac{\partial\overline{u_j}}{\partial x_i}\right)-\frac{2}{3}\rho k\,\delta_{ij}$
- The most commonly used values for the constants are:

$$C_\mu=0.09,\quad C_{\varepsilon 1}=1.44,\quad C_{\varepsilon 2}=1.92,\quad \sigma_k=1.0,\quad \sigma_\varepsilon=1.3$$

- Two new PDEs are relatively simple to implement (same form as NS)
  – But, time-scales for k - ε are much shorter than for the mean flow
- Other $k-\varepsilon$ models: Spalart-Allmaras $\nu-L$; Wilcox or Menter $k-\omega$; anisotropic $k-\varepsilon$'s; etc.

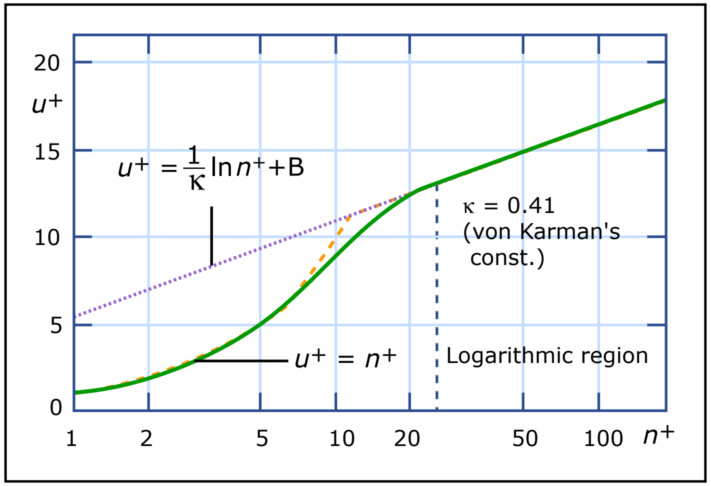
Turbulence Closures: k - ε Models, Cont'd

- Numerics for standard k - ε models
  - Since time-scales for k - ε are much shorter than for the mean flow, their equations are treated separately
    - Mean-flow NS outer iteration can be first performed using old k - ε
    - Strongly non-linear equations for k - ε are then integrated (outer-iteration) with smaller time-step and under-relaxation
  - Smaller space scales requires finer-grids near walls for $k - \varepsilon$ eqns
    - Otherwise, too low resolution can lead to wiggles and negative k - ε
    - If grids are the same, need to use schemes that reduce oscillations
- Boundary conditions for k - ε models
  - Similar than for other scalar eqns., except at solid walls
    - Inlet: k, ε given (from data or from literature)
    - Outlet or symmetry axis: normal derivatives set to zero (or other OBCs)
    - Free stream: k, ε given or zero-derivatives
    - Solid walls: depends on Re

Turbulence Closures: k - ε Models, Cont'd

- Solid-walls boundary conditions for k - ε models
  - No-slip BC would be standard:
    - Hence, appropriate to set $k = 0$ at the wall
    - But, dissipation not zero at the wall $\rightarrow$ use : $\varepsilon = \nu \left.\frac{\partial^2 k}{\partial n^2}\right|_{\text{wall}}$ or $\varepsilon = 2\nu \left.\left(\frac{\partial k^{1/2}}{\partial n}\right)^2\right|_{\text{wall}}$
  - At high-Reynolds numbers:
    - One can avoid the need to solve $k - \varepsilon$ right at the wall by using an analytical shape "wall function":
    - At high-Re, in logarithmic layer :

$$L \approx \kappa y \;\Rightarrow\; u^* \cong \kappa y \frac{\partial \bar{u}}{\partial y} \;\Rightarrow\; u^+ = \frac{\bar{u}}{u^*} = \frac{1}{\kappa} \ln y + \text{const.}$$



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    - If dissipation balances turbulence production, recall: $L \approx \frac{k^{3/2}}{\varepsilon}$; $\mu_t = C_\mu \rho \frac{k^2}{\varepsilon}$
    - Combining, one obtains: $\varepsilon \approx \frac{k^{3/2}}{L} = \frac{(u^*)^3}{\kappa y}$ and one can match: $\tau_{\text{wall}} = \rho (u^*)^2$ without resolving the viscous sub-layer
    - For more details, including low-Re cases, see references

Turbulence Closures: k - ε Models, Cont'd

- Example: Flow around an engine Valve (Lilek et al, 1991)
  - $k-\varepsilon$ model, 2D axi-symmetric
  - Boundary-fitted, structured grid
  - 2nd order CDS, 3-grids refinement
  - BCs: wall functions at the walls
  - Physics: separation at valve throat
  - Comparisons with data not bad
  - Such CFD study can reduce number of experiments/tests required

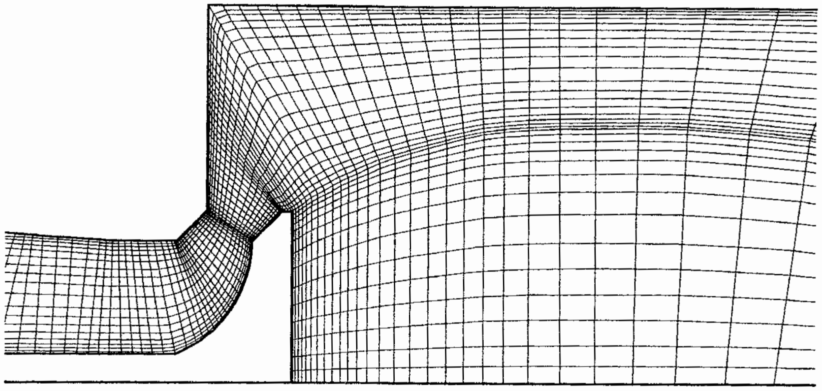


Fig. 9.12. Section of a grid (level two) used to calculate flow around a valve (from Lilek et al., 1991)

Please also see figures 9.13 and 9.14 from Figs 9.13 and 9.14 from Ferziger, J., and M. Peric. *Computational Methods for Fluid Dynamics*. 3rd ed. Springer, 2001.

Reynolds-Stress Equation Models (**RSMs**)

- Underlying assumption of "Eddy viscosity/diffusivity" models and of k - ε models is that of isotropic turbulence, which fails in many flows
  - Some have used anisotropic eddy-terms, but not common
- Instead, one can directly solve transport equations for the Reynolds stresses themselves: $-\rho \overline{u_i' u_j'}$ and $-\rho \overline{u_i' \phi'}$
  - These are among the most complex RANS used today. Their equations can be derived from NS
  - For momentum, the six transport eqs., one for each Reynolds stress, contain: diffusion, pressure-strain and dissipation/production terms which are unknown
    - In these "2^{nd} order models", assumptions are made on these terms and resulting PDEs are solved, as well as an equation for ε
    - Extra 6 + 1 = 7 PDEs to be solved increase cost. Mostly used for academic research (assumptions on unknown terms still being compared to data)

Reynolds-Stress Equation Models (RSMs), Cont'd

- Equations for $\tau_{ij}^{\mathrm{Re}} = -\rho\,\overline{u'_i u'_j}$

$$\frac{\partial \tau_{ij}^{\mathrm{Re}}}{\partial t} + \frac{\partial(\tau_{ij}^{\mathrm{Re}}\,\overline{u}_j)}{\partial x_j} = -\overline{p'\left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i}\right)} - \left(\tau_{im}^{\mathrm{Re}}\frac{\partial \overline{u}_j}{\partial x_m} + \tau_{jm}^{\mathrm{Re}}\frac{\partial \overline{u}_i}{\partial x_m}\right) + \rho\,\varepsilon_{ij} + \frac{\partial}{\partial x_j}\left(\nu\frac{\partial \tau_{ij}^{\mathrm{Re}}}{\partial x_j} + C_{ijm}\right)$$

Rate of change of Reynolds Stress + Advection of Reynolds Stress = Pressure-strain redistribution of Reynolds stresses + Rate of production of Reynolds stress + Rate of tensor dissipation of Reynolds stress - Rates of viscous and turbulent diffusions (dissipations) of Reynolds stress

where

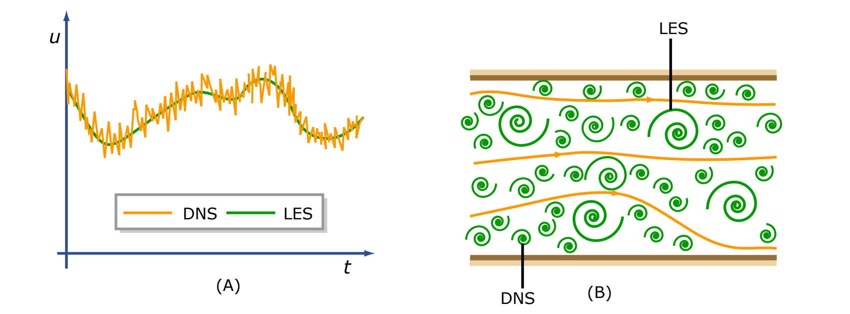
- The dissipation (as ε but now a tensor) is : $\varepsilon_{ij} = 2\nu\,\overline{e'_{ik}\,.\,e'_{jk}}$
- The 3rd order turbulence diffusions are: $C_{ijm} = \rho\,\overline{u'_i u'_j\,.u'_m} + \overline{p'u'_i}\,\delta_{jk} + \overline{p'u'_j}\,\delta_{ik}$

– Simplest and most common 3rd order closures:

- Isotropic dissipation: $\varepsilon_{ij} = \frac{2}{3}\varepsilon\,\delta_{ij} = \frac{4}{3}\nu\,\overline{e'_{ij}\,.\,e'_{ij}}\,\delta_{ij}$ $\rightarrow$ one ε PDE must be solved
- Several models for pressure-strain used (attempt to make it more isotropic), see Launder et al)
- The 3rd order turbulence diffusions: usually modeled using an eddy-flux model, but nonlinear models also used
- Active research

Large Eddy Simulation (LES)

- Turbulent Flows contain large range of time/space scales
- However, larger-scale motions often much more energetic than small scale ones
- Smaller scales often provide less transport



(A) The time dependence of a component of velocity at one point; (B) Representation of turbulent motion.

Image by MIT OpenCourseWare.

→ simulation that treats larger eddies more accurately than smaller ones makes sense ⇒ LES:

- Instead of time-averaging, LES uses spatial filtering to separate large and small eddies
- Models smaller eddies as a “universal behavior”
- 3D, time-dependent and expensive, but much less than DNS
- Preferred method at very high Re or very complex geometry

Large Eddy Simulation (LES), Cont'd

- Spatial Filtering of quantities
  - The larger-scale (the ones to be resolved) are essentially a local spatial average of the full field
  - For example, the filtered velocity is: $$\overline{u_i}(\mathbf{x},t) = \int_V G(\mathbf{x},\mathbf{x}';\Delta)\ u_i(\mathbf{x}',t)\ dV'$$

    where $G(\mathbf{x},\mathbf{x}';\Delta)$ is the filter kernel, a localization function of support/cutoff width Δ

    - Example of Filters: Gaussian, box, top-hat and spectral-cutoff (Fourier) filters
- When NS, incompressible flows, constant density is averaged, one obtains

$$\frac{\partial \rho \overline{u_i}}{\partial x_i} = 0$$

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

  - Continuity is linear, thus filtering does not change its shape
  - Simplifications occur if filter does not depend on positions: $G(\mathbf{x},\mathbf{x}';\Delta) = G(\mathbf{x}-\mathbf{x}';\Delta)$

Large Eddy Simulation (LES), Cont'd

- LES sub-grid-scale stresses
  - It is important to note that $\rho \overline{u_i u_j} \neq \rho \overline{u_i}\ \overline{u_j}$
  - This quantity is hard to compute
  - One introduces the sub-grid-scale Reynolds Stresses, which is the difference between the two:

$$\tau_{ij}^{SG} = -\rho\left(\overline{u_i u_j} - \overline{u_i}\ \overline{u_j}\right)$$

    - It represents the large scale momentum flux caused by the action of the small or unresolved scales (SG is somewhat a misnomer)
  - Example of models:
    - Smagorinsky: it is an eddy viscosity model

$$\tau_{ij}^{SG} - \frac{1}{3}\tau_{kk}^{SG}\,\delta_{ij} \cong \mu_t\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right) = 2\mu_t\,\overline{e_{ij}}$$

    - Higher-order SGS models
    - More advanced models: mixed models, dynamic models, deconvolution models, etc.
  - Mixed eqns, e.g. Partially-averaged Navier-Stokes (PANS): RANS → LES

Examples (see Durbin and Medic, 2009)

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Examples (see Durbin and Medic, 2009)

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