PROJECT:

Get a copy of the following papers:
[1] Kim, Moin and Moser JFM 1987 177, pp133-166
[2] Moin and Kim, JFM 1982, 118, pp 341-377
[3] IIHR report no. 413 by Cui, Patel and Lin

Raw data corresponding to two computations of the fully developed channel flow at $Re_\tau = u_\tau h/\nu = 180$ (2h=distance between channel walls in the y direction) are available on the class web site. The DNS computation was run on a 128*64*128 grid in (x,y,z) while the LES was run on a 32*64*32 grid. Ten sets of data containing u,v,w and p spaced $1.0h/u_\tau$ are available. The time step in the simulations was $0.001h/u_\tau$. The size of the domain in the streamwise direction is $4\pi h$ and in the spanwise direction is $4/3\pi h$. The nondimensionalization in the numerical simulations is such that h=1 and the mean friction velocity $u_\tau=1$, so $Re=1/\nu$. The points are uniformly distributed in x and z directions while in the y direction the grid is finer near the walls. The stretching function constant was 1.9 so that $y^+\sim 1.0$ at the first point off the wall in both DNS and LES (see formula 4.1 in [2]).

The data files were written using the following format that can be used to read it:

```
       open(32,file=sname)
       write(32,*) 'TITLE = "JET SOLN"'
       write(32,*) 'VARIABLES = X,Y,Z,UC,VC,WC,P'
       write(32,*) 'ZONE T="zone1", I=',N1+1, ' , J=',N2+1,',
     &  K=',N3+1,' , F=POINT'
           do k=0,N3
           do j=0,N2
           do i=0,N1
          Xc=i*HX
          Yc=Y2(j)
          Zc=k*HZ
          WRITE(32,*)Xc,Yc,Zc,Ucc(i,j,k),Vc(i,j,k),Wcc(i,j,k),Pc(i,j,k)
           end do
           end do
           end do
         close(32)
```

The ratio of the test filter to the grid filter was 2. Test filtering was applied only in homogeneous directions so in Germano's formula $(\hat{\Delta}/\Delta)^2=4$ was used. The test filter was a discrete approximation of the top-hat filter obtained using Simpson's rule. The width of the filter is 2Δ. In one dimension the filter is:

$$\overline{\phi_i} = 1/6\phi_{i-1} + 4/6\phi_i + 1/6\phi_{i+1} \qquad (1)$$

The mean distribution of the dynamic coefficient $C\Delta^2$ and eddy viscosity ν_t in the LES simulation can be obtained from the following file that is also provided

```
      OPEN(44,file='C_NIU_MEAN.dat')
      DO 340 J=0,N2+1
        YP=RE*( 1.D0-ABS(Y(J)) )
        WRITE(44,*) 'YP  Cdelta2   NIUT   J  Y '
        WRITE(44,4100) YP,CONSTM(J),VTM(J),J,Y(J)
340   CONTINUE
      CLOSE(44)
```

TASK1: Data exploration

Calculate Δx, Δz, min(Δy), max(Δy) from the files for both LES and DNS. What are their values in wall units? Using same levels for the contours and same range for the variables plot the instantaneous resolved u and v fields using contours using approximately 40 contours. Are there overall any differences between the LES and DNS fields?

TASK2: Statistics

Calculate statistics for DNS and LES using the whole data set provided (use all frames). Average in time and over the 2 homogeneous directions. Thus, all statistics can be presented in a plot S=S(y). Plot the distributions of the mean velocity component U and mean components of the Reynolds stresses (only resolved part for LES). Plot U/Uc vs. y and then U^+ vs. y^+. Also plot $U^+=y^+$ for $y^+<10$ and $U^+=2.5 \log y^+ +5.5$ (Uc is the centerline velocity). Calculate Uc as well as the average channel velocity, Um, and then the Reynolds numbers defined with Uc and Um and the ratio between these velocities and the friction velocity u_τ. Calculate the mean stress at the wall τ_w and then the friction coefficient Cf. What is the effective Reynolds number of the calculation? How does the DNS and LES values compare to Table 1 in [1]? How does Cf and Uc/Um compare to the values calculated using Dean's correlation (page 142 in [1])? Is the direct comparison between DNS and LES a fair one?

TASK3: Visualization of vortical structures

Read sections 3.7 to 3.10 from [3].

Plot the u contours in a x-z plane situated at ~ $y^+=6$ from one of the walls. You are going to observe some streaky structures of low/high streamwise velocity. Estimate the average width and length of these structures in both LES and DNS (use wall units).

Visualize the low-speed streaks in 3D using contours of the instantaneous fluctuation of the streamwise velocity (probably u'/Um=-0.2 is a good value, but you can play with that value; $u'=U(x,y,z)-\overline{U}(y)$) for both DNS and LES (use only one data set for each). Write a code to visualize the vertical structures of an instantaneous flow field using the λ_2

method of Jeong and Hussain (1995, JFM 285, page 66-94). A short description of the method is given in section 3.10.1. in [3]. Produce a figure showing the vertical structures from different angles similar to fig. 3.18 in [3].

Now let's focus on the flow structures in a (y,z) plane. Try to see how the vortices that are present in the resolved velocity field (as shown by the instantaneous velocity fluctuations v',w') correlate with contours of pressure minima, contours of the instantaneous resolved vorticity magnitude and, finally, contours of the vorticity structures as shown by the λ_2 method (similar to Fig 3.17 in [3]). What is the mean inclination angle of the structures relative to the streamwise direction in an (x,z) plane? What is their average penetration height in the channel? Comment on the results. Information about the average streak spacing can be obtained from the 2 point correlations $R_{uu}(y,r_1)$ and $R_{uu}(y,r_3)$.

$$R_{uu}(y,r_1)=\frac{< u'(x,y,z)u'(x+r1,y,z) >}{< u'^2(x,y,z) >} \qquad (2)$$

$$R_{uu}(y,r_3)=\frac{< u'(x,y,z)u'(x,y,z+r3) >}{< u'^2(x,y,z) >} \qquad (3)$$

Using only one data set (frame) calculate these correlations for both LES and DNS data at a location corresponding approximately to $y^+=10$ for $0<r1^+, r3^+<500$. Make sure when performing the summation over the homogeneous directions you include all terms, for points situated close to one of the lateral boundaries in x or z directions you will have to use the periodicity of the data to get the value, let's say at x+r1. Distance between the origin and the point where the $R_{uu}(y,r_3)$ correlation reaches a minimum represents the 'statistical mean' distance between low-speed and high-speed streaks. Twice that distance represents the average spacing between streaks. How does that distance for LES and DNS compare with the experimental measured value which is close to 100 wall units?

TASK4: Analysis of the primary shear stress

Plot the r.m.s. distribution of the velocity components (normalized by u_τ) vs y^+ (up to 100 wall units) and vs. y/h (across the channel). Do not forget to subtract the local mean from the u(x,y,z) values (the mean of v and w should be zero).
What are the maximum values for the 3 components and at what y^+ are they observed? Memorize those values.

Show that for a fully developed channel flow (DNS):

$$-\frac{\overline{u'v'}}{u_\tau^2} + \frac{du^+}{dy^+} = 1-\frac{y^+}{h^+} \qquad \text{where } h^+ = hu_\tau/\nu \qquad (4)$$

OBS: You should define the origin and direction of y axis such that both terms in the left hand side should be positive.

TURB VISC LINEAR VARIATION

In the following use the above nondimensionalization for the stresses.

Plot the distribution of the (mean) viscous shear stress, the turbulent shear stress and the total stress for DNS in both wall and global coordinates (see also fig 10 in [1] and fig 3.5 in [3]). Check if indeed the total stress varies linearly across the channel.
Repeat the same exercise for LES. Here you will have one extra term, the sub-grid term. You can use the values of ν_t from file `'C_NIU_MEAN.dat'` to estimate the subgrid term. Comment on the results.

TASK5: Additional statistics for DNS

For DNS data only:
Calculate the skewness and the flatness coefficients for the velocity fluctuations in all three directions:

$$S_i = \frac{<\overline{u_i'^3}>}{u_{i,rms}^3} \qquad F_i = \frac{<\overline{u_i'^4}>}{u_{i,rms}^4} \tag{5}$$

where <> denoted averages over time and homogeneous directions.

Plot S_i, F_i vs. y/h. Calculate and plot the correlation coefficient $<u'v'>/u_{rms}v_{rms}$. Compare with experimental data from fig 11 in [1]. Create a plot similar to fig 12 in [1]. This will allow you to check the behavior of the Reynolds stresses near the wall ($y^+<10$) compared to the asymptotic solutions.

Calculate the mean vorticity distribution ω_z as well as the r.m.s. distribution of the resolved vorticity for all 3 components. If you normalize them by the mean shear at the wall ($\omega_z \nu / u_\tau^2$) you should get a plot similar to fig 14 in [1].

TASK6: Turbulence kinetic energy budget for LES and DNS

k=$\overline{u}_i\overline{u}_i$ /2 where – denotes the resolved quantities, and

$$\frac{\partial k}{\partial t} + \frac{\partial k\overline{u}_j}{\partial x_j} = \overline{u}_i\overline{u}_j \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial}{\partial x_j}\left(-\overline{p}\overline{u}_j - \overline{u}_i\tau_{ij} + \nu\frac{\partial k}{\partial x_j}\right) - \nu\frac{\partial \overline{u}_i}{\partial x_j}\frac{\partial \overline{u}_i}{\partial x_j} + \tau_{ij}\frac{\partial \overline{u}_i}{\partial x_j} \tag{6}$$

uns+ adv = prod +press_diff+subgrid_diff+visc_diff+resolved_diss+SGS_diss

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j \qquad (7)$$

Flow is steady so <uns>=0. However, the mean (<>) of all the other terms is not zero. Calculate the mean of all the terms independently and check the energy balance for both LES and DNS (for DNS the subgrid diffusion and subgrid dissipation terms are absent as all the stresses are resolved on the grid). For LES you'll have to reconstruct the unresolved stresses using the dynamic Smagorinsky model for which you know the distribution of $C\Delta^2$. Use

$$\tau_{ij} - 1/3\delta_{ij}\tau_{kk} = -2\nu_t \bar{S}_{ij} \qquad (8)$$

$$\nu_t = C\Delta^2 |\bar{S}|$$
$$|\bar{S}| = \sqrt{2\bar{S}_{ij}\bar{S}_{ij}} \qquad (9)$$

Produce a plot similar to fig 3.8 in [3] (observation: The form of the resolved t.k.e. equation is changed compared to [3]).

OBS: You have the option to define k with the fluctuating component only –this is in fact the more popular definition- (for channel flow this will affect only the i=1 component), in which case you should use the modified form of (6), (8) and (9) consistent with this definition (see equations 6.1 to 6.3 and figure 17 in Moin and Kim).

TASK7: Quadrant analysis

For one of the 3D flow fields in LES and DNS perform a quadrant analysis similar to section 4.6 in [1] and 3.7 in [3]. In particular, plot the event frequency (sweep, ejection, outward interaction and inward interaction) vs. y/h (do not forget to subtract the mean U(y) from the instantaneous velocity component u). Then plot the fractional contribution of the four stresses normalized first by u_τ^2 and then by the local Reynolds shear stress (in this case the sum at all locations should be equal to 1) similar to fig 16 in [1] and figs 3.10 and 3.11 in [3].

TASK8: Filters

Define a filter of a function f(x) as:

$$\bar{f}(x) = \int_{-\infty}^{\infty} G(x - x') f(x') dx' \qquad (10)$$

The normalization condition for the filter is

$$\int_{-\infty}^{\infty} G(x - x', \Delta) dx' = 1 \qquad (11)$$

For the following filters show that the normalization condition is satisfied and calculate the filter function in wave space $\hat{G}(k)$ using Fourier transform $\hat{G}(k)$=F(G(x,Δ)). Plot the filter functions in physical space (one figure, for |x|<3.0) and in wave space (one figure, for |k|<30). Comment the results especially for the Fourier (sharp) cut-off filter.

a) Gaussian filter $G(x-x',\Delta)=\sqrt{\frac{6}{\pi\Delta^2}}\exp\left(-\frac{6(x-x')^2}{\Delta^2}\right)$ (12)

b) Top-hat filter $G(x-x',\Delta)=\begin{cases}\frac{1}{\Delta} & if \quad |x-x'|<\Delta/2 \\ 0 & otherwise\end{cases}$ (13)

c) Fourier cut-off filter $G(x-x',\Delta)=\frac{1}{\Delta}\left(\frac{\sin[k_c(x-x')]}{k_c(x-x')}\right) \qquad k_c=\pi/\Delta$

(14)

If we consider one mode of a velocity field, u=exp(ikx) and evaluate the one-dimensional sub-filter stress (SFS) as $\tau=\overline{u^2}-\bar{u}^2$ show that

1) the filtered velocity takes the form

$$\bar{u}=\mathrm{H}(\mathrm{k}\Delta)\exp(\mathrm{ikx}) \tag{15}$$

where

$$H_G(k\Delta)=\exp\left(-\frac{k^2\Delta^2}{24}\right) \text{ for Gaussian filter} \tag{16}$$

and

$$H_T(k\Delta)=\frac{\sin(k\Delta/2)}{k\Delta/2} \text{ for tophat filter} \tag{17}$$

2) Up to a truncation of O(Δ^6), the series expansion used to represent the unfiltered velocity field becomes

$$u^*=A(k\Delta)H(k\Delta)\exp(ikx) \tag{18}$$

where

$$A_G(k\Delta)=\left(1+\frac{k^2\Delta^2}{24}+\frac{k^4\Delta^4}{1152}\right) \text{ for the Gaussian filter} \tag{19}$$

and

$$A_T(k\Delta)=\left(1+\frac{k^2\Delta^2}{24}+\frac{7k^4\Delta^4}{5760}\right) \text{ for the tophat filter} \tag{20}$$

Hint: See also the discussion in task 9 which will allow you to prove the above expression for A_T and A_G.
In other words, u* should be an $O(\Delta^6)$ approximation for u=exp(ikx). Plot the amplitude $A(k\Delta)H(k\Delta)$ vs. kΔ for the two filters with different truncation errors (2, 4 and 6) of the expansion in A(kΔ). The order of accuracy is evidently 0, 2 and 4, respectively. The range of interest corresponds to wavenumbers k, such that $k\Delta<\pi$ (resolved range of wavenumbers on a grid of size Δ), but you can plot the functions up to $k\Delta<10$. Comment on the accuracy of the different filters with respect to the approximation to the full velocity u (that corresponds to $A(k\Delta)H(k\Delta)=1$).

3) Show that the exact form of the SFS stress $\tau = \overline{u^2} - \bar{u}^2$ for u=exp(ikx) is

$$\tau_G = \left[H_G(2k\Delta) - H_G^2(k\Delta)\right]\exp(2ikx) \tag{21}$$

$$\tau_T = \frac{1}{2}\left[1 - H_T^2(k\Delta)\right] - \frac{1}{2}\left[H_T(2k\Delta) - H_T^2(k\Delta)\right]\exp(2ikx) \tag{22}$$

Obs: For relation (22) assume u=sin(kx) and prove:

$$\tau_T = \frac{1}{2}\left[1 - H_T^2(k\Delta)\right] - \frac{1}{2}\left[H_T(2k\Delta) - H_T^2(k\Delta)\right]\cos(2ikx) \tag{22a}$$

Consider (22) just a generalization of (22a) which you do not have to prove.
Remember that (17) applies for u=exp(ikx), so in particular for both the real and imaginary parts meaning that $\overline{\cos(kx)} = \mathrm{H}(k\Delta)\cos(kx)$ and $\overline{\sin(kx)} = \mathrm{H}(k\Delta)\sin(kx)$.

4) Now consider two approximate forms to $\tau = \overline{u^2} - \bar{u}^2$ using u^* instead of u:

Model 1: $\tau_1 = \overline{u^{*2}} - \bar{u}^2$ (23)

Model 2: $\tau_2 = \overline{u^{*2}} - \overline{u^*}^2$ (24)

Show that:

$$\tau_{G1} = H_G^2(k\Delta)\left[A_G^2(k\Delta)H_G(2k\Delta) - 1\right]\exp(2ikx) \tag{25}$$

$$\tau_{T1} = \frac{1}{2}H_T^2(k\Delta)\left[A_T^2(k\Delta) - 1 - (A_T^2(k\Delta)H_T(2k\Delta) - 1)\exp(2ikx)\right] \tag{26}$$

$$\tau_{G2} = A_G^2(k\Delta)H_G^2(k\Delta)\tau_G \tag{27}$$

$$\tau_{T2} = A_T^2(k\Delta)H_T^2(k\Delta)\tau_T \tag{28}$$

Plot the amplitude of the oscillating part (the coefficient in front of the exp function) of $\tau_{G1}, \tau_{G2}, \tau_{T1}, \tau_{T2}$ vs. kΔ along with the amplitude of the oscillating part of the exact τ for the second-order (you retain only the first 2 terms in the expression for A) and the fourth-order model (retain all three terms).

TASK9: Estimation (reconstruction) of the unfiltered quantities from the filtered ones

Consider the multi-dimensional series expansion for any scalar variable (velocity component, pressure, etc.) at a point x_j=(x,y,z):

$$u_i(x_j^{'}) \approx u_i(x_j) + (x_m^{'} - x_m)\frac{\partial u_i(x_j)}{\partial x_m} + \frac{1}{2}(x_m^{'} - x_m)(x_n^{'} - x_n)\frac{\partial^2 u_i(x_j)}{\partial x_m \partial x_n} + \dots \tag{29}$$

where index notation (summation is implied for indices present in the same term) was used for compactness. Next, apply an anisotropic Gaussian filter:

$$\overline{u}_i(x,y,z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(x-x', y-y', z-z')u_i(x',y',z')dx'dy'dz' \tag{30}$$

with G defined as

$$G(x-x', y-y', z-z', \Delta_x, \Delta_y, \Delta_z) = \left(\sqrt{\frac{6}{\pi}}\right)^3 \frac{1}{\Delta_x \Delta_y \Delta_z} \exp\left(-\frac{6(x-x')^2}{\Delta_x^2} - \frac{6(y-y')^2}{\Delta_y^2} - \frac{6(z-z')^2}{\Delta_z^2}\right) \tag{31}$$

Show that:

$$\overline{u}_i(x,y,z) = u_i + \frac{\Delta_x^2}{24}\frac{\partial^2 u_i}{\partial x^2} + \frac{\Delta_y^2}{24}\frac{\partial^2 u_i}{\partial y^2} + \frac{\Delta_z^2}{24}\frac{\partial^2 u_i}{\partial z^2} + \frac{\Delta_x^4}{1152}\frac{\partial^4 u_i}{\partial x^4} + \frac{\Delta_y^4}{1152}\frac{\partial^4 u_i}{\partial y^4} + \frac{\Delta_z^4}{1152}\frac{\partial^4 u_i}{\partial z^4} + \frac{\Delta_x^2\Delta_y^2}{1728}\frac{\partial^4 u_i}{\partial x^2 \partial y^2} + \frac{\Delta_y^2\Delta_z^2}{1728}\frac{\partial^4 u_i}{\partial y^2 \partial z^2} + \frac{\Delta_z^2\Delta_x^2}{1728}\frac{\partial^4 u_i}{\partial z^2 \partial x^2} + O(\Delta^6) \tag{32}$$

Use the previous expression recursively to estimate $u_i = f(\overline{u}_i)$. Prove that:

$$u_i(x,y,z) \approx \overline{u}_i - \frac{\Delta_x^2}{24}\frac{\partial^2 \overline{u}_i}{\partial x^2} - \frac{\Delta_y^2}{24}\frac{\partial^2 \overline{u}_i}{\partial y^2} - \frac{\Delta_z^2}{24}\frac{\partial^2 \overline{u}_i}{\partial z^2} + \frac{\Delta_x^4}{1152}\frac{\partial^4 \overline{u}_i}{\partial x^4} + \frac{\Delta_y^4}{1152}\frac{\partial^4 \overline{u}_i}{\partial y^4} + \frac{\Delta_z^4}{1152}\frac{\partial^4 \overline{u}_i}{\partial z^4} +$$

$$\frac{5\Delta_x^2\Delta_y^2}{1728}\frac{\partial^4\overline{u}_i}{\partial x^2\partial y^2}+\frac{5\Delta_y^2\Delta_z^2}{1728}\frac{\partial^4\overline{u}_i}{\partial y^2\partial z^2}+\frac{5\Delta_z^2\Delta_x^2}{1728}\frac{\partial^4\overline{u}_i}{\partial z^2\partial x^2}+O(\Delta^6) \qquad (33)$$

At this point if u denotes the velocity, you partially reconstructed the total velocity from the filtered (resolved) value that is calculated in LES. So, you can then estimate, for instance, the turbulent stress $\overline{u_i u_j}$ which in fact is what you need to do in order to close the filtered Navier-Stokes equations. So basically you built a subfilter scale model using reconstruction (or defiltering) techniques. Essentially you estimated the inverse of the filter that is applied initially on the Navier-Stokes equations.

If the filter is isotropic then

$$u_i(x,y,z)\approx\overline{u}_i-\frac{\Delta^2}{24}\nabla^2\overline{u}_i+\frac{\Delta^4}{1152}\left(\frac{\partial^4\overline{u}_i}{\partial x^4}+\frac{\partial^4\overline{u}_i}{\partial y^4}+\frac{\partial^4\overline{u}_i}{\partial z^4}\right)+\frac{5\Delta^4}{1728}\left(\frac{\partial^4\overline{u}_i}{\partial x^2\partial y^2}+\frac{\partial^4\overline{u}_i}{\partial y^2\partial z^2}+\frac{\partial^4\overline{u}_i}{\partial z^2\partial x^2}\right)+O(\Delta^6) \qquad (34)$$

TASK10: Sub-filter scale models

Using the expression obtained in previous task, derive several models for $\tau_{ij}=\overline{u_i u_j}-\overline{u}_i\overline{u}_j$. Neglect the fourth and higher order terms in the expansion for u_i. Expand only the unclosed term $\overline{u_i u_j}$ and obtain the following model

Model 1

$$\tau_{ik}=\overline{\overline{u}_i\overline{u}_k}-\overline{u}_i\overline{u}_k-\frac{\Delta^2}{24}\overline{\overline{u}_i\nabla^2\overline{u}_k}-\frac{\Delta^2}{24}\overline{\overline{u}_k\nabla^2\overline{u}_i} \qquad (35)$$

Expand also the explicit term $\overline{u}_i\overline{u}_j$ to obtain

Model 2

$$\tau_{ik}=\overline{\overline{u}_i\overline{u}_k}-\overline{\overline{u}}_i\overline{\overline{u}}_k-\frac{\Delta^2}{24}\overline{\overline{u}_i\nabla^2\overline{u}_k}-\frac{\Delta^2}{24}\overline{\overline{u}_k\nabla^2\overline{u}_i}+\frac{\Delta^2}{24}\overline{\overline{u}}_k\nabla^2\overline{\overline{u}}_i+\frac{\Delta^2}{24}\overline{\overline{u}}_i\nabla^2\overline{\overline{u}}_k \qquad (36)$$

Observation: To second order in filter width Model 2 reduces to one of the most popular LES models: the Bardina scale-similarity model (Model 3)

Model 3

$$\tau_{ik}=\overline{\overline{u}_i\overline{u}_k}-\overline{\overline{u}}_i\overline{\overline{u}}_k \qquad (37)$$

Model 4 (Modified Clark model)

Start with the expression for Model 1 and use the fact that up to second order accuracy in the last expression of previous task $\overline{u}_i - \frac{\Delta^2}{24}\nabla^2\overline{u}_i$ can be replaced by the unfiltered variable u_i. Show that

$$\tau_{ik} = \overline{\overline{u}_i\overline{u}_k} - \overline{u}_i\overline{u}_k - \frac{\Delta^2}{24}\nabla^2\overline{\overline{u}_i\overline{u}_k} + \frac{\Delta^2}{12}\overline{\frac{\partial \overline{u}_k}{\partial x_j}\frac{\partial \overline{u}_i}{\partial x_j}} \tag{38}$$

and then use the same expression on the first and third terms to show that

$$\tau_{ik} = \frac{\Delta^2}{12}\overline{\frac{\partial \overline{u}_k}{\partial x_j}\frac{\partial \overline{u}_i}{\partial x_j}} + O(\Delta^4) \tag{39}$$

Obviously Clark's model is 2nd-order accurate in filter width.

TASK11: Mixed Models

It was observed that for most complex flows use of a scale-similarity model alone does not produce enough dissipation and the code becomes unstable. In practice scale similarity models are supplemented by a dissipative (Smagorinsky like) SGS model. There are several ways of doing that. Two examples are provided below, the so-called one coefficient model and the two-coefficient mixed models (Zang et al., Vreeman et al., Liu et al., etc).

a) $$\tau_{ik} = \overline{\overline{u}_i\overline{u}_k} - \overline{\overline{u}}_i\overline{\overline{u}}_k - 2C_d\Delta^2|\overline{S}|\overline{S}_{ik} \tag{40}$$

or more generally

$$\tau_{ik} = A_{ik} - 2C_d\alpha_{ik} \tag{41}$$

b) $$\tau_{ik} = C_{ss}(\overline{\overline{u}_i\overline{u}_k} - \overline{\overline{u}}_i\overline{\overline{u}}_k) - 2C_d\Delta^2|\overline{S}|\overline{S}_{ik} \tag{42}$$

or more generally

$$\tau_{ik} = C_{ss}A_{ik} - 2C_d\alpha_{ik} \tag{43}$$

Exactly as in the case of the determination of the C_d constant in the classical dynamic Smagorinsky model, minimize the error to obtain the following expressions for these constants in cases a) and b)

a) $$C_d = -\frac{1}{2}\frac{P_{LM} - P_{NM}}{P_{MM}} \tag{44}$$

b) $C_{ss} = \dfrac{P_{MN}P_{LM} - P_{MM}P_{LN}}{P_{MN}P_{MN} - P_{MM}P_{NN}}$ (45)

$$C_d = -\frac{1}{2}\frac{P_{MN}P_{LN} - P_{NN}P_{LM}}{P_{MN}P_{MN} - P_{MM}P_{NN}} \quad (46)$$

where $P_{EF} = \langle E_{ik}F_{ik} \rangle$ and $\langle\rangle$ denotes average over the homogeneous directions.

Hint: A basic introduction to the idea of dynamic modeling. Consider an arbitrary nonlinear term t(u), which is known function of the field variables, u, and suppose we wish to determine its filtered value by modeling the subgrid residual with an algebraic model m(u), which depends on the field variables but, in general, can also depend explicitly on space and time and on other parameters such as the filter width Δ. The value of the filtered term is then the sum of the filtered and modeled parts:

$$\overline{t(u)} = t(\overline{u}) + m(\overline{u}) \quad (47)$$

The basic idea behind the basic procedure is to consider how t(u) and m(u) vary with the filter width. In particular, an expression similar to the previous one for the value of the filtered term at a larger filter width, referred as test filter, can be written as:

$$\widetilde{\overline{t(u)}} = t(\tilde{\overline{u}}) + m(\tilde{\overline{u}}) \quad (48)$$

If relation (47) is test filtered and subtracted from (48) we get:

$$\widetilde{t(\overline{u})} - t(\tilde{\overline{u}}) = m(\tilde{\overline{u}}) - \widetilde{m(\overline{u})} \quad (49)$$

Remarkably, all the terms in this equation are computable from the resolved field. It represents the 'band-pass filtered' contribution to the nonlinear term in the scale range between the grid and the test filter levels. A consistent SGS model should contribute the same amount as the resolved field in this band. The key to the dynamic procedure is to use this identity as a constraint for calibration of SGS models. Note that while (49) is an exact identity when m(u) is the exact subgrid residual, it should only expected to hold in a statistical sense when m(u) is modeled.

Returning to our problem, choose t=u_iu_k and m($\overline{u}$) a model for the stress τ_{ik}. Remember also that by definition the subtest stress T_{ik} is just τ_{ik} with $\overline{}$ replaced by $\tilde{\overline{}}$ ($T_{ik} = \widetilde{\overline{u_iu_k}} - \tilde{\overline{u}}_i\tilde{\overline{u}}_j$). The test filter width is taken normally larger than the width of the test filter). So from (49) we get:

$$\widetilde{\overline{u}_i\overline{u}_k} - \tilde{\overline{u}}_i\tilde{\overline{u}}_k = T_{ik} - \tilde{\tau}_{ik} \quad (50)$$

where, for instance, in case (a) $T_{ik} = B_{ik} - 2C_d\beta_{ik}$ To be more specific, in our case $B_{ik} = \overline{\tilde{\tilde{u}}_i\tilde{\tilde{u}}_k} - \tilde{\tilde{u}}_i\tilde{\tilde{u}}_k$ and $\beta_{ik} = \tilde{\Delta}^2\left|\tilde{\tilde{S}}\right|\tilde{\tilde{S}}_{ik}$. The other important observation is that the left hand side of (50) is just the resolved stress denoted L_{ik}. Upon introduction of the proposed expressions for T_{ik} and τ_{ik} (50) can be satisfied only approximately. Also (50) contains in fact a system of 6 independent equations that have to be used to determine only one or two constants. A least-square procedure can be determined to minimize the error in (50). For instance, in case (a)

$$e_{ik} = L_{ik} - T_{ik} + \tilde{\tilde{\tilde{\tau}}}_{ik} = L_{ik} - (B_{ik} - \hat{A}_{ik}) + 2C_d(\beta_{ik} - \hat{\alpha}_{ik}) = L_{ik} - N_{ik} + 2C_d M_{ik} \qquad (51)$$

where to simplify the calculation we used

$$\begin{aligned} N_{ik} &= B_{ik} - \hat{A}_{ik} \\ M_{ik} &= \beta_{ik} - \alpha_{ik} \end{aligned} \qquad (52)$$

So all what you have to do is to minimize $E^2 = e_{ik}e_{ik}$. Typically, the final expression is averaged (44-46) over the homogeneous directions in the flow (if they exists) to improve the robustness of the predictions (the coefficient C_d should be positive for stability reasons, something that is not guaranteed by the dynamic procedure).

TASK12: A priori evaluation of sub-grid and sub-filter stress models.

In a priori tests data from DNS are filtered and compared to the model. A priori tests indicate the degree of correlation between the modeled and exact SGS/SFS model and are useful indications of the expected performance of the model in actual LES computations (a posteriori tests). Though a high correlation (close to one) with the exact value is not a sufficient condition for a good SGS/SFS model, it is a desirable feature. A posteriori tests are necessary to obtain complete information on the model performance and, in particular, on the level of energy dissipation introduced by the model (most SFS models do not introduce enough dissipation to keep the simulations stable if not supplemented by a dissipative (generally, Smagorinsky type) model as discussed in TASK 11).

Choose one data sample (file) for DNS. Remember that $4\Delta_{DNS}=\Delta_{LES}$ in the x and z directions, while the mesh is identical in the nonhomogeneous direction. The filters are thus going to be applied ONLY in the homogeneous directions. There are several ways to do the data transformation and the filtering. Here we are going to adopt a simplified procedure. Sample the DNS data on the scale of the LES grid, and filter it using a discrete top-hat filter of width $2\Delta_{LES}$ to obtain the LES field $\overline{u}_i$. The expression for that filter using trapezoidal rule is:

$$\overline{\phi}_i = 1/4\phi_{i-1} + 2/4\phi_i + 1/4\phi_{i+1} \qquad (53)$$

Make sure you are using the periodicity of the data near boundaries.

Since the DNS data represent the exact velocity field, the exact SFS stress can be computed at each point on the grid. To do that you just have to estimate $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$ in the same way you obtained $\bar{u}_i$. The modeled SFS stress can be computed from the LES field $\bar{u}_i$ defined on the LES grid, and compared to the exact stress at the same points on the LES grid. Remember that all quantities related to LES should be derived starting from $\bar{u}_i$, not from DNS, in other words one can use information residing only at the coarser mesh locations. Use central differences to estimate the different LES velocity derivatives involved in the expressions of the SFS stress in Models 1 to 4 and in the Smagorinsky model. Take into account that the grid spacing is different in the two directions, so for instance in Model 1 the term $\frac{\Delta^2}{24}\overline{\bar{u}_i \nabla^2 \bar{u}_k}$ should be written as $\frac{\Delta_x^2}{24}\overline{\bar{u}_i \frac{\partial^2 \bar{u}_k}{\partial x^2}} + \frac{\Delta_z^2}{24}\overline{\bar{u}_i \frac{\partial^2 \bar{u}_k}{\partial z^2}}$. In the SFS model expressions there are additional explicit filtering operations that have to be carried out on the LES fields. Use the same top hat filter of size 2 Δ_{LES} for these operations.

Compute the modeled SFS stress $\tau_{12} = \tau_{xy}$ for Models 1 to 4 defined in Task 10, as well as for the dynamic Smagorinsky model $\tau_{ik} = 2C\Delta_{LES}{}^2 |\bar{S}| \bar{S}_{ij}$ with $C\Delta_{LES}{}^2$ determined from `file='C_NIU_MEAN.dat'`.

Plot the distribution of the instantaneous stress τ_{12} (exact+estimated using the different models considered) in an (x,z) plane at around 20 wall units from the wall. Then, average the results in the (x,z) directions and plot the averaged exact SFS stress vs. the one predicted by each of the four models. Ideally, the data should be close to the line at 45^0. Compute the correlation coefficient $\rho(y^+)$ and the ratio r(y^+) of the rms values of the exact and predicted stress τ_{12}.

$$\rho_\tau(y^+) = \frac{<(\tau_M - <\tau_M>)(\tau_E - <\tau_E>)>}{<(\tau_M - <\tau_M>)^2>^{1/2} <(\tau_E - <\tau_E>)^2>^{1/2}} \qquad (54)$$

where M refers to model value, E to exact value, and <> represents average in the (x,z) directions. The correlation coefficient measures the degree of linearity in the relationship between the modeled and the exact SFS stress, while the ratio gives information about the coefficient of proportionality. Comment on the results. Repeat the same exercise for the SFS/SGS dissipation $\varepsilon = \tau_{ij}\bar{S}_{ij}$.

Why do you think the SGS dynamic Smagorinsky model does poorer than the SFS models?

Comments:
You could obtain the LES field $\bar{u}_i$ by filtering the DNS data on the DNS grid with a filter of size $2\Delta_{LES} = 8\ \Delta_{DNS}$. However, the explicit filtering in the LES Models should be done with the discrete top-hat filter of width $2\Delta_{LES}$. You can use a discrete top-hat filter (derive its expression), or you can use a discrete Gaussian filter (make sure that the coefficients of the discrete approximation add exactly to one). Deduce an expression for such a Gaussian filter knowing that the coefficients are practically zero for distances larger than 3 times the width of the filter. For extra points you can use the discrete Gaussian filter in the above analysis. Do you see any important differences?
The most correct way of doing this operation is to go to wave space using Fast Fourier Transform (FFT) in the periodical directions, apply the Gaussian filter in wave space, then a sharp cut-off filter to eliminate all frequencies larger than the LES grid size $G(x - x', \Delta) = 0 \quad for \quad k > k_c = \pi / \Delta$ and, finally, go back to physical space. You can try to do this for additional extra points.

TASK13: Estimate the performance of the dynamic Smagorinsky SGS model used in the LES based on the DNS results on a finer mesh (this is part of an a posteriori analysis).

The analysis is similar to what was required for the Smagorinsky model in Task12, but here the filter width should be the grid size in the LES grid (Δ_{LES}). The test filter used in the LES calculation was a discrete top-hat filter derived using Simpson's rule:

$$\tilde{\phi}_i = 1/6\phi_{i-1} + 4/6\phi_i + 1/6\phi_{i+1} \qquad (55)$$

Calculate using only the velocity data from the LES simulation the dynamic constant

$$C\Delta^2 = \frac{1}{2}\frac{< L_{ij} M_{ij} >}{< M_{ij} M_{ij} >} \qquad (56)$$

$$L_{ik} = -\widetilde{\bar{u}_i \bar{u}_k} + \tilde{\bar{u}}_i \tilde{\bar{u}}_k \qquad M_{ik} = \left(\tilde{\Delta}/\Delta\right)^2 \left|\tilde{\bar{S}}\right| \tilde{\bar{S}}_{ik} - \widetilde{\left|\bar{S}\right| \bar{S}_{ik}} \qquad (57)$$

where in our case the filter width ratio is 2. Compare the obtained distribution of $C\Delta^2$ (y) with the one given in the file `'C_NIU_MEAN.dat'`. Calculate the distribution of the total (resolved + modeled) shear stress τ_{xy}. Use the filtered DNS data to predict the 'correct' distribution of τ_{xy}. Comment on the results. You can do a similar analysis for some of the other statistics. Is the agreement between LES and the statistics obtained using the filtered DNS data on the LES grid better? In any case this is a much fair comparison to make when one SGS/SFS model is evaluated.

TASK14: Well resolved DNS compared to our DNS.

Compare your statistics with those obtained by Kasagi et al at the same and/or similar Reynolds number on finer meshes. The statistics are available at http://www.thtlab.t.u-tokyo.ac.jp/ .