Handout: Large Eddy Simulation III

Other subgrid scale models:

1. Structure-function model (SFM)

It is a transposition of the spectral-space model of Metais and Lessieur

$$\nu_T = C(E(k_c)/k_c)^{1/2}$$

k_c = cutoff wavenumber ($\pi/\Delta x$)

into physical space and can be interpreted as a model based on the energy at cutoff expressed in physical space.

Eddy viscosity can be written using dimensional analysis arguments as:

$$\nu_T \sim \Delta U_T \sim \Delta(q_{sgs}^2(x))^{1/2} \quad \text{or}$$

$$\nu_T = C\Delta(F(\Delta x))^{1/2}$$

where q_{SGS}^2 is the SGS energy and F is the second-order structure function defined as power of velocity difference at two points:

$$F(r) = \overline{\|\vec{u}(\vec{x}) - \vec{u}(\vec{x}+r)\|^2}$$

Obviously, F is related to two-point correlation spectrum. Main hypothesis is that the subgrid energy (k=q_{sgs}^2) is proportional to the squared of the velocity gradient at the smallest resolved scales:

$$q_{sgs}^2 = 1/2\overline{(u_i(\vec{x},t) - \overline{u}_i(\vec{x},t))^2} \sim F(r)$$

In three dimensions:

$$F = \frac{F_1 + F_2 + F_3}{3}:$$

$$F_k = \frac{1}{6}\sum_{i=1}^{3}(\overline{u_k(\vec{x}) - u_k(\vec{x} + \Delta x_i \vec{e}_i)} + \overline{u_k(\vec{x}) - u_k(\vec{x} - \Delta x_i \vec{e}_i)})$$

Analyze by using Taylor series:

$$u_j(\vec{x}) - u_j(\vec{x} + \Delta x_i \vec{e}_i) = -\Delta x_i \frac{\partial u_j}{\partial x_i} + HOT$$

If only one term is retained in F_k, then

$$\big((u_j(\vec{x}) - u_j(\vec{x} + \Delta x_i \vec{e}_i)\big)\big(u_j(\vec{x}) - u_j(\vec{x} + \Delta x_i \vec{e}_i)\big) \approx \Delta x_i \Delta x_k \frac{\partial u_j}{\partial x_i}\frac{\partial u_j}{\partial x_k}$$

But

$$\frac{\partial u_j}{\partial x_i} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right) + \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} - \frac{\partial u_i}{\partial x_j}\right) = S_{ij} + \Omega_{ij}$$

Recall vorticity vector is related to the rotation tensor:

$$\omega_{ij} = \varepsilon_{ijk}\Omega_{jk}$$

When this is plugged into eddy viscosity expression (1-D form for simplicity):

$$F(\Delta x) \approx (\Delta x)^2 (S_{ij} S_{ij} + \frac{1}{2} \omega_i \omega_i)$$

where we neglected $S_{ij}\omega_{ij}$~0.

So, SFM ($\nu_T = C\Delta\sqrt{F}$) is similar to Smagorinsky ($\nu_T = C\Delta^2 S$) with

$$S \rightarrow \sqrt{S^2 + \omega^2 / 2}$$

Improved results reported; why?

- Explanation offered: $S \rightarrow \sqrt{S^2 + \omega^2 / 2}$ helps improve results
- In isotropic turbulence: $\overline{S^2} = \overline{\omega^2 / 2}$ so difference in models is small
- Thus, this is not a very satisfactory explanation
- If we keep two terms in the Taylor series expansion:

$$\nu_T = C\left[(\Delta x)^2 \sqrt{S^2 + \omega^2 / 2} + (\Delta x)^4 \frac{\sum_{ijk} \left(\frac{\partial^2 u_j}{\partial x_i \partial x_k} \right)^2}{\sqrt{S^2 + \omega^2 / 2}} \right]$$

- Last term similar to fourth-order viscosity Smagorinsky like model
  - May explain success compared to the classical Smagorinsky model (which is a second order viscosity model). This gives idea for improved Smagorinsky model to be described next.

2. Fourth Order Viscosity Models

They are in fact mixed fourth-order / second-order models in which both coefficients can be calculated dynamically (dynamic 2-4 model).

$$\tau_{ij} = -(\upsilon_4 \nabla^2 S_{ij} + \upsilon_2 S_{ij})$$

where ν_4 is usually called hyperviscosity and must be modeled. Dimensional analysis suggests $\nu_4 = C_4 \Delta^4 |S|$. So the new expression is:

$$\tau_{ij} = -(C_4 \Delta^4 |S| \nabla^2 S_{ij} + C_2 \Delta^2 |S| S_{ij})$$

The hyper-viscosity term is similar to the 4-th order term in the SFM model.

For best results, use both 2nd and 4th order viscosities

- Use dynamic procedure to determine the two constants C_2 and C_4
- Least square method
- Potential problem

  - Order of N-S equations increased (fourth-order PDE system instead of second order) so we may need more boundary conditions (two on each boundary). To avoid this, one has to require that $\nu_4 \rightarrow 0$ near boundary.

Applied to:

- 2D and 3D (decay) isotropic turbulence
- Channel flow

<u>Advantages/disadvantages</u>

- Works well for flows mentioned above
- Increased cost ≈ 20%
- More accurate and more stable than 2nd order model
- 4th order term important

  - Dynamic model makes it go to zero at wall automatically (so the problem of satisfying additional boundary conditions is eliminated automatically)

3. **One equation SGS models** (Yoshizawa, 1986, Ghosal et al., 1994, Menon and Kim, 1996)

The Smagorinsky model does not contain any information regarding the total amount of energy in the subgrid scales, k=q_{sgs}^2. Therefore, if the model coefficient becomes negative in any part of the domain, the model does not have any information on the available energy in the subgrid scales and is therefore unable to provide a mechanism to saturate the reverse flow of energy. A model that keeps track of k will address this problem. Define eddy viscosity as:

$$\nu_t = C_d \Delta k^{1/2}$$

Solution: solve PDE for subgrid scale energy

- One equation enough

  - No need for length scale equation in LES (use Δ)

  - Simpler than k-ε model, especially that the modeling of the unclosed terms in the ε equation is much more uncertain than the ones in the k equation.

In this model the resulting model coefficient can still have either sign, but it was observed that numerical computations using this kind of models are much more stable when the coefficient is negative. In other words, these models can account for relatively large amounts of backscatter in a numerically stable way. The energy flows back and forth between the resolved and subgrid scales while their sum decays monotonically due to viscous effects in the absence of external input of energy.

In this approach the stresses are modeled as (using simple dimensional analysis and using k for the velocity scale characterizing the unresolved turbulence fluctuations):

$$\tau_{ik} = -2C_d \Delta k^{1/2} \overline{S}_{ik}$$

As already mentioned, as opposed to RANS where the turbulence length scale is unknown and there is no simple way to determine it, in LES using SGS models (typically with implicit filtering) the turbulence length scale is the local grid space Δ. This was used to obtain the previous expression for the modeled SGS stresses.

Typically, the equation for k is similar to the one used in RANS models, but the form of the dissipation term is different. In the original **model of Yoshizawa** the following equation was used:

$$\frac{\partial k}{\partial t} + \frac{\partial}{\partial x_j}(\overline{u}_j k) = \frac{\partial}{\partial x_j}\left[(\nu + \nu_t)\frac{\partial k}{\partial x_j}\right] + 2\nu_t \overline{S}_{ij}\overline{S}_{ij} - C_\varepsilon \frac{k^{3/2}}{\Delta}$$

The SGS viscosity was obtained using a constant coefficient Smagorinsky model ($\Delta = \min\{\Delta x, \Delta y, \Delta z\}$). The model constants are:

C_d=0.07
C_ε=1.05

A more advanced variant was proposed by **Menon and Kim (1996).** In this model using a second test filter of wider width than the filter at the grid level, the model coefficient is calculated dynamically, in a manner similar to the classical dynamic Smagorinsky model. The transport equation solved in their model is:

$$\frac{\partial k}{\partial t} + \frac{\partial}{\partial x_j}(\overline{u}_j k) = \frac{\partial}{\partial x_j}\left[(\nu + \nu_t)\frac{\partial k}{\partial x_j}\right] + 2\nu_t \overline{S}_{ij}\overline{S}_{ij} - C_* \frac{k^{3/2}}{\Delta}$$

where

$$C_d = \frac{1}{2}\frac{L_{ij}\sigma_{ij}}{\sigma_{ij}\sigma_{ij}}$$

$$\sigma_{ij} = -\widetilde{\Delta} k_{test}^{1/2} \widetilde{\overline{S}}_{ij}$$

$$L_{ij} = \widetilde{\overline{u}_i \overline{u}_j} - \widetilde{\overline{u}}_i \widetilde{\overline{u}}_j$$

$$k_{test} = \frac{1}{2} L_{ii}$$

$$C_* = \frac{\widetilde{\Delta}}{k_{test}^{3/2}} (\nu + \nu_t) \left(\widetilde{\frac{\partial \overline{u}_i}{\partial x_j} \frac{\partial \overline{u}_i}{\partial x_j}} - \frac{\partial \widetilde{\overline{u}}_i}{\partial x_j} \frac{\partial \widetilde{\overline{u}}_i}{\partial x_j} \right)$$

A different variant that also estimates dynamically the model constants using the dynamic localization model was proposed by Ghosal et al, 1995. This variant guarantees positive viscosity.

<u>Advantages of the one-equation SGS models over the standard dynamic Smagorinsky model:</u>

- One-equation models **can predict backscattering**. In the standard dynamic model the model coefficient must be averaged in the homogeneous directions and/or clipped in an adhoc manner to prevent the solution from diverging due to the local presence of negative diffusion. This averaging and clipping often implies that $\nu + \nu_t > 0$, i.e., the production term should be larger than $-2\nu \overline{S}_{ij} \overline{S}_{ij}$. Obviously this greatly restricts the backscattering in the dynamic Smagorinsky model.

- In one-equation models, when estimating dynamically the model coefficients, there is **no need to average locally or in the homogeneous directions**.

- Although in one-equation models it is necessary to solve one extra transport equation, because these models are numerically more stable, one **can generally use larger time**

steps and thus in the end these models may be computationally cheaper than the standard dynamic model. One should also point out that by using the transport equation to determine k, **memory effects are included** into the resulting SGS model, something that is also lacking in the standard dynamic model.

<u>Problems:</u>

- Parameters (constants) in the k equation not known. In many cases the values determined from RANS models are used.
- Does not address major issue
  - Problem is not the value of the eddy viscosity
  - It is the fact that the SGS Reynolds stresses and resolved strain principal axes are not aligned.
    * One can eventually address this deficiency by using a Reynolds stress model for the subgrid stresses, but the modeling of the unclosed terms and the determination of the constants is even a tougher problem.

4. Deconvolution models

A - 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):

$$u_i(x_j') \approx u_i(x_j) + (x_m' - x_m)\frac{\partial u_i(x_j)}{\partial x_m} + \frac{1}{2}(x_m' - x_m)(x_n' - x_n)\frac{\partial^2 u_i(x_j)}{\partial x_m \partial x_n} + \ldots \qquad (1)$$

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

$$\bar{u}_i(x,y,z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(x-x', y-y', z-z')u_i(x',y',z')dx'dy'dz' \qquad (2)$$

with G (Gaussian filter in 3D) defined as

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

Using series expansion one can show that:

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

This is in fact a differential equation for u_i. Then one can use the previous expression recursively to estimate $u_i = f(\overline{u}_i)$. One obtains:

$$u_i(x,y,z) \approx \overline{u}_i - \frac{\Delta_x^2}{24}\frac{\partial^2 \overline{u}_i}{\partial x^2} - \frac{\Delta_y^2}{24}\frac{\partial^2 \overline{u}_i}{\partial y^2} - \frac{\Delta_z^2}{24}\frac{\partial^2 \overline{u}_i}{\partial z^2} + \frac{\Delta_x^4}{1152}\frac{\partial^4 \overline{u}_i}{\partial x^4} + \frac{\Delta_y^4}{1152}\frac{\partial^4 \overline{u}_i}{\partial y^4} + \frac{\Delta_z^4}{1152}\frac{\partial^4 \overline{u}_i}{\partial z^4} + \frac{5\Delta_x^2\Delta_y^2}{1728}\frac{\partial^4 \overline{u}_i}{\partial x^2 \partial y^2} + \frac{5\Delta_y^2\Delta_z^2}{1728}\frac{\partial^4 \overline{u}_i}{\partial y^2 \partial z^2} + \frac{5\Delta_z^2\Delta_x^2}{1728}\frac{\partial^4 \overline{u}_i}{\partial z^2 \partial x^2} + O(\Delta^6) \tag{5}$$

At this point if u denotes the velocity in equation (5), **we partially reconstructed the total (filtered plus fluctuating part) velocity from the filtered (resolved) value that is calculated in LES**.

So, one can then estimate, for instance, the turbulent stress $\overline{u_i u_j}$ which in fact is what one need to do in order to close the filtered Navier-Stokes equations.

To compute SGS Reynolds stress:

- Substitute approximate u_i into definition of τ_{ij}, compute it
- Model defined, self-contained
- Contains no parameters!
- Model is nonlinear

In other words we built a **subfilter scale model using reconstruction (or defiltering or deconvolution) techniques**. Essentially we estimated the inverse of the filter that is applied initially on the Navier-Stokes equations.

If the Gaussian filter is isotropic then equation (5) simplifies to:

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

Similar formulas can be obtained for other filters, in particular the top-hat filter.

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

1) the filtered velocity takes the form

$$\overline{u} = \mathrm{H(k\Delta)exp(ikx)} \tag{7}$$

where

$$H_G(k\Delta) = \exp\left(-\frac{k^2\Delta^2}{24}\right) \text{ for Gaussian filter} \tag{8}$$

and

$$H_T(k\Delta) = \frac{\sin(k\Delta/2)}{k\Delta/2} \text{ for tophat filter} \tag{9}$$

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

$$u^* = A(k\Delta)H(k\Delta)\exp(ikx) \tag{10}$$

where

$$A_G(k\Delta) = \left(1 + \frac{k^2\Delta^2}{24} + \frac{k^4\Delta^4}{1152}\right) \text{ for the Gaussian filter} \tag{11}$$

and

$$A_T(k\Delta) = \left(1 + \frac{k^2\Delta^2}{24} + \frac{7k^4\Delta^4}{5760}\right) \text{ for the tophat filter} \tag{12}$$

The range of interest corresponds to wavenumbers k, such that $k\Delta<\pi$ (resolved range of wavenumbers on a grid of size Δ).

B - Sub-filter scale (SFS) models
(models obtained by partially reconstructing the total velocity)

Using the expression (6) for the partially reconstructed velocity one can derive several models for $\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j$. Neglecting the fourth and higher order terms in equation (6) and expanding only the unclosed term $\overline{u_i u_j}$ one can obtain the following model:

Model 1

$$\tau_{ik} = \overline{\bar{u}_i \bar{u}_k} - \bar{u}_i \bar{u}_k - \frac{\Delta^2}{24} \overline{\bar{u}_i \nabla^2 \bar{u}_k} - \frac{\Delta^2}{24} \overline{\bar{u}_k \nabla^2 \bar{u}_i} \tag{13}$$

Expanding also the explicit term $\bar{u}_i \bar{u}_j$ one obtains

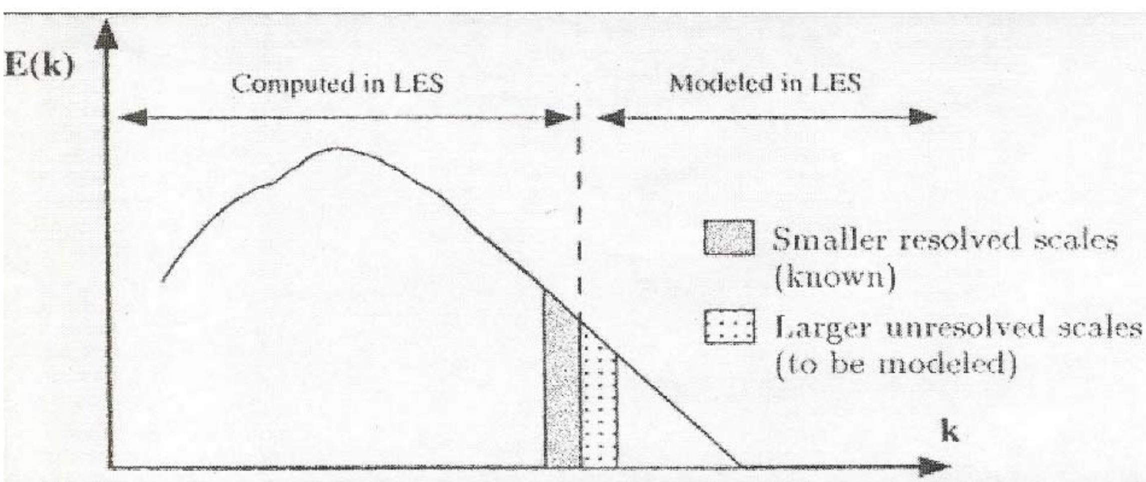
Model 2

$$\tau_{ik} = \overline{\bar{u}_i \bar{u}_k} - \bar{\bar{u}}_i \bar{\bar{u}}_k - \frac{\Delta^2}{24} \overline{\bar{u}_i \nabla^2 \bar{u}_k} - \frac{\Delta^2}{24} \overline{\bar{u}_k \nabla^2 \bar{u}_i} + \frac{\Delta^2}{24} \bar{\bar{u}}_k \nabla^2 \bar{\bar{u}}_i + \frac{\Delta^2}{24} \bar{\bar{u}}_i \nabla^2 \bar{\bar{u}}_k \tag{14}$$

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) which was originally defined based on other considerents.

Model 3 (Bardina's scale-similarity model)

$$\tau_{ik} = \overline{\bar{u}_i \bar{u}_k} - \bar{\bar{u}}_i \bar{\bar{u}}_k \tag{15}$$



Bardina's assumption: the resolved and unresolved stresses behave similarly, i.e., the subgrid scales near the filter cutoff can be extrapolated from the resolved scales near the cutoff.

Model 4 (Modified Clark model)

Starting with the expression for Model 1 and using the fact that up to second order accuracy in equation (6) $\bar{u}_i - \frac{\Delta^2}{24}\nabla^2\bar{u}_i$ can be replaced by the unfiltered variable u_i, one can show that

$$\tau_{ik} = \overline{\bar{u}_i\bar{u}_k} - \bar{u}_i\bar{u}_k - \frac{\Delta^2}{24}\overline{\bar{u}_i\bar{u}_k} + \frac{\Delta^2}{12}\overline{\frac{\partial\bar{u}_k}{\partial x_j}\frac{\partial\bar{u}_i}{\partial x_j}} \tag{16}$$

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

$$\tau_{ik} = \frac{\Delta^2}{12}\overline{\frac{\partial\bar{u}_k}{\partial x_j}\frac{\partial\bar{u}_i}{\partial x_j}} + O(\Delta^4) \tag{17}$$

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

Further remarks:

SGS Reynolds stresses and resolved strain principal axes not necessarily aligned.

- In a priori tests, correlation between filtered DNS stress and SFS stress is very high compared to any Smagorinsky based model
- Need to distinguish subgrid and subfilter scales
  - Reconstruction of field only possible for resolved (SFS) scales
  - Scales below grid size (actually, twice grid size) not represented – need SGS model
- Add a Smagorinsky term (possibly dynamic) to represent SGS
- This is in fact a dynamic mixed model to be discussed later

5. The Approximate Deconvolution Model (Stolz and Adams, 1999)

The main idea behind this model is the approximation of the non-filtered velocity field by truncated series expansion of the inverse filter operator. The approximate deconvolution of the filtered velocity is obtained by repeated filtering operations (the filter is G) applied to the filtered quantities using van Cittert (1931) deconvolution method. If the unfiltered velocity is u_i and the filtered velocity is denoted $\overline{u}_i$ then:

$$\overline{u}_i = G * u_i \qquad (18)$$

or, if we invert it

$$u_i = G^{-1} * \overline{u}_i \qquad (19)$$

But formally, if G has an inverse then it can be expanded as an infinite series that can be truncated up to an arbitrary order (let's denote the approximate inverse using the truncated series up to order N by Q_N), let's say N.

$$G^{-1} = \frac{1}{G} = \frac{1}{I-(I-G)} = I + (I-G) + (I-G)^2 + \ldots = \sum_{m=0}^{\infty} (I-G)^m \qquad (20)$$

$$Q_N = \sum_{m=0}^{N} (I-G)^m \qquad (21)$$

The series expansion provides an estimate for the inversion of the filter G. This series converges if $\|I-G\| < 1$, where I is the identity matrix. If G is positive in Fourier space for all wavenumbers, the exact inverse can be obtained by simply inverting the filter kernel in wave space. If G crosses from positive to negative values in wave space at any wavenumber, exact inversion becomes impossible due to division by zero. Therefore, the series reconstruction over all wavenumbers of such a filtered field is approximate. The exact reconstruction can be obtained as long as the filter kernel is positive in wave space.

Thus, it is preferable to choose an explicit filter function that is positive for at least all the wavenumbers that are represented on the grid (up to the Nyquist frequency). Then the approximate deconvolution is given simply by:

$$u_i^* = Q_N * \overline{u}_i = \overline{u}_i + (I - G) * \overline{u}_i + (I - G) * ((I - G) * \overline{u}_i) + ... \qquad \text{(N terms)} \qquad (22)$$

One can show that if one retains N terms in (21) then the level (order) of the reconstruction is N-1. The expression (22) for the unfiltered velocity is only used to calculate the term $\overline{u_i^* u_j^*}$ in τ_{ij}. In practical calculations N is typically taken equal to 5 and the ADM model is often combined with a dynamic Smagorinsky model to produce extra dissipation at the small scales (this is a common problem with practically all models based on reconstructing the turbulent stresses or the non-filtered velocity fields including the scale-similarity and the tensor-diffusivity models discussed previously).

6. The multiscale model (Hughes et al., 2001)

The main justification behind this model is that most of the shortcomings associated with Smagorinsky based models are due to their inability to differentiate between large and small scales. Recall that the SGS model is supposed to act only on the smallest scales not on all of them. So, if a separation of scales is possible (this is indeed the case if we are using a fully spectral method where the Navier-Stokes equations are solved in wavenumber space in all three directions) then one can add the SGS Smagorinsky term only to the equations corresponding to the small scales (high wavenumbers), while the equations corresponding to the low wavenumbers are unchanged (like in DNS). In other words, modeling is confined only to the equations governing the small scales. The limit between the small and large scales is somewhat arbitrary, let's say N/2, if N is the total number of modes supported by the grid.

So starting with the Navier Stokes equations in physical space:

$$\frac{\partial u}{\partial t} + \nabla \cdot (u \otimes u) + \nabla p = \nu \Delta u$$
$$\nabla u = 0 \qquad (23)$$

where u is the velocity vector. If the solution is periodic in all three directions (e.g., simulations of isotropic turbulence in a box) then the Fourier series representation of the solution is

$$u(x,t) = \sum_k \hat{u}_k(t) e^{ik \cdot x}$$
$$p(x,t) = \sum_k \hat{p}_k(t) e^{ik \cdot x} \qquad (24)$$

where k=(k_1, k_2, k_3) is the wavenumber vector , x=(x_1, x_2, x_3), $\hat{u}_k$ and $\hat{p}_k$ are the Fourier coefficients of u and p, respectively. One can easily show that the Fourier transform of the Navier Stokes equations are:

$$\left(\frac{d}{dt} + \nu |k|^2 \right) \hat{u}_k = -ik\hat{p}_k - ik\overline{(u \otimes u)}_k$$
$$ik \cdot \hat{u}_k = 0 \qquad (25)$$

where $\overline{(u \otimes u)}_k$ is the k Fourier coefficient of the convective term (recall this term is nonlinear so its Fourier transform involves interactions with all the other modes; this is how the momentum equations for the coefficients $\hat{u}_k$ are coupled in wave space). On a grid of size N^3, the above equations are truncated to $-N/2 \le k_j \le N/2 - 1$ for j=1,2,3.

Next, the solution is decomposed into large scale and small-scale components:

$$u = \overline{u} + u'$$
$$p = \overline{p} + p' \qquad (26)$$

where

$$
\begin{aligned}
\overline{u}(x,t) &= \sum_{|k|<N/2} \hat{u}_k(t) e^{ik\cdot x} \\
\overline{p}(x,t) &= \sum_{|k|<N/2} \hat{p}_k(t) e^{ik\cdot x} \\
u'(x,t) &= \sum_{|k|\geq N/2} \hat{u}_k(t) e^{ik\cdot x} \\
p'(x,t) &= \sum_{|k|\geq N/2} \hat{p}_k(t) e^{ik\cdot x}
\end{aligned}
\tag{27}
$$

and $|k| = \left(k_1^2 + k_2^2 + k_3^2\right)^{1/2}$. The modeling is confined to the small scales. In physical space the Smagorinsky term is:

$$
T = 2\nu_t' \nabla^s u' \tag{28}
$$

where as usual the rate of strain tensor is

$$
\begin{aligned}
\nabla^s u &= \frac{1}{2}\left(\nabla u + (\nabla u)^T\right) \\
\left|\nabla^s u\right| &= \left(2\nabla^s u \cdot \nabla^s u\right)^{1/2}.
\end{aligned}
\tag{29}
$$

However, for the eddy viscosity we can use the modulus of the rate of strain tensor corresponding to either the small scales or the large scales (both options were shown to produce similar results at least for decay of isotropic turbulence):

$$
\nu_t' = C_d' \Delta^2 \left|\nabla^s u'\right| \tag{30}
$$

or

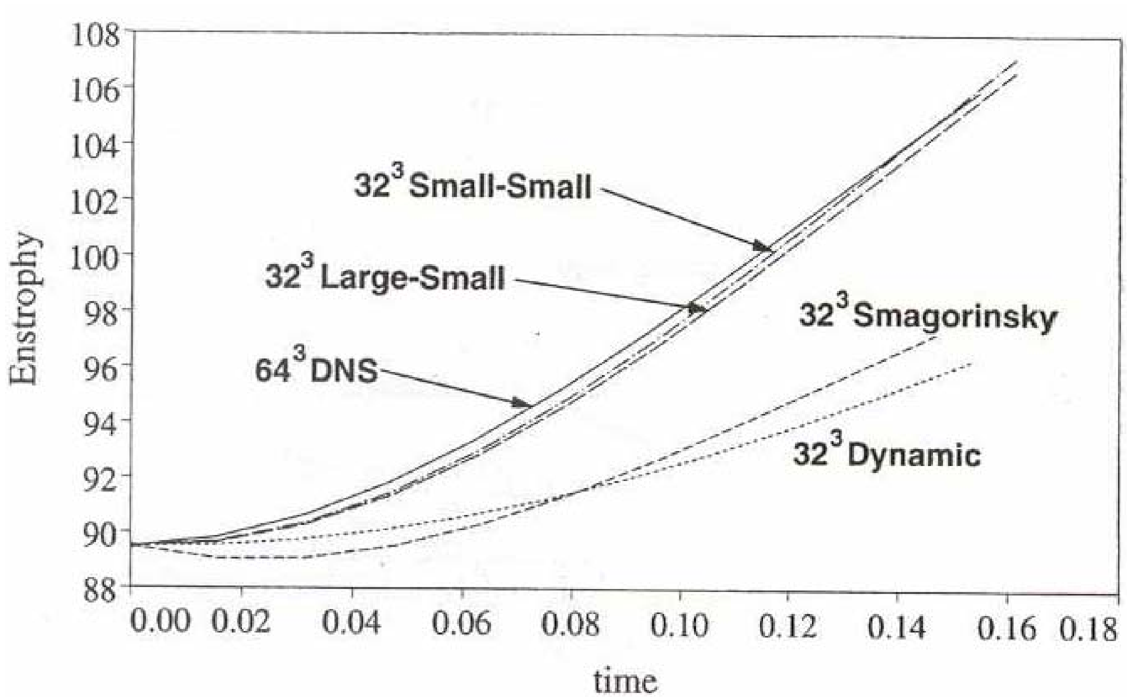
$$
\nu_t' = C_d' \Delta^2 \left|\nabla^s \overline{u}\right| \tag{31}
$$

The resulting form of the momentum equations in the wave space for the multiscale model is:

$$\left(\frac{d}{dt}+\nu|k|^2\right)\hat{u}_k = -ik\hat{p}_k - ik\overline{u\otimes u}_k \qquad |k| < N/2 \tag{32}$$

$$\left(\frac{d}{dt}+\nu|k|^2\right)\hat{u}_k = -ik\hat{p}_k - ik(\overline{u\otimes u}_k - \hat{T}_k) \quad |k| \geq N/2 \tag{33}$$

It was shown that simulations using a constant coefficient Smagorinsky model in the multiscale model produced more correct solutions for the decay of isotropic turbulence compared to solutions obtained using the dynamic model applied at all scales. The dynamic procedure can of course be applied to the multiscale model. There are attempts to propose multiscale models in physical space based on an approximate separation of scales.



7. Dynamic mixed models

It was observed that for most complex flows use of a scale-similarity (deconvolution based) model alone does not produce enough dissipation and the code becomes unstable. In practice deconvolution models are supplemented by a dissipative (Smagorinsky like) SGS model.

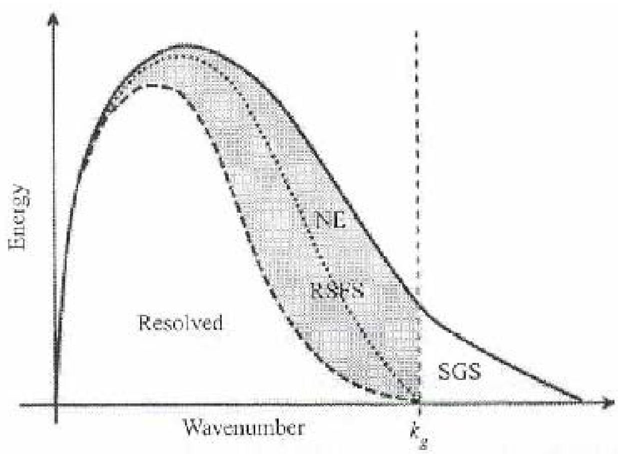


FIGURE 1. Schematic of velocity energy spectrum showing partitioning into resolved, subfilter-scale, and subgrid-scale motions. The numerical error region is also shown. The grid is indicated by the vertical dashed line, and the filter by the curved dashed line.

In particular, in the case of the scale similarity model (Model 3)

- Two versions
    - a. Consider coefficient of scale similarity term fixed (usually unity)
        - *Determine Smagorinsky parameter by least squares method (Zang & Street)
    - b. Two parameter dynamic model (Salvetti & Banerjee)
        - *Smagorinsky, scale similarity parameters both determined dynamically

a) $\tau_{ik} = \overline{\bar{u}_i \bar{u}_k} - \bar{\bar{u}}_i \bar{\bar{u}}_k - 2C_d \Delta^2 \left|\bar{S}\right| \bar{S}_{ik}$ (34)

or more generally

$$\tau_{ik} = A_{ik} - 2C_d \alpha_{ik} \quad (35)$$

$$A_{ik} = \overline{\overline{u}_i \overline{u}_k} - \overline{\overline{u}}_i \overline{\overline{u}}_k \qquad \alpha_{ik} = \Delta^2 \left|\overline{S}\right| \overline{S}_{ik}$$

$$\text{b)} \ \tau_{ik} = C_{ss}(\overline{\overline{u}_i \overline{u}_k} - \overline{\overline{u}}_i \overline{\overline{u}}_k) - 2C_d \Delta^2 \left|\overline{S}\right| \overline{S}_{ik} \quad (36)$$

or more generally

$$\tau_{ik} = C_{ss} A_{ik} - 2C_d \alpha_{ik} \quad (37)$$

Exactly as in the case of the determination of the C_d constant in the classical dynamic Smagorinsky model, by minimizing the error one can obtain the expressions of the model constants in both models. For instance, in case (a): $T_{ik} = B_{ik} - 2C_d \beta_{ik}$, $B_{ik} = \overline{\widetilde{\overline{u}}_i \widetilde{\overline{u}}_k} - \widetilde{\overline{\overline{u}}}_i \widetilde{\overline{\overline{u}}}_k$, $\beta_{ik} = -2C_d \widetilde{\Delta}^2 \left|\widetilde{\overline{S}}\right| \widetilde{\overline{S}}_{ik}$ and $L_{ik} = -\widetilde{\overline{u}_i \overline{u}_k} + \widetilde{\overline{u}}_i \widetilde{\overline{u}}_k$ is the usual Leonard term. Thus the error can be calculated as:

$$e_{ik} = L_{ik} - T_{ik} + \widetilde{\tau_{ik}} = L_{ik} - (B_{ik} - \widetilde{A}_{ik}) + 2C_d (\beta_{ik} - \widetilde{\alpha}_{ik}) = L_{ik} - N_{ik} + 2C_d M_{ik} \quad (38)$$

where to simplify the calculation we used

$$N_{ik} = B_{ik} - \widetilde{A}_{ik}$$

$$M_{ik} = \beta_{ik} - \widetilde{\alpha}_{ik} \quad (39)$$

So all what has to be done is to minimize $E^2 = e_{ik} e_{ik}$ in a least square sense to obtain:

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

b) $C_{ss} = -\frac{P_{MN}P_{LM} - P_{MM}P_{LN}}{P_{MN}P_{MN} - P_{MM}P_{NN}}$ (40)

$$C_d = -\frac{1}{2}\frac{P_{MN}P_{LN} - P_{NN}P_{LM}}{P_{MN}P_{MN} - P_{MM}P_{NN}} \quad (41)$$

where $P_{EF} =< E_{ik}F_{ik} >$ and $<>$ denotes average over the homogeneous directions.

Performance

- Variation of Smagorinsky part coefficient C_d very much reduced
- Without averaging, program is much more stable
  - But can still be unstable
- One parameter version as good as two parameter version
- Gives good results for several flows

8. Filtering and commutation

- Filtering defines large scale field and its governing equations
- Virtually all Smagorinsky based LES calculations to date have ignored explicit filtering of the Navier Stokes equations.
- If deconvolution (or, in general SFS) based models are used then the quality of the explicit filter is essential in the accuracy of the final simulation
- Filtering and differentiation do not in general commute for non-uniform filters

$$\overline{\frac{\partial f}{\partial x}} \neq \frac{\partial \bar{f}}{\partial x}$$

- Commuting filters for non-uniform filter widths and unstructured grids were recently proposed (Vasilyev & Moin, JCP, 1998, Marsden et al., JCP, 2002, Haselbacher & Vasilyev, JCP, 2003)

When using **explicit filtering**:

- Filter width should not be tied to grid spacing. Preferably:

$$\Delta_{\text{filter}} > \Delta_{\text{grid}}$$

- LES solution should converge to true solution of the LES equations with grid refinement, and not to DNS

9. The dynamic model without test filtering (Chester, Charlette and Meneveau, 2001)

This model was motivated by the fact that the construction of accurate test filters in complex geometry flows, in particular in codes that are using unstructured grids with large non-uniform variations between element sizes, is very difficult. Moreover, just choosing the neighboring elements that have to be used in the local construction of the filter is a challenging problem in itself that is needed to maintain a good shape for the resulting filter. The idea behind the present model is to **replace the actual test filtering of the solution by estimating higher order derivatives of the resolved velocity field in the general expression for the dynamic Smagorinsky coefficient**:

$$C_d \Delta^2 = \frac{1}{2} \frac{< L_{ij} M_{ij} >}{< M_{ij} M_{ij} >} \tag{42}$$

$$L_{ik} = -\widetilde{\bar{u}_i \bar{u}_k} + \tilde{\bar{u}}_i \tilde{\bar{u}}_k \qquad M_{ik} = \left(\tilde{\Delta}/\Delta\right)^2 \left|\tilde{\bar{S}}\right| \tilde{\bar{S}}_{ik} - \widetilde{\left|\bar{S}\right| \bar{S}_{ik}} \tag{43}$$

These derivatives can be estimated in a much easier way and relatively accurately using least square algorithms on unstructured meshes. The proposed method is also based on

Taylor series expansions of the resolved velocity field, as was the case in the models based on reconstructing the unfiltered velocity from the filtered one.

Let's define a function f and its filter (grid filter) as:

$$\bar{f}(x) = \int_{-\infty}^{\infty} G_{\Delta}(x - x') f(x') dx' \qquad (44)$$

where

$$x = (x_1, x_2, x_3)$$

The test filtering operation (denoted by tilde) is defined in a similar way, except that the filter acts on a larger scale $\tilde{\Delta}$ (typically the ratio is equal to 2).

$$\tilde{\bar{f}}(x) = \int_{-\infty}^{\infty} G_{\tilde{\Delta}}(x - x') \bar{f}(x') dx' \qquad (45)$$

Let's replace $\bar{f}(x')$ by its Taylor series expansion about the point x. This leads to simple integrations that are performed analytically. The result is:

$$\tilde{\bar{f}}(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \partial^n_{i_1 \ldots i_n} \bar{f} \,|_x < y_{i_1} \cdots y_{i_n} >$$

y=x-x'

$$< y_{i_1} \cdots y_{i_n} >= \int y_{i_1} \cdots y_{i_n} G_{\tilde{\Delta}}(y) dy \qquad (46)$$

For an isotropic filter, all terms with n odd vanish, so one can take m=2n. Since derivatives can only be calculated to a limited accuracy, and the Taylor series are truncated, the method yields an approximation to the filtered operation. By varying the number of terms in the Taylor expansion and the way the derivatives are calculated, the accuracy of the approximation can be varied.

Let's choose the Gaussian filter as the grid and test filters (others filters such as the box filter can be used but the final expression will be different):

$$G(x-x',y-y',z-z',\Delta_x,\Delta_y,\Delta_z)=\left(\sqrt{\frac{6}{\pi}}\right)^{3/2}\frac{1}{\Delta_x\Delta_y\Delta_z}\exp\left(-\frac{6(x-x')^2}{\Delta_x^2}-\frac{6(y-y')^2}{\Delta_y^2}-\frac{6(z-z')^2}{\Delta_z^2}\right) \tag{47}$$

Introducing (47) into (45) one can show using the properties of the moments for the Gaussian filter that

$$\tilde{\bar{f}}(x)=\sum_{m=0}^{\infty}\frac{(\tilde{\Delta})^{2m}}{24^m m!}\left(\nabla^2\right)^m\bar{f}(x) \tag{48}$$

where $(\nabla^2)^m$ represents m applications of the Laplacian operator. This expression allows to replace test-filtered quantities that appear in the dynamic model by expressions involving resolved (grid-filtered) quantities and their derivatives.

Application of (48) to $\bar{u}_i, \bar{u}_j, \bar{u}_i\bar{u}_j$, $\bar{S}_{ij}, |S|\bar{S}_{ij}$ yields the approximation (up to four order in Δ):

$$L_{ij}=-\frac{\tilde{\Delta}^2}{12}\frac{\partial\bar{u}_i}{\partial x_k}\frac{\partial\bar{u}_j}{\partial x_k} \tag{49}$$

$$M_{ij}=-2\Delta^2\left\{\left(|\bar{S}|\bar{S}_{ij}-\frac{\tilde{\Delta}^2}{\Delta^2}|\bar{S}^t|\bar{S}_{ij}\right)+\frac{\tilde{\Delta}^2}{24}\left[\nabla^2(|\bar{S}|\bar{S}_{ij})-\frac{\tilde{\Delta}^2}{\Delta^2}|\bar{S}^t|\nabla^2\bar{S}_{ij}\right]\right\} \tag{50}$$

where $\left|\bar{S}^{t}\right|$ is the derivative based approximation to $\left|\tilde{\bar{S}}\right|$

$$\left|\bar{S}^{t}\right| = \left[2\left(\bar{S}_{ij} + \frac{\tilde{\Delta}^2}{24}\nabla^2\bar{S}_{ij}\right)\right]^{1/2} \tag{51}$$

The last three expressions are introduced in the definition of the model coefficient (42).

10. Numerical methods in LES

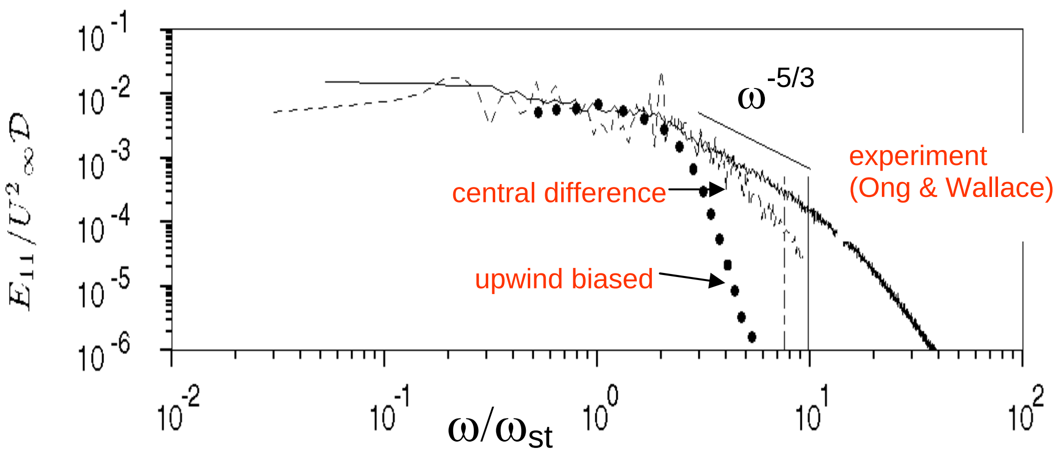
- It is important for LES calculations to predict accurately the quantities that led to choosing LES in the first place (e.g., turbulent fluctuations, acoustic sources, mixing,…)

- Numerical dissipation present in most RANS codes is inadequate for LES (c.f. flow over cylinder)

- Ideally in LES nondissipative discretizations (central differencing as opposed to low order upwinding or any extra added numerical dissipation) must be used.

Numerical dissipation in LES of cylinder @ Re=3,900

Mittal & Moin (AIAA J., 1997, 8:1415 – 1417)



One-dimensional streamwise velocity spectra E11 along the wake centerline

Vertical lines indicate the grid cutoff:
—— central difference
_ . _ upwind biased

11. Model free LES

<u>High-Re 'Direct Simulation'</u>

Claim- DNS of complex high Re flows

- High Reynolds number flows simulated (10^6)
- Complex geometries: e.g. Automobiles, reasonable qualitative results

Important to note

- Third order upwind differencing used (several types)
- This means that in fact the coarse DNS was an LES with 4^{th} order dissipation that looks like hyperviscosity, but the local amount of dissipation is controlled by the grid size and discretization of the convection operator. This is bad as, for instance, one cannot get grid independent results.

For LES simulations one can think similarly. Why not **discretize the convective terms in a way to be consistent with a SGS model**?

<u>Model-Free LES</u>

- Use numerical error (dissipation introduced by the discretization) as model
- Example: **monotonically integrated LES (MILES)**
- Another version recently given by Los Alamos
  - Use scheme that eliminates wiggles
  - Similar to schemes used in aerodynamics
  - Has nonlinear limiters

Performance:

- Produces reasonable looking simulations
- Quantative comparisons rarely made
- Model has lots of parameters that can be adjusted to produce better looking results but they are highly flow dependent. No dynamic way to estimate them.
- Results are grid dependent. Value not proven. To be avoided.

12. SGS Models for Transition

Prediction of transition important

- Difficult for boundary layer
  - Processes are very complex
- Free shear flows easier
  - Instabilities are inviscid

DNS difficult, expensive

- Small scales develop far from wall in boundary layer
  - Hard to determine location in advance
- Numerically unstable without very fine grid

LES desirable

- Constant coefficient Smagorinsky model behaves poorly; relaminarizes flow
  - Too much viscosity introduced too early
- Need other models

More successful Models:

- Ramped Smagorinsky
  - Increase parameter C_d slowly starting from zero
  - Arbitrary; unclear how fast to increase parameter
- Dynamic model
- Deconvolution based models