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Large Eddy Simulations:

A Note on Derivation of the Equations

for the Subgrid Turbulent Kinetic Energies

by

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Abstract

In Large Eddy Simulations the turbulent stresses are defined as the difference between the filtered product of velocities $\overline{u_i u_j}$ and the product of the filtered velocities $\bar{u}_i \bar{u}_j$. Unlike in traditional Reynolds averaging this is *not* equal to the tensor of the fluctuations $\overline{u_i' u_j'}$. This also has some consequences on the transport equations for the turbulent kinetic energies. In the present note, transport equations for the turbulent kinetic energy of the subgrid energy are derived.

1. Filters

In the Dynamic model of Germano [1], two different filters are used. The grid filter Δ where the equations are filtered with as (box-filter are used in the present study)

$$\bar{\Phi}(x,t) = \int_{x-0.5\Delta x}^{x+0.5\Delta x} \Phi(\xi,t)d\xi \tag{1}$$

We can then apply a second, coarse filter (test filter) $\widehat{\Delta}$ where $\widehat{\Delta}/\Delta = 2$ defined as

$$\widehat{\bar{\Phi}}(x,t) = \int_{x-0.5\widehat{\Delta x}}^{x+0.5\widehat{\Delta x}} \bar{\Phi}(\xi,t)d\xi. \tag{2}$$

Associated with these filters we have subgrid turbulent kinetic energies k_{sgs} (for filter Δ) and K (for filter $\widehat{\Delta}$).

2. Derivation of the transport equation for k_{sgs}

The incompressible Navier-Stokes equations reads

$$\frac{\partial u_i}{\partial t} + (u_i u_j)_{,j} = -\frac{1}{\rho} p_{,i} + \nu u_{i,jj}. \tag{3}$$

The momentum equation for the filtered velocity $\bar{u}_i$ reads

$$\frac{\partial \bar{u}_i}{\partial t} + (\bar{u}_i \bar{u}_j)_{,j} = -\frac{1}{\rho} \bar{p}_{,i} + \nu \bar{u}_{i,jj} - \tau_{ij,j} \tag{4}$$

where

$$\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j. \tag{5}$$

Multiply Eq. 3 by u_i and filter the equation, multiply Eq. 4 by $\bar{u}_i$ and subtract the latter from the former and we get

$$\begin{aligned} &\underbrace{\overline{u_i \frac{\partial u_i}{\partial t}} - \bar{u}_i \frac{\partial \bar{u}_i}{\partial t}}_{\text{term 1}} + \underbrace{\overline{u_i (u_i u_j)_{,j}} - \bar{u}_i (\bar{u}_i \bar{u}_j)_{,j}}_{\text{term 2}} = \\ &- \underbrace{\frac{1}{\rho} \left(\overline{u_i p_{,i}} - \bar{u}_i \bar{p}_{,i} \right)}_{\text{term 3}} + \underbrace{\nu \overline{u_i u_{i,jj}} - \nu \bar{u}_i \bar{u}_{i,jj}}_{\text{term 4}} + \underbrace{\bar{u}_i \tau_{ij,j}}_{\text{term 5}}. \end{aligned} \tag{6}$$

Term 1 gives

$$\overline{u_i \frac{\partial u_i}{\partial t}} - \bar{u}_i \frac{\partial \bar{u}_i}{\partial t} = \frac{\partial \frac{1}{2} \overline{u_i u_i}}{\partial t} - \frac{\partial \frac{1}{2} \bar{u}_i \bar{u}_i}{\partial t} = \frac{\partial k_{sgs}}{\partial t} \tag{7}$$

where we have defined

$$k_{sgs} \equiv \frac{1}{2} (\overline{u_i u_i} - \bar{u}_i \bar{u}_i) = \frac{1}{2} \tau_{ii} \tag{8}$$

Defining

$$\bar{k} \equiv \frac{1}{2} \bar{u}_i \bar{u}_i, \; k \equiv \frac{1}{2} \overline{u_i u_i}$$

where

$$k = \bar{k} + k_{sgs} \tag{9}$$

term 2 can be rewritten as

$$\begin{aligned} &\overline{u_i (u_i u_j)_{,j}} - \bar{u}_i (\bar{u}_i \bar{u}_j)_{,j} = \frac{1}{2} \left\{ \overline{u_i u_i u_j} - \bar{u}_i \bar{u}_i \bar{u}_j \right\}_{,j} = \\ &\left\{ \frac{1}{2} \overline{u_i u_i u_j} - \bar{k} \bar{u}_j \right\}_{,j} = \left\{ \frac{1}{2} \overline{u_i u_i u_j} - (k - k_{sgs}) \bar{u}_j \right\}_{,j} \end{aligned} \tag{10}$$

For **Term 3** we get

$$\frac{1}{\rho} \left(\overline{u_i p_{,i}} - \bar{u}_i \bar{p}_{,i} \right) = \frac{1}{\rho} \left[\overline{u_i p} - \bar{u}_i \bar{p} \right]_{,i} \tag{11}$$

Term 4 can be rewritten as

$$\begin{aligned} \nu \left\{ \overline{u_i u_{i,jj}} - \bar{u}_i \bar{u}_{i,jj} \right\} &= \nu \left\{ \overline{(u_i u_{i,j})_{,j} - u_{i,j} u_{i,j}} - \left[(\bar{u}_i \bar{u}_{i,j})_{,j} - \bar{u}_{i,j} \bar{u}_{i,j} \right] \right\} \\ &= \nu \left\{ \overline{\frac{1}{2} (u_i u_i)_{,jj} - u_{i,j} u_{i,j}} - \left[\frac{1}{2} (\bar{u}_i \bar{u}_i)_{,jj} - \bar{u}_{i,j} \bar{u}_{i,j} \right] \right\} \\ &= \nu (k_{sgs})_{,jj} - (\overline{u_{i,j} u_{i,j}} - \bar{u}_{i,j} \bar{u}_{i,j}) \end{aligned} \tag{12}$$

Finally, **Term 5** reads

$$\bar{u}_i\tau_{ij,j} = \left(\bar{u}_i\tau_{ij}\right)_{,j} - \bar{u}_{i,j}\tau_{ij} \tag{13}$$

The equation for the subgrid kinetic energy k_{sgs} can now be assembled as

$$\begin{aligned}\frac{\partial k_{sgs}}{\partial t} + (\bar{u}_j k_{sgs})_{,j} = -\bar{u}_{i,j}\tau_{ij} - \left\{\frac{1}{2}\overline{u_iu_iu_j} - k\bar{u}_j + \frac{1}{\rho}\overline{u_jp} - \frac{1}{\rho}\bar{u}_j\bar{p} - \bar{u}_i\tau_{ij}\right\}_{,j} \\ +\nu(k_{sgs})_{,jj} - \nu\left(\overline{u_{i,j}u_{i,j}} - \bar{u}_{i,j}\bar{u}_{i,j}\right)\end{aligned} \tag{14}$$

Note that if we follow Germano [2] and introduce *generalized* central moments (as we, in fact, already have done for the stresses in Eq. 5)

$$\begin{aligned}\mathcal{T}_f(u_i,u_j) &\equiv \tau_{ij} = \overline{u_iu_j} - \bar{u}_i\bar{u}_j \\ \mathcal{T}_f(u_i,u_j,u_k) &= \overline{u_iu_ju_k} - \bar{u}_i\tau_{jk} - \bar{u}_j\tau_{ik} - \bar{u}_k\tau_{ij} - \bar{u}_i\bar{u}_j\bar{u}_k \\ \mathcal{T}_f(u_i,p/\rho) &= \frac{1}{\rho}\left(\overline{u_ip} - \bar{u}_i\bar{p}\right)\end{aligned} \tag{15}$$

In the equation for turbulent kinetic energy the diffusion term includes a term like $\frac{1}{2}\overline{u_iu_iu_j}$. The second equation can for $i=k$ re-written as

$$\frac{1}{2}\mathcal{T}_f(u_i,u_i,u_j) = \frac{1}{2}\overline{u_iu_iu_j} - \bar{u}_i\tau_{ij} - \frac{1}{2}\bar{u}_j\tau_{ii} - \frac{1}{2}\bar{u}_i\bar{u}_i\bar{u}_j \tag{16}$$

Eq. 14 can be written on the form we are used to see the equation for turbulent kinetic energy, i.e.

$$\begin{aligned}\frac{\partial k_{sgs}}{\partial t} + (\bar{u}_j k_{sgs})_{,j} = -\bar{u}_{i,j}\mathcal{T}_f(u_i,u_j) - \left\{\frac{1}{2}\mathcal{T}_f(u_j,u_i,u_i) + \mathcal{T}_f(u_j,p/\rho)\right\}_{,j} \\ +\nu(k_{sgs})_{,jj} - \nu\mathcal{T}_f(u_{i,j},u_{i,j})\end{aligned} \tag{17}$$

3. Derivation of the transport equation for K

Apply the (coarse) test filter to Eq. 4 so that

$$\frac{\partial\widehat{\bar{u}}_i}{\partial t} + \left(\widehat{\bar{u}}_i\widehat{\bar{u}}_j\right)_{,j} = -\frac{1}{\rho}\widehat{\bar{p}}_{,i} + \nu\widehat{\bar{u}}_{i,jj} - T_{ij,j} \tag{18}$$

where

$$T_{ij} = \widehat{\overline{u_iu_j}} - \widehat{\bar{u}}_i\widehat{\bar{u}}_j. \tag{19}$$

The stresses L_{ij} with length scales ℓ between the two filters ($\Delta < \ell < \widehat{\Delta}$) are related to τ_{ij} and T_{ij} as [1,3]

$$L_{ij} = T_{ij} - \widehat{\tau}_{ij} \tag{20}$$

Equations 5,19,20 give

$$L_{ij} = \widehat{\bar{u}_i\bar{u}_j} - \widehat{\bar{u}}_i\widehat{\bar{u}}_j \tag{21}$$

and we see that L_{ij} is *computable* from the resolved velocities.

Now we repeat the procedure in Section 2, but for the test level, i.e. we multiply Eq. 3 by u_i and filter the equation twice (both grid and test filter), and multiply Eq. 18 by $\widehat{\bar{u}}_i$ and take the difference and we get the transport equation for $K \equiv \frac{1}{2}T_{ii}$

$$\begin{aligned}\frac{\partial K}{\partial t} + (\widehat{\bar{u}}_j K)_{,j} = -\widehat{\bar{u}}_{i,j}T_{ij} - \left\{\frac{1}{2}\widehat{\overline{u_iu_iu_j}} - \widehat{k}\widehat{\bar{u}}_j + \widehat{\overline{u_jp/\rho}} - \widehat{\bar{u}}_j\widehat{\bar{p}/\rho} - \widehat{\bar{u}}_iT_{ij}\right\}_{,j} \\ +\nu K_{,jj} - \nu\left(\widehat{\overline{u_{i,j}u_{i,j}}} - \widehat{\bar{u}}_{i,j}\widehat{\bar{u}}_{i,j}\right)\end{aligned} \tag{22}$$

or, using generalized moments (see Eq. 15), we get

$$\begin{aligned}\frac{\partial K}{\partial t} + \left(\widehat{\bar{u}}_jK\right)_{,j} = -\widehat{\bar{u}}_{i,j}\mathcal{T}_{fg}\left(u_i, u_j\right) \\ -\left\{\frac{1}{2}\mathcal{T}_{fg}\left(u_j, u_i, u_i\right) + \mathcal{T}_{fg}\left(u_j, p/\rho\right)\right\}_{,j} + \nu K_{,jj} - \mathcal{T}_{fg}\left(u_{i,j}, u_{i,j}\right)\end{aligned} \tag{23}$$

where $\mathcal{T}_{fg}$ denotes that both the grid and the test filter have been applied. For the stresses, for example, we have

$$\mathcal{T}_{fg}(u_i, u_j) \quad \equiv \quad T_{ij} = \widehat{\overline{u_iu_j}} - \widehat{\bar{u}}_i\widehat{\bar{u}}_j \tag{24}$$

4. A One-Equation Dynamic Subgrid Model

In the dynamic subgrid model the subgrid stresses are computed from

$$\tau_{ij}^a = -2C\Delta^2|\bar{S}|\bar{S}_{ij} \tag{25}$$

where τ_{ij}^a denotes the anisotropic part of τ_{ij}, and $\bar{S}_{ij}$ is the strain tensor of the resolved velocities. The coefficient C is computed dynamically [2,4,5].

If we solve a transport equation for k_{sgs}, the stress tensor can be expressed as [6]

$$\tau_{ij}^a = -2C\Delta k_{sgs}^{\frac{1}{2}}\bar{S}_{ij} \tag{26}$$

where k_{sgs} is obtained from its transport equation. Below we derive a transport equation for k_{sgs} where the unknown terms are modelled.

Equations 17,23 can be written on symbolic form

$$C_{k_{sgs}} - D_{k_{sgs}} \quad = \quad P_{k_{sgs}} - \varepsilon_{k_{sgs}} \tag{27}$$

$$C_K - D_k \quad = \quad P_K - \varepsilon_K \tag{28}$$

(29)

where we have convection ($C_{k_{sgs}}$, C_K), diffusion ($D_{k_{sgs}}$, D_k), production ($P_{k_{sgs}}$, P_K) and dissipation ($\varepsilon_{k_{sgs}}$, ε_K) and where (see Eqs. 17,23)

$$
\begin{aligned}
C_{k_{sgs}} &= \frac{\partial k_{sgs}}{\partial t} + (\bar{u}_j k_{sgs})_{,j} \\
D_{k_{sgs}} &= -\left\{\frac{1}{2}\mathcal{T}_f(u_j,u_i,u_i) + \mathcal{T}_f(u_i,p)\right\}_{,j} + \nu(k_{sgs})_{,jj} \\
P_{k_{sgs}} &= -\bar{u}_{i,j}\mathcal{T}_f(u_i,u_j) \\
\varepsilon_{k_{sgs}} &= \nu\mathcal{T}_f(u_{i,j},u_{i,j}) \\
C_K &= \frac{\partial K}{\partial t} + \left(\widehat{\bar{u}}_j K\right)_{,j} \\
D_K &= -\left\{\frac{1}{2}\mathcal{T}_{fg}(u_j,u_i,u_i) + \mathcal{T}_{fg}(u_i,p)\right\}_{,j} + \nu K_{,jj} \\
P_K &= -\widehat{\bar{u}}_{i,j}\mathcal{T}_{fg}(u_i,u_j) \\
\varepsilon_K &= -\mathcal{T}_{fg}(u_{i,j},u_{i,j})
\end{aligned}
$$

If we estimate the dissipation as

$$
\varepsilon_{k_{sgs}} = C_* \frac{k_{sgs}^{\frac{3}{2}}}{\Delta}, \quad \varepsilon_K = C_* \frac{K^{\frac{3}{2}}}{\widehat{\Delta}} \tag{30}
$$

we obtain

$$
C_{k_{sgs}} - D_{k_{sgs}} = P_{k_{sgs}} - C_* \frac{k_{sgs}^{\frac{3}{2}}}{\Delta} \tag{31}
$$

$$
C_K - D_K = P_K - C_* \frac{K^{\frac{3}{2}}}{\widehat{\Delta}} \tag{32}
$$

The subgrid turbulent kinetic energy, k_{sgs}, is essentially a local quantity. Indeed, the Smagorinsky model is based on the assumption of local equilibrium of k_{sgs} [7], i.e. $P_{k_{sgs}} - \varepsilon_{k_{sgs}} = 0$. A better assumption would be to set the filtered right-hand side of k_{sgs} equation (Eq. 31) to that of the K equation (Eq. 32), i.e.

$$
\widehat{P}_{k_{sgs}} - \frac{1}{\Delta}\widehat{C_* k_{sgs}^{\frac{3}{2}}} = \left(P_K - C_* \frac{K^{\frac{3}{2}}}{\widehat{\Delta}}\right) \Rightarrow C_*^{n+1} = \left(P_K - \widehat{P}_{sgs} + \widehat{C_*^n k_{sgs}^{\frac{3}{2}}}/\Delta\right)\frac{\widehat{\Delta}}{K^{\frac{3}{2}}} \tag{33}
$$

In Eq. 33, C_*^n is kept inside the filtering process. Following Piomelli and Liu [8], the dynamic coefficient under the filter is taken at the old time step. The modelled k_{sgs} equation can now be written [9]

$$
\frac{\partial k_{sgs}}{\partial t} + \frac{\partial}{\partial x_j}(\bar{u}_j k_{sgs}) = \frac{\partial}{\partial x_j}\left(\langle C\rangle_{xyz}\Delta k_{sgs}^{\frac{1}{2}}\frac{\partial k_{sgs}}{\partial x_j}\right) + 2\nu_{sgs}\bar{S}_{ij}\bar{S}_{ij} - C_*\frac{k_{sgs}^{\frac{3}{2}}}{\Delta} \tag{34}
$$

To ensure numerical stability, a *constant* value of C in space ($\langle C \rangle_{xyz}$) is used in the momentum equations as well as in the diffusion term in the k_{sgs} equation. This is determined by requiring that the production in the whole computational domain should remain the same, i.e.

$$\langle 2C\Delta k_{sgs}^{\frac{1}{2}} \bar{S}_{ij}\bar{S}_{ij}\rangle_{xyz} = 2\langle C\rangle_{xyz}\langle \Delta k_{sgs}^{\frac{1}{2}} \bar{S}_{ij}\bar{S}_{ij}\rangle_{xyz} \tag{35}$$

The idea is to include all local dynamic information through the source terms of the transport equation for k_{sgs}. This is probably physically more sound since large local variations in C appear only in the source term, and the effect of the large fluctuations in the dynamic coefficients will be smoothed out in a natural way. In this way, it turns out that the need to restrict or limit the dynamic coefficient is eliminated altogether.

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