DETERMINISTIC LARGE-EDDY SIMULATION OF ISOTROPIC TURBULENCE

Robert Rubinstein
Computational AeroSciences Branch,
NASA Langley Research Center
Hampton, Virginia 23681-2199, USA
r.rubinstein@larc.nasa.gov

Timothy T. Clark
Northrop Grumman Information Technology,
Advanced Technology Division
Albuquerque, New Mexico 87106, USA
tim.clark@ngc.com

ABSTRACT

By 'deterministic large-eddy simulation' we mean the simulation of a reduced number of modes in a spectral closure with a simpler model representing the effect of the unresolved modes. The physical ideas behind standard subgrid models translate into this deterministic setting, in which testing and validation become particularly easy. We reformulate the Smagorinsky model and the one-equation subgrid model of Yoshizawa and Horiuti in this setting and apply them to the transient evolution of forced turbulence. We also formulate (stochastic) LES models in which the subgrid model is a spectral closure.

INTRODUCTION

Large eddy simulation computes a reduced number of degrees of freedom in a turbulent flow, the resolved large scales, and models the effects of the unresolved scales. The justification is that while the resolved large scales are determined by flow-specific features like boundaries and instability mechanisms, the unresolved small scales may have universal features that make them susceptible to modeling strategies, generally based on Kolmogorov's theory of the universal small scales of motion in turbulent flows.

The problem of modeling small scales can also be posed in an entirely deterministic setting: starting with a spectral closure model and a given number of modes, we can ask whether the number of modes can be reduced by replacing the unresolved modes by some simpler model. This program is reasonable theoretically because no property of turbulence that is invoked to formulate models is not a property of the spectral closure we use; it is reasonable practically because it makes testing of the physical ideas behind subgrid models becomes very simple. We will show that some basic subgrid models: the Smagorinsky model and the one-equation subgrid model of Yoshizawa and Horiuti (1985), can be reformulated in this deterministic setting. We will also propose a deterministic reformulation of the dynamic Smagorinsky model and briefly outline the use of spectral closure as a subgrid model.

DETERMINISTIC SUBGRID MODELING IN GENERAL

We use an analytically simple closure, the CMSB model of (Rubinstein and Clark, 2004), in which the spectral evolution equation is

$$\dot{E}(k,t) = P(k,t) - \frac{\partial \mathcal{F}}{\partial k} - 2\nu k^2 E(k,t) \tag{1}$$

where

$$\mathcal{F}(k) = C_H \left\{ \int_0^k d\kappa\ \kappa^2 E(\kappa) \int_k^\infty dp\ \theta(p) E(p) - \int_0^k d\kappa\ \kappa^4 \int_k^\infty dp\ \theta(p) \frac{E(p)^2}{p^2} \right\} \tag{2}$$

and the time scale θ satisfies

$$\dot{\theta}(k) = 1 - \eta(k)\theta(k) - \nu k^2 \theta(k) \tag{3}$$

with eddy damping

$$\eta(k) = C_\eta \theta(k) \int_0^k dp\ p^2 E(p) \tag{4}$$

Suppose that we compute with this model, up to some scale k_∞ at which E is vanishingly small. The analog of LES is a computation on a reduced space of explicitly resolved modes $k \le k_m \ll k_\infty$ with some model accounting for interactions with the unresolved modes $k \ge k_m$. In view of this connection, the scale k_m may be called the *filter scale.* It is possible to imitate the basic physical idea of any LES model in this context.

Decomposing the transfer term into resolved and unresolved components,

$$\frac{\partial \mathcal{F}}{\partial k} = C_H \left\{ \left[\int_k^{k_m} dp\ \theta(p) E(p) \right] k^2 E(k) - \left[\int_0^k d\kappa\ \kappa^2 E(\kappa) \right] \theta(k) E(k) - k^4 \left[\int_k^{k_m} dp\ \theta(p) E(p)^2 p^{-2} \right] \right.$$

$$+\left[\int_0^k d\kappa\, \kappa^4\right] \theta(k)E(k)^2 k^{-2}\Bigg\}$$
$$+\nu_m k^2 E(k) - f_m k^4 \tag{5}$$

For this spectral closure, the effect of the subgrid scales enters entirely through the two quantities:

$$\nu_m = C_H \int_{k_m}^{\infty} dp\ \theta(p)E(p) \tag{6}$$
$$f_m = C_H \int_{k_m}^{\infty} dp\ \theta(p)E(p)^2 p^{-2} \tag{7}$$

an eddy viscosity and a forcing term respectively.

In general, subgrid modeling will also require the flux through the filter scale, $\mathcal{F}_m = \mathcal{F}(k_m)$ which is expressed in terms of ν_m and f_m as

$$\begin{aligned}\mathcal{F}_m &= C_H \left\{ \int_0^{k_m} d\kappa\ \kappa^2 E(\kappa) \int_{k_m}^{\infty} dp\ \theta(p)E(p) \right. \\ &\quad \left. - \int_0^{k_m} d\kappa\ \kappa^4 \int_{k_m}^{\infty} dp\ \theta(p) \frac{E(p)^2}{p^2} \right\} \\ &= \nu_m \int_0^{k_m} d\kappa\ \kappa^2 E(\kappa) - \frac{1}{5} k_m^5 f_m \end{aligned} \tag{8}$$

The integral on the right side of this equation defines the resolved strain

$$\bar{S}^2 = \int_0^{k_m} d\kappa\ \kappa^2 E(\kappa) \tag{9}$$

so that more simply,

$$\mathcal{F}_m = \nu_m \bar{S}^2 - \frac{1}{5} k_m^5 f_m \tag{10}$$

THE DETERMINISTIC SMAGORINSKY MODEL

The simplest subgrid model is the *Smagorinsky model*, which postulates that the subgrid scales are in a local Kolmogorov steady state in which

$$E(k) = C_K \epsilon^{2/3} k^{-5/3} \tag{11}$$

and

$$\theta(k) = C_\theta \left[k^3 E(k)\right]^{-1/2} \tag{12}$$

Eqs. (11) and (12) express the subgrid quantities ν_m and f_m in terms of ϵ and k_m. Whereas k_m is the known resolution limit, ϵ is a new quantity requiring closure. The Smagorinsky model closes ϵ by assuming an instantaneous flux balance

$$\epsilon = \mathcal{F}(k_m) \tag{13}$$

between the resolved and unresolved scales.

Using Eqs. (11), (12), and (13) to close ν_m and f_m in Eqs. (6)–(7) leads to

$$\nu_m = c_1 \mathcal{F}_m^{1/3} k_m^{-4/3} \tag{14}$$
$$f_m = c_2 \mathcal{F}_m k_m^{-5} \tag{15}$$

To lighten the notation, the various model constants which arise are always written in the form c_i but not given explicitly; for example, in Eq. (14) $c_1 = 3C_H C_K / 4C_\theta$, and in Eq. (15), $c_2 = C_H C_K^2 / 5C_\theta$.

Substituting Eqs. (14)–(15) in the expression for the flux through the filter scale Eq. (5) leads to

$$\mathcal{F}_m = c_3 \mathcal{F}_m^{1/3} k_m^{-4/3} \bar{S}^2 - c_4 \mathcal{F}_m \tag{16}$$

consequently

$$\mathcal{F}_m = c_5 |\bar{S}|^3 k_m^{-2} \tag{17}$$

As in the classical Smagorinsky model, the flux depends on the resolved strain. Note also that the flux $\mathcal{F}_m$ is necessarily positive; although f_m appears in Eq. (10) with a negative sign, indicating that this term represents the *backscatter* of energy from small to large scales, the assumptions of the Smagorinsky model lead to the expression Eq. (17) which is necessarily positive, so that the net energy flux is always from resolved to subgrid scales.

The basic subgrid quantities in the deterministic Smagorinsky model can also be expressed in terms of the cutoff scale $\Delta_m \sim k_m^{-1}$ and $\bar{S}$ by replacing $\mathcal{F}_m$ by Eq. (17) as

$$\nu_m = c_1' \Delta_m^2 |\bar{S}| \tag{18}$$
$$f_m = c_2' |\bar{S}|^3 \Delta_m^7 \tag{19}$$
$$\mathcal{F}_m = c_5' \Delta_m^2 |\bar{S}|^3 \tag{20}$$

The expression for ν_m in Eq. (18) recovers the usual Smagorinsky model. Similarly, the expression for f_m coincides with the random force proposed by Leith (1990).

YOSHIZAWA-HORIUTI ONE-EQUATION MODEL

The Smagorinsky model makes two assumptions: Kolmogorov scaling of the subgrid scales, and a local flux balance. It can be generalized, either by retaining the assumption of a local flux balance and dropping Kolmogorov scaling (Bataille *et al.*, 2005), or by assuming Kolmogorov scaling but dropping the flux balance. We consider the one-equation model of Yoshizawa and Horiuti (1985) from the latter viewpoint. Assume that $\mathcal{F}_m$ and ϵ are independent and that ϵ satisfies the phenomenological relaxation equation

$$\dot{\epsilon} = C_Y \epsilon^{1/3} k_m^{2/3} (\mathcal{F}_m - \epsilon) \tag{21}$$

where $\mathcal{F}_m$ is defined by Eq. (17). This equation proves to be equivalent to the subgrid energy equation $\dot{k} = \mathcal{F}_m - k^{3/2}/L$ used by Yoshizawa and Horiuti. In steady state conditions, $\epsilon = \mathcal{F}_m$, as in the Smagorinsky model, but in general, a flux imbalance can exist.

VALIDATION OF THE SUBGRID MODELS

To test the subgrid models we begin with a sanity check by verifying that they can correctly maintain a Kolmogorov steady state. We run the CMSB model with 500 modes to a forced steady state beginning from a nearly zero spectrum. After 80000 time steps, an approximately steady state is achieved. Noting that the spectrum is nearly Kolmogorov already at 64000 time steps, we switch on the models with 20 mode resolution at 66000 time steps.

Figure 1 shows that the spectra computed using the deterministic Smagorinsky model can indeed be made to overlay the full model when the cutoff scale is set to $k_m = 20$. Figure 2 compares the resolved kinetic energy, the energy in the first 20 modes, with the energy predicted by the deterministic Smagorinsky model. When the subgrid model is turned on at 66000 time steps, the total energy immediately drops and correctly equals the energy of the resolved motion.

Finally, Figure 3 compares the dissipation rate with the energy flux predicted by the deterministic Smagorinsky model. When the model is turned on, the dissipation drops immediately to nearly zero because the dissipation scales are no longer resolved. But Figure 3 shows that the deterministic Smagorinsky model immediately supplies an energy flux through the cutoff scale exactly equal to the dissipation rate, thereby maintaining the correct energy balance. This result is of course consistent with the behavior of the resolved energy in Figure 2.

Similar verification is possible for the one-equation model.

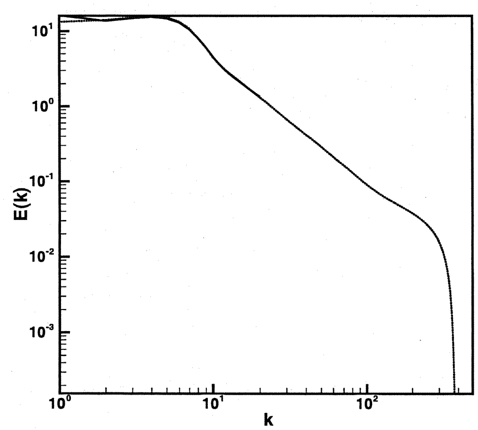

Figure 1: Spectra after 80000 time steps for CMSB model with 500 modes (dotted) and Smagorinsky model with 20 modes (solid). The graphs nearly superpose where both are defined ($k \leq k_m = 20$).

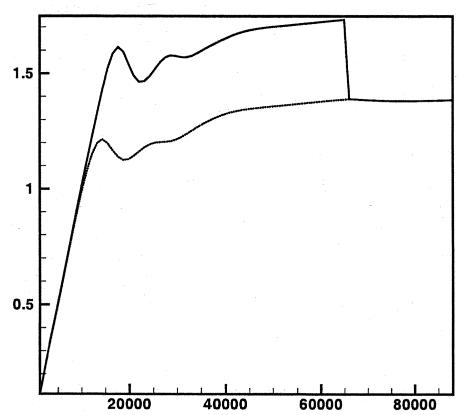

Figure 2: Kinetic energy computed by Smagorinsky model (solid) compared to resolved energy (dotted).

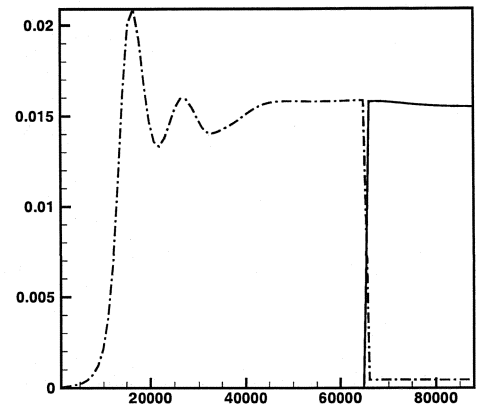

Figure 3: Dissipation (dot-dash) and subgrid flux from Smagorinsky model (solid).

TRANSIENT FORCED TURBULENCE

We next test the two subgrid models in transient forced turbulence by turning the models on at the beginning of the simulation instead of during the steady state. The subgrid models attempt to reproduce the resolved kinetic energy and the flux through the cutoff scale; the time evolution of the resolved kinetic energy is shown above in Figure 2 and the energy flux through k_m is shown in Figure 4. Both quantities exhibit strong dynamic behavior rather than simple relaxation: note in particular that the energy growth is not even monotonic. There is also a very distinct transient imbalance between dissipation and energy flux, although this imbalance cannot be captured by a subgrid model.

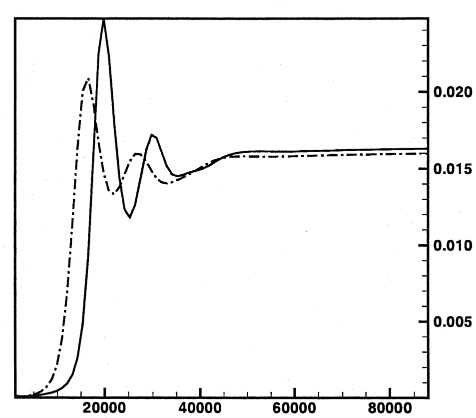

Figure 4: total dissipation (solid) and energy flux through filter scale (dot-dash).

Smagorinsky model

Figure 5 shows that the energy and dissipation evolution are very smooth; the overshoots in both which are evident in

Figures 2 and 4 are entirely absent. This smoothing effect corresponds to the frequently repeated observation that the Smagorinsky model is 'too diffusive.' The effect of increasing the number of resolved modes to 100 is shown in Figure 6. As expected, the evolution is closer to the original closure model but is still somewhat too smooth. But even this accuracy is available only at the expense of a rather highly resolved simulation. We emphasize that this comparison is not intended to discredit the Smagorinsky model; it simply suggests what may be lost by using such a simple subgrid model.

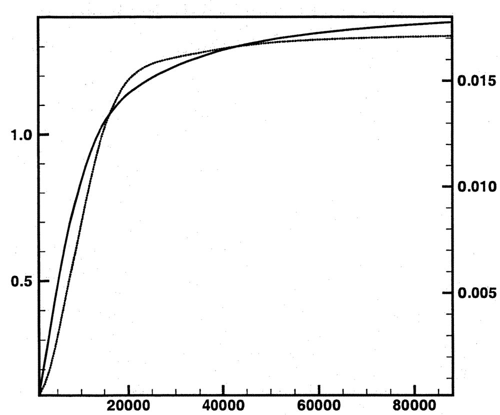

Figure 5: resolved kinetic energy (solid, left scale) and energy flux through filter scale (dotted, right scale) in deterministic Smagorinsky model at resolution 20.

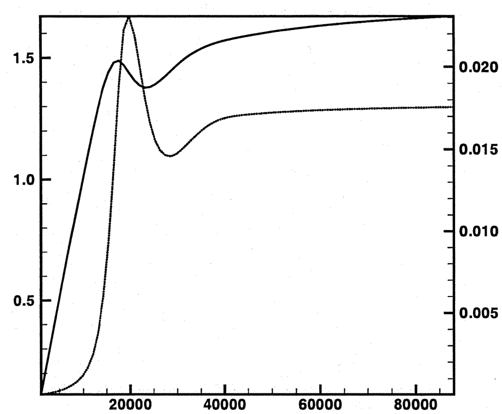

Figure 6: resolved kinetic energy (solid, left scale) and energy flux through filter scale (dotted, right scale) in deterministic Smagorinsky model at resolution 100.

Yoshizawa-Horiuti single-equation model

A limitation of this model in this test case is that the subgrid energy cannot build up if it vanishes initially. The model was only satisfactory when initiated after the subgrid energy had grown to some extent. In this test case, as few as 10 time steps could be used. The results are shown in Figure 7. Initiating the deterministic Smagorinsky model after the same number of time steps led to an insignificant change in the predictions.

The Yoshizawa-Horiuti model is superior to the Smagorinsky model in this test case because the evolution of both the resolved energy and the flux exhibit some dynamic behavior; although the simple linear relaxation postulated in Eq. (21) is far from accurate, it does at least capture the overshoot in the dissipation rate. Certainly, the linear relaxation assumption is preferable to the much cruder assumption of an instantaneous flux balance made in the Smagorinsky model.

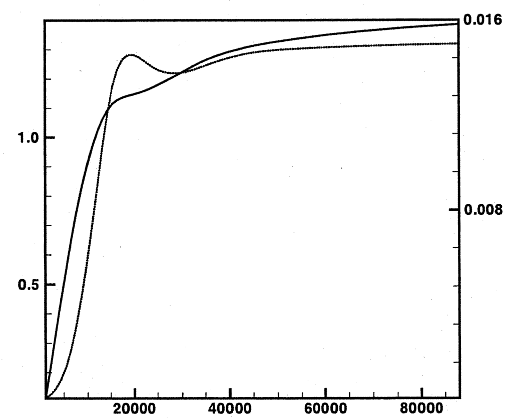

Figure 7: resolved kinetic energy (solid, left scale) and energy flux through filter scale (dotted, right scale) in Yoshizawa's single equation model

DYNAMIC SMAGORINSKY MODEL

Although there is no meaningful Germano identity in the deterministic setting, we can imitate the idea of the dynamic model as follows. Assume the Smagorinsky model in the form $\nu(k_m) = C k_m^{-2} \bar{S}(k_m)$ in which the constant C is unknown: we recall that its value follows from the flux balance on which the model is based. We can also obtain its value by comparing the viscosity at two different filter sizes, say k_m and $k_m/2$. Writing

$$\begin{aligned} \nu(k_m/2) &= C_H \int_{k_m/2}^{\infty} dp\ \theta(p) E(p) \\ &= C_H \int_{k_m/2}^{k_m} dp\ \theta(p) E(p) + \nu(k_m) \end{aligned} \tag{22}$$

and substituting the value of $\nu(k_m)$, then solving for C,

$$C = \frac{C_H \int_{k_m/2}^{k_m} dp\ \theta(p) E(p)}{(k_m/2)^{-2} \bar{S}(k_m/2) - (k_m)^{-2} \bar{S}(k_m)} \tag{23}$$

An important property of this deterministic dynamic model is that if the resolved energy spectrum is Kolmogorov, the constant C will revert to its 'equilibrium' value in Eq. (18). By allowing a departure from this equilibrium value, this model appears, like the Yoshizawa-Horiuti model, to relax the condition of a flux balance between resolved and unresolved scales: compare in this respect (Yoshizawa *et al.*, 1996). Unlike the Yoshizawa-Horiuti model, however, this model attempts to characterize the imbalance in terms of resolved quantities alone.

SPECTRAL CLOSURES AS SUBGRID MODELS

In the previous sections, the spectral closure has been substituted for the Navier-Stokes equations. We next describe the possibility of using the spectral closure as a subgrid model. The goal of this program is to model the interaction between resolved and unresolved scales more accurately. Replacing the spectral closure by simpler models permits systematic derivation of families of subgrid models.

CMSB LES model

We reconsider Eq. (1) with the closure assumption Eq. (5), written in terms of resolved and unresolved parts. This time, instead of replacint the small scales by a deterministic model, we replace the closure for the large scales by the exact equations of motion, with the unresolved terms reformulated as a Langevin model following Kraichnan (1971). The result is

$$\begin{aligned}\dot{u}_i(\mathbf{k}) = &-\frac{i}{2}P_{imn}(\mathbf{k})\int_{\Delta'} u_m(\mathbf{p})u_n(\mathbf{q})\\ &-\nu_m k^2 u_i(\mathbf{k}) + f_i(\mathbf{k})\end{aligned} \tag{24}$$

where

$$\int_{\Delta'} = \int_{p,q\leq k_m} d\mathbf{p}d\mathbf{q}\ \delta(\mathbf{k}-\mathbf{p}-\mathbf{q}) \tag{25}$$

restricts the nonlinear interaction to resolved modes alone, ν_m is defined by Eq. (6), and the random force f_i has the components (Kraichnan, 1971)

$$f_\alpha(\mathbf{k}) = \sqrt{C_B}w(t)k\int_{k_m}^{\infty} dp\ \theta(p)^{1/2}\frac{1}{p}v_\alpha(\mathbf{p})w_\alpha(\mathbf{p}) \tag{26}$$

where $w(t)$ is white noise with unit variance, and v_α and w_α are independent Gaussians with variance

$$\langle v_\alpha(\mathbf{k})v_\alpha(-\mathbf{k})\rangle = \langle w_\alpha(\mathbf{k})w_\alpha(-\mathbf{k})\rangle = \frac{1}{2\pi k^2}E(k) \tag{27}$$

It is straightforward to verify that the subgrid model defined by Eqs. (24)–(27) reproduces the original CMSB model provided that the triple correlations are replaced by the CMSB model on resolved scales.

Evidently, the subgrid quantities are defined in terms of the subgrid spectrum $E(p)$ and time scale $\theta(p)$. Again, we reverse our earlier procedures by taking their equations of motion to be the CMSB model equations with resolved quantities replaced by their values from the simulation. The resolved field enters these equations only through the resolved strain of Eq. (9); this quantity can be computed from the resolved field independently of spectral information as

$$\bar{S}^2 = \left\langle\left[\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right]^2\right\rangle \tag{28}$$

The subgrid equations are

$$\begin{aligned}\dot{E}(k) = &-C_B\left\{k^2E(k)\int_k^\infty dp\ \theta(p)E(p)\right.\\ &+\theta(k)E(k)\left[\bar{S}^2+\int_{k_m}^k d\kappa\ \kappa^2E(\kappa)\right]\\ &\left.-\frac{1}{5}k^3\theta(k)E(k)^2+k^4\int_k^\infty dp\ \frac{1}{p^2}\theta(p)E(p)^2\right\}\\ &-2\nu k^2E(k)\\ \dot{\theta}(k) = &\ 1-C_\eta\left[\bar{S}^2+\int_{k_m}^k d\kappa\ \kappa^2E(\kappa)\right]\theta(k)^2\end{aligned} \tag{29}$$

It is reasonable to interpret the term in the subgrid spectral evolution equation that contains $\bar{S}$ as the production of subgrid energy by the resolved field.

The main features of this model are that the couplings between resolved and unresolved quantities show both damping and forcing and that no assumptions about Kolmogorov scaling, scale separation or the like have been made. We have assumed that the unresolved motion is isotropic, however.

Heisenberg LES model

We obtain it from the previous model by dropping the random force contribution, and closing $\theta(k) = [k^3E(k)]^{-1/2}$. The relevant equations are

$$\begin{aligned}\dot{u}_i(\mathbf{k}) = &-\frac{i}{2}P_{imn}(\mathbf{k})\int_{\Delta'} u_m(\mathbf{p})u_n(\mathbf{q})\\ &-\nu_m k^2 u_i(\mathbf{k}) - 2\nu k^2E(k)\end{aligned} \tag{30}$$

where

$$\nu_m = C'_H\int_{k_m}^\infty dp\sqrt{\frac{E(p)}{p^3}} \tag{31}$$

The subgrid energy spectrum $E(p)$ satisfies

$$\begin{aligned}\dot{E}(k) = &\ C'_H\left\{-k^2E(k)\int_k^\infty dp\ \sqrt{\frac{E(p)}{p^3}}\right.\\ &\left.+\sqrt{\frac{E(k)}{k^3}}\left[\bar{S}^2+\int_{k_m}^k d\kappa\ \kappa^2E(\kappa)\right]\right\}\\ &-2\nu k^2E(k)\end{aligned} \tag{32}$$

The structure of this model is very simple: the subgrid scales act as an eddy viscosity in Eq. (30); they evolve according to Eq. (32) in which the resolved scales contribute to production of the subgrid motion through $\bar{S}$.

Smagorinsky model

The Smagorinsky model is obtained by two steps: first, assume that the subgrid energy spectrum is Kolmogorov, so that the eddy viscosity formula Eq. (31) becomes

$$\nu_m = c_6\epsilon^{1/3}k_m^{4/3} \tag{33}$$

Second, determine the new quantity ϵ, the subgrid dissipation rate, by assuming that the spectrum is in an (instantaneous) steady state, that is, by setting the left side of Eq. (32) to zero. The result is

$$c_7\epsilon^{2/3}k_m^{3/4} = \bar{S}^2 \tag{34}$$

Substituting this value of ϵ in Eq. (33) and expressing the filter size Δ_m in terms of k_m through $\Delta_m = 2\pi/k_m$, we recover the Smagorinsky model in the form Eq. (18).

Yoshizawa-Horiuti one-equation model

We reverse the logical order by considering a model more complex than the Smagorinsky. Integrating Eq. (32) over all subgrid scales gives the subgrid energy balance

$$\dot{K} = C_H \left[\int_{k_m}^{\infty} \sqrt{\frac{E(k)}{k^3}} dk \right] \bar{S}^2 - \epsilon \tag{35}$$

where ϵ is the subgrid dissipation rate. Assume, as in the Smagorinsky model, that $E(p)$ is Kolmogorov. We obtain

$$\dot{K} = \frac{3}{4} C_H C_K^{1/2} \epsilon^{1/3} k_m^{-4/3} \bar{S}^2 - \epsilon \tag{36}$$

but under our assumptions, K and ϵ are related through $K = (3/2)C_K \epsilon^{2/3} k_m^{-2/3}$; accordingly Eq. (36) can be written in terms of the subgrid dissipation rate alone as

$$\dot{\epsilon} = c_8 \epsilon^{1/3} k_m^{2/3} \left\{ c_9 \epsilon^{1/3} k_m^{-4/3} S^2 - \epsilon \right\} \tag{37}$$

which coincides with Eq. (21). The Smagorinsky model is simply the steady form of this equation obtained by setting the term in braces to zero.

REFERENCES

Bataille, F., Rubinstein, R., and Hussaini, M. Y., 2005, "Eddy viscosity and diffusivity modeling," preprint.

Germano, M., Piomelli, U., Moin, P., and Cabot, W. H., 1991, "A Dynamic Subgrid-scale Eddy Viscosity Model," *Phys. Fluids A* Vol. 3, p. 1760.

Kraichnan, R. H., 1971, "An Almost-Markovian Galilean-Invariant Turbulence Model," *J. Fluid Mech.*, Vol. 47, p. 513.

Leith, C. E., 1990, "Stochastic Backscatter in a Subgrid-scale Model: Plane Shear Mixing Layer," *Phys. Fluids A*, Vol. 2, p. 297.

Rubinstein, R., and Clark, T. T., 2004, "A Generalized Heisenberg Model for Turbulent Spectral Dynamics," *Theor. Comput. Fluid Dynamics* Vol. 17, p. 249.

Smagorinsky, J., 1963, "General Circulation Experiments with the Primitive Equations. I. The Basic Experiment," *Mon. Weather Rev.* Vol. 91, p. 99.

Yoshizawa, A., and Horiuti, K., 1985, "A Statistically-derived Subgrid-scale Kinetic-energy Model for the Large-Eddy Simulation of Turbulent Flows," *J. Phys. Soc. Japan*, Vol. 54, pp. 2834–2839.

Yoshizawa, A., Tsubokura, M., Kobayashi, T., and Taniguchi, N., 1996, "Modeling of the Dynamic Subgrid-Scale Viscosity in Large Eddy Simulation," *Phys. Fluids* Vol. 8, p. 2254.