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SUB-GRID SCALE MODELING: CORRECT MODELS AND OTHERS

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ABSTRACT

One approach to studying turbulent convection in stars is through the use of large computers with a technique called Large Eddy Simulation (LES). Since no computer presently available, or even projected in the foreseeable future, can resolve all of the scales that characterize a fully developed turbulent flow, the LES technique resolves the largest scales, while it models the "unresolved" scales with a sub-grid scale (SGS) model. In the astrophysical literature, two such models have been used.

It is the purpose of this paper to show that the first of the SGS models (1) contradicts Galilei invariance, (2) employs an incorrect timescale (Eulerian instead of Lagrangean), (3) contradicts the Kolmogorov inertial law and the Richardson diffusion law, (4) misinterprets dynamical and kinematic effects, and (5), from the numerical view point, gives rise to a turbulent viscosity much larger than it ought to be.

The second SGS model has none of the above problems, the only shortcoming being its incompleteness, since it was originally devised for shear rather than buoyancy dominated flows. Thus, it must be improved—a process that present knowledge of turbulence allows us to carry out quite systematically.

In conclusion, the first SGS should be avoided, while the second should be used and improved.
Subject headings: convection — methods: numerical — stars: interiors — turbulence

1. INTRODUCTION

Historically, the one-point closure model, also known as the Reynolds stress approach (Speziale 1991; Shih & Shabbir 1992; Lumley 1978), has been widely and successfully used to describe all types of turbulent flows—except, thus far, the ones of astrophysical interest where the model is only recently being considered, in spite of its more than 50 yr of successes in other fields where convection, shear, and rotational effects are present. Since compressibility effects can be incorporated into these models (Sarkar 1990; Canuto 1996), the only outstanding feature differentiating astrophysical settings are the radiative losses, which, however, are a separate issue from the heart of the nonlinear problems that constitute the major hurdle in constructing a reliable model of turbulence.

While the Reynolds stress models (also called second-order closure [SOC]) are being continuously improved, in the last decade a new methodology has come to the fore, based on the use of large computers that attempt to solve the Navier-Stokes equations (NSE) themselves: a technique known as Large Eddy Simulation (LES). Such techniques are presently employed in astrophysics (Canuto 1994). The LES method, however, faces a basic difficulty: a fundamental and model-independent law of turbulence (Landau & Lifshitz 1982; Lesieur 1991; McComb 1990) shows that the number of degrees of freedom of a fully developed three-dimensional turbulent flow, or alternatively, the number of grid points N, scales with the Reynolds number Re as

$$N \sim \mathrm{Re}^{9/4} . \tag{1a}$$

Since today's fastest computers can handle at most $N \sim 10^9$, the Re that one is really able to resolve is

$$\mathrm{Re}_{\max} \sim 10^4 , \tag{1b}$$

which is several orders of magnitude smaller than the one encountered in either geophysics ($\mathrm{Re} \sim 10^8$) or astrophysics ($\mathrm{Re} \sim 10^{10}$). In other words, one can fully resolve a flow that is considerably less turbulent than the real flow one needs to study. To quantify the problem in terms of convective parameters, we recall that, since the Reynolds number Re, the Prandtl number σ, and the Rayleigh number Ra are related by

$$\sigma \mathrm{Re}^2 \sim \mathrm{Ra}(\Phi S^{-1/2})^{2/3} , \tag{2a}$$

where Φ is a dimensionless function representing the ratio between turbulent and molecular conductivity, and S is given by

$$\Phi = \frac{\chi_t}{\chi} , \quad S = \sigma \mathrm{Ra} . \tag{2b}$$

We also have

$$N \sim \mathrm{Re}^{9/4} \sim \sigma^{-9/4} S^{9/8} (\Phi S^{-1/2})^{3/4} . \tag{2c}$$

We must distinguish two cases:

1. *Laboratory convection.*—In this case, one usually employs substances with

$$\sigma \sim 1 \tag{2d}$$

(Kerr 1996; Castaing et al. 1989). For a fully developed, highly efficient turbulent regime, $\Phi \sim S^{1/2}$, and so the maximum Ra one can resolve is

$$(\mathrm{Ra})_{\max} \sim 10^8 . \tag{2e}$$

Indeed, the latest numerical approach to turbulent convection (Kerr 1996) has resolved all the scales up to $\mathrm{Ra} \sim 10^7$. Since one of the major goals of this calculation was to study the newly discovered (Castaing et al. 1989) transition to "hard turbulence," that is, the change in the Nusselt number (Nu) versus Ra relationship

$$\mathrm{Nu} \sim (\mathrm{Ra})^{1/3} \rightarrow \mathrm{Nu} \sim (\mathrm{Ra})^{2/7} , \tag{2f}$$

and since the latter is known to set in at the *lowest* Ra ($\sim 10^4$), in the case of the *largest* aspect ratio, the calculations were carried out for an aspect ratio of ~ 7 and, indeed, they confirmed the existence of such a transition. Thus, the numerical approach known as direct numerical simulation (DNS) and the laboratory data confirmed each other quite convincingly. There is no need to employ an LES unless a transition to a new exponent of Ra is found at even higher values of Ra.

2. *Stellar convection.*—In the middle of the convective zone (CZ) of a star, turbulence is so efficient,

$$\nabla = \nabla_{ad} + O(10^{-8}) , \tag{3a}$$

that one hardly needs a sophisticated turbulence model. The interesting and challenging case is near the borders of the CZ, where convection is inefficient and therefore

$$\nabla = \nabla_{ad} + O(1) . \tag{3b}$$

The interpretation of the most recent helioseismological data (Baturin & Miranova 1995; Monteiro, Christensen-Dalsgaard, & Thompson 1996) depend critically on the proper quantification of $O(1)$, that is, on the convective model one employs. In this region, we have ($\Phi \sim S^2$)

$$S \leq 1 , \tag{3c}$$

and so equation (2c) becomes ($\sigma \sim 10^{-10}$) ,

$$N \sim 10^{-4}\sigma^{-9/4}S^{9/4} \approx 10^{16} , \tag{3d}$$

which is $\sim 10^7$ larger than the maximum $N_{max} \sim 10^9$ one can resolve with today's computers (even with the upcoming teraflop machines, one is still some 8 orders of magnitude short of what is required). Thus, the behavior of the most important region of a stellar CZ cannot and will not be fully describable by a numerical approach alone, since a huge number of scales remain unresolved. One can easily be convinced that, with $N_{max} \sim 10^9$, *one actually resolves a few percent of all the scales.* This has two consequences: (a) one must supplement the LES with a physical model to represent the subgrid scales, and (b) the LES results depend on how complete a physical model one adopts for the SGS.

In this paper, we shall discuss the two SGS models used in astrophysical LES calculations and show that the first is physically incorrect on several accounts, while the second is physically correct, but its physical content needs to be improved.

2. THE SGS PROBLEM

At the level of the fundamental dynamic equations, it can be said very succinctly that an LES resolve not the full NSE but the truncated version,

$$\left[\frac{\partial}{\partial t} + \nu k^2 + \tau^{-1}(k\,|\,k_*)\right]u^<_\alpha(\boldsymbol{k}) = \sum_j M^<_{\alpha\beta\gamma}(\boldsymbol{k})u^<_\beta(\boldsymbol{j})u^<_\gamma(\boldsymbol{k}-\boldsymbol{j}) , \tag{4a}$$

where the symbol " < " indicates that one resolves the scales smaller than a limiting wavenumber

$$k < k_* \sim \Delta^{-1} . \tag{4b}$$

The effect of the unresolved scales is represented by $\tau(k\,|\,k_*)$, which can also be represented as a dynamical, subgrid viscosity,

$$\tau^{-1}(k\,|\,k_*) = k^2\nu_d(k\,|\,k_*) . \tag{4c}$$

The choice of this timescale is therefore a crucial matter.

2.1. *Incorrect SGS Model*

Suppose one identifies τ with the Eulerian timescale τ_E, given by

$$\tau_E^{-1} \sim e^{1/2}k \sim Vk , \tag{5a}$$

where e is the turbulent kinetic energy, which, being contributed mostly by the large scales, justifies the second expression, where V is the velocity of the largest eddies. The choice (eq. [5a]) physically means that the SGS are governed not by dynamical effects, which are local and therefore entail only on local properties like k and ϵ (the rate of energy input), but rather by kinematic effects, also known as *sweeping effects.* This presents an immediate problem because kinematic effects cannot govern the small scales, since they are in effect a Doppler shift

$$\omega - kV , \tag{5b}$$

which, once integrated, cannot affect the eddy energy spectrum. This has been amply discussed in the appropriate literature on turbulence (Orszag 1973; L'vov 1991), where it is shown that the effect of large scales is akin to a uniform convection that cannot distort an eddy and transfer energy, therefore defeating the very purpose of an SGS of representing the energy drawn by the small scales from the large ones. Being a purely kinematic rather than a dynamic effect, equation (5a) cannot represent the basis for a SGS. In addition, the use of uniform convection as per equation (5a) would contradict Galilei invariance of the many times moments, since, for example, the correlation timescale t–t' of two-time energy spectrum would be dominated by τ rather than by local dynamical effects.

In the development of theories of turbulence (Kraichnan 1958, 1959; Leslie 1973), the use of equation (5a) and the implication of large-scale convective effects on small scales was recognized as the main reason for the failure to obtain the Kolmogorov law,

$$E(k) \sim \epsilon^{2/3}k^{-5/3} , \tag{6a}$$

which is an amply validated law in turbulence. Rather, equation (5a) yields

$$E(k) \sim \epsilon^{1/2}V^{1/2}k^{-3/2} , \tag{6b}$$

which is not found experimentally and which we shall discuss in § 3. The law (eq. [6a]), even if taken as an empirical law, indicates the absence of effects of kinematic origin that are represented in equation (6b) by the presence of V. Kolmogorov law indicates instead that the convective effects of the large scale are dynamically unimportant, since an eddy that is superimposed on a uniform velocity field is convected without exchange of energy. One can say that the message of equation (6a) is that small eddies are statistically independent of the large eddies. Alternatively but equivalently, the energy transfer among small eddies is local; that is to say, it cannot depend on the large-scale peculiarities of the flow. Equation (5a) contradicts these facts.

Finally, one can also see that equation (5a) contradicts the Richardson diffusion law (Lesieur 1991; McComb 1990; Leslie 1973). In general, one has that the diffusion coefficient D is defined as

$$D = \frac{1}{2}\frac{d}{dt}X^2(t) = \langle v^2\rangle\tau , \tag{6c}$$

where $X^2(t)$ represent the mean square distance $X(t)$ traveled by a diffusing particle in a turbulent medium. We have purposely written the last equality in such a way as to allow more generality. Suppose we choose $\tau = \tau_L$ and therefore $\langle v^2\rangle = e$. We get a diffusion coefficient that is

$$D \sim e^{1/2}l , \tag{6d}$$

where l represents the largest scales. Such a law does not reproduce the well-known Richardson law,

$$D \sim \epsilon^{1/3}l^{4/3} . \tag{6e}$$

In conclusion, equation (5a) is not physically acceptable. For an astrophysical LES, see Nordlund (1982).

2.2. *Correct SGS Model*

In a turbulent flow, the smallest scale one strives to resolve is the dissipation length scale, given by

$$k_d \equiv (\nu^3\epsilon^{-1})^{-1/4} . \tag{7a}$$

Since the ratio of k_d to k_0 (smallest wavenumber) is

$$\frac{k_d}{k_0} = \frac{L}{l} = \mathrm{Re}^{3/4} , \tag{7b}$$

a full numerical simulation must resolve all the scales from L all the way down to l. Since this is not possible in a large Re situation, one resolves all of the scales up to, for instance, k_*, where

$$k_0 \le k_* \ll k_d . \tag{7c}$$

To mimic a DNS, an LES must try to extend k_* as close as possible to k_d. This means that the ν that appears in the original equations should actually be as close as possible to the one obtained from inverting (eq. [7a]), that is,

$$\nu_d \sim \epsilon^{1/3} k_*^{-4/3} . \tag{7d}$$

The corresponding timescale is then

$$\tau^{-1} \sim k_*^{2/3}\epsilon^{1/3} , \tag{7e}$$

which is quite different from equation (5a) in that it no longer contains any memory of the convective effects of the large scales. In fact, it is an entirely local expression, in agreement with the general arguments that only dynamical, rather than kinematic, effects ought to govern the eddy energy distribution.

An alternative, more formal, way to derive equation (7e) is by way of avoiding the choice of a Eulerian timescale, and instead, use the Lagrangean timescale

$$\tau_{\mathrm{L}}^{-1} = \left[\int_0^k E(q) dq q^2\right]^{1/2} , \tag{8a}$$

which we recognize as the timescale based on the square vorticity. If one substitutes Kolmogorov law eq. [6a], one obtains

$$\tau_{\mathrm{L}}^{-1} \sim k_*^{2/3}\epsilon^{1/3} , \tag{8b}$$

which is identical to equation (7e). It is important to recall that once the failure to derive Kolmogorov law was recognized as being due to the choice of a Eulerian timescale, the same theory was reformulated in Lagrangean terms (Kraichnan 1965, 1996). This resulted, as expected, in the derivation of the correct Kolmogorov law. One can also interpret equation (7d) as a function that removes kinetic energy at the resolved scales (Leith 1996) that would otherwise attempt to cascade to unresolved scales, creating an erratic behavior in the numerical simulation.

In practical terms, one can also say that, since on general grounds

$$\tau_{\mathrm{E}} < \tau_{\mathrm{L}} , \tag{8c}$$

The dynamical viscosity generated by Eulerian timescale overestimates the true value of ν_d, notwithstanding the fact that it is not the correct physical representation of the SGS physics.

Finally, let us note that if in equation (6c) we interpret v^2 and τ as

$$v^2 = v^2(k) = kE(k) \sim k^{-2/3}\epsilon^{2/3} \tag{8d}$$

$$\tau^{-1} = \tau_{\mathrm{L}}^{-1} \sim kv(k) \sim k[kE(k)]^{1/2} \sim k^{2/3}\epsilon^{1/3} , \tag{8e}$$

respectively, we obtain

$$D \sim \epsilon^{1/3}k^{-4/3} \sim \epsilon^{1/3}l^{4/3} , \tag{8f}$$

which coincides with the Richardson law (eq. [6f]).

Equation (7d) was used in Sofia & Chan (1984), Hossian & Mullan (1991), Fox, Sofia, & Chan (1991), Fox, Theobald, & Sofia (1991), and Xie & Toomre (1991).

2.3. *Smagorinsky Model*

In actual LES calculations (Sofia & Chan 1984; Hossian & Mullan 1991; Fox et al. 1991a, 1991b; Xie & Toomre 1991), the SGS is not used in the form (7d) but in an equivalent expression, as we now show. If we assume that locally production equals dissipation, we have

$$\epsilon = -\tau_{ij} S_{ij} , \tag{9a}$$

where τ_{ij} is the Reynolds stress and S_{ij} the shear generated by the largest scales on the SGS. If we write

$$\tau_{ij} = -2\nu_d S_{ij} , \tag{9b}$$

we derive

$$\epsilon = \nu_d S^2 , \tag{9c}$$

where $S^2 \equiv 2S_{ij}S_{ij}$ is the mean rate of shear. Thus, substituting in equation (7d) yields

$$\nu_d \sim k_*^{-2} S \sim \Delta^2 S , \tag{9d}$$

which is the well-known Smagorinsky model (Lesieur 1991; McComb 1990), widely used in a large variety of LES.

3. KOLMOGOROV LAW; EULERIAN AND LAGRANGEAN TIMESCALES

We have stated that depending on which timescale one chooses, one may or may not obtain Kolmogorov law. Here we suggest a proof of such a statement. Consider the NSE written in the $k, \omega \equiv \kappa$ representation:

$$(-i\omega + \nu k^2)u_i(\kappa) = f_i(\kappa) + P_{ijl}(\boldsymbol{k})M_{jl}(\kappa) , \tag{10a}$$

where f_i represents an arbitrary external force and $\boldsymbol{M}$ represents the nonlinear terms

$$M_{ij}(\kappa) \equiv \int d\kappa' u_i(\kappa')u_j(\kappa - \kappa') . \tag{10b}$$

Here P_{ijl} is the standard projection operator. We are interested in the correlation function

$$\langle u_i(\kappa)u_j(\kappa')\rangle \equiv Q_{ij}(\kappa, \kappa') = P_{ij}(k)Q(k, \omega)\delta(\kappa + \kappa') . \tag{10c}$$

The energy spectrum E(k) is given by

$$E(k) = 4\pi k^2 \int Q(\kappa) d\omega . \tag{10d}$$

In the absence of nonlinear interactions, we have simply

$$Q(\kappa) \to Q_0(\kappa) = \frac{\phi(\kappa)}{\omega^2 + \nu^2 k^4} , \tag{11a}$$

where ϕ is the correlation function of the external force f_i—that is, $\phi_{ij} \sim f_i f_j$. In the presence of nonlinearities, we can use the formal solution of the NSE first given by Wyld

(1961) and usually referred to as the Wyld-Dyson solution. Equation (11a) becomes

$$Q(\kappa) = \frac{\phi + \tilde{\phi}}{\omega^2 + \tau_d^{-2}} . \tag{11b}$$

This is formally interpreted as implying that the effects of the nonlinearities are twofold: on the one hand, they renormalize the external forcing by introducing a new forcing $\tilde{\phi}$; and they also renormalize the viscosity by introducing a new timescale, τ_d (d for dynamical). The Wyld-Dyson solution is formal in that it does not provide the expressions for $\tilde{\phi}$ or τ_d. In the region of interest in the construction of an SGS, we can neglect ϕ by definition—since the external force is no longer acting—the dynamical behavior of the small scales being governed by the ghost forcing $\tilde{\phi}$. Since, of course, the knowledge of $\tilde{\phi}$ and τ_d is equivalent to the full knowledge of the turbulent solution, we shall employ a form for $\tilde{\phi}$ suggested in Monin & Yaglom (1971) that corresponds to the case of a turbulent forcing that is delta correlated in time. Though not the most general case, it serves the purpose of the present case. The expression is

$$\tilde{\phi} \sim -k^{-2}\Pi(k)E^{-1}(k)\frac{\partial}{\partial k}E(k) , \tag{12a}$$

where $\Pi(k)$ is the energy flux (the derivative of which is the transfer), which, in the present situation, is constant and equal to the rate of energy input ϵ. Thus, using equations (10d) and (11b), we obtain

$$E(k) \sim -\tau_d(k)E^{-1}(k)\frac{\partial}{\partial k}E(k) , \tag{12b}$$

which can be integrated to yield

$$E(k) \sim \epsilon\left[\int \tau_d^{-1}(k)dk\right]^{-1} . \tag{12c}$$

At this point, we must choose the variable τ_d. Let us begin with the Lagrangean case,

$$\tau_d^{-1} \equiv \tau_{\rm L}^{-1} \sim k^{2/3}\epsilon^{1/3} . \tag{13a}$$

Equation (12c) yields

$$E(k) \sim \epsilon^{2/3}k^{-5/3} , \tag{13b}$$

which is Kolmogorov law (eq. [6a]). On the other hand, if we choose the Eulerian timescale

$$\tau_d^{-1} \equiv \tau_{\rm E}^{-1} \sim ke^{1/2} , \tag{13c}$$

we obtain from equation (12c)

$$E(k) \sim V^{1/2}\epsilon^{1/2}k^{-3/2} , \tag{13d}$$

since $\epsilon \sim ke^{3/2}$. Equation (13d) is the spectrum first obtained by Kraichnan (1958), and it does not conform to the observed law (eq. [13b]).

4. CONCLUSIONS

LES methodology has clear advantages and equally clear limitations. The advantage is that it circumvents one of the major problems presented by any type of turbulence—the occurrence of a huge number of scales—by separating them into two broad categories, which are then treated differently:

1. The largest eddies, which are sensitive to the boundary conditions, the details of the stirring mechanisms, etc., and, which therefore lack universality, are treated (resolved) numerically without introducing adjustable parameters. The downside is that the number of such scales is only a fraction of the total.
2. Therefore, the remaining, unresolved scales are assumed, without a real proof, to be more homogeneous, more isotropic, less dependent on the geometry and injection peculiarities, and therefore more amenable to a theoretical model. That is the goal of the SGS.

We have already suggested (Canuto 1994) a hierarchy of SGS models that include stable stratification, rotation, shear, convection, etc. The simplest possible model coincides with the Smagorinsky model, upon which one builds physically more complete models. Such procedure ought to be implemented since the background model is physically sound though incomplete.

The other SGS model we have discussed and that has been used in stellar/solar LES calculations, is physically unacceptable at a rather basic level because it contradicts several well-established laws, ranging from fundamental ones such as Galilei invariance to Kolmogorov inertial law. Irrespective of how "reasonable" the ensuing LES results might appear, they are the result of a flawed representation of a large fraction of eddies.

The construction of a new SGS model based on a recent model of fully developed turbulence (Canuto & Dubovikov 1996a, 1996b, 1996c), and that is parameter free, is under way.

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