An *ad hoc* operational method to compensate for absent turbulence modes in an insufficiently resolved numerical simulation.

A.J. Young and W.D. McComb
Department of Physics, University of Edinburgh, Mayfield Road, Edinburgh, Scotland, EH9 3JZ
(June 22, 1999)

If the largest resolved wavenumber in a numerical simulation of isotropic turbulence is too small, then it is well known that the energy spectrum will depart from its expected monotonic decrease with increasing wavenumber and will instead begin to increase. By detecting this increase, and making it the basis of a feedback loop, we show that an operational method is capable of modifying the instantaneous velocity field such that the unphysical features of the spectrum are suppressed. When this procedure is interpreted in terms of an effective viscosity, it agrees well with the usual result obtained by comparison with a fully resolved direct numerical simulation.

The numerical simulation of systems with many degrees of freedom has been of great interest in physics for some time and in practice there is often a requirement to reduce the number of degrees of freedom which have to be explicitly simulated. In fluid dynamics, the recognition that numerical simulation could be employed if one reduced the number of degrees of freedom goes back to meteorological work in the 1960s, when the idea of a large-eddy simulation (LES) was first put forward: for a recent review, see [?].

In applying the concept of LES to spectral simulations, the conventional approach is to resolve Fourier modes with wavenumbers up to some $k = K_C$, and to model the nonlinear transfer to the (now nonexistent) modes with $k \geq K_C$ by means of some additional viscosity acting on the resolved modes. In general one may expect such a subgrid viscosity to depend on both the local wavenumber k and on the cutoff wavenumber K_C. (Also one may expect some other nonlinear effects to be present, in addition to the Newtonian-type effective viscosity.) In this paper we introduce a novel method of compensating for the absence of nonlinear transfers.

We begin by restricting our attention to the numerical simulation of stationary, homogeneous, isotropic turbulence of an incompressible fluid [?,?,?,?,?,?,?,?,?,?]. We work in Fourier wavenumber space where the degrees of freedom are the Fourier modes $\boldsymbol{u}(\boldsymbol{k},t)$ of the velocity field as defined in terms of the velocity field $\boldsymbol{u}(\boldsymbol{x},t)$ by

$$\boldsymbol{u}(\boldsymbol{x},t) = \sum_{\boldsymbol{k}} \boldsymbol{u}(\boldsymbol{k},t) e^{i\boldsymbol{k}\cdot\boldsymbol{x}}. \tag{1}$$

In this situation, the main quantity of interest is the energy spectrum, as given by

$$E(k,t) = 2\pi k^2 \left\langle \boldsymbol{u}(\boldsymbol{k},t)\cdot\boldsymbol{u}(-\boldsymbol{k},t)\right\rangle, \tag{2}$$

where $\langle\cdots\rangle$ denotes an ensemble average.

We have carried out a numerical simulation with a resolution of $N = 256$ and at a Taylor-Reynolds number of $R_\lambda \approx 190$. For this simulation we chose the fluid kinematic viscosity to be $\nu = 10^{-3}$ with dissipation rate $\varepsilon = 0.149$ (in arbitrary units), giving $L_B/L(t) \approx 5$ where the computational box side is L_B and the integral length scale is L; and $K_{\max}/k_d \approx 1.2$, where k_d is the Kolmogorov dissipation wavenumber. These values are reasonably well in line with current practice [?]. The forcing, which is necessary to maintain a steady state, takes the following form:

$$\boldsymbol{f}(\boldsymbol{k},t) = \begin{cases} \varepsilon \boldsymbol{u}(\boldsymbol{k},t)/(2E_f(t)) & \text{if } 0 < k < k_f \\ 0 & \text{otherwise,} \end{cases} \tag{3}$$

where $E_f(t)$ is the energy contained within the forced modes and $k_f = 1.5$. This forcing scheme is the same as that used by Machiels [?].

The idea underlying the proposed operational procedure may be explained by first considering what happens in a truncated simulation where the maximum wavenumber is significantly less than the dissipation wavenumber. As is well known, one of the most obvious effects of such a truncation is an upturn at the high wavenumber end of the energy spectrum, corresponding to a local build up of energy. This is illustrated in Fig. ?? where we have plotted an energy spectrum taken from a truncated (i.e. unresolved) simulation after several integration steps. Our aim is to locate this upturn and to correct it in some way. In general terms, the proposed algorithm may be described as follows. First, we identify the onset of the upturn with the minimum of the derivative, $\mathrm{d}(\ln E)/\mathrm{d}(\ln k)$, and denote the corresponding wavenumber by $k = k_{\text{upturn}}$. Second, we use the value of this derivative at k_{upturn} to generate a corrected energy spectrum by extrapolating forward from this point. The intended result of this operation is shown in Fig. ?? as a dashed line. We note that, although our present method is believed to be new, the idea of conducting such direct experiments on a numerical simulation is now of growing interest [?,?,?,?].

The following algorithm is carried out after each time-integration step:

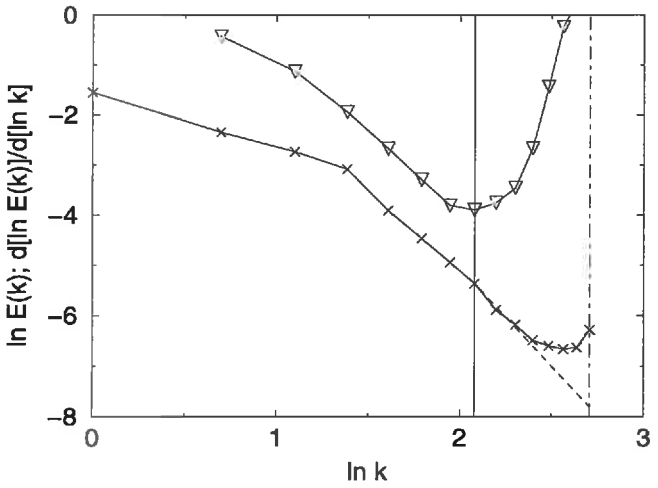

FIG. 1. An energy spectrum with an upturn (crosses), its derivative, $\mathrm{d}(\ln E)/\mathrm{d}(\ln k)$ (triangles) and a schematic indication of what the corrected energy spectrum should look like after application of the operational feedback procedure (dashed line). The vertical solid and dot-dashed lines indicate the positions of k_{upturn} and K_C respectively.

1. A smoothed spectrum E_S is obtained by fitting a polynomial in $\ln k$ to $\ln E$, where $E(k)$ is the usual energy spectrum obtained from the velocity field by shell-averaging. A fourth-order polynomial was used for this, as it was found that lower-orders do not reproduce the upturn, while significantly higher-orders follow the spectrum too closely to give adequate smoothing.

2. The minimum of the derivative, $\mathrm{d}(\ln E_S)/\mathrm{d}(\ln k)$, is obtained analytically.

3. The gradient, $\mathrm{d}(\ln E_S)/\mathrm{d}(\ln k) = \Gamma$, at $k = k_{\mathrm{upturn}}$ is used to extrapolate the original shell-averaged spectrum, E, forward in wavenumber from k_{upturn} in order to give the corrected spectrum:

$$E_C(k) = \begin{cases} E(k) & \text{if } k \le k_{\mathrm{upturn}}; \\ E(k_{\mathrm{upturn}})(k/k_{\mathrm{upturn}})^{\Gamma} & \text{if } k \ge k_{\mathrm{upturn}}. \end{cases} \tag{4}$$

4. The ratio of the corrected spectrum to the shell-averaged spectrum then provides the basis for a correction of the velocity field, thus:

$$\boldsymbol{u}_C(\boldsymbol{k}) = \boldsymbol{u}(\boldsymbol{k})\sqrt{E_C(k)/E(k)}. \tag{5}$$

As a first test for this procedure, we compared three cases: a resolved simulation with $N = 256$, an unresolved simulation with $N = 64$ (i.e. without compensation for the missing modes) and a compensated simulation with $N = 64$ (following the procedure outlined above). All simulations were allowed to run for approximately 24 evolved eddy turnover times.

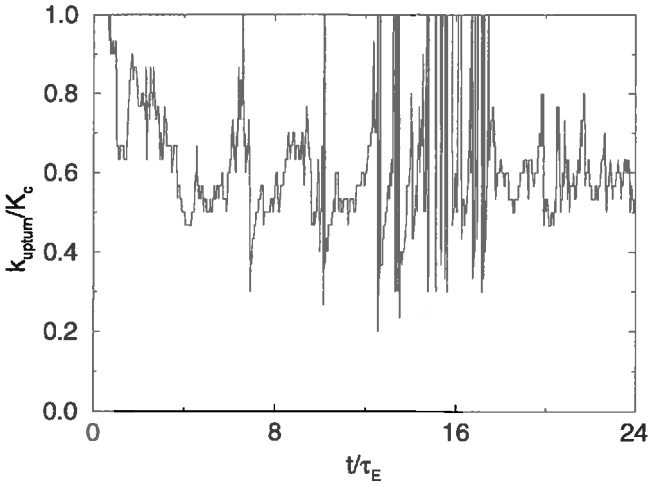

FIG. 2. k_{upturn}/K_C plotted as a function of time. A value of $k_{\mathrm{upturn}} = K_C$ indicates that the operational method has not amended the velocity field in any way. The time axis has been scaled on τ_E, the eddy turnover time.

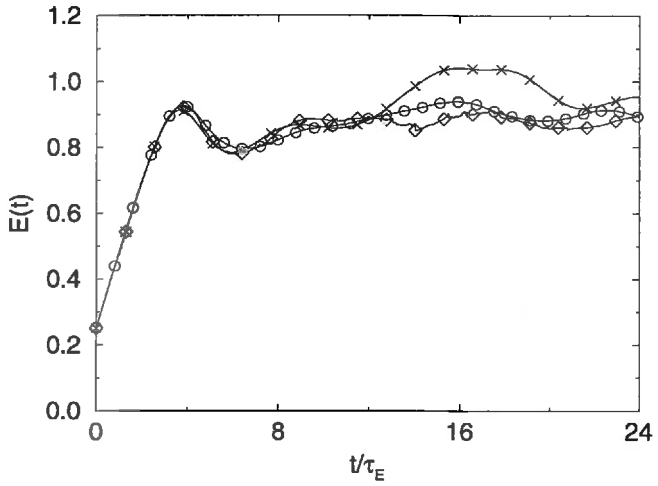

FIG. 3. Evolution of total energy showing the results from the resolved 256^3 simulation (circles), the unresolved 64^3 simulation (crosses) and the compensated 64^3 simulation (diamonds).

In Fig. ?? we have plotted k_{upturn}/K_C against time. We see that it appears to fluctuate around a value of $k_{\mathrm{upturn}}/K_C \approx 0.5$, and we note a period of rapid fluctuations between 12 and 18 eddy turnover times.

Figure ?? shows the evolution with time of the total energy for each of the three simulations. The mean values found by averaging over time, with error estimates given by twice the standard deviation, were: resolved simulation with $N = 256$, $E = 0.90 \pm 0.04$; unresolved simulation with $N = 64$, $E = 0.96 \pm 0.12$; and compensated simulation with $N = 64$, $E = 0.89 \pm 0.03$. Evidently, despite the large number of eddy turnover times, there is no significant difference between the mean levels (the fluctuations are a different matter).

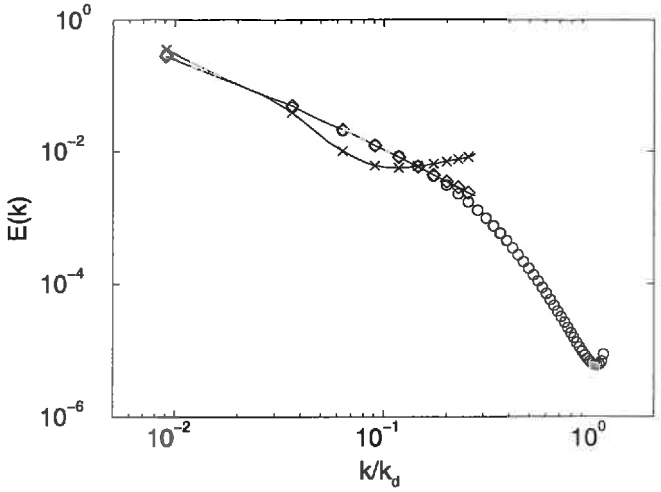

FIG. 4. Average evolved energy spectra, showing the results from the resolved 256^3 simulation (circles), the unresolved 64^3 simulation (crosses) and the compensated 64^3 simulation (diamonds).

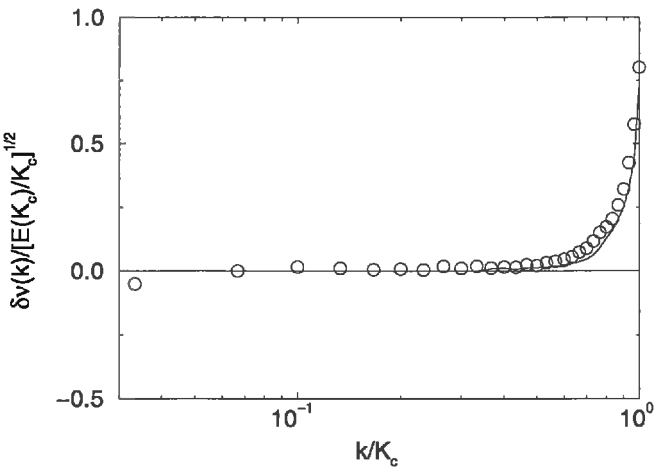

FIG. 5. Average equivalent eddy viscosity computed from the compensated 64^3 simulation (line) compared with the 'empirical' eddy viscosity computed from the resolved 256^3 simulation (circles).

However, when we turn to 'microscopic' effects, the picture is quite different. Energy spectra, time-averaged over the final 15 eddy turnover times of the simulations, are given in Fig. ??. Here, the problems in the unresolved simulation are clearly seen, with the upturn dominating the energy spectrum. In contrast, the spectrum obtained from the compensated simulation, shows a good match with that obtained from the resolved simulation.

We have also investigated the effect of this feedback procedure on the velocity derivative skewness $S(t)$. The time-averaged value obtained from the resolved simulation, with an estimate of the error (given by twice the standard deviation) is $S = -0.50 \pm 0.07$ in agreement with experiment [?]. However, as noted by Dubois, Jauberteau and Zhou [?], the simple act of truncating a velocity field in Fourier space — and hence removing the small scales — will cause a reduction in the skewness. Therefore, in order to make a fair comparison with the results of our two 64^3 simulations, we have also computed the skewness based on a number of truncated 256^3 velocity fields. This gave a value of $S = -0.33 \pm 0.04$. The unresolved simulation with $N = 64$ gave a value of $S = -0.12 \pm 0.04$, indicating a distribution closer to the Gaussian case than for the resolved 256^3 result, while the compensated simulation gave a value of $S = -0.30 \pm 0.05$ in agreement with the result obtained from the truncated 256^3 fields.

Furthermore, it is interesting to relate our operational approach to the more conventional use of an effective viscosity to represent the effect of high-k modes, which has its origins in the work of Heisenberg [?]. It was Kraichnan [?] who first expressed the eddy viscosity as,

$$\delta\nu(k) = -\frac{T_{\rm SG}(k)}{2k^2E(k)}, \qquad (6)$$

where $T_{\rm SG}(k)$ represents energy transfers due to interactions with subgrid modes. Kraichnan used an analytical turbulence theory — the test-field model — to obtain an eddy viscosity which exhibited the now familiar characteristics of a constant asymptotic value for $k \ll K_C$ and a cusp at $k = K_C$, and this approach inspired much other work of this type.

It is possible to interpret the compensated simulation presented here in terms of the usual spectral large-eddy simulation by generating an effective eddy viscosity, $\delta\nu(k, t_n)$, at each time step, which would give an enhanced dissipation rate equivalent to the rate of energy removal due to the operational procedure. It is readily shown that in going from t_n to t_{n+1} this takes the form:

$$\delta\nu(k, t_n) \equiv \frac{E(k, t_{n+1}) - E_C(k, t_{n+1})}{2k^2\delta t E(k, t_n)}. \qquad (7)$$

The time-averaged result is plotted in Fig. ?? alongside an empirical eddy viscosity, computed from a resolved velocity field (see [?] for details of this type of calculation). There is good agreement between the two.

The operational procedure outlined here appears to give promising results at the relatively low Reynolds number we have explored. But, it must be borne in mind that it depends on an assumption about the form of the spectrum, if we truncate the high-wavenumber modes. Under the present restricted circumstances, there is only one possible outcome. In the absence of nonlinear transfer to higher-k modes, the energy must increase at the cutoff wavenumber. This guarantees the stability of the feedback process. However, we should remind ourselves that although this is true for the simple spectral method used here, and for isotropic turbulence, it is not necessarily true for more realistic flows. This is a matter which would require further investigation.

Moreover, even with the present idealized turbulence, at higher Reynolds numbers we might expect the eddy

viscosity to have a significant non-zero asymptote as $k \to 0$ which this operational procedure, by its very nature, will be unable to reproduce. It may be possible to overcome this limitation by combining the operational procedure with an enhanced viscosity, thus generating a hybrid approach. One possible candidate for this would be a renormalization group (RG) calculation recently reported [?].

Of course RG methods have had great success in comparable problems involving many length scales in microscopic physics [?], but there is now considerable pessimism about their use in turbulence [?]. To the present writers, such pessimism seems entirely justified if one seeks (as is usually the case) to apply field-theoretic methods to a macroscopic deterministic system such as fluid turbulence. However, we have previously argued elsewhere [?] that the basic RG algorithm may be applied to turbulence as an example of deterministic chaos exhibiting scaling behaviour. More recently we have concluded that such an application has heuristic validity, in that it seems to represent the turbulent energy transfers quite accurately; but, like all eddy-viscosity models, is incapable of adequately representing the phase effects which dominate interscale momentum transfers [?]. Nevertheless, this implies that the RG viscosity can represent the dissipation rate correctly, a result which is in line with current thinking on subgrid modelling from other points of view [?,?,?]. As the two methods have complementary ranges of validity in wavenumber space, there is a case for investigating their joint use, and again this kind of approach is in tune with other investigations of subgrid modelling. This is the subject of current work.

Both authors acknowledge the support and facilities provided by the Edinburgh Parallel Computing Centre. A.Y. acknowledges the financial support of the Engineering and Physical Sciences Research Council. W.D.McC. thanks Bernard Geurts and Javier Jiménez for helpful discussions and is happy to acknowledge the hospitality and support of the Isaac Newton Institute.

[1] M. Lesieur and O. Metais, Ann. Rev. Fluid Mech. **28**, 45 (1996).
[2] R.M. Kerr, J. Fluid Mech. **153**, 31 (1985).
[3] P.K. Yeung and S.B. Pope, J. Fluid Mech. **207**, 531 (1989).
[4] A. Vincent and M. Meneguzzi, J. Fluid Mech. **225**, 1 (1991).
[5] Z.-S. She, S. Chen, G. Doolen, R.H. Kraichnan, and S.A. Orszag, Phys. Rev. Lett. **70**, 3251 (1993).
[6] L.-P. Wang, S. Chen, J.G. Brasseur, and J.C. Wyngaard, J. Fluid Mech. **309**, 113 (1996).
[7] S. Chen, K.R. Sreenivasan, and M. Nelkin, Phys. Rev. Lett. **79**, 1253 (1997).
[8] P.K. Yeung and Y. Zhou, Phys. Rev. E **56**, 1746 (1997).
[9] J. Jiménez and A.A. Wray, J. Fluid Mech. **373**, 255 (1998).
[10] K.R. Sreenivasan, Phys. Fluids **10**, 528 (1998).
[11] L. Machiels, Phys. Rev. Lett. **79**, 3411 (1997).
[12] J. Jiménez, *'Energy transfer and constrained simulations in isotropic turbulence'*, in 'Fluid Physics' (Eds. M.G. Velarde and C.I. Christov) World Scientific 543–547 (1995).
[13] J.A. Domaradzki and E.M. Saiki, Phys. Fluids **9**, 2149 (1997).
[14] B.J. Geurts, Phys. Fluids **9**, 3585 (1997).
[15] S. Stolz and N.A. Adams, Phys. Fluids **99**, 1699 (1999).
[16] A. Tsinober, E. Kit, and T. Dracos, J. Fluid Mech **242**, 169 (1992).
[17] T. Dubois, F. Jauberteau, and Y. Zhou, Physica D **79**, 390 (1997).
[18] W. Heisenberg, Proc. R. Soc. A **195**, 402 (1948).
[19] R.H. Kraichnan, J. Atmos. Sci. **33**, 1521 (1976).
[20] J.A. Domaradzki, R.W. Metcalfe, R.S. Rogallo, and J.J. Riley Phys. Rev. Lett. **58**, 547 (1987).
[21] W.D. McComb and C. Johnston, Newton Institute Preprint NI99005-TRB, submitted for publication.
[22] K.G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[23] G.L. Eyink, Phys. Fluids **6**, 3063 (1997).
[24] W.D. McComb and A.G. Watt, Phys. Rev. Lett. **65**, 3281 (1990); W.D. McComb, W. Roberts, and A.G. Watt, Phys. Rev. A **45**, 3507 (1992); W.D. McComb and A.G. Watt, Phys. Rev. A **46**, 4797 (1992).
[25] J. Jiménez and R.D. Moser, AIAA Paper 98-2891 (1998).
[26] B. Vreman, B. Geurts, and H. Kuerten, J. Fluid Mech. **339**, 357 (1997).