Explicit-Scales Projections of the Partitioned Non-Linear Term in Direct Numerical Simulation of the Navier-Stokes Equation

David McComb and Alistair Young
Department of Physics and Astronomy
University of Edinburgh
James Clerk Maxwell Building
Mayfield Road
Edinburgh EH9 3JZ
United Kingdom

Abstract
In this paper we consider the properties of the internal partitions of the nonlinear term, obtained when a filter with a sharp cutoff is introduced in wavenumber space. We see what appears to be some degree of independence of the choice of the position of the cutoff wavenumber for both instantaneous and time-integrated partitioned nonlinearities. We also investigate the basic idea of an eddy-viscosity model for subgrid terms and have found that while phase modelling will be very poor, amplitude modelling can be far more successful.

Introduction
As is well known, full numerical simulation of any significant turbulent flow lies far beyond the scope of current computational resources, the main problem being the large number of degrees of freedom involved in the problem. As these degrees of freedom may be represented by, for instance, the number of independently excited modes in wavenumber space, the problem becomes one of eliminating modes, in some statistical sense, in order to bring the reduced number of degrees of freedom within the capacity of current (or even future) computers. One such way by which we may systematically obtain such a reduction in the number of modes is by the use of a Renormalization Group (RG) calculation. A general account of the background to this work has been given in the review by McComb (1995).

In this study, we are undertaking direct numerical simulations (DNS) of homogeneous, isotropic, incompressible turbulence in a box with periodic boundary conditions, in order to assess the underlying feasibility of using RG to reduce the size of the computational problem. We have already reported some results on the use of conditional averages (McComb et al. 1997, Machiels 1997) as previously formulated by McComb et al. (1992) and McComb and Watt (1992). In the present paper we concentrate on the Hilbert space partitions of the nonlinear terms and their filtered projections in order to assess the appropriateness of the ‘eddy viscosity’ concept. Results of this study should have direct relevance to large eddy simulations (LES) in general, as well as to RG.

The Partitioned Nonlinear Term
Consider the forced Navier-Stokes equation for stationary turbulence,

\[ \left( \frac{\partial}{\partial t} + \nu \mathbf{k}^2 \right) \mathbf{u}(\mathbf{k}, t) = M_{\alpha \beta \gamma} \mathbf{k} \int d^3 j u_\beta(j, t) u_\gamma(k - j, t) + f_\alpha(k, t), \]

where \( \mathbf{u}(\mathbf{k}, t) \) is the velocity field in Fourier-space, \( \nu \) is the kinematic viscosity, \( M_{\alpha \beta \gamma} \mathbf{k} \) is given by

\[ M_{\alpha \beta \gamma}(\mathbf{k}) = (2i)^{-1} [\kappa_{\beta} D_{\alpha \gamma}(\mathbf{k}) + \kappa \delta_{\alpha \beta}](\mathbf{k}) \],

where

\[ D_{\alpha \beta}(\mathbf{k}) = \delta_{\alpha \beta} - \frac{k_\alpha k_\beta}{|\mathbf{k}|^2} \]

and \( f(k, t) \) is a forcing term used to achieve stationarity. We may rewrite equation (1) in a highly symbolic form as

\[ L_0 \mathbf{u} = M \mathbf{u} + f. \]

The nonlinear term \( M \mathbf{u} \mathbf{u} \) in our shorthand notation may be partitioned by introducing a cutoff at \( k = k_0 \) and defining \( \mathbf{u}^- \) and \( \mathbf{u}^+ \) such that \( u_\alpha(k, t) = u_\alpha^- (k, t) \) for \( 0 < k < k_1 \) and \( u_\alpha(k, t) = u_\alpha^+ (k, t) \) for \( k_1 < k < k_0 \). The maximum cutoff wavenumber, \( k_0 \), is of the same order of magnitude as the Kolmogorov dissipation wavenumber and is defined via the dissipation integral,

\[ \varepsilon = \int_0^\infty \nu k^2 E(k) dk \approx \int_0^{k_0} \nu k^2 E(k) dk \]

where \( \varepsilon \) is the dissipation rate.

Equation (1) can now be expanded to give

\[ L_0 \mathbf{u} = \psi^- + \psi^- + \psi^+ + f \]

where the partitions are defined by

\[ \psi^- = M \mathbf{u}^- \mathbf{u}^- \]
\[ \psi^+ = 2 M \mathbf{u}^- \mathbf{u}^+ \]
\[ \psi^+ = M \mathbf{u}^+ \mathbf{u}^+ \]
and we further define
\[ \psi = \psi^- + \psi^+ + \psi^{++} = M_{uu}. \] (10)

We may now ‘solve’ equation (9) by introducing \( G_0 \)
where, for some field \( \phi \),
\[ G_0 X(k, t) = L_0^{-1} X(k, t) = \int e^{-i k^2 (t-t')} X(k, t') dt' \] (11)

so that
\[ u = \phi^- + \phi^+ + \phi^{++} + G_0 \phi, \] (12)

where
\[ \phi^- = G_0 \psi^- \] (13)
\[ \phi^+ = G_0 \psi^+ \] (14)
\[ \phi^{++} = G_0 \psi^{++} \] (15)

and we also define
\[ \phi = \phi^- + \phi^+ + \phi^{++} = G_0 \psi = G_0 M_{uu}. \] (16)

We have carried out direct numerical simulations to calculate \( \psi \)- and \( \phi \)-fields in order to investigate their properties.

**NUMERICAL SIMULATIONS**

We started from an existing, well validated code for the direct numerical simulation (DNS) of turbulence, constructed at the University of Edinburgh and running on the Cray T3D administered by the Edinburgh Parallel Computing Centre. In Figure 1 we have plotted a number of the standard DNS outputs generated by our code, running on a 256 \(^3 \) grid.

For the fundamentals of direct numerical simulations, the reader is directed to the pioneering work of Orszag (1969 and 1971). Time integration is performed by way of a second-order Runge-Kutta scheme and partial dealiasing is achieved through application of a random-shifting method (see, for example, Rogallo, 1981). At each time-step, the nonlinear term, \( \psi \), is calculated by a pseudospectral method involving a number of fast Fourier transforms. \( \psi^- \) and \( \psi^+ \) may be computed by carrying out the same procedure having first zeroed the \( u^+ \) and \( u^- \) fields respectively while \( \psi^{++} \) may be calculated simply by subtracting \( \psi^- \) and \( \psi^+ \) from the total nonlinear term.

**Forcing**

Stationarity is obtained by use of a deterministic forcing term given by,
\[ f_a(k, t) = \begin{cases} \varepsilon_0 u_a(k, t)/[2E_f(t)] & \text{if } 0 < k < k_f, \\ 0 & \text{otherwise}, \end{cases} \] (17)

where \( \varepsilon_0 \) is the desired mean dissipation rate (supplied as an input parameter to the simulation), and
\[ E_f(t) = \int_0^{k_f} E(k, t) dk \] (18)

with \( E(k, t) \) defined as the energy spectrum. \( k_f \) is chosen to be 1.5 so that the forcing is applied to only the first shell of wavenumbers. With this forcing, we have observed over many simulations that after a sufficient number of time steps the velocity field reaches a statistically stationary form, as desired.

**Computing the \( \phi \)-fields**

The evolution of \( \phi \) and its partitions, as defined in equations (13)-(16), is a costly exercise as it must be performed in parallel with the evolution of the velocity field. We use a simple trapezoidal method to carry out the necessary time integrals, but the need to calculate each of the partitions of \( \psi \) at each time step leads to a code that is roughly three times as computationally expensive as a straightforward DNS.

Further problems arise out of the necessity to choose suitable initial \( \phi \)-fields with which to begin the computation. Here, we have chosen to begin by zeroing each of the \( \phi \)-fields for all values of \( k \), in the expectation that after a sufficient number of time steps the initial conditions will have been forgotten. To this end, we run the DNS code until the four \( \phi \)-fields have reached a statistically stationary state, and assume that this indicates convergence to their true values. Further evidence may be provided by keeping in mind the fact that our forcing is only being applied to a single shell in wavenumber space, so that we have
\[ u = \phi \text{ for } k_f < k < k_0. \] (19)

We note that \( \langle |u|^2 \rangle \approx \langle |\phi|^2 \rangle \) from our evolved data but carry out an additional test by computing the correlation between the two fields. We define the general correlation between two fields, \( a \) and \( b \), by
\[ R(a, b; k) = \frac{\langle a_a(k)b_b(-k) \rangle}{\langle |a(k)|^2 \rangle^{1/2} \langle |b(k)|^2 \rangle^{1/2}} \] (20)
and plot $R(u, \phi; k)$ in Figure 2 for six different time steps. We see that by the final time step, the level of correlation is excellent for $k > 5$ and good for $k > 1$. The increasing quality of correlation with increasing $k$ is to be expected as this is outside the valid range of equation (15).

Finally we note that in order to compute $\phi$-fields for different cutoff wavenumbers, $k_1$, we must reperform the entire DNS from initial conditions up to the fully evolved state.

**Experimental Details**

We have computed $\psi$-fields for a number of different cutoff wavenumbers at resolutions of $64^3$ and $256^3$ grid points. The high cost of calculating the $\phi$-fields means that for these we have been restricted to a resolution of $64^3$ grid points and only two cutoff wavenumbers.

Our $64^3$ simulation achieved a microscale Reynolds number of $R_\lambda \approx 70$ while our $256^3$ simulation reached $R_\lambda \approx 190$.

**RESULTS**

**Low Reynolds Number**

The results given in this section correspond to our $64^3$ simulation. We begin by presenting results for the $\phi$-fields with cutoff wavenumbers $k_1 = 16.5$ and $k_1 = 24.5$. Throughout this work, the cutoff wavenumbers are chosen to be half-integers so that they lie between two distinct shells. For each data set, we compute the correlation between $\phi$ and each of its partitions using equation (21) and also a measure of their relative magnitudes, $r(k)$, given by

$$r(a; b; k) = \frac{\langle |b(k)|^2 \rangle}{\langle |a(k)|^2 \rangle}.$$  

(21)

Results are plotted in Figures 3 and 4 with both functions plotted against $k/k_1$. We first note that, once scaled in this way, the exact choice of $k_1$ seems to have little effect on the shape of the graphs. We believe that the peaky
Figure 7: **Low Reynolds number** ($R_\lambda \approx 70$) 
$R(\psi, \psi^-; k)$ for cutoff wavenumbers $k_1 = 4.5, 8.5, 12.5, 16.5, 20.5, 24.5, 28.5$ with $k_0 = 32$. The dot-dashed line indicates $k = k_1$. 

Figure 10: **High Reynolds number** ($R_\lambda \approx 190$) 
$R(\psi, \psi^-; k)$ for cutoff wavenumbers $k_1 = 16.5, 32.5, 48.5, 64.5, 80.5, 96.5, 112.5$ with $k_0 = 128$. The dot-dashed line indicates $k = k_1$. 

Figure 8: **Low Reynolds number** ($R_\lambda \approx 70$) 
$R(\psi, \psi^+; k)$ for cutoff wavenumbers $k_1 = 4.5, 8.5, 12.5, 16.5, 20.5, 24.5, 28.5$ with $k_0 = 32$. The dot-dashed line indicates $k = k_1$. 

Figure 11: **High Reynolds number** ($R_\lambda \approx 190$) 
$R(\psi, \psi^+; k)$ for cutoff wavenumbers $k_1 = 16.5, 32.5, 48.5, 64.5, 80.5, 96.5, 112.5$ with $k_0 = 128$. The dot-dashed line indicates $k = k_1$. 

Figure 9: **Low Reynolds number** ($R_\lambda \approx 70$) 
$R(\psi, \psi^+; k)$ for cutoff wavenumbers $k_1 = 4.5, 8.5, 12.5, 16.5, 20.5, 24.5, 28.5$ with $k_0 = 32$. The dot-dashed line indicates $k = k_1$. 

Figure 12: **High Reynolds number** ($R_\lambda \approx 190$) 
$R(\psi, \psi^+; k)$ for cutoff wavenumbers $k_1 = 16.5, 32.5, 48.5, 64.5, 80.5, 96.5, 112.5$ with $k_0 = 128$. The dot-dashed line indicates $k = k_1$. 


behaviour observed for \(k/k_1 < 0.5\) in Figure 3 is an effect caused by the presence of the forcing term.

The general picture which seems to emerge from both correlation and magnitude information, is that for \(k < k_1\), the \(\phi^+\) partition is the dominant part of \(\phi\). For \(k > k_1\), it is \(\phi^-\) which is dominant while \(\phi^{++}\) is broadly insignificant for all values of \(k\).

It was at this point in our work that it became apparent that the computational cost involved in calculating the \(\phi\)-fields was too high and so attention was turned to the \(\psi\)-fields which are far easier to calculate. For these, a single velocity field realization is enough to calculate \(\psi\) and its partitions for any cutoff wavenumber, \(k_1\). We begin by duplicating the calculations performed on the \(\phi\)-fields for the same resolution grid, and for the same cutoff wavenumbers. Results are shown in Figures 5 and 6 where we see a very similar picture to that presented in Figures 3 and 4.

We now consider a hypothetical large eddy simulation, and that there is good correlation for all values of \(k_1\) as we move beyond the cutoff. Above the cutoff, this correlation decays rapidly away to zero. We also note that, mathematically, \(\psi^-\) (\(k = 0\) for \(k > 2k_1\)) so that the occurrence of a non-zero correlation in this region points to the existence of small numerical and aliasing errors.

This picture is reversed when we consider \(R(\psi, \psi^+; k)\) as shown in Figure 8. The collapse of data is not so good, particularly in the low-wavenumber region, and we see that as \(k/k_1\) increases, the correlation begins to tail away from unity.

A pattern is even more difficult to discern when we compute \(R(\psi, \psi^-; k)\), shown in Figure 9. We see that overall, \(\psi^-\) does not correlate well with \(\psi\); although the level of correlation increases with \(k/k_1\) as we move beyond the cutoff.

**Moderate Reynolds Number**

We now extend our work by applying the ideas outlined in previous sections to \(\psi\)-field data from our 256\(^3\) simulations. Figures 10–12 show correlations of \(\psi\) with each of its partitions from this data. As can be easily seen, the picture has changed very little from our 64\(^3\) data, the biggest difference being that the results seem better behaved, which is expected due to there being more data points available for shell averaging in the region \(k < k_1\).

In the following sections, all results are generated using the \(\psi\)-fields taken from our 256\(^3\) simulation.

**Eddy-viscosities with Sharp Cutoffs**

We begin by rewriting our Navier-Stokes equation (1) for the low-wavenumber modes as

\[ L_0 u_\perp = \tilde{\phi}^- + \psi^{(-)} + f_\perp \]  \hspace{1cm} (22)

where the subscript ‘\(\perp\)’ indicates that we are only concerned with \(k < k_1\) and where

\[ \psi^{(-)} = \psi^+ + \psi^{++}. \]  \hspace{1cm} (23)

In a large eddy simulation, wavenumbers \(k > k_1\) will not be available and so we introduce some model for \(\psi^{(-)}\), which we will denote \(\tilde{\psi}^{(-)}\). A standard form for \(\tilde{\psi}^{(-)}\) is an eddy-viscosity model, whereby

\[ \tilde{\psi}^{(-)} = -\delta \nu(k) \Delta u_\perp \]  \hspace{1cm} (24)

for some viscosity increment, \(\delta \nu(k)\).

We now consider a hypothetical large eddy simulation, based around the idea of our wavenumber cutoffs introduced in previous sections.

![Figure 13: \(R(\psi^{(-)}(\perp); \psi(\perp); k)\) for cutoff wavenumbers \(k_1 = 16.5\) (―), \(32.5\) (—), \(48.5\), \(64.5\), \(80.5\), \(96.5\), \(112.5\) (—) with \(k_0 = 128\).](image)

![Figure 14: \(T^{(-)}(k)\) (—) and \(T^{(-)}(k)\) (—) for cutoff wavenumber \(k_1 = 96.5\) with \(k_0 = 128\).](image)

We can now compute the correlation between the exact subgrid terms and the model, \(R(\psi^{(-)}, \tilde{\psi}^{(-)}; k)\). Because of \(\tilde{\psi}^{(-)}\)'s relationship with \(u\) and assuming only that \(\delta \nu(k)\) is positive for all values of \(k\) this is equal to \(R(\psi^{(-)}, -u_\perp; k)\). The results are plotted in Figure 13. We see immediately that the correlation is, in general, quite poor. We also see what appears to be a difference in behaviour between cutoffs \(k_1 \geq 48.5\) where there appears to be some degree of universality and cutoffs \(k_1 \leq 32.5\). In general, however, we can state quite categorically that, for the case of a sharp cutoff in wavenumber space, no eddy-viscosity model (subject to the reasonable constraint \(\delta \nu(k) \geq 0\)) can perfectly reproduce the missing nonlinear terms. But, as we shall see, our conclusion will be modified somewhat when we consider phase and amplitude information separately.

Returning to equation (22), we can generate an energy balance equation by multiplying through by \(u_\perp\) and averaging. Multiplying this through by \(2\pi k^2\) then gives,

\[ \frac{\partial}{\partial t} E_\perp + 2 \nu k^2 E_\perp = T^{(-)}_\perp + T^{(++)}_\perp + W_\perp \]  \hspace{1cm} (25)

where \(T^{(-)}_\perp\) describes energy transfer to and from the low-wavenumber modes through exclusively low-wavenumber couplings while \(T^{(++)}_\perp\) describes energy transfer to and from the low-wavenumber modes through coupling involving at least one high-wavenumber mode. \(W_\perp\) is the energy input due to the forcing. For interest's sake, the two en-
Separating out Phase and Amplitude Effects

In this section we look at what happens if we separate our data into those contributions due to phase and those contributions due to amplitude. For each point in our field given by the wavevector, \( \mathbf{k} \), we choose some unit vector perpendicular to \( \mathbf{k} \) which we call \( \hat{\mathbf{n}} \). We may then generate a transverse component of the velocity field,

\[
u_T = u_T \hat{\mathbf{n}}.
\]

We note that \( u_T \) provides us with a statistically complete picture of our system. This is because, through continuity, \( u_L \), the component parallel to \( \mathbf{k} \) will be zero and due to isotropy, the statistical properties of \( u_T \) are independent of the exact choice of \( \hat{\mathbf{n}} \).

Since we are working in Fourier space, \( u_T \) will be a complex scalar and so may be rewritten in the form

\[
u_T = u_T e^{i u_T},
\]

and similarly for our \( \psi \)-fields. We may now consider correlations based solely on phase or amplitude information (note that as we are now working with scalar fields, equation (29) must be modified by the removal of the sum over components, \( \omega \)).

In Figures 13—15, we have plotted correlations corresponding to Figures 10—12 but concerning ourselves only with phase information. We see a picture which is largely similar to that seen when considering all parts of the \( \psi \)-fields, but note that in places — most obviously for \( k > k_1 \) in the \( \psi^{<} \)-data — the correlations are less good.

Moving on to Figures 16—18, where we have considered only amplitude information, we see a different picture. Here, while the regions of excellent correlation remain more or less untouched, for the rest of the data we see that the level of correlation does not drop below about 0.75 and indeed seems to remain approximately constant at some value between 0.75 and 0.80.

We can shed some light on the reasons for this by considering the statistical nature of the \( \psi \)-fields. In Figures 19—21, where we have considered only amplitude information, we see a different picture. Here, while the regions of excellent correlation remain more or less untouched, for the rest of the data we see that the level of correlation does not drop below about 0.75 and indeed seems to remain approximately constant at some value between 0.75 and 0.80.

We can shed some light on the reasons for this by considering the statistical nature of the \( \psi \)-fields. In Figures 19—21, where we have considered only amplitude information, we see a different picture. Here, while the regions of excellent correlation remain more or less untouched, for the rest of the data we see that the level of correlation does not drop below about 0.75 and indeed seems to remain approximately constant at some value between 0.75 and 0.80.
Figure 16: Phase-correlation.
$R(\psi_0, \psi_0^{-}; k)$ for cutoff wavenumbers $k_1 = 16.5, 32.5, 48.5, 64.5, 80.5, 96.5, 112.5$ with $k_0 = 128$. The dot-dashed line indicates $k = k_1$.

Figure 17: Phase-correlation.
$R(\psi_0, \psi_0^{+}; k)$ for cutoff wavenumbers $k_1 = 16.5, 32.5, 48.5, 64.5, 80.5, 96.5, 112.5$ with $k_0 = 128$. The dot-dashed line indicates $k = k_1$.

Figure 18: Phase-correlation.
$R(\psi_r, \psi_r^{-}; k)$ for cutoff wavenumbers $k_1 = 16.5, 32.5, 48.5, 64.5, 80.5, 96.5, 112.5$ with $k_0 = 128$. The dot-dashed line indicates $k = k_1$.

Figure 19: Amplitude-correlation.
$R(\psi_0, \psi_0^{-}; k)$ for cutoff wavenumbers $k_1 = 16.5, 32.5, 48.5, 64.5, 80.5, 96.5, 112.5$ with $k_0 = 128$. The dot-dashed line indicates $k = k_1$.

Figure 20: Amplitude-correlation.
$R(\psi_r, \psi_r^{-}; k)$ for cutoff wavenumbers $k_1 = 16.5, 32.5, 48.5, 64.5, 80.5, 96.5, 112.5$ with $k_0 = 128$. The dot-dashed line indicates $k = k_1$.

Figure 21: Amplitude-correlation.
$R(\psi_r, \psi_r^{+}; k)$ for cutoff wavenumbers $k_1 = 16.5, 32.5, 48.5, 64.5, 80.5, 96.5, 112.5$ with $k_0 = 128$. The dot-dashed line indicates $k = k_1$. 
Figure 22: PDF for $\psi_r$ (---); $\psi_r^-$ (----); $\psi_r^+$ (-----) at $k = 32$ with $k_1 = 64.5$.

Figure 23: PDF for $\psi_\theta$ (---); $\psi_\theta^-$ (----); $\psi_\theta^+$ (-----) at $k = 32$ with $k_1 = 64.5$.

Figure 24: Phase-correlation. $R(\{\psi_r^{(-)}\}_r, \{\psi_r^{(-)}\}_r; k)$ for cutoff wavenumbers $k_1 = 16.5$ (-----), 32.5 (-----), 48.5, 64.5, 80.5, 96.5, 112.5 (-----) with $k_0 = 128$.

Figure 25: Amplitude-correlation. $R(\{\psi_\theta^{(-)}\}_r, \{\psi_\theta^{(-)}\}_r; k)$ for cutoff wavenumbers $k_1 = 16.5$ (-----), 32.5 (-----), 48.5, 64.5, 80.5, 96.5, 112.5 (-----) with $k_0 = 128$.

computers of the Edinburgh Parallel Computing Centre. The research of A. Young is supported by the Engineering and Physical Sciences Research Council.

REFERENCES

Kraichnan, R.H., “Eddy viscosity in two and three dimensions,” J. Atmos. Sci., Vol. 33, pp. 1521–1536.

Lesieur, M. and Rogallo, R., 1989, “Large-eddy simulation of passive scalar diffusion in isotropic turbulence,” Phys. Fluids A, Vol. 1, No. 4, pp. 718–722.

McComb, W.D., 1995, “Theory of turbulence”, Rep. Prog. Phys., Vol. 58, pp. 1117-1206.

McComb, W. D., Roberts, W. and Watt, A. G., 1992, “Conditional-averaging procedure for problems with mode-mode coupling”, Phys. Rev. A, Vol. 45, pp. 3507–3515.

McComb, W. D. and Watt, A.G., 1992, “Two-field theory of incompressible-fluid turbulence”, Phys. Rev. A, Vol. 46, pp. 4797–4812.

McComb, W.D., Yang, T.-J., Young, A.J. and Machiels, L., 1997, “Investigation of renormalization group methods for the numerical simulation of isotropic turbulence,” Proc. 11th Symposium on Turbulent Shear Flows, Grenoble, pp. 4-23–4-27.

Machiels, L., 1997, “Predictability of small-scale motion in isotropic fluid turbulence,” Phys. Rev. Lett., Vol. 79, No. 18, pp. 3411–3414.

Orszag, S., 1969, “Numerical Methods for the Simulation of Turbulence,” Phys. Rev. Lett., Vol. 79, No. 18, pp. 3411–3414.

Orszag, S., 1969, “Numerical Methods for the Simulation of Turbulence.” Phys. Fluids (suppl. 2), Vol. 12, pp. 250–257.

Orszag, S., 1971, “Numerical Simulation of Incompressible Flows Within Simple Boundaries. I. Galerkin (Spectral) Representations,” Stud. Appl. Maths., Vol. 50, No. 4, pp. 293–327.

Rogallo, R.S., 1981, “Numerical Experiments in Homogeneous Turbulence,” NASA TM-81315.