Computation of large-scale statistics in decaying isotropic turbulence

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1. Motivation and objectives

The most basic result in a study of decaying isotropic turbulence is the evolution of the kinetic energy as a function of time. By postulating a self-similar decay of the energy spectrum based on an exact invariant $B_0$ of the flow, Saffman (1967a,b) determined the high Reynolds number decay law

$$\langle u^2 \rangle \propto B_0^1 t^{-\frac{5}{3}}$$

where $B_0$ is the leading coefficient of the energy spectrum near $k = 0$

$$E(k) \sim 2\pi B_0 k^2 \quad k \to 0.$$  \hspace{1cm} (2)

Saffman's determination of the high Reynolds number decay exponent was based on earlier work by Kolmogorov (1941) in which it was assumed that a self-similar decay of the spectrum could be based on the invariance of the Loitsianski integral $B_2$ (Loitsianski, 1939), yielding the decay law

$$\langle u^2 \rangle \propto B_2^1 t^{-\frac{1}{2}}$$

where now

$$E(k) \sim 2\pi B_2 k^4 \quad k \to 0.$$  \hspace{1cm} (4)

However, it was later shown (Proudman & Reid, 1954; Batchelor & Proudman, 1956) that $B_2$ was in fact not invariant and depended on time during the turbulence decay.

However, one may still postulate an exact self-similar decay of the energy spectrum at large-scales (Lesieur, 1990). If it is assumed that

$$B_2(t) = \beta t^\gamma,$$

then (3) still holds but with $B_2(t)$ given by (5). When $\gamma$ is positive, as is indicated by numerical simulations and quasi-normal closure models, this results in a less rapid decay of the energy as $t^{-10/7+2\gamma/7}$.

We have performed large-eddy simulations of decaying isotropic turbulence (Chasnov, 1994) to test the prediction of self-similar decay of the energy spectrum and to compute the decay exponents of the kinetic energy. In general, good agreement between the simulation results and the assumption of self-similarity were obtained. However, the statistics of the simulations were insufficient to compute the value of $\gamma$ which corrects the decay exponent when the spectrum follows a $k^4$ wavenumber behavior near $k = 0$. To obtain good statistics, it was found necessary to average over a large ensemble of turbulent flows. We report on this work here as well as in a recent Physics of Fluids A letter (Chasnov, 1993).
2. Computation of the Loitsianski integral

The coefficient $B_2$ above, the so-called Loitsianski integral, can be written as an integral over the infinite flow volume as

$$B_2 = -\frac{1}{48\pi^3} \lim_{r \to \infty} \int_V (u_i(x)u_i(x+r)) r^2 \, dr.$$  \hspace{1cm} (6)

To compute $B_2$ by numerical simulation, we assume that the velocity field is periodic in three directions with periodicity length $L = 2\pi$. The velocity field may then be expanded in a Fourier series as

$$u(x) = \sum_k \hat{u}(k) \exp(i k \cdot x),$$  \hspace{1cm} (7)

where the components of $k$ in the sum span the set of integers. A good approximation to homogeneous turbulence is thus obtained when the integral scale of the turbulence is much less than $\pi$. Treating the average in (6) as a volume average, and substituting the Fourier expansion (7) into (6), we obtain after one integration over the volume

$$B_2 = -\frac{1}{48\pi^3} \sum_k \hat{u}_i(k)\hat{u}_i(-k) \int_V \exp(i k \cdot r) r^2 \, dr.$$  \hspace{1cm} (8)

The remaining volume integral in (8) may be evaluated analytically, and making use of $\hat{u}_i(-k) = \hat{u}_i(k)^*$, where $^*$ denotes the complex conjugate, and $\hat{u}_i(0,0,0) = 0$ we obtain

$$B_2 = -\frac{2}{3} \sum_{k=1}^{\infty} \frac{(-1)^k}{k^2} \left[ |\hat{u}(k,0,0)|^2 + |\hat{u}(0,k,0)|^2 + |\hat{u}(0,0,k)|^2 \right].$$  \hspace{1cm} (9)

There are two main difficulties in the direct use of (9) to compute $B_2$ in a numerical simulation. Firstly, the correlation $(u_i(x)u_i(x+r))$ in (6) decreases in general as $O(r^{-5})$ in homogeneous turbulence (Batchelor & Proudman, 1956) – although it decreases faster as $O(r^{-6})$ in isotropic turbulence – so that the integral scale of the turbulence must be small enough for the integral in (6) to converge within the computational domain. Secondly, as the value of $r$ in (6) becomes comparable to $\pi$, the replacement of the ensemble average in (6) by a volume average becomes inaccurate because of a lack of sample of the largest computed scales. Explicit computation has shown that direct use of (9) to compute $B_2$ in a single realization of a turbulent flow is highly inaccurate. We are thus led to average $B_2$ over an ensemble of such flows. This is equivalent to treating the original average in (6) as a combination of a volume and ensemble average.

In this research brief, we report on a computation of $B_2(t)$ accomplished by performing 1024 independent simulations of resolution $64^3$. The size of this ensemble is sufficient to compute $B_2(t)$ to a statistical accuracy better than 5% over the entire time-evolution considered. The computations are performed on an Intel
iPSC/860 hypercube parallel machine containing 128 processors. The machine had eight megabytes RAM per processor which allowed 64 realizations to be performed in parallel with each independent realization computed on 2 processors. Communication between processors computing different realizations is minimal so that the simulation of an ensemble of turbulent flows makes very efficient use of parallel computer architectures. Sixteen independent runs — each of 800 total time-steps — were performed. With each time-step taking approximately 10.6 seconds of cpu time, a total of 38 hours of dedicated machine use was required.

Our main goal in computing $B_2(t)$ is to determine its long time, high Reynolds number behavior. Under the constraints imposed by $64^3$ resolution simulations, this necessitates the use of a large-eddy simulation with the initial peak of the energy spectrum placed at as large a value of $k$ magnitude as possible (Chasnov, 1994). Here, the initial energy spectrum is taken to be

$$E(k,0) = 2\pi B_2(0)k^4 \exp \left[-2\left(k/k_p\right)^2\right], \tag{7}$$

with $k_p = 25$ and $B_2(0) = 6.934 \times 10^{-8}$, so that $\langle u^2 \rangle = 1$. As we have done previously, an eddy-viscosity subgrid scale model (Kraichnan, 1976; Chollet & Lesieur, 1981) is used to model the unresolved small-scale turbulence. Although the inclusion of a stochastic backscatter term in the subgrid model (Chasnov, 1991) can directly affect the time-variation of $B_2$, this effect is negligible at the later times of the turbulence evolution of interest to us here.

The finite resolution of the simulation results in a spherical truncation of the Fourier series in (7) at $k_m$, the maximum wavenumber of the simulation, so that the sum to $\infty$ in (9) is replaced by a sum to $k_m/\sqrt{3}$. At small times when the peak of the energy spectrum is near $k_m$, this sharp cutoff results in errors in the computed value of $B_2$. We have shown that these errors can be easily removed by applying an additional Gaussian filter of the form $\exp[-(k/k_f)^2]$ with $k_f = 12$ to $\hat{u}(k)$ before computing (9). At the later evolution times of interest to us here, the effect of this additional filter is negligible.

The results obtained from the simulations are shown in figures 1-3. In figure 1, we plot the time-evolution of the ensemble-averaged energy spectrum obtained from the large-eddy simulations by summing the contributions of $|\hat{u}(k)|^2$ into wavenumber shells of thickness $\Delta k = 1$ in the usual way, i.e.,

$$E(k,t) = \frac{2\pi k^2}{S_k} \sum_{k-\frac{1}{2} \leq |q| < k+\frac{1}{2}} \hat{u}_i(q,t)\hat{u}_i(-q,t),$$

where $S_k$ is the number of Fourier modes in each wavenumber shell and $k = 1.5, 2.5, 3.5, \ldots, 29.5$. A good approximation to the homogeneous turbulence energy spectrum is thus obtained at high wavenumbers, while the approximation is less accurate at low wavenumbers. Nevertheless, the increase in time of the low wavenumber $k^4$ coefficient is clearly evident from the plot.
The coefficient $B_2(t)/B_2(0)$ versus time, in units of the initial large-eddy turnover time $\tau(0)$ where $\tau(0) = 1.38/(k_p^2 B_2(0))^{1/2}$, is plotted in figure 2. The points represent the statistical mean of the ensemble while the pluses represent one standard deviation from the mean. The standard deviation of the distribution of $B_2$ itself, which we have shown from the simulation data to be approximately Gaussian, varies somewhat over the course of the simulation but at the latest time plotted is 80% of the mean. With 1024 realizations, the statistical uncertainty of the mean at the latest time is 2.5%.
Large-scale statistics in isotropic turbulence

In figure 3, we plot the logarithmic derivative of $B_2$ with respect to time in order to determine the validity of (5) and to compute a value of $\gamma$ from the simulation. In agreement with the EDQNM model, we find that $B_2(t)$ follows an approximate power-law at large times. From figure 3, we estimate the power law exponent to be $\gamma \approx 0.25$, with a statistical uncertainty of 6% at the latest time. The straight line drawn on the log-log plot of figure 2 represents this result. The value of $\gamma$ we obtain from the simulation is about 50% larger than that estimated previously (Lesieur & Schertzer, 1978; Lesieur, 1990). Using our computed value for $\gamma$, the Kolmogorov decay exponent becomes $-1.36$ instead of $-1.43$, a difference of 5%.

The statistical uncertainty of our asymptotic result for $\gamma$ can be reduced further by computing additional realizations. However, there may be other errors in our result associated with the deviation of "periodic turbulence" from homogeneous turbulence at the latest times of evolution, as well as the expected slow approach of the turbulence to asymptotics (Chasnov, 1994). The evident trend of figure 3 is towards a somewhat smaller asymptotic value for $\gamma$ than we have estimated. It would be of interest to repeat the present computation at higher resolution with a larger ensemble after parallel machines have become substantially more powerful.

We also note here another approach to the current computation. Rather than simulate 1024 $64^3$ turbulent fields, we could have simulated 16 $256^3$ fields with slightly more computer time due to the need for inter-processor communication. To obtain similar statistics between these two simulations, we would have to increase the initial peak of the energy spectrum $k_p$ by a factor of four and truncate the volume integration in (8) to $1/64$ the volume of the entire periodic domain. It is unclear which simulation would result in a more accurate computation of $B_2(t)$, but we chose the former mainly to illustrate the efficiency of performing realization averages of turbulent flows on parallel machines.
3. Conclusions

This work has demonstrated the capability of numerical simulations to compute large-scale statistics of turbulent flows by means of an ensemble average over a large number of independent realizations of the flow. Such a technique is "embarrassingly parallel" and is ideally suited for the new parallel computer architectures. This technique may also be applicable to turbulence simulation on virtual parallel machines in which many powerful workstations are connected together over a local network. If the memory of each workstation is sufficiently large so that each realization can be performed independently on each workstation, then the only communication required between workstations is to perform the ensemble average.

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