LETTERS

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Relative diffusion of a pair of fluid particles in the inertial subrange of turbulence

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Turbulent diffusion of a pair of fluid particles in 3-dimensional homogeneous and isotropic turbulence was studied using a high-resolution direct numerical simulation (DNS) with 1024^3 grid points. The DNS showed that the mean square of the distance $\delta\mathbf{x}$ between the two fluid particles grows with time t as $\langle|\delta\mathbf{x}|^2\rangle \sim C\epsilon t^3$ in the inertial subrange, which is in agreement with Richardson (1926) and Obukhov (1941), where $C \approx 0.7$ and ϵ is the mean dissipation rate per unit mass. A simple Lagrangian closure approximation for $\langle|\delta\mathbf{x}|^2\rangle$ is shown to be in good agreement with the DNS. [DOI: 10.1063/1.1508443]

One of the characteristic features of turbulence is its ability to disperse and mix heat, particles, etc. A turbulent admixture cloud that contains a large number of particles is spread by the motion of the fluid, i.e., by turbulent diffusion. Such a phenomenon is well characterized by the statistics of the evolution with respect to time t of the distance vector $\delta\mathbf{x}(t)$ between a pair of fluid particles moving with the fluid. Richardson[1] suggested that the mean square separation of a pair of particles that are initially close to each other grows with t as $\langle|\delta\mathbf{x}(t)|^2\rangle \propto t^3$ over an appropriate time interval. Later, Obukhov[2] showed that this scaling is consistent with dimensional analysis based on Kolmogorov's idea of a universal inertial subrange, which gives

$$\langle|\delta\mathbf{x}(t)|^2\rangle \sim C\epsilon t^3, \tag{1}$$

where ϵ is the rate of energy dissipation per unit mass and C is a universal constant.

There have been extensive studies to confirm or test (1) as reviewed by Monin and Yaglom,[3] Fung *et al.*,[4] and a recent paper by Ott and Mann[5] (hereafter referred to as OM). Many experiments that support the scaling in (1) have been reported. However, there is a great deal of scatter in the measured C values in the literature. This is presumably because of experimental or observational uncertainties in quantities such as ϵ. It is therefore interesting to study the statistics using direct numerical simulation (DNS) at high Reynolds numbers that is free from such uncertainties and may provide more details about the turbulence field.

We have recently performed a high resolution DNS with 1024^3 grid points, of quasi-stationary homogeneous and isotropic, incompressible, three-dimensional turbulence. This Letter reports some of the results, and proposes a simple closure approximation for the mean square separation $\langle|\delta\mathbf{x}(t)|^2\rangle$.

In the DNS, the Navier–Stokes equations are solved under periodic boundary conditions using a fourth order Runge–Kutta method to advance time and an alias free spectral method. The periodic boundary conditions consist of a period 2π in each of the Cartesian coordinate directions. A negative viscosity is used to maintain quasi-steady turbulence. It is wavenumber-independent and non-zero only in the wavenumber range $k<2.5$ and is adjusted every time step so as to keep the total kinematic energy constant. The kinematic viscosity ν is so chosen that $k_{max}\eta \sim 2$ in the statistically quasi-steady state, where $k_{max}=483$ is the maximum wavenumber of the retained wavevectors in the DNS and $\eta = (\nu^3/\epsilon)^{1/4}$ is the Kolmogorov length scale. The other parameter values used in the DNS are listed in Table I.

Lagrangian statistics are computed by tracing $O(10^5)$ fluid particles using a cubic spline interpolation and a fourth order Runge–Kutta method with a time increment twice as large as that used to advance the flow field. The particles are released after the turbulence attains its statistically quasi-stationary state. The micro-scale Reynolds number is then $R_\lambda \sim 283$. The velocity structure function $D(r) = \langle|\mathbf{u}(\mathbf{x}+\mathbf{r}) - \mathbf{u}(\mathbf{x})|^2\rangle$, where $\mathbf{u}(\mathbf{x})$ is the velocity at position $\mathbf{x}$, is close to $b\epsilon^{2/3}r^{2/3}$ with $b \sim 7.5$, in $50 \lesssim r/\eta \lesssim 200$, while the energy spectrum $E(k)$ is close to $C_K\epsilon^{2/3}k^{-5/3}$ with $C_K \sim 1.7$, in the wavenumber range $4 \lesssim k \lesssim 16$, where the energy flux through k is almost equal to ϵ. At time t_0, when the particles are released, they are positioned in a systematic manner such that there are at least 32^3 pairs of particles that have the same initial displacement $\delta\mathbf{x}_0 = (r_0, 0, 0)$ with $r_0/\Delta x = 4, 8, \ldots, 32$. Here, $\Delta x = 2\pi/1024$ is the grid width of the DNS, and $\eta/\Delta x \approx 0.7$, $\lambda/\Delta x \approx 23$, and $L/\Delta x \approx 197$ (see Table I).

TABLE I. DNS parameters and turbulence characteristics at time t_0; u': rms of a single component of velocity, $L=(\pi/2u'^2)\int_0^\infty E(k)/k dk$: integral length scale, $\lambda=(15\nu u'^2/\epsilon)^{1/2}$: Taylor microscale, $T=L/u'$: eddy turnover time, $\tau_\eta=(\nu/\epsilon)^{1/2}$: Kolmogorov time scale.

u'	ν	ϵ	R_λ	L	λ	η	Δx	T	τ_η	Δt
0.577	0.000289	0.0719	283	1.21	0.142	0.00429	0.00614	2.18	0.0635	0.00625

Figure 1 shows the DNS values of $\langle|\delta\mathbf{x}|^2\rangle^{1/3}$ vs $\tau=t-t_0$ for several values of the initial separation r_0, where the brackets denote an ensemble average. It is seen that $\langle|\delta\mathbf{x}|^2\rangle^{1/3}$ increases almost linearly in time τ for $\tau>\tau_0\equiv(r_0^2/\epsilon)^{1/3}$, irrespective of the initial separation under consideration. This is in agreement with the t^3 scaling implied by (1). It is tempting to determine the value of C by fitting the curves in Fig. 1 to straight lines, as in OM. The values of C by such a fitting for $\tau>\tau_0$ are plotted in Fig. 2. This gives $C\approx 0.7$ for $\lambda\lesssim r_0 \ll L$, which is in fairly good agreement with the recent experimental value $C=0.5\pm 0.2$ reported by OM. Figure 2 shows that C approaches asymptotically to a constant for large r_0, and is close to the constant already at r_0 as small as $\sim 25\eta=O(\lambda)$.

One might think that the t^3-law (1) holds only for $\tau \gg \tau_0$, and the slope in the linear region of Fig. 1, where $\tau\sim\tau_0$, may be not related simply to C. It is therefore of interest to get some more idea on $\langle|\delta\mathbf{x}|^2(t)\rangle$. For this purpose, let us consider the Lagrangian correlation $R(s,s')\equiv\langle\delta\mathbf{v}(s+t_0)\cdot\delta\mathbf{v}(s'+t_0)\rangle$, where $\delta\mathbf{v}(t)$ is the velocity difference between a pair of fluid particles defined as

$$\delta\mathbf{v}(t)=\mathbf{v}(\mathbf{x}+\delta\mathbf{x}_0,t_0;t)-\mathbf{v}(\mathbf{x},t_0;t),$$

in which $\mathbf{v}(\mathbf{y},t;s)$ is the velocity at time s of the fluid particle that was at $\mathbf{y}$ at time t. The relative separation vector $\delta\mathbf{x}(t)$ between the pair particles is given by

$$\delta\mathbf{x}(t)=\delta\mathbf{x}_0+\int_{t_0}^{t}\delta\mathbf{v}(s)\mathrm{d}s, \tag{2}$$

so that we have

$$\langle\delta x_i(t)\delta x_j(t)\rangle=\langle\delta x_i(t_0)\delta x_j(t_0)\rangle+\Delta_{ij}(t), \tag{3}$$

for turbulence with zero mean velocity, where

$$\Delta_{ij}(t)=\int_{t_0}^{t}\mathrm{d}s\int_{t_0}^{s}\mathrm{d}s'\{\langle\delta v_i(s')\delta v_j(s)\rangle+\langle\delta v_i(s)\delta v_j(s')\rangle\}. \tag{4}$$

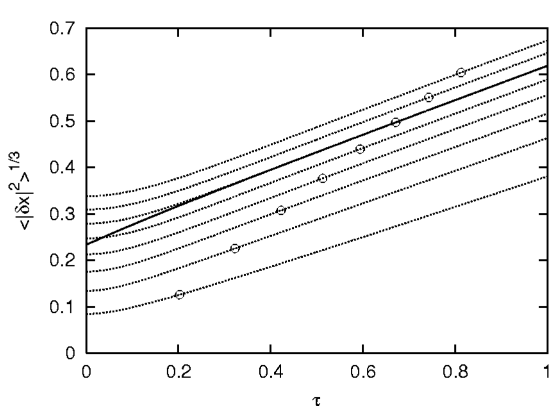

FIG. 1. DNS values of $\langle|\delta\mathbf{x}(\tau)|^2\rangle^{1/3}$ for initial separations $r_0/\Delta x=4,8,\ldots,32$ from bottom to top (dotted lines). On each curve ○ is at $\tau=\tau_0$. Solid line is $[2D(a\tau+b)^3/(3a)+\alpha]^{1/3}$ obtained from (6).

In particular,

$$\langle|\delta\mathbf{x}|^2(\tau)\rangle=r_0^2+2\int_0^\tau\mathrm{d}s\int_0^s\mathrm{d}s'R(s,s'). \tag{5}$$

Figure 3 shows the DNS value of $R(s,s')$ for $r_0=24\Delta x\approx 35\eta$, which is chosen as a representative value of r_0 in view of Fig. 2. For this value of r_0, $\tau_0=0.67$. It is seen that $R(s,s')\sim R(0,0)$ holds only in a small range (say, the range S with $s,s'<0.1$). The so-called ballistic relation $\langle|\delta\mathbf{x}|^2(\tau)\rangle\sim r_0^2+R(0,0)\tau^2$ therefore holds only in S. Figure 3 suggests that the dominant contribution to the integral in (5) is from the range (say, the range E with s and $s'>0.25$), where the time dependence of $R(s,s')$ is quite different from that in S, and

(i) $R(s,s)$ is almost linear in s, i.e., $R(s,s)\sim as+b$, and
(ii) the s'-dependence of $R(s,s')$ is similar for various values of s,

in which a and b are time independent constants. The least square fitting of $R(s,s)$ in Fig. 3 to $as+b$ for $\tau_0(=0.67)<s<1$ gives $(a,b)=(0.37,0.26)$. Regarding (ii), a close inspection of the data for Fig. 3 shows that the plots of the normalized correlation $F(s,t)\equiv R(s,s-tA)/A$ vs t for various values of s overlap quite well for $A=R(s,s)$ (figures omitted), and therefore supports

(ii′) $F(s,t)\equiv R(s,s-tA)/A$ with $A=as+b$ almost independent of s in the range E.

Applying (i) and (ii′), we have

$$\int_0^s\mathrm{d}s'R(s,s')=A^2\int_0^{s/A}\frac{R(s,s-tA)}{A}\mathrm{d}t\sim D(as+b)^2, \tag{6}$$

where $D=\int_0^{s/A}F(s,t)\mathrm{d}t$. Since Fig. 3 shows that $R(s,s')$ is small at $s'=0$ $(t=A/s)$ for $s>\tau_0$, D may be regarded approximately constant for $s>\tau_0$. This fact and (5) suggest to fit the DNS values of $\langle|\delta\mathbf{x}|^2(\tau)\rangle$ for $\tau>\tau_0$ to a function of the form $2D(a\tau+b)^3/(3a)+\alpha$, where α is a constant. The use of $(a,b)=(0.37,0.26)$, and the least square fitting for

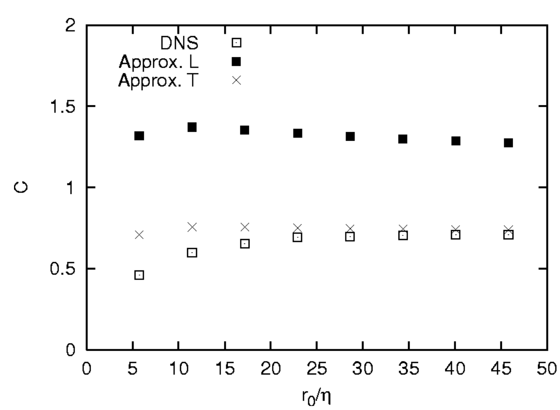

FIG. 2. Plots of C vs the initial separation r_0.

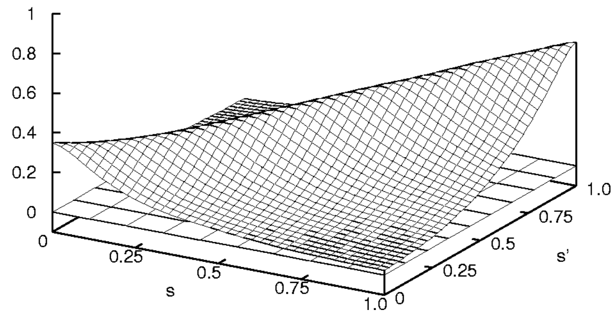

FIG. 3. Bird's view of the DNS value of the Lagrangian correlation $R(s,s')\equiv\langle\delta\mathbf{v}(s+t_0)\cdot\delta\mathbf{v}(s'+t_0)\rangle$ for $r_0=24\Delta x$.

$\tau_0<\tau<1$ then gives $(D,\alpha)=(0.54,-0.004)$ and C $(=2Da^2/(3\epsilon))\sim0.67$. The result $C\sim0.67$ is close to the value 0.7 obtained above, which suggests that the linearity for $\tau>\tau_0$ observed in Fig. 1 is closely related to (1), i.e., the asymptotic behavior for $\tau\gg\tau_0$.

It is a challenging problem to derive the statistics of such pair-particle diffusion theoretically. Previous attempts include those based on Lagrangian closure approximations: the abridged Lagrangian history direct interaction approximation (ALHDIA)[6] and the Lagrangian renormalized approximation (LRA).[7] These closures are free from any *ad hoc* adjusting parameter and are applicable to a number of turbulence problems, including turbulent diffusion. The ALHDIA and LRA, respectively, give $C=5.5$ and 4.7 for $R_\lambda\to\infty$, after the correction noted by OM. Comparing the ALHDIA value 5.5 with their experimental value 0.5, OM concluded that "...it is therefore discouraging that the predicted value of C is ten times too large...."

It may be however worthwhile to note here that such a comparison may give an overestimate for the disagreement between the theory and experiments, because the theoretical ALHDIA value 5.5 is for $R_\lambda\to\infty$, whereas R_λ is only 100 or so in the experiments by OM. It would be fair to compare the theory and experiment or DNS at the similar R_λ. Our recent analysis motivated by these considerations shows that the LRA gives $C\approx2.7$, instead of $C\approx4.7$, at $R_\lambda\sim283$. (The details of the analysis will be reported elsewhere.) The value 2.7 is substantially smaller, and closer to the DNS value 0.7, than the value 4.7 cited above. However, the agreement with the DNS is still unsatisfactory. It is therefore interesting to derive a better approximation for $\langle|\delta\mathbf{x}(t)|^2\rangle$.

In the following, we try to derive such an approximation. For the purpose, we first note

$$\langle\delta v_i(s')\delta v_j(s)\rangle=2[V_{ij}(0,t_0,s',s)-V_{ij}(\delta\mathbf{x}_0,t_0,s',s)],$$
$$V_{ij}(\delta\mathbf{x}_0,t_0,s',s)\equiv\langle v_i(\mathbf{x}+\delta\mathbf{x}_0,t_0;s')v_j(\mathbf{x},t_0;s)\rangle, \quad (7)$$

and use the exact expression for V_{ij} in (7):

$$V_{ij}=\int d^3\mathbf{r}\langle\delta^3(\mathbf{r}-\delta\mathbf{x}(s'))v_i(\mathbf{y}+\mathbf{r},s';s)v_j(\mathbf{y},s';s')\rangle,$$

where δ^3 is the three-dimensional delta function, $\mathbf{y}=\mathbf{z}(\mathbf{x},t_0;s')$, $\mathbf{z}(\mathbf{x},s_1;s_2)$ is the position at time s_2 of the fluid particle that was at $\mathbf{x}$ at time s_1, and $\delta\mathbf{x}(t)$ is given by (2).

Since $\mathbf{d}(s',t_0)\equiv\delta\mathbf{x}(s')-\delta\mathbf{x}_0$ is given by the integration of the velocity difference $\delta\mathbf{v}(\tau)$ over the time interval $t_0\leq\tau\leq s'$ (see (2)), it is natural to assume that for large enough $s'-t_0$, the instantaneous separation $\delta\mathbf{x}(s')$ is statistically independent from the instantaneous velocity at time s and $s'(<s)$. We assume here that one may extend this approximation of statistical independence also to not very large $s'-t_0$. Then (7) is reduced to

$$V_{ij}=\int d^3\mathbf{r}\langle\delta^3(\mathbf{r}-\delta\mathbf{x}(s'))\rangle Q_{ij}(\mathbf{r},s';s), \quad (8)$$

where Q is the Lagrangian two-point two-time velocity correlation defined as

$$Q_{ij}(\mathbf{r},s';s)=\langle v_i(\mathbf{x}+\mathbf{r},s';s)v_j(\mathbf{x},s';s')\rangle, \quad (s\geq s'),$$

in which the argument $\mathbf{x}$ in Q_{ij} is omitted because the turbulence is assumed here to be homogeneous. The approximation (8) is similar to Corrsin's conjecture[8] in the sense that they both assume statistical independence between the particle displacement and the instantaneous velocity field, although Corrsin's conjecture is for single particle diffusion whereas (8) is for relative diffusion. The statistical independence was assumed only for small time separation in Corssin's conjecture, and one may question the validity of its extension to not very large time separation. However, it is to be recalled that for the problem of single particle diffusion, its extension has been examined and shown to yield reasonable approximations.[9–11] This encourages us to examine such an approximation applied to the problem of relative diffusion.

Equation (8) may be further simplified by noting that (2) suggests that the probability distribution function (PDF) of $\mathbf{d}(s',t_0)$ is Gaussian for a time separation $s'-t_0$ much larger than the characteristic time scale of $\delta\mathbf{v}$. Although the Gaussianity unlikely holds for not large enough time separation, it is tempting to assume that the integral in Eq. (8) is not sensitive to the exact form of the PDF or $\langle\delta^3(\mathbf{r}-\delta\mathbf{x}(s'))\rangle$, and to apply the Gaussian approximation also to smaller $s'-t_0$, in order to simplify (8). The idea of Gaussian approximation has been tested and shown to work well for problems of single particle diffusion (see, e.g., Refs. 11 and 12). It therefore seems worthwhile to try and examine the approximation for the problem of relative diffusion. The approximation with (8) then results in

$$\langle\delta^3(\mathbf{r}-\delta\mathbf{x}(s'))\rangle=\frac{1}{(2\pi)^3}\int d^3\mathbf{k}\exp[i\mathbf{k}\cdot(\mathbf{r}-\delta\mathbf{x}_0)]\times\exp\left[-\frac{1}{2}k_\alpha k_\beta\Delta_{\alpha\beta}(s')\right]. \quad (9)$$

Equations (4), (7)–(9) give the following closed set of equations for Δ_{ij}:

$$\Delta_{ij}(t)=4\int_{t_0}^{t}ds'\int_{s'}^{t}ds\int d^3\mathbf{k}\hat{Q}_{ij}(\mathbf{k},s';s)\times\left\{1-\exp(-i\mathbf{k}\cdot\delta\mathbf{x}_0)\exp\left[-\frac{1}{2}k_\alpha k_\beta\Delta_{\alpha\beta}(s')\right]\right\}, \quad (10)$$

for any given $\delta\mathbf{x}_0$ and the Lagrangian correlation Q_{ij}, where $\hat{Q}_{ij}$ is the Fourier transform of Q_{ij}.

In order to solve (10) one needs to know Q_{ij} (or $\hat{Q}_{ij}$). In principle, one can estimate Q_{ij} (i) from DNS or experimental data or (ii) by using an appropriate approximation. Since (i) is practically difficult, we adopt here (ii). Among various possible approximations in (ii), we use here one of the following two approximations L and T; (L) apply the LRA to the velocity field, and (T) use the Taylor expansion of $\hat{Q}_{ij}$ in powers of $\tau = s - s'$.

In approximation L, $\hat{Q}_{ij}$ is computed as follows: specify the quasi-stationary energy spectrum $E(k)$ from the DNS data, substitute it into the LRA equations,[7] and solve the LRA equations.

In approximation T, $\hat{Q}(k,\tau) \equiv \hat{Q}_{ii}(\mathbf{k}, t+\tau, t)$ is approximated by

$$\hat{Q}(k,\tau) = \hat{Q}(k,t,t)\exp[a(k)\tau + b(k)\tau^2], \tag{11}$$

where $2\pi k^2 \hat{Q}(k,t,t) = E(k)$, and $a(k)$ and $b(k)$ are determined so that (11) is consistent to $O(\tau^2)$ with the exact Taylor expansion of $\hat{Q}(k,\tau)$ in powers of τ for the isotropic turbulence under consideration. The summation convention has been used here for repeated indices. Details about the Taylor expansions and approximations similar to (11) can be found in Kaneda *et al.*[13] These approximations have been shown to agree well with DNS data. Approximation T requires the spectra of the fourth-order moments, in addition to the energy spectrum. Therefore, it is more expensive than approximation L, but it contains more information on exact turbulence statistics.

Once Q_{ij} is known by approximation L or T as discussed above, one can estimate Δ_{ij} by solving (10) for any given initial separation $\delta\mathbf{x}_0$. Figure 2 shows the values of C estimated in such a way. They, especially the one by approximation T, are in good agreement with the DNS data.

We were informed of a theoretical expression relating C to the Kolmogorov constant b in the velocity structure function $D(r)$.[14,15] It is based on (4), (7) and a few approximations for V_{ij}, and gives $C = (2b/3)^{3/2}$. Substituting the DNS value $b \sim 7.5$ or $b \sim 7.8$ as reported by Sreenivasan[16] yields $C \sim 11$ or 12, which seems too high as compared to the value 0.7 in our DNS or 0.5 ± 0.2 by OM. (According to the theory, the correction due to the finiteness of R_λ is small provided that the so-called intermittency factor μ is small. This factor μ is known to be in fact small,[16] so that the correction is unlikely significant within the theory.)

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