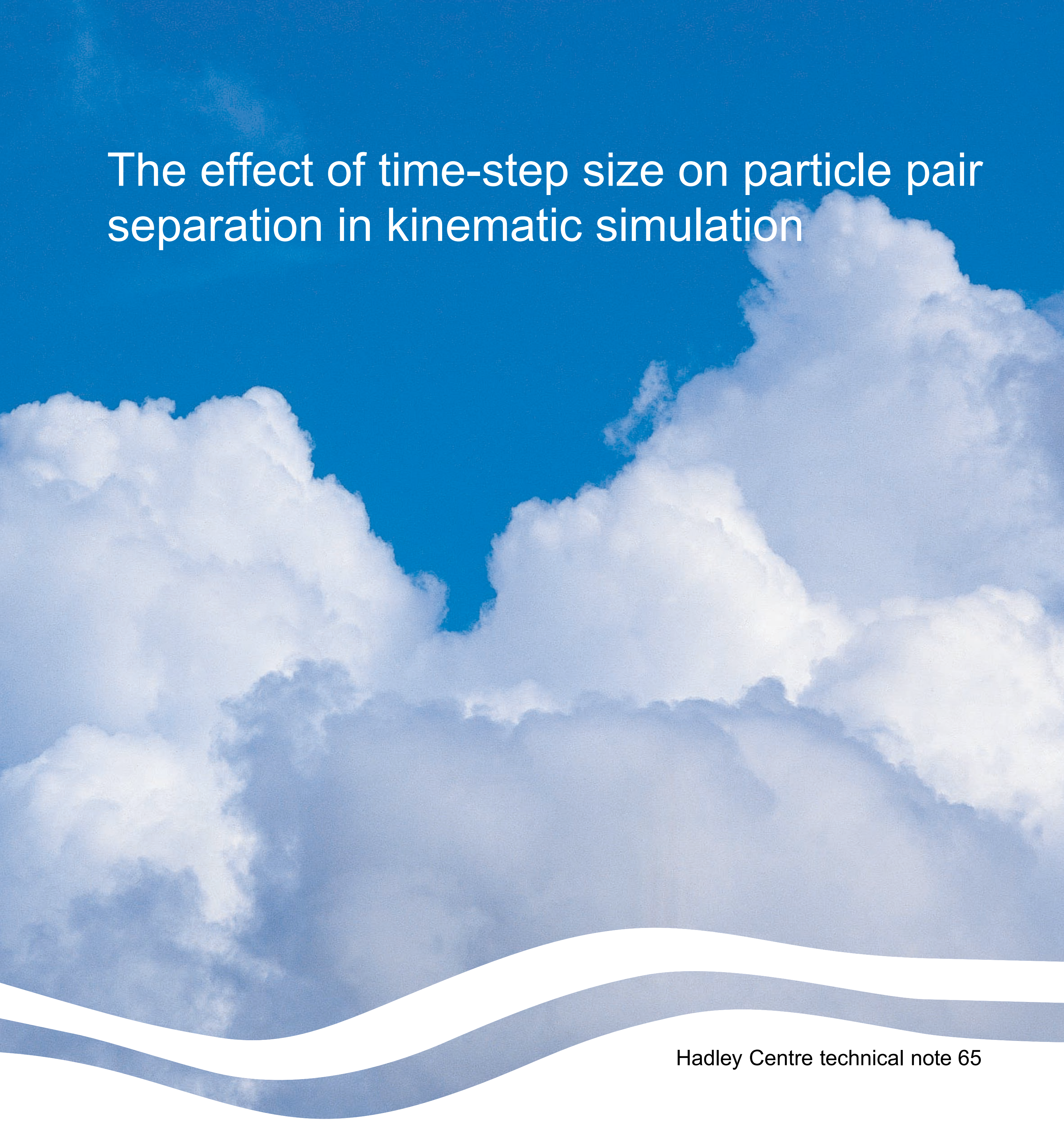

The effect of time-step size on particle pair separation in kinematic simulation

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Abstract

An understanding of the rate of separation of particle pairs in turbulent flows is crucial for predicting the variability and extremes of concentration in turbulent dispersion problems. In a previous study (Thomson and Devenish, 2005, *J. Fluid Mech.* **526**, 277-302) we explored the ability of the kinematic simulation approach to represent the separation process and concluded that it did not correctly reproduce the t^3 Richardson law which is expected to hold in reality in the turbulent inertial subrange. The simulations presented in that study used a time step which varied with the particle pair separation. This choice of time step was made to reduce the cost of the simulations, but is a source of some doubt over the validity of the conclusions. Here we repeat some of the simulations with a small fixed time-step. These new simulations show similar results, enabling us to confirm that the previous study was not compromised by the variable time-step used.

1 Background

Mathematically one can consider the problem of turbulent dispersion for an arbitrary stochastic flow field, and not just for realistic flows obeying the Navier-Stokes equation. This can be useful, for example, for developing and testing ideas using simpler flows than those generated by Navier-Stokes, for understanding what aspects of the flow are important for the dispersion, and for searching for flows which, while not completely realistic, may be useful models for real turbulence. One class of flows which has been much studied in this connection is the class of flows generated by 'kinematic simulation' (see e.g. Kraichnan, 1970; Fung, Hunt, Malik and Perkins, 1992). Such flows consist of a superposition of random independent Fourier modes and can be regarded as approximations to Gaussian random flows.

An important question in turbulent dispersion is the way pairs of particles separate, a question which was first studied by Richardson (1926). An understanding of the rate of separation is crucial for predicting the variability in the concentration of dispersing material. This is important, for example, in atmospheric dispersion problems involving toxic, flammable or odorous substances — here assessment of the hazard should take account of the variability and extremes — and in chemically reacting flows in the atmosphere or in engineering — here the reaction rate depends on the instantaneous concentrations and so the speed of the reaction can be limited by the time to mix the materials together rather than by the reaction rate which would apply for pre-mixed materials.

Particle pair separation has been explored extensively in the context of kinematic simulation (Sabelfeld and Kurbanmuradov, 1990; Fung, Hunt, Malik and Perkins 1992; Elliott and Majda, 1996; Kurbanmuradov, Sabelfeld and Koluhin, 1997; Fung and Vassilicos, 1998; Malik and Vassilicos, 1999; Flohr and Vassilicos, 2000). Recently we argued that, in kinematic simulation of 3-D flow with an inertial subrange spectrum proportional to $\varepsilon^{2/3}k^{-5/3}$, the mean square pair separation does not follow the Richardson law $\langle r^2 \rangle \sim \varepsilon t^3$ as expected in real flows (see Thomson and Devenish 2005). [Here ε is the notional energy dissipation rate per unit mass in the kinematic simulation, k is wave number, r is the particle separation and t is time.] Instead we argued that, because of the lack of 'sweeping' (i.e. advection) of the small scale modes by larger modes in kinematic simulation, the separation should, in the limit of a long inertial subrange, grow like t^6 if a strong mean flow is present, and like $t^{9/2}$ for no mean flow. These predictions were supported by numerical simulations. Note that, by a strong mean flow, we mean that a strong mean flow is simply added to a $k^{-5/3}$ velocity field, without advection of the $k^{-5/3}$ velocity field by the mean flow. This is clearly unrealistic, but exaggerates the sweeping problem and is useful to help understand the limitations of kinematic simulation as a realistic model for turbulence. If the arguments and simulation results in Thomson and Devenish (2005) are correct, this indicates that kinematic simulation does not treat the pair separation problem realistically, at least in the 3-D turbulence inertial subrange.

The simulations which were carried out in support of our arguments used an adaptive time-step in calculating the particle pair trajectories through the turbulent velocity field. This time step was determined separately for each pair and depended on the pair separation. The aim here was to reduce the computational effort. A justification was offered for the choice of time step on the basis that the eddies much smaller than the pair separation have negligible effect on the separation process and so do not need to be resolved by the time step. We believe this is correct and it was supported by some simulations using a fixed small time-step. However these simulations, for reasons of computational cost, extended over only a small fraction of the time required for the pair separation to reach the integral scale of the turbulence. This leaves some room for doubt over the validity of the results. Note that the adaptive time-step was chosen to resolve the time scale of what we believe to be the key physics of the separation process in kinematic simulation, namely the sweeping of a pair with separation r through an eddy of size $\sim r$ by the sweeping velocity, the latter being the larger of the standard deviation of the velocity (at a fixed point) and the mean flow velocity. When the separation is much less than the integral scale, this yields a time step which is much smaller than the expected time-scale of the physics in real Navier-Stokes flows, which is of order $r^{2/3}/\varepsilon^{1/3}$.

Our aim in this short note is to repeat some of the simulations presented in Thomson and Devenish (2005) with the adaptive time-step replaced by a fixed small time-step, in order to confirm that the use of an adaptive step did not lead to incorrect conclusions.

2 Simulations

The method used to generate the random flows is identical to that used by Thomson and Devenish (2005) and closely follows that used by e.g. Fung and Vassilicos (1998) and Malik and Vassilicos (1999). The velocity at position $\mathbf{x}$ at time t is given by

$$\mathbf{u}(\mathbf{x},t) = \overline{\mathbf{U}} + \sum_{n=1}^{N} \mathbf{A}_n \cos(\mathbf{k}_n.\mathbf{x} + \omega_n t) + \mathbf{B}_n \sin(\mathbf{k}_n.\mathbf{x} + \omega_n t)$$

where $\overline{\mathbf{U}} = (\overline{U}, 0, 0)$ is the mean velocity, N is the number of modes, $\mathbf{k}_n$ and ω_n are the wave number vector and frequency of the nth mode, and $\mathbf{A}_n$ and $\mathbf{B}_n$ are the mode amplitudes. The wave number vector $\mathbf{k}_n$ is chosen as $k_n\hat{\mathbf{k}}_n$ where $\hat{\mathbf{k}}_n$ is a unit vector in a random direction and k_n is chosen as described below. The amplitudes $\mathbf{A}_n$ and $\mathbf{B}_n$ are chosen to have random directions perpendicular to $\hat{\mathbf{k}}_n$ and magnitudes A_n and B_n given by

$$A_n^2 = B_n^2 = 2E(k_n)\Delta k_n.$$

Here $E(k)$ is a prescribed energy spectrum

$$E(k) = \begin{cases} \alpha\varepsilon^{2/3}k^{-5/3} & \text{for } 2\pi/L \le k \le 2\pi/\eta \\ 0 & \text{otherwise} \end{cases}$$

where L and η are proportional to the integral length scale and the Kolmogorov dissipation length scale respectively, and α is the Kolmogorov constant. The energy spectrum is defined here so that

$$\int_0^\infty E(k)\,\mathrm{d}k$$

is the turbulent energy per unit mass. The interval Δk_n is defined by

$$\Delta k_n = \begin{cases} (k_2 - k_1)/2 & \text{for } n = 1 \\ (k_{n+1} - k_{n-1})/2 & \text{for } 2 \le n \le N-1 \\ (k_N - k_{N-1})/2 & \text{for } n = N \end{cases}$$

where $k_1 = k_L = 2\pi/L$ and $k_N = k_\eta = 2\pi/\eta$. The wavenumbers are discretized according to the geometric sequence

$$k_n = k_L a^{n-1}, \quad n = 1, \ldots, N$$

where $a = (L/\eta)^{1/(N-1)}$.

The frequency ω_n determines the unsteadiness associated with the nth mode. Some of our simulations involve a frozen velocity field with $\omega_n = 0$. However we also conduct some simulations with ω_n proportional to the eddy-turnover time of the nth mode, that is,

$$\omega_n = \lambda\sqrt{k_n^3 E(k_n)}\xi$$

where λ is a dimensionless constant of order one and ξ is either one or a random number uniformly distributed in $[0, 2]$.

With the above form for $E(k)$ we have $\sigma_u^2 = \alpha(\varepsilon/2\pi)^{2/3}(L^{2/3} - \eta^{2/3})$ where σ_u is the r.m.s. value of any one component of the velocity fluctuations. In all our simulations we have $\eta \ll L$ and so $\sigma_u^2 = \alpha(\varepsilon/2\pi)^{2/3}L^{2/3}$ to quite high accuracy. We choose $\sigma_u = L = 1$ for all our simulations, but present results in non-dimensional form so that this is transparent to the reader.

Particle pairs are released with separation r_0 and tracked through the flow using a forward Euler method. In the adaptive time-step simulations presented by Thomson and Devenish (2005), the time step was given by

$$\Delta t = \min\left(0.1\frac{\min(r, L)}{\max(\overline{U}, \sigma_u)}, 0.01\frac{[\min(r, L)]^{2/3}}{\lambda\sigma_u/L^{1/3}}\right).$$

The justification offered for this choice was that it should ensure that the time step is small enough to resolve the changes in particle velocity due to (i) the sweeping of particles through the eddies that dominate the separation process, and (ii) the temporal change of such eddies caused by λ. In addition some sensitivity tests and comparisons with short-duration fixed-time-step simulations were presented in support of the choice of time step. The new longer-duration fixed-time-step simulations presented here are designed to test this more rigorously. For these simulations, we use a time step given by

$$\Delta t = \min\left(0.1\frac{\eta}{\max(\overline{U}, \sigma_u)}, 0.01\frac{\eta^{2/3}}{\lambda\sigma_u/L^{1/3}}\right).$$

This should be small enough to resolve the effect of even the smallest eddies throughout the evolution of the pair separation.

For the adaptive time-step simulations presented in Thomson and Devenish (2005), a number of pairs were tracked in each realisation of the flow and the initial positions of the pairs were chosen by placing one particle from each pair on a uniform cubic lattice of side L and placing the other particle at a distance r_0 in a random direction. For the new simulations we only follow one pair in each realisation of the velocity field to maximise the statistical accuracy for the available computing time (following a pair is far more expensive than generating a flow field, and so it makes sense to ensure the pairs are completely independent).

Figures 1-4 show comparisons between the adaptive time-step simulations presented in Thomson and Devenish (2005) and the new fixed time-step simulations. The new simulations stop at times significantly smaller than the adaptive simulations; however the time covered is much longer than that in the fixed time-step simulations presented in Thomson and Devenish (2005) and is long enough for $\langle r^2 \rangle$ to reach the point of transition towards a diffusive regime proportional to t. There is significant noise in the new results because the computational cost of the simulations makes it prohibitive to follow as many particle pairs as we would like. However the results are close enough (on the log-log plots) to those with the adaptive time-step to confirm that the deductions about power law behaviour made previously were not compromised by the use of an adaptive time-step.

The results do not show a clear t^6 power law for the strong mean flow cases (see figures 1 and 2). Because t^6 would take one from r_0^2 to L^2 in less than two decades of time this should not be expected, even for the small values of r_0/L used here. However, taken with the other evidence given in Thomson and Devenish (2005), which includes simulations with even smaller values of r_0/L and/or η/L, it provides support for t^6 being approached

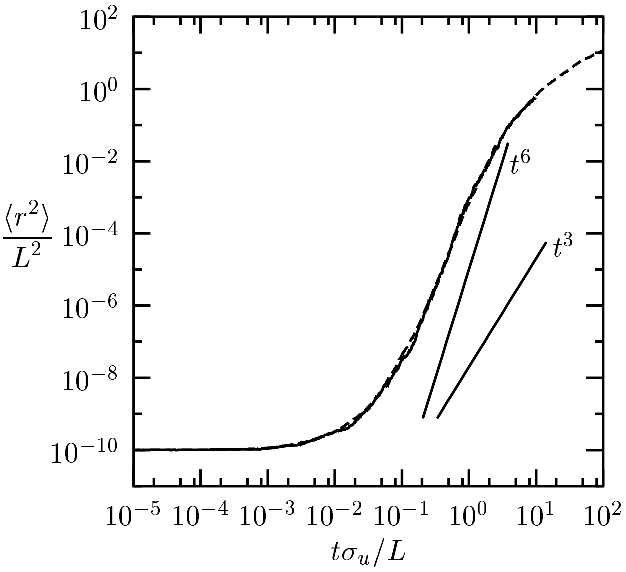

Figure 1: Comparison of adaptive and fixed time-step simulations for the case with a strong mean flow and frozen turbulence. Dashed curve: adaptive time-step (from Thomson and Devenish, 2005, figures 1a and 5); solid curve: fixed time-step. Parameters: $\overline{U}/\sigma_u = 10$, $\eta/L = 10^{-6}$, $r_0/L = 10^{-5}$, 1200 modes, $\lambda = 0$. The adaptive (fixed) time-step simulation used 5 (100) realisations of the flow with 125 (1) pairs per realisation. The straight lines are proportional to t^6 and t^3.

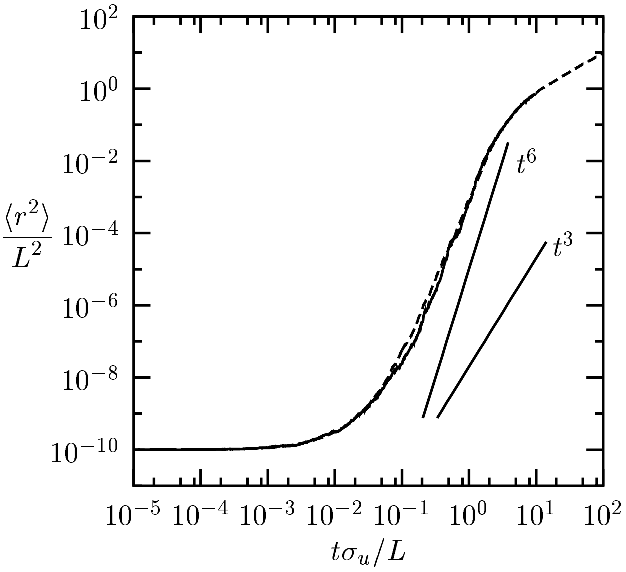

Figure 2: Comparison of adaptive and fixed time-step simulations for the case with a strong mean flow and unsteady turbulence. Dashed curve: adaptive time-step (from Thomson and Devenish 2005, figure 10); solid curve: fixed time-step. Parameters: $\overline{U}/\sigma_u = 10$, $\eta/L = 10^{-6}$, $r_0/L = 10^{-5}$, 1200 modes, $\lambda = 5$ with $\xi = 1$. The adaptive (fixed) time-step simulation used 5 (100) realisations of the flow with 125 (1) pairs per realisation. The straight lines are proportional to t^6 and t^3.

asymptotically as the inertial subrange becomes very long (see discussion in Thomson and Devenish). The support for $t^{9/2}$ for the steady no mean flow case (see figure 3) is more clear cut. Figure 3 itself shows results very close to $t^{9/2}$ and, by combining (i) the evidence

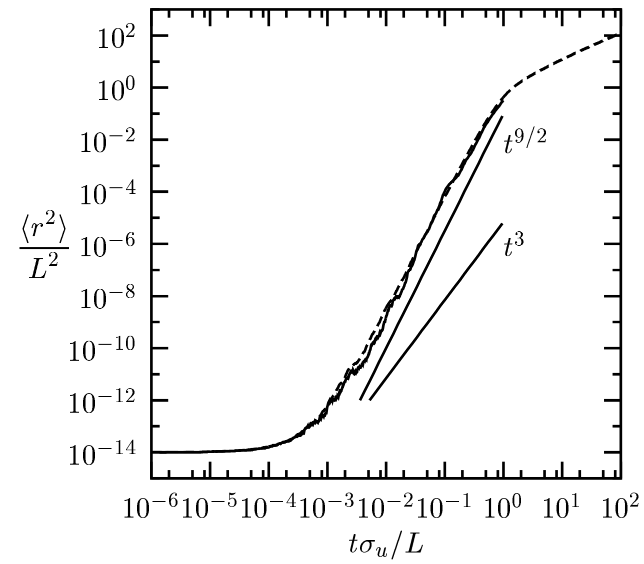

Figure 3: Comparison of adaptive and fixed time-step simulations for the case with no mean flow and frozen turbulence. Dashed curve: adaptive time-step (from Thomson and Devenish 2005, figures 12 and 13); solid curve: fixed time-step. Parameters: $\overline{U} = 0$, $\eta/L = 10^{-8}$, $r_0/L = 10^{-7}$, 1600 modes, $\lambda = 0$. The adaptive (fixed) time-step simulation used 20 (80) realisations of the flow with 125 (1) pairs per realisation. The straight lines are proportional to $t^{9/2}$ and t^3.

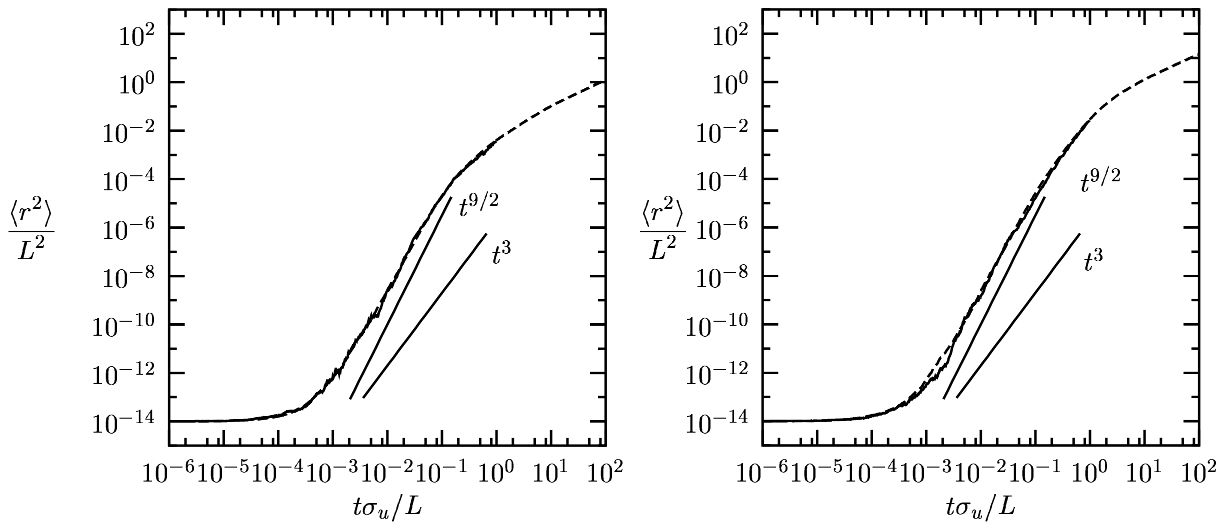

Figure 4: Comparison of adaptive and fixed time-step simulations for the case with no mean flow and unsteady turbulence. (a) shows the case with $\xi = 1$ (deterministic ω_n), while (b) shows the case with ξ uniformly distributed in $[0, 2]$. Dashed curve: adaptive time-step (from Thomson and Devenish 2005, figure 15); solid curve: fixed time-step. Parameters: $\overline{U} = 0$, $\eta/L = 10^{-8}$, $r_0/L = 10^{-7}$, 1600 modes, $\lambda = 5$. The adaptive (fixed) time-step simulations used 20 (80) realisations of the flow with 125 (1) pairs per realisation. The straight lines are proportional to $t^{9/2}$ and t^3.

in figure 3 that the adaptive time-step numerics are reliable with (ii) the adaptive time-step results given in Thomson and Devenish (2005) for even smaller r_0/L and/or η/L, it seems clear that $t^{9/2}$ is at least very close to the true asymptotic behaviour. The unsteady no mean flow cases are more complicated (see figure 4). As t increases, the growth rate increases towards a $t^{9/2}$ power law but, before really reaching this, the growth rate slows back down as the effects of unsteadiness become important (see discussion in Thomson and Devenish).

To summarise, we have repeated some of the simulations presented in Thomson and Devenish (2005) with the adaptive time-step replaced by a fixed small time-step, with a view to assessing if the deductions made by Thomson and Devenish were compromised by the use of an adaptive time-step. We conclude that they were not.

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