Direct numerical simulation on strained turbulent flows and particles within

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Abstract. We present results from direct numerical simulations of strained turbulent flows. Our focus is twofold. One is to improve our understanding of the interactions of large and small scale dynamics in strained turbulent flow; another focus is to understand the influence of the straining on the motions of passive and inertial particles of varied Stokes numbers. We seek to emphasize the effects of the strain geometry and strain rate on the particles' behaviors. Eulerian flow field results and the Lagrangian particle velocity and acceleration statistics will be discussed. The Rogallo algorithm is applied for simulating the flow field in a non-cubical domain.

1. Introduction

Strained turbulence occurs in various natural phenomena and engineering applications such as in external flows over bluff or streamlined bodies and in internal flows of varied cross sections, such as the flow through nozzles and diffusers (Hunt, 1973; Hunt & Carruthers, 1990). Straining flows are ideally suited for studying interactions of various turbulence scales due to the scale dependent effects of the straining (Kida & Hunt, 1989), and these flows have therefore been studied in detail both theoretically and experimentally, e.g. see (Lee & Reynolds, 1985; Ayyalasomayajula & Warhaft, 2005; Chen et al., 2006; Gylfason & Warhaft, 2009; Gaultieri & Meneveau, 2010). The motions of passive and inertial particles in turbulence have also been studied extensively, (Barré et al., 2001; Mordant et al., 2001; Voth et al., 2002; Ayyalasomayajula et al., 2006; Bec et al., 2006; Xu et al., 2006; Gaultieri et al., 2009), motivated by applications such as the spread of pollutants or bio-agents in atmosphere and oceans, the formation of clouds, and the transport of sediments.

Our work employs the Direct Numerical Simulation (DNS) to study strained turbulence seeded with passive and inertial particles. We investigate these flows from the Eulerian and Lagrangian viewpoints, with the aim of improving our understanding of the interactions of the different scales present, in addition to understand the effects of straining on the dynamics of inertial particles present in such flows.
2. Simulation of strained turbulence

The motion of a constant property, incompressible fluid is described by the momentum and continuity equations

\[
\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla \rho = \nu \nabla^2 \mathbf{u},
\]

\[
\nabla \cdot \mathbf{u} = 0,
\]

where \( \mathbf{u} \) and \( \rho \) are the instantaneous flow velocity and pressure respectively, \( \nu \) is the kinematic viscosity of the fluid, and \( \partial_t = \partial / \partial t \) is the derivative operator with respect to \( t \). By applying Reynolds decomposition and taking the curl of the resulting momentum equation we obtain the velocity-vorticity relation:

\[
\partial_t \mathbf{ω} - \nabla \times (\mathbf{u} \times \mathbf{ω}) + \nabla \times (\mathbf{U} \cdot \nabla \mathbf{u}) + \nabla \times (\mathbf{u} \cdot \nabla \mathbf{U}) = \nu \nabla^2 \mathbf{ω},
\]

(2)

Here, \( \mathbf{U} \) refers to the mean velocity, and \( \mathbf{u} \) to the velocity fluctuation. The vorticity, \( \mathbf{ω} \), is defined as \( \mathbf{ω} = \nabla \times \mathbf{u} \). Since the velocity fluctuation is solenoidal, Helmholtz’s decomposition theorem allows us to represent \( \mathbf{u} \) in terms of a vector potential, \( \mathbf{b} \), with \( \mathbf{u} = \nabla \times \mathbf{b} \). As a result, the vorticity is given by \( \mathbf{ω} = -\nabla^2 \mathbf{b} \).

In this work we are concerned with axisymmetrically expanding flow where the mean flow field is defined as \( \mathbf{U} = (-2Sx, Sy, Sz) \). Here \( S \) is mean strain rate \( S = \frac{1}{\nu} (\mathbf{S}_{ij}\mathbf{S}_{ij})^{1/2} \), and \( \mathbf{S}_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \) is the mean rate of strain tensor. Equation (2) can be rewritten as

\[
-\partial_t \nabla^2 \mathbf{b} - \nabla \times (\mathbf{u} \times \mathbf{ω}) + 2Sx \partial_x \nabla^2 \mathbf{b} - Sy\partial_y \nabla^2 \mathbf{b} - Sz\partial_z \nabla^2 \mathbf{b} + 3S \nabla^2 \mathbf{b} - 3S \nabla^2 \mathbf{b}_1 \hat{e}_1 = -\nu \nabla^4 \mathbf{b},
\]

(3)

where \( \mathbf{b}_1 \) is the first component of \( \mathbf{b} \), \( \hat{e}_1 \) is the unit vector in the \( x \)-direction.

Rogallo’s algorithm (Rogallo, 1981) is used to solve our system of flow equations, and the straining geometry is introduced by deforming the system coordinates. Specifically, we apply the following variable transformations:

\[
x' = e^{2St}x, \quad y' = e^{-St}y, \quad z' = e^{-St}z, \quad t' = t,
\]

and hence the vector potential of the velocity fluctuation satisfies

\[
-\partial_t \nabla^2 \mathbf{b} - \nabla \times (\mathbf{u} \times \mathbf{ω}) + 2Sx \partial_x \nabla^2 \mathbf{b} - Sy\partial_y \nabla^2 \mathbf{b} - Sz\partial_z \nabla^2 \mathbf{b} + 3S \nabla^2 \mathbf{b}_1 \hat{e}_1 = -\nu \nabla^4 \mathbf{b},
\]

(4)

where \( \nabla' = (e^{2St} \partial_x', e^{-St} \partial_y', e^{-St} \partial_z') \). By adopting this new coordinate system, the physical domain deforms with time while the computational lattice grid is time independent. The pseudo-spectral method is applied by taking the Fourier transform of the vector potential equations (4), resulting in the following equation

\[
-\partial_t \hat{\mathbf{b}}_k - \frac{\partial_t |\mathbf{k}'|^2}{|\mathbf{k}'|^2} \hat{\mathbf{b}}_k + i \mathbf{k}' \times \mathcal{F}(\mathbf{u} \times \mathbf{ω})_k + S\hat{\mathbf{b}}_k - 3S\hat{\mathbf{b}}_1 \hat{e}_1 - \nu |\mathbf{k}'|^2 \hat{\mathbf{b}}_k,
\]

(5)

where \( \hat{\mathbf{b}}_k \) represents the Fourier coefficient at wave number \( \mathbf{k} \), \( \mathcal{F} \) indicates Fourier Transform, and \( \mathbf{k}' = (k_x e^{2St}, k_y e^{-St}, k_z e^{-St}) \). If we define \( N_k = (N_{1k}, N_{2k}, N_{3k}) = \frac{i \mathbf{k}' \times \mathcal{F}(\mathbf{u} \times \mathbf{ω})_k}{|\mathbf{k}'|^2} \), equation (5) has the componentwise form

\[
\partial_t \hat{b}_{jk} + [\partial_t (\ln |\mathbf{k}'|^2) + S_j + \nu |\mathbf{k}'|^2] \hat{b}_{jk} = N_{jk}, \quad j = 1, 2, 3,
\]

(6)

where \( S_1 = 2S, S_2 = S_3 = -S \). Let \( H_j(t') \) be the integrating factor of the ordinary differential equations in (6) and \( \hat{b}_{jk} = H_j(t') \hat{b}_{jk} \), above componentwise equation is equivalent to

\[
\partial_t \hat{b}_{jk} = H_j(t') N_{jk}, \quad j = 1, 2, 3.
\]

(7)

Numerical time integration (7) is carried out using the second order Adams-Bashforth method.
3. Simulation of particle movements

The fluid is seeded with small tracers and inertial particles (compared to the smallest length scales present in the flow) of densities considerably higher than the fluid density. The particle number densities are assumed to be sufficiently low so that particle-particle interactions can be ignored. Furthermore, our simulation allow only for one-way coupling between the flow and particle fields. The Lagrangian equation of inertial particle motion is derived from Newton’s second law, and represents the balance between the forces acting on the particles (inertia and Stokes drag). The equations describing the motion of a particle of diameter \( d_p \) and density \( \rho_p \), located at \( x_p \) and with instantaneous velocity \( \vec{v}_p \) are:

\[
\frac{dx_p}{dt} = \vec{v}_p, \quad (8)
\]

\[
\frac{d\vec{v}_p}{dt} = \frac{1}{\tau_p} (\vec{u}(x_p) - \vec{v}_p), \quad (9)
\]

where \( \tau_p = \beta d_p^2 / 18 \nu \) is the Stokes relaxation time for the particle and \( \beta = (\rho_p - \rho_f) / \rho_f \) is the relative density ratio between the particle and the fluid. The Stokes number \( St = \tau_p / \tau_\eta \) characterizes the inertia of a particle in the flow; \( \tau_\eta \) is the Kolmogorov timescale.

The ordinary differential equations (8) and (9) are solved numerically by the second order Adams-Bashforth method. In equation (9), the instantaneous flow velocity at the particle location, \( x_p \), is evaluated as

\[
\bar{u}(x_p) = U(x_p) + u(\mathbf{x}_p);
\]

that is, the mean flow velocity is evaluated at the location of the particle through the formula \( U(x_p) = (-2Sx_p, Sy_p, Sz_p) \), and the flow velocity fluctuation is evaluated at the congruent location in the computational domain \( \mathbf{x}_p \), where \( \bar{x}_p \equiv x_p \mod \) (domain length in \( x \)), \( \bar{y}_p \equiv y_p \mod \) (domain length in \( y \)), and \( \bar{z}_p \equiv z_p \mod \) (domain length in \( z \)). The velocity fluctuation at the congruent location is interpolated from the nearest grid points by a trilinear polynomial.

4. Results

Homogeneous isotropic turbulent flow, seeded with tracers and inertial particles, is subjected to constant axisymmetric expansion at constant rate of strain. The flow is simulated over the domain \([0, 8\pi] \times [0, 2\pi] \times [0, 2\pi]\) with \(1024 \times 256 \times 256\) grid points. To accommodate the flow deformation, due to the straining, the computational domain is initially longer in the \( x \)-direction to maintain a reasonable aspect ratio of the domain during the simulation. The initial flow configuration is derived from stationary homogeneous isotropic flow simulations, which have evolved for approximately 40 large-eddy turnover times. Flow parameters at the beginning of straining are listed in Table 1.

Figure 1 shows the energy spectra for the flow with \( S = 16 \) at different time instants. The energy at wave number \( k' \), which deforms with time, is measured and collected according to the magnitude of \( k' \). Due to the deformation of our computational domain with time the spectra are stretched to higher wave numbers. Effects of the straining are more evident in the one-dimensional spectra, here the \( x \) component, shown in the insert.

Figure 2 shows the turbulent kinetic energy \( k \equiv \frac{1}{2} (\langle u_1(t)^2 \rangle + \langle u_2(t)^2 \rangle + \langle u_3(t)^2 \rangle) \), in our simulations with strain rates \( S = 0.5, 1, 1.5, 10 \) in addition to showing the evolution of the kinetic energy in our homogeneous isotropic flow (between 4 and 40 eddy turnover times) used to initialize each strain run. Each curve is obtained by taking the average over ten simulations. The flows are simulated from \( S \times t = 0 \) to \( S \times t = 1.5 \) except for the case \( S = 10 \), which is simulated from \( S \times t = 0 \) to \( S \times t = 1 \). The straining simulation are terminated at a given aspect ratio (1:5:5 for the case \( S = 10 \) and 1:22:22 for the other cases) of the physical
**Table 1.** Flow parameters at the beginning of the straining

| Parameter                              | Value         |
|----------------------------------------|---------------|
| Turbulent kinetic energy, $k$          | $4.6 \pm 0.4$ |
| Taylor scale, $\lambda$               | $1.75 \pm 0.07$ |
| rms velocity $u_{rms}$                 | $0.34 \pm 0.02$ |
| Kolmogorov length scale, $\eta$       | $0.0163 \pm 0.0006$ |
| Dissipation rate, $\epsilon$          | $2.18 \pm 0.15$ |
| Viscosity, $\nu$                      | $0.0052$      |
| Turbulent Reynolds number, $R_\lambda$| $117 \pm 5$   |
| Integral length scale, $\ell$         | $2.68 \pm 0.25$ |

**Figure 1.** The energy spectra for a flow experiencing a constant strain rate $S = 16$ at different times. Black solid line: at the early stage of the straining cycle $S \times t = 0.08$. Blue dashed line: $S \times t = 0.32$. Green dashed-dotted line: $S \times t = 0.56$. Red solid line with solid circle: $S \times t = 0.8$. $k'$ is the deformed wave number. The insert shows the one-dimensional spectra $E_1(k')$ at the same instant.

**Figure 2.** Turbulent kinetic energy, $k$, for flows with different strain rates normalized by the initial value vs. $S \times t$. In addition, the normalized energy of homogeneous isotropic turbulence is shown. Initial energy values are $k = 4.54$ for $S = 10$ and $k = 4.71$ for other cases. Black solid line: homogeneous isotropic turbulence. Blue dashed line: $S = 0.5$. Green dots: $S = 1$. Red squares: $S = 1.5$. Cyan triangles: $S = 10$. Inside figure: a blow up view for energy between $0 \leq t \leq 0.6$. 

$k = \frac{1}{2} \left( \langle u_1'^2 \rangle + \langle u_2'^2 \rangle + \langle u_3'^2 \rangle \right)$
domain to prevent loss of resolution. Further limits are set on the velocity magnitudes to ensure numerical convergence.

Figure 3 shows the diagonal entries of the anisotropy tensor, $b_{ii}$, defined as

$$b_{ij} \equiv \frac{\langle u_i u_j \rangle}{\langle u_k u_k \rangle} - \frac{1}{3} \delta_{ij}$$

for the various rates of strains simulated. Additionally, we show the initial response of the flow predicted by Rapid Distortion Theory (RDT) (Pope, 2000). The diagonal elements of the production, $P_{ii}$, are $P_{11} = 4\langle u_1^2 \rangle S$ and $P_{33} = -2\langle u_3^2 \rangle S$. The curves for the individual strain rates are virtually identical due to the limited range of strain rates simulated. The initial anisotropy displayed in the graph would be eliminated by averaging over a larger number of simulations; the statistics presented here are based on 10 simulations for each strain rate.

**Figure 3.** The diagonal entries of the anisotropy tensor from the flows of three different strain rates are plotted against the strain time $S \times t$. Blue symbols: $b_{11}$; green symbols: $b_{22}$; red symbols: $b_{33}$. Circles: strain rate = 0.5; boxes: strain rate = 1; triangles: strain rate = 1.5. The solid lines represent the early-time predictions of RDT for isotropic initial conditions.

![Figure 3](image)

**Figure 4.** Sample particle trajectories for tracers and inertial particles in flows with strain rates 0.5, 1, 1.5. Left figure: tracers. Middle figure: particles with $\tau_p = 0.015$. Right figure: particles with $\tau_p = 0.1$. The blue, green and red symbols refer to strain rates $S = 0.5, 1, 1.5$, respectively.

Figure 4 shows a few sample trajectories of tracers, particles with $\tau_p = 0.015$ and particles with $\tau_p = 0.1$. The vertical direction undergoes compression, whereas the flow expands in the horizontal directions. The stagnation point is located at the origin.
Figure 5. Probability density functions (pdf) of velocities of tracers and particles with $\tau_p = 0.025$, 0.05, 0.1 at time $S \times t = 0.6$. Upper figures: $S = 0.5$. Lower figures: $S = 1.5$. Left figures: $x$ component of acceleration fluctuation. Right figures: $y$ component of acceleration fluctuation. Black dots: tracer. Blue circle: $\tau_p = 0.025$. Green square: $\tau_p = 0.05$. Red triangle: $\tau_p = 0.1$. Black solid line is the standard Gaussian pdf.

Figure 5 shows the probability density functions (pdf) of the $x$ and $y$ components of velocities for tracers and particles with $\tau_p = 0.025$, 0.05, and 0.1, corresponding to initial particle Stokes numbers of $St = 0.5, 1, 2$, at the time instant when $S \times t = 0.6$. The $z$ component is omitted due to symmetry. In an effort to remove the signature of the mean flow from the pdfs, we subtract a local estimate of the mean particle velocity. For tracers, the mean field is calculated directly from the mean velocity, but for inertial particles the situation is more complex. There is no clear way for defining the mean inertial particle velocity field, due to sensitivity to initial conditions. In this work we employ the concept of “local mean”, where the computational domain is divided into rectangular boxes (here $32^3$ computational lattice points), and the average of particle velocities is evaluated in each box as the local mean velocity for particles in the box. Probability density functions of the inertial particle velocities are thus computed from particle velocities with the local mean removed.

For both strain rates, the pdfs of the $x$ component of velocity (the compression direction) appear to be narrower than the $y$ component.

In Figure 6 we plot the pdfs of tracers and particles with $\tau_p = 0.025$ and 1 at three time instants the correspond to $S \times t = 0, 0.6, 1$ in flows with $S = 1.5$. The pdfs of the $x$ component of the tracers become systematically narrower with time, whereas the $y$ component expands with time. For the inertial particles the trends appear to be more complex, with possible dependence on Stokes number, rate of strain and time.

Figure 7 shows the pdfs of the $x$ and $y$ components of accelerations for tracers and particles with $\tau_p = 0.025, 0.05, 0.1$ at $S = 0.5$ and $S = 1.5$. The stretched tails of the pdfs are
Figure 6. Probability density functions (pdf) of velocities of tracers and particles with $\tau_p = 0.025, 0.1$ in flows with strain rate $S = 1.5$ at $S \times t = 0, 0.6, 1$. Top row: $x$ component of velocity. Bottom row: $y$ component of velocity. Left figure: tracers. Middle figure: $\tau_p = 0.025$. Right figure: $\tau_p = 0.1$. Black dots, green squares and red crosses refer to different time instants of straining.

systematically narrower with higher particle inertia, as expected. It is furthermore evident that at $S = 1.5$, the pdf of the $x$ component are narrower than corresponding $y$ component. For the lower strain rate, this is either not the case, or the effect is too small to be noted.

In order to calculate the acceleration pdfs we apply the same method as for the particle velocities. Initially we calculate the full particle acceleration by $\frac{d\vec{v}_p}{dt} = \frac{1}{\tau_p} (\vec{u}(x_p) - \vec{\nu}_p)$. For tracers we use finite difference on their velocities to approximate the accelerations, and their means are calculated directly from the mean flow. The local mean of accelerations is computed by averaging particle accelerations in $32^3$ sub-boxes.

Figure 8 displays pdfs of accelerations of tracers and particles with $\tau_p = 0.025$ and $0.1$ at time $S \times t = 0, 0.6, 1$ (corresponding to Figure 6). The tails of the $x$ component of the tracers becomes narrower with time, but the effect on the $y$ component is small. The $\tau_p = 0.025$ do not seem to have changes in either components at different time instants. In pdfs of $\tau_p = 0.1$, shape changes from the beginning of strain is observed in both components, but between $S \times t = 0.6$ and $1$, the changes are not as clear.
5. Conclusion

We present numerical methods to simulate axisymmetrically strained turbulence and particle movements in the flow on a non-cubical domain. Basic Eulerian flow statistics are presented. When analyzing the velocities and accelerations of inertial particles in the flow, the issue of separating the mean and fluctuating components arises. We divide the computational domain into lattice point boxes and find local velocity and acceleration means. With these local means, we compute and compile the probability density functions of particle velocities and accelerations. The results indicate that both velocity and acceleration pdfs of tracer and inertial particles are affected by the straining, indicating direct effect on the intermittent small scales in the flows. Further simulations are required to fully realize the nature of the effect, such as the rates of strain, Reynolds numbers, and particle Stokes numbers.

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Figure 8. Probability density functions (pdf) of accelerations of tracers and particles with $\tau_p = 0.025, 0.1$ in a flow with $S = 1.5$ at $S \times t = 0, 0.6, 1$. Top row: $x$ component. Bottom row: $y$ component. Left figure: tracers. Middle figure: $\tau_p = 0.025$. Right figure: $\tau_p = 0.1$. Black dots, green squares and red crosses refer to different time instants of straining.

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