Effects of Forcing Scheme on the Flow and the Relative Motion of Inertial Particles in DNS of Isotropic Turbulence

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Motivation for Current Problem
Particle-laden turbulent flows are important both in natural and engineering applications such as:

- **Warm-Cloud Precipitation**: Atmospheric scientists are investigating if turbulence augments water-droplet growth rates by increasing droplet collision rates, which may hasten rainfall initiation.

- **Planetesimal Formation**: Astrophysicists are interested in knowing if turbulence-driven dispersion, sedimentation, and collisional coalescence of dust particles impact planetesimal formation.
Volcanic Eruption: Understanding dispersion of volcanic particles in the atmosphere is of interest

Spray Dynamics in Engines: Effects of turbulence on atomization, dispersion, and evaporation of fuel droplets is the relevant physics

In these applications, we are interested in quantifying the effects of turbulence on particle-pair relative motion.
Particle-Pair Relative Motion

- Pair relative motion refers to the temporal and spatial dynamics of pair separations $r$ and relative velocities $U$.

- Turbulence is known to spatially homogenize passive scalars.

- However, it induces strong inhomogeneities in inertial particle relative motion, which are of two kinds:
  - **Spatial Inhomogeneities**: Particle preferential concentration, quantified by Radial Distribution Function (RDF) $g(r)$.
  - **Relative Velocity Inhomogeneities**: Non-Gaussian relative velocity distribution, described by pair relative velocity PDF $P(U_r)$.

- Through these two statistics, one can study the role of turbulent fluctuations in driving particle collision frequency:

  \[
  N_c = 4\pi \sigma^2 g(\sigma) \int_{-\infty}^{0} U_r P(U_r|\sigma) \, dU_r
  \]
Particle response to turbulence is controlled by its inertia, as quantified by the Stokes number \( St = \tau_v / \tau_{\text{flow}} \)

- \( \tau_v \) is particle viscous relaxation time and \( \tau_{\text{flow}} \) is a flow time scale

When particle Stokes number \( St_\eta = \frac{\tau_v}{\tau_\eta} \approx 1 \)

- Denser-than-fluid particles accumulate in regions of excess strain-rate over rotation-rate, i.e. where \( S^2 - \Omega^2 > 0 \)
DNS of isotropic turbulence by Reade and Collins\textsuperscript{1} demonstrates the effects of $St_\eta$ on clustering.

$h(r) > 0$ is indicative of particle preferential concentration.

DNS of Sundaram and Collins\textsuperscript{2} illustrates the nature of relative velocity PDF at various separations:

- Gaussian relative velocity PDF at integral-scale pair separations
- Non-Gaussian relative velocity PDF with a peak and a long tail at smaller separations; $\sigma = \text{sum of particle radii (at contact)}$

Therefore, a closure theory should capture both preferential concentration and Gaussian to Non-Gaussian PDF transition

Background
In a recent study\textsuperscript{3}, we derived a closure for diffusion current in the PDF kinetic equation for the relative motion of high-Stokes-number particle pairs in isotropic turbulence.

For $St_r \gg 1$ particles, the pair PDF $\Omega(r, U)$ is governed by:

$$\frac{\partial \Omega}{\partial t} + \nabla_r(U\Omega) - \frac{1}{\tau_v} \nabla U \cdot (U\Omega) - \nabla U \cdot (D_{UU} \cdot \nabla U \Omega) = 0$$

\textsuperscript{3}Rani, Dhariwal, and Koch, JFM, Vol. 756, 2014
Stochastic Theory \((St_r = \tau_v/\tau_r \gg 1)\)

- For \(St_r \gg 1\) particles, it was shown that diffusivity

\[
D_{UU} = \frac{1}{\tau_v^2} \int_{-\infty}^{0} \langle \Delta u(r, x, 0) \Delta u(r, x, t) \rangle \, dt
\]

- In \(St \gg 1\) regime, pair separation \(r\) and center of mass position \(x\) remain essentially fixed during fluid time scales

- Therefore, \(\langle \Delta u(r, x, 0) \Delta u(r, x, t) \rangle\) is a Eulerian two-time correlation

- \(D_{UU}\) can be closed by computing Eulerian two-time relative velocity correlation \(\langle \Delta u(r, x, 0) \Delta u(r, x, t) \rangle\) from DNS

- In our prior study, \(D_{UU}\) was closed by converting the two-time relative velocity correlation into two-point correlation in the limit of \(St_r \gg 1\)
Evaluating \( \langle \Delta u(r, x, 0) \Delta u(r, x, t) \rangle \) using DNS is computationally very expensive

Important parameters: \( N_{\text{pairs}} \) and \( \Delta r \) (pair separation bin size)

Considered \( 5 \times 10^{11} \) stationary particle pairs and \( \Delta r = \eta / 8 \)
  
  \( \eta \) is Kolmogorov length scale

Correlations computed using 20,000 processors

Binning of \( \Delta u(r, x, t) \Delta u(r, x, t + \tau) \) according to \( r \) for all the pairs separated by a time interval \( \tau \) required 40 hours of wall-clock time
Parallel Performance of DNS code
1D Domain Decomposition

- Domain decomposition along one direction
- $N^3$ simulations can be run on up to $N$ processors
- Limited to small $Re_\lambda$

Figure: (a) XZ slabs; (b) YZ slabs
2D Domain Decomposition

- Domain decomposition along two directions
- $N^3$ simulations can be run on up to $N^2$ processors
- Allows higher flow $Re_\lambda$

Figure: (a) $X$; (b) $Y$; (c) $Z$ pencils
Strong Scaling

- Strong scaling for 2D parallel code

![Graph showing strong scaling for 2D parallel code. The graph compares ideal speedup with measured speedup across different processor counts. The ideal speedup is represented by a dashed line, and the measured speedup is represented by a solid line with data points. The x-axis represents the number of processors, while the y-axis represents the speedup compared to 1024 processors. The graph demonstrates a linear relationship between the number of processors and the speedup.]
Effects of Forcing Scheme in DNS on Motion of Inertial Particles
Governing Equations

- Fluid phase governing equations

\[ \nabla \cdot \mathbf{u} = 0 \]
\[ \frac{\partial \mathbf{u}}{\partial t} + \boldsymbol{\omega} \times \mathbf{u} = -\nabla \left( \frac{p}{\rho_f} + \frac{\mathbf{u}^2}{2} \right) + \nu \nabla^2 \mathbf{u} + \mathbf{f}_f \]

- \( \mathbf{f}_f \) is external forcing to maintain a statistically stationary turbulence

- Particle phase governing equations

\[ \frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p \]
\[ \frac{d\mathbf{v}_p}{dt} = \frac{\mathbf{u}(\mathbf{x}_p, t) - \mathbf{v}_p}{\tau_v} \]

- \( \mathbf{u}(\mathbf{x}_p, t) \) obtained using 8\(^{th}\) order Lagrange interpolation
Recall, large scale external forcing is added to N-S equation to maintain statistically stationary turbulence.

**Deterministic forcing**\(^4\): Turbulent kinetic energy dissipated during a time step is added back to the velocity field.

**Stochastic forcing**\(^5\): Random forcing acceleration based on Ornstein-Uhlenbeck process is added to the velocity components.

- Two important parameters: acceleration variance, \(\sigma_f^2\) and forcing time-scale, \(T_f\).

Both forcing schemes add energy to a low-wavenumber band.

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\(^4\)Witkowska et al., J Comput Acoust 1997;5:317–36

\(^5\)Eswaran & Pope, Comput Fluids 1988;16:257–78
Deterministic Forcing (DF) Scheme

- Turbulence is initialized with a certain amount of turbulent kinetic energy (TKE).
- In our DF, we maintain TKE constant as turbulence evolves temporally.
- Energy dissipated during $\Delta t$ is resupplied to the spectral velocity components in the range $\kappa \in (0, \sqrt{2}]$.
- This is done by scaling velocity components in the forcing wavenumber band:

$$\hat{u}(\kappa, t + \Delta t) = \hat{u}(\kappa, t + \Delta t) \sqrt{1 + \frac{\Delta E_{\text{diss}}(\Delta t)}{\int_{\kappa_{\text{min}}}^{\kappa_{\text{max}}} E(\kappa, t + \Delta t) d\kappa}}$$

$\kappa = |\kappa|$ such that $\kappa \in (0, \sqrt{2}]$, $[\kappa_{\text{min}}, \kappa_{\text{max}}]$ is the entire wavenumber range of the DNS.
Here TKE is not kept constant in the stochastic scheme

Instead, a random acceleration term $\hat{f}$ is added to N-S equations

$\hat{f}$ computed from six independent Uhlenbeck-Ornstein processes

\[
\hat{f} = \hat{b}(\kappa, t) - \kappa \kappa \cdot \hat{b}(\kappa, t)/(\kappa \cdot \kappa)
\]

\[
\hat{b}(\kappa, t + \Delta t) = \hat{b}(\kappa, t) \left(1 - \frac{\Delta t}{T_f}\right) + \theta \left(\frac{2\sigma^2 \Delta T}{T_f}\right)^{1/2}
\]

$\hat{b}(\kappa, t)$ is an UO process having $\sigma^2$ as the variance and $T_f$ time-scale

Forcing time-scale $T_f$ is a key parameter, whose effects are studied

$\hat{f}$ non-zero only for $\kappa \in (0, \sqrt{2}]$
DNS parameters

- Three grid resolutions considered: $128^3$, $256^3$ and $512^3$
- $Re_\lambda$ achieved: 76, 131 and 196
- Twelve particle $St_\eta$ ranging from 0.05 to 40 considered
- Particles per $St_\eta$
  - 262,144 for $128^3$ and $256^3$
  - 2,097,152 for $512^3$
- Forced wave-numbers range for both schemes, $|\kappa| \in (0, \sqrt{2}]$
- Five $T_f$ considered: $T_e/4$, $T_e/2$, $T_e$, $2T_e$ and $4T_e$
  - $T_e$ is the eddy turnover time obtained using deterministic forcing
- Thus a total of $6 \times 3 = 18$ DNS runs were performed
Effects of Forcing on RDF for $St_\eta \geq 1$ at $Re_\lambda = 80$. 

DNS of Inertial Particles

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Effects of Forcing on RDF for $St_\eta \geq 1$ at $Re_\lambda = 210$
Blue: \( r = 2\eta \) and Green: \( r = L/2 \)

DF, SF3 and SF4 are compared
Effects of $St_\eta$ at $r = 2\eta$ and $r = L/2$ are shown

PDFs shown only for DF
Conclusions

- Computed diffusivity tensor using DNS
- Pair statistics obtained using the analytical model are in good agreement with DNS statistics
- Studied the effects of large scale forcing in DNS on pair relative motion statistics
- The computational resources of Blue Waters allowed us to perform these computationally intensive DNS simulations