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

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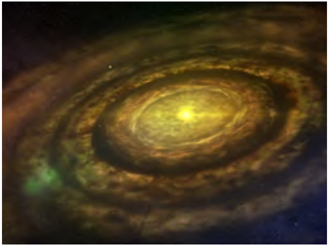
Outline

Motivation for Current Problem

Particle-Laden Turbulent Flows I

- 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

Warm-Cloud Precipitation



Planetesimal Formation

Particle-Laden Turbulent Flows II

- 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

Volcanic Eruption

Spray Dynamics in Engines

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

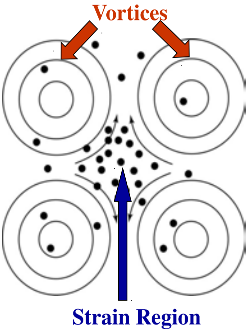
Particle-Pair Relative Motion

- Pair relative motion refers to the temporal and spatial dynamics of pair separations $\mathbf{r}$ and relative velocities $\mathbf{U}$
- 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:

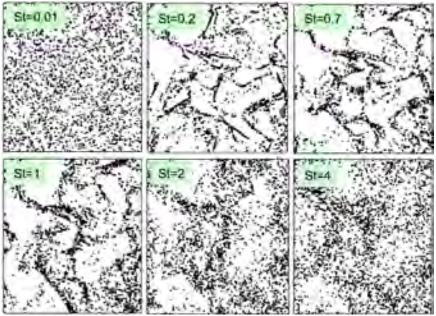
$$\text{Collision frequency} \quad N_c = 4\pi\sigma^2 g(\sigma) \int_{-\infty}^{0} U_r \; P(U_r|\sigma) \; dU_r$$

Particle Preferential Concentration I

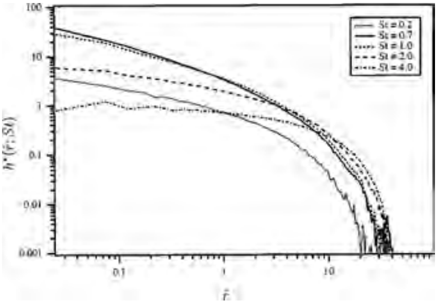
- Particle response to turbulence is controled by its inertia, as quantified by the Stokes number $St = \tau_v / \tau_{\text{flow}}$
  - τ_v is particle viscous relaxation time and τ_{flow} is a flow time scale
- When particle Stokes number $St_\eta = \frac{\tau_v}{\tau_\eta} \lesssim 1$
  - Denser-than-fluid particles accumulate in regions of excess strain-rate over rotation-rate, i.e. where $\mathbf{S}^2 - \mathbf{\Omega}^2 > 0$



- DNS of isotropic turbulence by Reade and Collins[1] demonstrates the effects of St_η on clustering
- $h(r) > 0$ is indicative of particle preferential concentration



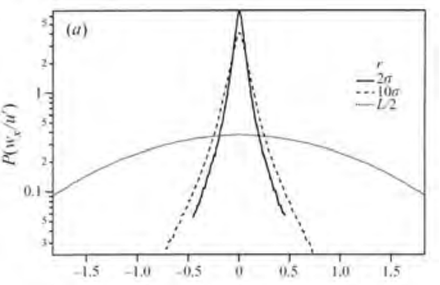
DNS of isotropic turbulence



Residual RDF $(g(r)-1)$**vs** $\widehat{r}$

[1]Reade and Collins, Phys. Fluids, Vol. 12, 2000.

- DNS of Sundaram and Collins[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; σ = sum of particle radii (at contact)



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

[2] Sundaram and Collins, JFM, Vol. 335, 1997.

Background

- In a recent study[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 $\Omega(\mathbf{r}, \mathbf{U})$ is governed by:

$$\frac{\partial \Omega}{\partial t} + \boldsymbol{\nabla}_{\boldsymbol{r}}(\boldsymbol{U}\Omega) - \frac{1}{\tau_v}\boldsymbol{\nabla}_{\boldsymbol{U}}\cdot(\boldsymbol{U}\Omega) - \boldsymbol{\nabla}_{\boldsymbol{U}}\cdot(\mathbf{D}_{UU}\cdot\boldsymbol{\nabla}_{\boldsymbol{U}}\Omega) = 0$$

[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

$$\mathbf{D}_{UU} = \frac{1}{\tau_v^2} \int_{-\infty}^{0} \langle \Delta \boldsymbol{u}(\boldsymbol{r}, \boldsymbol{x}, 0)\ \Delta \boldsymbol{u}(\boldsymbol{r}, \boldsymbol{x}, t) \rangle\, dt$$

  - In $St \gg 1$ regime, pair separation **r** and center of mass position **x** remain essentially fixed during fluid time scales
  - Therefore, $\langle \Delta \boldsymbol{u}(\boldsymbol{r}, \boldsymbol{x}, 0)\ \Delta \boldsymbol{u}(\boldsymbol{r}, \boldsymbol{x}, t) \rangle$ is a Eulerian two-time correlation

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

- In our prior study, $\mathbf{D}_{UU}$ was closed by converting the two-time relative velocity correlation into two-point correlation in the limit of $St_r \gg 1$

- Evaluating $\langle \Delta \boldsymbol{u}(\boldsymbol{r}, \boldsymbol{x}, 0)\ \Delta \boldsymbol{u}(\boldsymbol{r}, \boldsymbol{x}, t) \rangle$ using DNS is computationally very expensive
- Important parameters: N_{pairs} and Δr (pair separation bin size)
- Considered 5×10^{11} stationary particle pairs and $\Delta r = \eta/8$
  - η is Kolmogorov length scale
- Correlations computed using 20,000 processors
- Binning of $\Delta \boldsymbol{u}(\boldsymbol{r}, \boldsymbol{x}, t)\ \Delta \boldsymbol{u}(\boldsymbol{r}, \boldsymbol{x}, t + \tau)$ according to r for all the pairs separated by a time interval τ required 40 hours of wall-clock time

Parallel Performance of DNS code

1D Domain Decomposition

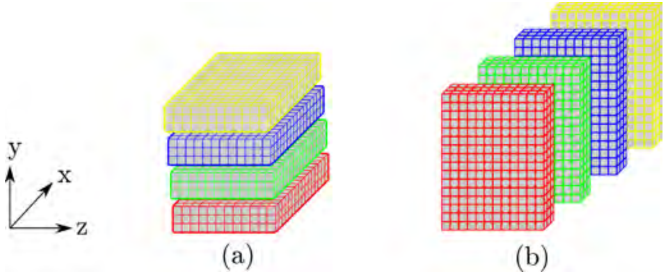


Figure: (a) XZ slabs; (b) YZ slabs

- Domain decomposition along one direction
- N^3 simulations can be run on up to N processors
- Limited to small Re_λ

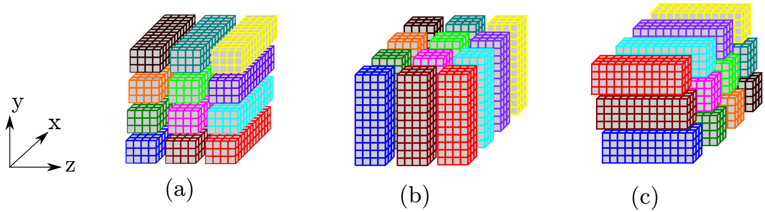
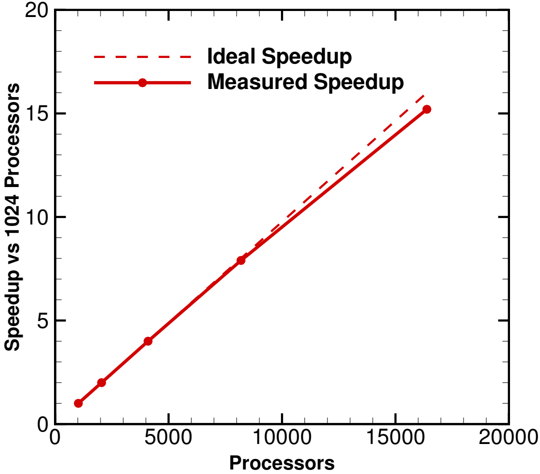


Figure: (a) X ; (b) Y; (c) Z pencils

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

- Strong scaling for 2D parallel code



Effects of Forcing Scheme in DNS on Motion of Inertial Particles

Governing Equations

- Fluid phase governing equations

$$\begin{aligned} \nabla \bullet \mathbf{u} &= 0 \\ \frac{\partial \mathbf{u}}{\partial t} + \boldsymbol{\omega} \times \mathbf{u} &= -\nabla \left(p/\rho_f + \mathbf{u}^2/2 \right) + \nu \nabla^2 \mathbf{u} + \mathbf{f}_f \end{aligned}$$

- $\mathbf{f}_f$ is external forcing to maintain a statistically stationary turbulence
- Particle phase governing equations

$$\begin{aligned} \frac{d\mathbf{x}_p}{dt} &= \mathbf{v}_p \\ \frac{d\mathbf{v}_p}{dt} &= \frac{\mathbf{u}(\mathbf{x}_p, t) - \mathbf{v}_p}{\tau_v} \end{aligned}$$

- $\mathbf{u}(\mathbf{x}_p, t)$ obtained using 8^{th} order Lagrange interpolation

Forcing Schemes

- 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, σ_f^2 and forcing time-scale, T_f
- Both forcing schemes add energy to a low-wavenumber band

[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 Δt 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

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

$\kappa = |\boldsymbol{\kappa}|$ such that $\kappa \in (0, \sqrt{2}]$, $[\kappa_{\min}, \kappa_{\max}]$ is the entire wavenumber range of the DNS

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- Here TKE is not kept constant in the stochastic scheme
- Instead, a random acceleration term $\widehat{\mathbf{f}}$ is added to N-S equations
- $\widehat{\mathbf{f}}$ computed from six independent Uhlenbeck-Ornstein processes

$$\widehat{\mathbf{f}} = \widehat{\mathbf{b}}(\boldsymbol{\kappa}, t) - \boldsymbol{\kappa}\boldsymbol{\kappa} \cdot \widehat{\mathbf{b}}(\boldsymbol{\kappa}, t)/(\boldsymbol{\kappa} \cdot \boldsymbol{\kappa})$$

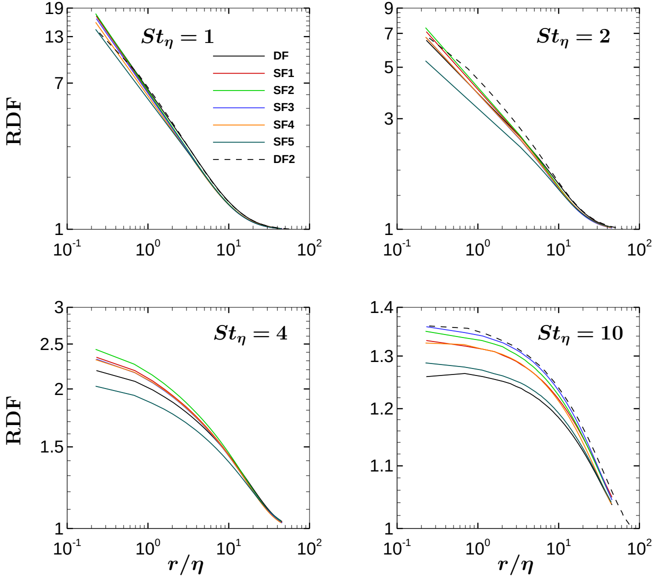
$$\widehat{\mathbf{b}}(\boldsymbol{\kappa}, t + \Delta t) = \widehat{\mathbf{b}}(\boldsymbol{\kappa}, t)\left(1 - \frac{\Delta t}{T_f}\right) + \boldsymbol{\theta}\left(\frac{2\sigma^2 \Delta T}{T_f}\right)^{1/2}$$

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

- Forcing time-scale T_f is a key parameter, whose effects are studied
- $\widehat{\mathbf{f}}$ non-zero only for $\kappa \in (0, \sqrt{2}]$

- Three grid resolutions considered: 128^3, 256^3 and 512^3
- Re_λ achieved: 76, 131 and 196
- Twelve particle St_η ranging from 0.05 to 40 considered
- Particles per St_η
  - 262,144 for 128^3 and 256^3
  - 2,097,152 for 512^3
- Forced wave-numbers range for both schemes, $|\boldsymbol{\kappa}| \in (0, \sqrt{2}]$
- 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 $Re_\lambda = 80$



Effects of Forcing on RDF for $St_\eta \geq 1$ at $Re_\lambda = 210$

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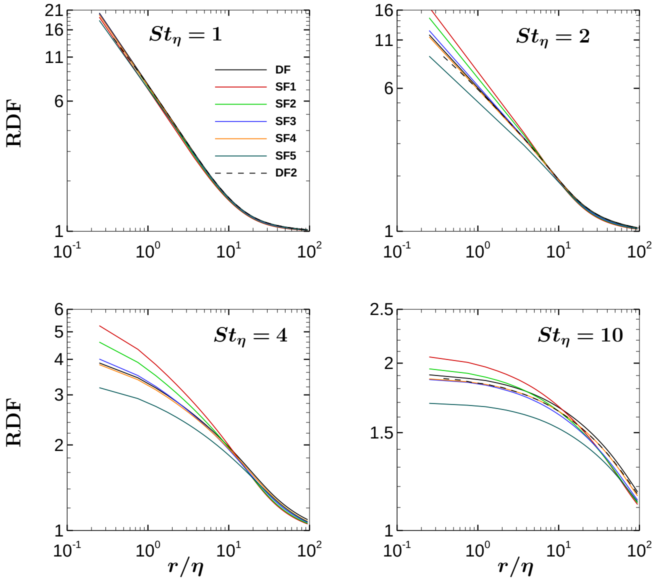

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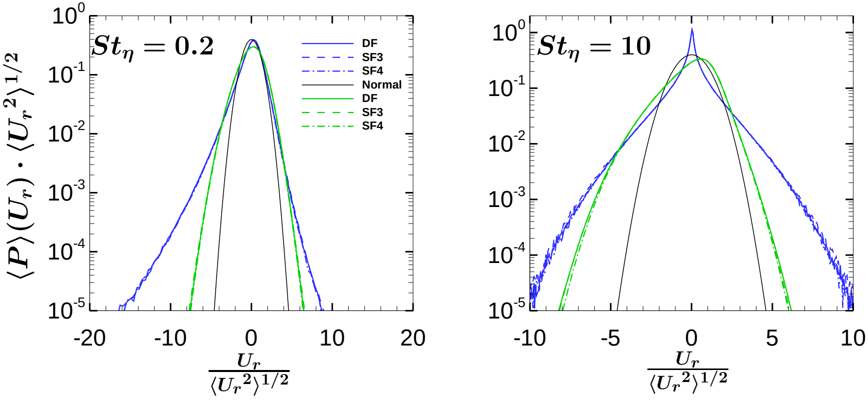
- Blue: $r = 2\eta$ and Green: $r = L/2$
- DF, SF3 and SF4 are compared



PDF $\langle P\rangle(U_r)$ for $Re_\lambda = 210$

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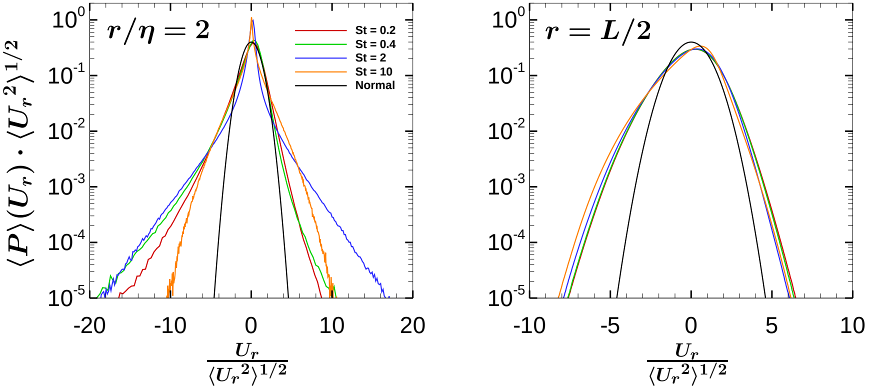
- Effects of St_η at $r = 2\eta$ and $r = L/2$ are shown
- PDFs shown only for DF



Conclusions

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- 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