New insights from comparing statistical theories for inertial particles in turbulence: I. Spatial distribution of particles

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Abstract
In this paper, we contrast two theoretical models for the spatial clustering of inertial particles in isotropic turbulence, one by Chun et al (2005 J. Fluid Mech. 536 219) and the other by Zaichik et al (2007 Phys. Fluids 19 113308). Although their predictions for the radial distribution function are similar in the regime $St \ll 1$, they appear to describe the physical mechanism responsible for the clustering in quite different ways. We demonstrate why the theories generate such similar results in the regime $St \ll 1$ by showing that the clustering mechanism in the Chun et al theory captures the leading order effects of the clustering mechanism in the Zaichik et al theory for $St \ll 1$. However, outside of this regime, the similarity between the predictions of the theories breaks down, and we consider the sources of the differences as well as the physical meaning and implications of the differences. Using DNS data we then show that the clustering mechanism described by the Zaichik et al theory accurately describes the clustering up to $St \approx 1$, and we identify a possible source of error for some of the slight quantitative discrepancies at larger $St$. We then compare these theories with others in the literature and attempt to reconcile as many of the physical explanations for clustering as we can. Finally, we consider the relationship between clustering in isotropic turbulence and the near-wall accumulation of...
inertial particles in a turbulent boundary layer, and how they scale with the Stokes number in the weak inertia limit.

Keywords: isotropic turbulence, inertial particles, multiphase flows, clustering, preferential concentration, statistical theory

1. Introduction

It is well known that an initially uniform distribution of inertial particles in isotropic turbulence will cluster under the right conditions [1], and this clustering can profoundly impact aerosol processes such as gravitational settling [2, 3], turbulence modulation [4, 5] and the rate particles collide [6, 7]. This has relevance to numerous industrial processes such as aerosol manufacturing [8], drug delivery [9] and spray combustion [10], among many other examples, as well as to natural processes such as sediment and plankton distribution in oceans [11] and even the formation of planets in the early universe [12]. The system of most interest to us is the formation of clouds in the atmosphere [13–16]. In particular, improving our understanding of turbulence enhancement of cloud droplet collision rates could help improve microphysical models of clouds that currently neglect the effect of turbulence [17].

The collision kernel for a monodisperse population of particles in isotropic turbulence can be written as follows [6, 7]

$$K = 4\pi\sigma^2 g(\sigma) \int_{-\infty}^{0} - w_p w_p d\|w\|,$$  \hspace{1cm} (1)

where $\sigma$ is the particle diameter, $g(\sigma)$ is the radial distribution function (RDF) evaluated at contact, $w_\|\|$ is the longitudinal projection of the particle pair relative velocity, and $p(w_\|\|\sigma)$ is the probability density function (PDF) for the longitudinal relative velocity at contact. Equation (1) is an exact kinematic relationship for the collision kernel, but it requires two external statistical inputs: the RDF and the relative velocity PDF. The RDF is a statistical measure of the spatial distribution of the inertial particles throughout the volume. It is defined as the ratio of the number of particle pairs found at a given separation distance to the number that would be expected if the particles were uniformly distributed throughout the flow field [18]

$$g(r) = \frac{N^i/\delta V^i}{N/V}, \hspace{1cm} (2)$$

where $N^i$ is the average number of particles found in an elemental shell with volume $\delta V^i$ at a distance $r \equiv |r|$ from the primary particle, $V$ is the total volume of the system and $N$ is the total number of particle pairs in the flow. The RDF has been normalized such that its value reduces to unity for a uniform distribution of particles.

Much of the early evidence for the clustering of inertial particles in turbulence came from direct numerical simulations (DNS) that yielded dramatic images of the highly non-uniform particle concentration field [19–21]. Clustering has also been observed in a variety of experiments [22–27] confirming that it is not a numerical artifact but a real physical phenomena, and detailed comparisons of DNS and experiments in [25] show good quantitative agreement. The focus of most of this work has been on the RDF and its dependence on the system parameters, particularly the particle Stokes number, $St$, which is a dimensionless measure of the
particle inertia. Here and throughout, $St = \tau_p/\tau_\eta$ where $\tau_p$ is the particle response time and $\tau_\eta$ is the Kolmogorov time scale. There are two aspects of clustering that are important to keep in mind. First, clustering peaks at Stokes numbers near unity and rapidly falls off for smaller or larger values. Second, clustering continues to increase at separation distances below the Kolmogorov length scale (the smallest scale of motion of the turbulence), implying no inner cutoff of the mechanism driving the particles together.

Theories that describe and predict inertial particle clustering are simultaneously under development. Some, based on a phenomenological description of the process, capture clustering reasonably well [28, 29], but do not yield new physical insights into the phenomenon. Others make assumptions about the turbulence that cannot be fully justified, such as white noise in time [30] or finite-time correlations that are significantly shorter than in real turbulence [31]. Two theories by Chun et al [32] and Zaichik et al [33] (hereafter CT and ZT, respectively) are based on similar descriptions of the turbulence, focus on sub-Kolmogorov scale clustering, and for small particles yield similar predictions in comparison with DNS. They are arguably the most comprehensive theories to date since they account for the finite spatiotemporal correlations of turbulent flows, and are free of adjustable parameters. CT was derived in the limit $St \ll 1$ and hence made several simplifying assumptions that were not made in ZT, which is applicable over the entire range of Stokes numbers.

This paper was motivated in part by comments made in [15, 34] that the CT and ZT theories for predicting the RDF are fundamentally different in the way they describe the physical mechanisms governing the clustering of the inertial particles in turbulence. In this paper, we explore this statement, not primarily from the perspective of the accuracy of the two theories (although this is of course of great importance and necessarily arises in the discussion), but rather to contrast the physical mechanisms for clustering underlying the two theories. This contrast provides insight into competing physical mechanisms for clustering. Additionally, we compare the mechanisms in the CT and ZT to alternative explanations in the literature such as ‘centrifuging’ [2, 20], ‘ergodic versus non-ergodic’ [31] and ‘sweep-stick’ [35–37] mechanisms, and attempt, to the extent possible, to reconcile them all.

The collision kernel in (2) also requires information on the relative velocity statistics. As this will be the primary topic of Part II of this paper, we leave the bulk of the discussion there; however as will become apparent, the RDF itself is influenced by the statistical properties of the relative velocity, and so we include some discussion of relative velocities here as well. Of particular interest is the argument put forth in Wilkinson and Mehlig [38] that ‘caustics’ may form, whereby a multiplicity of point particles can possess the same configuration space coordinate, but with differing velocities. This phenomenon, also referred to as the ‘sling effect’ [39, 40] and ‘random uncorrelated motion’ [41–43] (although it should be noted that random uncorrelated motion is really a statistical manifestation of the occurrence of caustics, which are in fact instantaneous events), has been observed in DNS [44]. Caustics tend to reduce the clustering (i.e., the RDF), even though they may enhance the overall collision kernel due to the compensating effect they have on the inward relative velocity [45].

The paper is organized as follows. In section 2 the theories are reviewed and a discussion of the physical mechanisms described by the theories is given, and differences between the theories are highlighted. In section 3 we demonstrate why the theories generate such similar results in the regime $St \ll 1$ by showing that the clustering mechanism in the CT captures the leading order effects of the clustering mechanism in the ZT for $St \ll 1$. Outside of this regime
the similarity between the predictions of the theories breaks down and we consider the sources of the differences as well as the physical meaning and implications of the differences. In section 4 we compare the predictions for clustering based on the ZT clustering mechanism with DNS data and find that it accurately describes the clustering up to $St \approx 1$ both qualitatively and quantitatively, and we identify a possible source of error for some of the slight quantitative discrepancies at larger $St$. In section 5 the theories are compared with other works in the literature with respect to the explanations given for the physical mechanisms governing particle clustering in isotropic turbulence. Finally, in section 6 we consider the relationship between clustering in isotropic turbulence and the near-wall accumulation of inertial particles in a turbulent boundary layer, and examine their dependencies on the Stokes number in the weak inertia limit.

2. Comparing the theories

The CT and ZT theories consider the relative motion of two identical inertial particles moving under the Stokes drag force only that do not interact with each other through physical collisions or hydrodynamic interactions and that do not affect the turbulence (i.e., ‘one-way coupling’). The particles are suspended in a turbulent flow that is incompressible, stationary and statistically homogeneous and isotropic. The starting point for both theories is the equation for the relative motion between a ‘primary’ particle fixed at the origin (of its Lagrangian reference frame) and a ‘satellite’ particle. The equation describing their relative motion under Stokes drag forcing is

$$\frac{d^2}{dt^2} r_p^i = \frac{d}{dt} w_p^i = \frac{1}{St \tau_\eta} (\Delta u_p^i - w_p^i),$$

where $r_p(t)$ is the relative position vector, $w_p(t)$ is the relative velocity vector, $\Delta u_p$ is the difference between the fluid velocity evaluated at the positions of the primary and satellite particles, $\tau_\eta$ is the fluid Kolmogorov timescale, $St = \tau_p / \tau_\eta$ is the particle Stokes number and $\tau_p$ is the particle momentum response time. For relative motion in the dissipation regime of the turbulence, i.e. $r \ll \eta$, where $\eta$ is the Kolmogorov length scale, we can approximate the fluid velocity difference by

$$\Delta u_p^i = \Gamma_{ij}^p r_p^j,$$

where $\Gamma^p = \Gamma (x^p(t), t)$ is the fluid velocity gradient tensor evaluated along the primary particle trajectory and $\text{tr} [\Gamma] = 0$ because of incompressibility. Here and throughout, the superscript ‘$p$’ on $r$ and $w$ denotes the time-dependent, Lagrangian variable defined along particle trajectories, and whenever such superscripts are absent (i.e. $r$ and $w$) these denote the independent variables associated with a ‘fixed’ reference coordinate system (i.e. either the configuration space $r$ or the phase-space $[r, \dot{r}]$).

2.1. Chun et al theory

Chun et al [32] derived a theory for inertial particle clustering in the regime $St \ll 1$. The main goal of the theory was to explain the power-law form of the RDF in the dissipation range that was found in an earlier investigation [47]
\[ \lim_{r/\eta \ll 1} g(r) = c_0 \left( \frac{\eta}{r} \right)^{c_1}, \]  

and to predict the dependence of the power, \( c_1 \), on the Stokes number.

CT constructed the following closed equation for the RDF

\[ \frac{\partial g}{\partial t} + \frac{\partial}{\partial r_i} \left( d_i g + D_{ij} \frac{\partial}{\partial r_j} g \right) = 0, \]  

where \( d \) is the drift velocity and \( D \) is the diffusion tensor. Details on the derivation of their result can be found in appendix B. The general expression for the drift velocity is

\[ d_i(r, t) = - \int_{-\infty}^{t'} \left\{ W_i(r, t) \frac{\partial}{\partial r_j} W_j(r^p(s), s) \right\} ds, \]  

where \( W \) is a particle velocity field whose precise definition is given in appendix B, and \( \langle \cdot \rangle \), denotes an ensemble average conditioned on \( r^p(t) = r \). They were able to close the drift velocity for \( S t \ll 1 \) by performing a perturbation expansion of the relative velocity \( w^p(t) \) (from which \( W \) is constructed), retaining only the zeroth- and first-order terms, and averaging the result over an ensemble of particle pair trajectories at a specified separation \( r \). The result for the drift velocity \( d \) for \( S t \ll 1 \) is

\[ d_i = - \frac{1}{3} S t \tau_{t f} \left\{ S^2(x^p(t), t) - R^2(x^p(t), t) \right\}, \]  

where \( \Gamma = S + R \), \( S^2 = S : S \), \( R^2 = R : R \), \( S \) being the strain-rate tensor, \( R \) being the rotation-rate tensor and \( x^p(t) \) the position of the primary particle. The average on the rhs of (8) is zero for fully mixed fluid particles and ballistic particles which uniformly sample the statistics of the turbulent flow field because \( \langle S^2(x, t) \rangle = \langle R^2(x, t) \rangle \) for incompressible, isotropic turbulence. But inertial particles sample more strain than rotation along their trajectory, which, according to (8), then leads to a net inward drift. This biased sampling mechanism for \( S t \ll 1 \) is represented in the more general result for \( d \) in (7) through the compressibility of the particle relative velocity field along the pair trajectory \( \nabla_r \cdot W(r^p(s), s) \), and it is the nature of this compressibility that causes the particles to preferentially accumulate in the straining regions of the turbulent velocity field.

They also showed that

\[ \left\{ S^2(x^p(t), t) - R^2(x^p(t), t) \right\} \propto S t, \quad \text{for } S t \ll 1, \]  

such that for \( S t \ll 1 \), \( d \propto S t^2 \). CT further analyzed \( \langle S^2(x^p(t), t) - R^2(x^p(t), t) \rangle \) in the limit \( S t \ll 1 \) and showed by perturbation analysis that, to leading order, the drift velocity can be expressed in terms of statistics prescribed along fluid particle trajectories \( (x^f(t)) \)

\[ d_i = - \left( \frac{\tau_{t f}}{3} \right) \int_{-\infty}^{t'} \left\{ \left[ S^2(x^f(t), t) - R^2(x^f(t), t) \right] \left[ S^2(x^f(t'), t') - R^2(x^f(t'), t') \right] \right\} dt', \]  

for which they derive a closed expression by relating these statistics to known statistics of the fluid dissipation and enstrophy.
The diffusion tensor, $\mathbf{D}$, for spherical particles in isotropic turbulence must be isotropic (i.e., proportional to the Kronecker delta function), hence only a single diffusion coefficient is required. Brunk et al. [48] showed that in the dissipation range the diffusion coefficient takes the form $D = -B^4 r^2 / \tau_y^3$, where $\tau_y$ is the Kolmogorov time scale, and $B^4 = 0.15$. Their analysis assumed the velocity gradient (along the particle trajectory) was white noise in time, which later they showed was false [49, 50]. CT modified the analysis in Brunk et al. [48] to account for so-called ‘non-local diffusion.’ The result was an integral form for the diffusion coefficient that they then re-expressed in differential form, but with a modified non-local coefficient $B_{NL} = 0.0926$ to make it consistent with the integral formulation.

Inserting these expressions into (6), CT were able to show that the steady state solution for $g(r)$ was a power law with a power $c_0 = A / B_{NL}^2$, where $A$ is the coefficient in the drift expression $d = -Ar / \tau_y$. In the regime $St \ll 1$, they derived $c_0 = 6.558 St^2$. Detailed comparisons with DNS were found to be in good agreement for $St \leq 0.2$.

According to CT, the physical explanation for drift is the oversampling of strain over rotation that leads to $\langle S^2 (x^p (t), t) - \mathbf{R}^2 (x^p (t), t) \rangle > 0$ and a net inward drift of particles. The mechanism is an extension of the argument made by Maxey [2]. We will return to this point below.

2.2. Zaichik et al. theory

In a series of papers [33, 51, 52], Zaichik and co-workers evolved a general theory for inertial particles in turbulence that would be valid for all $St$ and all $r$. As a consequence of its intended generality, ZT began with the joint PDF for $r^p (t)$ and $w^p (t)$ in the phase-space $\mathbf{r}, \mathbf{w}$

$$ p(r, w, t) = \langle \mathcal{P}(r, w, t) \rangle = \langle \delta \left( r^p (t) - r \right) \delta \left( w^p (t) - w \right) \rangle. $$

For relative motion governed by (3) the exact transport equation for $p(r, w, t)$ is

$$ \frac{\partial}{\partial t} p = - \frac{\partial}{\partial r^i} [wp] + \left( St_{\tau} \right)^{-1} \frac{\partial}{\partial w_j} [wp] - \left( St_{\tau} \right)^{-1} \frac{\partial}{\partial w_j} \langle \Delta u^p \mathcal{P} \rangle. \tag{10} $$

The unclosed term

$$ \langle \Delta u^p \mathcal{P} \rangle, $$

is the phase-space diffusion current that describes the effect of the turbulent velocity difference field $\Delta \mathbf{u}$ on dispersing the particles throughout the phase-space $\mathbf{r}, \mathbf{w}$. In order to close this term, ZT applied the Furutsu–Novikov correlation splitting technique (e.g., see [53, 54]) which relates the diffusion current to a series expansion involving the cumulants of the field $\Delta \mathbf{u}$ and the functional derivatives of $\mathcal{P}$ with respect to $\Delta \mathbf{u}$. To truncate this expansion, ZT further assumed the field $\Delta \mathbf{u}$ is a spatially and temporally correlated Gaussian field, for which the series expansion formally reduces to an exact expression involving only the second-order cumulant of $\Delta \mathbf{u}$. With this closure, the PDF equation becomes

$$ \frac{\partial}{\partial t} p = - \frac{\partial}{\partial r^i} [wp] + \left( St_{\tau} \right)^{-1} \frac{\partial}{\partial w_j} [wp] + \frac{\partial}{\partial w_j} \left[ \frac{\partial}{\partial r^j} \lambda^\mu p + \frac{\partial}{\partial w^j} \mu^\mu p - \kappa p \right], \tag{11} $$
where $\lambda(r, w, t)$ and $\mu(r, w, t)$ are dispersion tensors defined as

$$
\lambda_{\mu}(r, w, t) = \left( Str_n \right)^{-1} \int_0^t \left\langle G_{ji}(t; t') \Theta_{ji}(r^p(t'), t'; r, t) \right\rangle_{r, w} \, dt',
$$

(12)

$$
\mu_{\mu}(r, w, t) = \left( Str_n \right)^{-1} \int_0^t \left\langle G_{ji}(t; t') \Theta_{ji}(r^p(t'), t'; r, t) \right\rangle_{r, w} \, dt',
$$

(13)

and $\kappa(r, w, t)$ is a drift tensor defined as

$$
\kappa_{\mu}(r, w, t) = \left( Str_n \right)^{-1} \int_0^t \left\langle G_{ji}(t; t') \partial_{ji} \Theta_{ji}(r^p(t'), t'; r, t) \right\rangle_{r, w} \, dt'.
$$

(14)

In these expressions $t' \leq t$ and the subscripts to the angled brackets indicate a conditioned ensemble average, such that only values of $G$ and $\Theta$ which are evaluated along trajectories satisfying $r^p(t) = r$ and $w^p(t) = w$ contribute to the ensemble average. The tensor $\Theta(r', t'; r, t)$ is the two-point, two-time correlation tensor for the fluid velocity difference field $\Delta u(r, t)$

$$
\Theta_{ji}(r', t'; r, t) = \left\langle \Delta u_k(r', t') \Delta u_i(r, t) \right\rangle,
$$

(15)

and $G(t; t')$ is the functional derivative

$$
G_{ji}(t; t') = \frac{\delta r^p_j(t)}{\delta \Delta u_k(r^p(t'), t')} \, dt',
$$

(16)

which describes the effect of a perturbation in the field $\Delta u$ at the particle pair position at time $t'$ upon the particle pair position at a later time $t$. Note that in (13)

$$
\dot{G}_{ji}(t; t') = \frac{d}{dt} G_{ji}(t; t') = \frac{\delta w^p_j(t)}{\delta \Delta u_k(r^p(t'), t')} \, dt'.
$$

The PDF equation in (11) may be regarded as a generalized Fokker–Planck equation [54], and reduces to the classical Fokker–Planck equation in the limit where $\Theta(r', t'; r, t) \propto \delta(t - t')$. It should be noted that (11) differs from the equation derived by ZT in that their formulation implicitly assumed $\nabla \cdot \lambda \equiv \kappa$. Strictly speaking, this assumption is false [55], however it will be shown in section 4 that in the present context of small-scale clustering in isotropic turbulence, the approximation is reasonably accurate (see also appendix C).

ZT [51] recognized that the velocity difference $\Delta u$ is far from Gaussian at small $r$, with the PDFs exhibiting stretched tails due to internal intermittency [56]. However, ZT argued that the contribution of these tails would have little effect on the low-order moments of $p(r, w, t)$ of primary concern to their theory (such as the RDF and second-order structure functions), and hence a Gaussian approximation for $\Delta u$ could yield an acceptable result. This argument is supported by other works [16, 57].
The closed expressions for the equilibrium forms of $\lambda$ and $\mu$ are

$$\lambda_{ji} = \begin{cases} \frac{r_m r_n \langle S_{jm} S_{in} \rangle}{\text{Str}_{ji} \tau_{ji}^{-1} \left(1 + \text{Str}_{ji} \tau_{ji}^{-1}\right)} + \frac{r_m r_n \langle R_{jm} R_{in} \rangle}{\text{Str}_{ji} \tau_{ji}^{-1} \left(1 + \text{Str}_{ji} \tau_{ji}\right)} & \text{for } r \ll \eta, \\ \frac{\langle \Delta u_i \Delta u_j \rangle}{\text{Str}_{ji} \tau_{ji}^{-1} \left(1 + \text{Str}_{ji} \tau_{ji}\right)} & \text{for } r \gtrsim \eta, \end{cases}$$

(17)

$$\mu_{ji} = \begin{cases} \frac{r_m r_n \langle S_{jm} S_{in} \rangle}{\text{Str}_{ji} \left(1 + \text{Str}_{ji} \tau_{ji}\right)} + \frac{r_m r_n \langle R_{jm} R_{in} \rangle}{\text{Str}_{ji} \left(1 + \text{Str}_{ji} \tau_{ji}\right)} & \text{for } r \ll \eta, \\ \frac{\langle \Delta u_i \Delta u_j \rangle}{\text{Str}_{ji} \left(1 + \text{Str}_{ji} \tau_{ji}\right)} & \text{for } r \gtrsim \eta. \end{cases}$$

(18)

Where $S$ and $R$ are the rate-of-strain and rate-of-rotation tensors, respectively, $\tau_s$ and $\tau_r$ are the strain rate and rotation rate timescales, $\tau_\eta$ is a Lagrangian timescale given by

$$\tau_\eta = \begin{cases} 0.3 \langle e \rangle^{-1/3} r^{2/3} & \text{for } \eta \ll r \ll L_j, \\ \tau_j & \text{for } r \gtrsim L_j, \end{cases}$$

(19)

and $\tau_j$, $L_j$ are the integral timescale and lengthscale of the flow. It should be noted that ZT’s original formulation [51] made the incorrect assumption $\tau_s \approx \tau_r \approx \sqrt{5} \tau_\eta$, which led to significant errors in the predictions. In subsequent papers [33, 52], they corrected this error and instead used DNS data to specify $\tau_s \approx 2.3 \tau_\eta$ and $\tau_R \approx 7.2 \tau_\eta$. We only consider the corrected formulation.

Note that in [33, 58] $\lambda$ and $\mu$ are made continuous functions of $r$ by specifying curve fits for $S_{ji}^2$ and $\tau_\eta$ that connect their various ranges in a continuous way. Since in this paper the focus is on the small scale clustering of the inertial particles, and since we are comparing the ZT with the CT (which only describes the dissipation scale behavior of the particles) we shall henceforth only consider the forms of $\lambda$ and $\mu$ for $r \ll \eta$. In Part II we consider the ZT at all scales of the turbulence.

ZT did not actually solve the PDF equation directly, but rather used it as a master equation to derive transport equations for the moments of the PDF. The momentum equation governing the RDF is obtained by multiplying (11) by $w$ and then integrating over all $w$. At equilibrium, and for an isotropic flow, the result is

$$0 = -\text{Str}_\eta \left(S_{ji}^{\eta} + \lambda_{ji}\right) \frac{\partial}{\partial r_j}\rho - \text{Str}_\eta \rho \left(\frac{\partial}{\partial r_j} S_{ji}^{\eta} + \frac{\partial}{\partial r_j} \lambda_{ji} - \lambda_{ji}\right),$$

(20)

where $S_{ji}^{\eta} (r, t) = \langle w^{\eta} (t) w^{\eta} (t) \rangle_{\eta}$ is the second-order particle velocity structure function and

$$\rho (r, t) = \int_w p (r, w, t) dw = \left\{ \delta (r^{\eta} (t) - r) \right\}. \quad (21)$$

For a statistically stationary, homogeneous and isotropic system the PDF $\rho$ is related to the RDF $g$ by [47]
where \( N \) is the total number of particles lying within the control volume \( V \) and \( n = N/V \) is the number density of particles.

For statistically stationary, homogeneous and isotropic turbulence, the transport equation obtained from (11) for the second-order velocity structure function is

\[
S_{2ij} = S_{\tau\eta} \bar{\rho}_{ij} - \frac{S_{\tau\eta}}{2\rho} \frac{\partial}{\partial \rho} \left( \rho S_{\eta ij} \right),
\]

where \( S_{i}^p (r, t) = \langle w^p(t)w^p(t) \rangle_r \) is the third-order particle velocity structure function. ZT closes the hierarchy of moment equations by introducing a ‘quasi-Gaussian’ approximation for the fourth-order moments [33, 58], yielding

\[
S_{ijk}^p = -\frac{S_{\tau\eta}}{3} \left[ (S_{2in} + \bar{\lambda}_n) \frac{\partial}{\partial \rho} S_{2jk}^p + (S_{2im} + \bar{\lambda}_m) \frac{\partial}{\partial \rho} S_{2ik}^p + (S_{2jn} + \bar{\lambda}_n) \frac{\partial}{\partial \rho} S_{2ij}^p \right].
\]

We will discuss this quasi-Gaussian approximation and its implications in more detail in Part II.

In equations (20), (23) and (24), \( \bar{\lambda}, \bar{\mu}, \bar{\kappa} \) are the integrals of equations (12), (13) and (14) over all \( \rho \); however, with the ZT closures we have \( \bar{\lambda} = \lambda, \bar{\mu} = \mu \) and \( \bar{\kappa} = \kappa \). For simplicity of notation we shall henceforth drop the ‘overline’ on these tensors.

Let us now consider the physical mechanisms governing the clustering according to (20). The diffusion tensor in (20) contains two contributions, \( S_{\tau\eta} \hat{\lambda} \) which describes the diffusion due to the turbulent field \( \Delta u \) and a second contribution \( S_{\tau\eta} S_{2}^p \) which describes the diffusion due to the particle relative velocities. In the regime \( St \ll 1 \) the particle velocity dynamics are strongly coupled to the underlying field \( \Delta u \) and \( \lambda \gg S_{2}^p \). The resulting diffusion tensor in the regime \( St \ll 1 \) is then simply \( -S_{\tau\eta} \hat{\lambda} \) and is effectively equivalent to the diffusion tensor in CT (there are subtle differences between the two, but under standard closure approximations they become the same for \( St \ll 1 \)). In the regime \( St \gg 1 \) the particle dynamics are decoupled from the underlying field \( \Delta u \) and the diffusion tensor reduces to \( -S_{\tau\eta} S_{2}^p \).

Since ZT further assumes \( V \cdot \vec{\lambda} \equiv \kappa \), the drift velocity in (20) reduces to

\[
-\frac{S_{\tau\eta}}{\rho} \frac{\partial}{\partial \rho} S_{2ij}^p,
\]

and is referred to by ZT as a ‘turbophoretic drift’, due to its similarity with the turbophoretic drift that occurs for one particle dispersion in inhomogeneous turbulent flows [59] (indeed, as has been noted in [34], there is an analogy between the clustering of inertial particles in isotropic turbulence and the near wall accumulation of inertial particles in a turbulent boundary layer, something we will return to in section 6). Beyond this simple analogy though, the papers provide little physical insight into this term. Here we attempt to explain the physical origin and meaning of the drift velocity.

The first term on the rhs of (23) is a purely ‘local’ contribution arising from the velocity space diffusion induced by the local turbulence. This local contribution to \( S_{2}^p \) makes a contribution to the drift velocity as
\[-\left(\text{St} \tau_\eta\right)^2 \frac{\partial}{\partial r_j} \mu_{ij} = -\text{St} \tau_\eta \left( \left\{ \frac{S_m(x)S_m(x)}{1 + \text{St} \tau_\eta \tau_s^{-1}} \right\} + \left\{ \frac{R_m(x)R_m(x)}{1 + \text{St} \tau_\eta \tau_r^{-1}} \right\} \right) \frac{\partial}{\partial r_j} \left( r_m r_n \right) \]
\[= -\frac{\text{St} \tau_\eta r_s^3}{3} \left( S^2(x) \right) \left( (1 + \text{St} \tau_\eta \tau_s^{-1})^{-1} - (1 + \text{St} \tau_\eta \tau_r^{-1})^{-1} \right).\]  

(25)

Introducing the DNS values \( \tau_s \approx 2.3 \tau_\eta \) and \( \tau_r \approx 7.2 \tau_\eta \) into (25) yields a positive drift velocity\(^2\). Consequently, the inward (negative) drift responsible for clustering comes entirely from the second term on the rhs of (23). In the regime \( \text{St} \ll 1 \) this term has a local scaling \( \propto r^2 \) in the dissipation regime. However at larger \( \text{St} \) the non-local contribution to the pair velocity dynamics causes deviations from this local scaling. The third-order structure function is non-zero both because \( p(r, \Delta u) \) is skewed for scales below the integral scale, and because of the history effect resulting from the particle inertia. This history effect gives rise to a symmetry break in the particle inward and outward motions, resulting in a negative skewness, even if \( p(r, \Delta u) \) happened to be symmetric. The solution to \( w_p(t) \) for a pair passing through \( r \), \( t \) is (setting \( w_p(0) = 0 \), for the sake of simplicity)

\[ w_p(t|s) = \frac{1}{\tau_\eta} \int_0^t \Delta u_s(r^p(s), s, r, t) \exp \left[ -\tau_\eta^{-1}(t-s) \right] ds. \]  

(26)

Now consider particle pairs that arrive at separation \( r \) at time \( t \); pairs that have come from larger separations will, statistically speaking, have experienced larger values of \( \Delta u(r^p(s), s, r, t) \) in their path history compared with pairs which have come from smaller separations. Consequently, according to (26), this path history asymmetry results in inwardly moving particles having larger relative velocities than outwardly moving particles, and hence \( S^p \neq 0 \).

Furthermore, since \( r^p \) is functionally dependent upon \( \Delta u(r^p(s), s, r, t) \) there may also exist a relationship between the way the pairs sample the turbulent velocity field and whether the pairs are moving together or apart, yielding a second source of symmetry breaking. These history effects give rise to a net inward drift that is responsible for the clustering.

In general, the RDF in the ZT is given by the solution to a set of coupled differential equations, specifically equations (20), (23) and (24). ZT derived a simplification for \( \text{St} \ll 1 \) by introducing an algebraic expression with unknown coefficients and powers that were determined by enforcing consistency with equations (20) and (23). The result is

\[ c_1 = 6 \text{St}^2 - 9.8 \text{St}^2 + 6.2 \text{St}^4 \]

Recall that the CT derived a similar first term, which in this limit reduced to \( c_1 = 6.558 \text{St}^2 \). It is suprising that there is such a small difference in the lead coefficient (i.e., 6 versus 6.558) given that the theories appear to describe the physical mechanism for clustering in quite different ways. In the next section we explain the similarity of their prediction for \( c_1 \) in the regime \( \text{St} \ll 1 \), showing that the similarity is in fact not coincidental.

\(^2\) We expect that this positive drift is simply an artifact arising because of the somewhat artificial way ZT splits up the strain and rotation contributions to \( \Delta u \) in the dissipation regime. However, this positive drift is negligible compared to the overall inward drift and therefore is irrelevant.
3. Analyzing the theories

3.1. Why the theories are similar in the regime $St \ll 1$

In order to gain insight into the relative agreement of the two theories in the limit $St \ll 1$, it is instructive to consider the drift velocity for the ZT in this limit. Recall that the ZT drift velocity is given by

$$\tau_{ij} \frac{\partial}{\partial \tau_k} S^p_{2ik} = -\tau_{ij} \frac{\partial}{\partial \tau_k} \langle w^p_i(t) w^p_j(t) \rangle_r.$$ 

In the CT, perturbation theory is applied to the particle equation of motion to obtain the following approximate solutions for $St \ll 1$

$$r^p_i(t) = r^p_i[0] + St r^p_i[1],$$  \hspace{1cm} (27)

$$w^p_i(t) = \Gamma^p_{ij} r^p_j[0] + St r^p_i \left( \tau_{ij} \Gamma^p_{km} - \tau_{ij} \frac{d}{dt} \Gamma^p_{km} - \Gamma^p_{ij} \Gamma^p_{km} r^p_i[1] \right),$$  \hspace{1cm} (28)

where the superscripts $[0]$ and $[1]$ denote the zeroth and first order terms in the perturbation expansion for $r^p(t)$. CT used (27) and (28) to derive the $St \ll 1$ form of their drift velocity in (8). Substituting (28) into the ZT drift velocity and invoking the conditioning approximation made in the CT $r = r^p \approx r^p[0]$ and $r[1] = 0$ we obtain

$$-\tau_{ij} \frac{\partial}{\partial \tau_k} S^p_{2ik} \approx -\tau_{ij} \frac{\partial}{\partial \tau_k} \left( r^p_j \langle \Gamma^p_{ij} \Gamma^p_{km} \rangle_r \right) + \left( \tau_{ij} \frac{\partial}{\partial \tau_k} \right) \left( r^p_j \langle \frac{d}{dt} \Gamma^p_{km} \rangle_r \right)$$

$$+ \left( \tau_{ij} \frac{\partial}{\partial \tau_k} \right) \left( r^p_j \langle \frac{d}{dt} \Gamma^p_{km} \rangle_r \right) + \left( \tau_{ij} \frac{\partial}{\partial \tau_k} \right) \left( r^p_j \langle \Gamma^p_{km} \Gamma^p_{km} r^p_i \rangle_r \right)$$

$$+ \left( \tau_{ij} \frac{\partial}{\partial \tau_k} \right) \left( r^p_j \langle \Gamma^p_{km} \Gamma^p_{km} r^p_i \rangle_r \right) + O\left( \tau_{ij} \frac{\partial}{\partial \tau_k} \right).$$  \hspace{1cm} (29)

Furthermore, the introduction of the approximation $r = r^p \approx r^p[0]$ and $r[1] = 0$ means that the density weighted averages $\langle \cdot \cdot \rangle_r$ in (29) are equivalent to unconditioned ensemble averages $\langle \cdot \cdot \rangle$ (since the distribution of $r^p[0]$ is uniform). Applying this to (29)

$$-\tau_{ij} \frac{\partial}{\partial \tau_k} S^p_{2ik} \approx -St \langle \Gamma^p_{ij} \Gamma^p_{km} \rangle \frac{d}{dt} \left( r^p_j \right) + \left( St \frac{d}{dt} \Gamma^p_{km} \right) \frac{d}{d\tau_k} \left( r^p_j \right)$$

$$+ \left( St \frac{d}{dt} \Gamma^p_{km} \right) \frac{d}{d\tau_k} \left( r^p_j \right) + \left( St \frac{d}{dt} \Gamma^p_{km} \Gamma^p_{km} \right) \frac{d}{d\tau_k} \left( r^p_j \right)$$

$$+ \left( St \frac{d}{dt} \Gamma^p_{km} \Gamma^p_{km} \right) \frac{d}{d\tau_k} \left( r^p_j \right).$$  \hspace{1cm} (30)
Evaluating each of the terms and simplifying yields (see appendix A for details)

\[-\text{Str}_\eta \frac{\partial}{\partial r_i} S_{\text{SS}} \approx -\text{Str}_\eta \left\langle \Gamma_{ij}^{p} \Gamma_{km}^{p} \right\rangle \frac{\partial}{\partial r_i} \left( r_j r_m \right) - \frac{2}{3} \left( \text{Str}_\eta \right)^2 r_i \left\langle \Gamma_{ij}^{p} \Gamma_{km}^{p} \Gamma_{lm}^{p} \right\rangle \]

\[
+ \frac{2}{3} \left( \text{Str}_\eta \right)^2 r_i \left\langle \Gamma_{ij}^{p} \Gamma_{km}^{p} \Gamma_{ml}^{p} \right\rangle 
= -\text{Str}_\eta \left\langle \Gamma_{ij}^{p} \Gamma_{km}^{p} \right\rangle \frac{\partial}{\partial r_i} \left( r_j r_m \right) 
= -\text{Str}_\eta \left\langle \Gamma_{ij}^{p} \Gamma_{km}^{p} \right\rangle \left( r_m \delta_{jk} + r_j \delta_{mk} \right) 
= -\text{Str}_\eta r_m \left\langle \Gamma_{ij}^{p} \Gamma_{km}^{p} \right\rangle - \text{Str}_\eta r_j \left\langle \Gamma_{ij}^{p} \Gamma_{mm}^{p} \right\rangle 
= -\frac{2}{3} \left( \text{Str}_\eta \right)^2 r_i \left\langle \Gamma_{ij}^{p} \Gamma_{km}^{p} \right\rangle 
= \frac{1}{3} \text{Str}_\eta r_i \left\langle S^2 \left( x^p(t), t \right) - \mathcal{R}^2 \left( x^p(t), t \right) \right\rangle. \tag{31}
\]

Comparing this with (8) from CT shows the equivalence of the two theories in the limit $\text{St} \ll 1$; that is, the drift velocity for ZT approaches that for the CT in this limit, suggesting conversely that CT captures the leading order contribution to the drift velocity in the ZT, in this limit. In addition to this, as explained in section 2, the diffusion tensors in CT and ZT are equivalent in the regime $\text{St} \ll 1$ and this, along with the drift velocity analysis above, explains the similarity in the theory predictions for $c_1$ for $\text{St} \ll 1$. The closed form predictions for $c_1$ differ slightly because of the way the two theories close the expression $\left\langle S^2 \left( x^p(t), t \right) - \mathcal{R}^2 \left( x^p(t), t \right) \right\rangle$, the CT closure being given through (9) and the ZT closure being contained within its transport equation for $S^p_{\text{SS}}$.

### 3.2. Why the theories differ outside the regime $\text{St} \ll 1$

In order to explain why the theories are different outside the regime $\text{St} \ll 1$, it is useful to first understand why the ZT reduces to the CT drift mechanism in the regime $\text{St} \ll 1$. In the dissipation regime (26) becomes

\[ w^p \left( t \mid r \right) = \frac{1}{\tau_p} \int_0^t \Gamma^p_{ij} \left( s \mid r, t \right) r_j^p \left( s \mid r, t \right) \exp \left[ -\tau_p^{-1} (t - s) \right] ds. \tag{32} \]

In the regime $\text{St} \ll 1$, $\Gamma^p$ and $r^p$ fluctuate on timescales much larger than $\tau_p$ and so

\[ w^p \left( t \mid r \right) \approx \Gamma^p_{ij} \left( t \mid r, t \right) r_j^p \frac{1}{\tau_p} \int_0^t \exp \left[ -\tau_p^{-1} (t - s) \right] ds \]

\[ = \Gamma^p_{ij} \left( t \mid r, t \right) r_j^p \left( \text{for } t \gg \tau_p \right). \tag{33} \]

It is this contribution at $\text{St} \ll 1$ that gives rise to the CT drift velocity and the result in (31) (since, as we have shown in section 3.1, the contributions to the drift velocity coming from the $O(\text{St})$ contributions to the perturbation expansion for $w^p(t)$ cancel each other out exactly), and
reflects the fact that at small $St$ the particle velocity field is single valued to leading order. Thus at low $St$ the symmetry breaking mechanism that gives rise to the inward drift and clustering comes not from the fact that, at a given separation, some pairs have come from larger separations and others from smaller separations (i.e. the path history symmetry breaking mechanism) but from the effect of the particles preferentially sampling the turbulence (this is the second source of symmetry breaking mentioned in section 2.2). How this breaks the symmetry is clear; the inertial particles respond differently to the straining and rotating motions of the turbulence giving rise to the traditional ‘centrifuge’ mechanism. Outside of the regime $St \ll 1$, the path history contribution to the pair velocity dynamics gives rise to an even stronger break in the particle inward and outward motion symmetry. The ZT captures this effect but the CT, because of its approximations $r = r^p \approx r^{[0]}$ and $r^{[1]} = 0$ (which makes $w^p$ single valued in the CT), does not.

Related to this is that the CT is unable to capture the influence of caustics on clustering. Recall that caustics are points in the fluid where multiple particles coexist with finite relative velocities at zero separation. At finite Stokes numbers this phenomenon has been observed in DNS [44]. The ZT predicts the existence of caustics through the second-order particle velocity structure function

$$S_{2ij}^p = St\tau_{ij} - \frac{Str_{ij}}{2\rho} \frac{\partial}{\partial r_i} \left( \rho S_{ijk}^p \right), \quad (34)$$

which contains both a smooth, local contribution (the first term, proportional to $r^2$ in the dissipation regime of the turbulence) and the second term, which captures the non-local dynamics and gives rise to $\lim_{r \to 0} S_{2}^p \neq 0$. In contrast, the CT approximation for the solution to $\langle w^p (t) \rangle$ generates $S_2^p \propto r^2$. Therefore the difference between CT and ZT outside $St \ll 1$ is also related to their ability to capture the influence of caustics on the clustering of particles in isotropic turbulence. We consider the role played by the formation of caustics on the behavior of the RDF in more detail in Part II.

4. Comparisons with DNS

We now evaluate the accuracy of the ZT by comparing its predictions to DNS. The exact equation governing the steady state RDF for an isotropic turbulent flow is

$$0 = \rho \left\langle \Delta u(r^p (t), t) \right\rangle_r - Str_{ij} \frac{\partial}{\partial r_i} \rho S_{ik}^p. \quad (35)$$

The ZT closes this expression by applying the Furutsu–Novikov closure and approximating $\Delta u$ as a spatio-temporally correlated Gaussian field, yielding (see section 2)

$$\rho \left\langle \Delta u(r^p (t), t) \right\rangle_r = -Str_{ij} \frac{\partial}{\partial r_i} \rho \lambda_{ji} + Str_{ij} \rho \kappa_{ij}. \quad (36)$$

That the closure in (36) only contains the gradient of $\rho$ and not higher order derivatives is a consequence of the Gaussian approximation for $\Delta u$. For non-Gaussian $\Delta u$ the closure for $\langle \Delta u (r^p (t), t) \rangle_r$ would contain, in addition to the gradient diffusion term $\lambda \cdot \nabla \rho$, an infinite sum of higher order derivatives of $\rho$, each with a corresponding diffusion tensor related to a successively higher order cumulant of the field $\Delta u$. Likewise, the closure for $\langle \Delta u (r^p (t), t) \rangle_r$
with non-Gaussian $\Delta u$ would contain not only the drift $\nabla \cdot \lambda - \kappa$ (associated with the second-order cumulant of the field $\Delta u$), but also an infinite sum of drift terms, each associated with successively higher order cumulants of the field $\Delta u$. In addition to neglecting these higher order cumulants, the ZT further assumes $\nabla \cdot \lambda \equiv \kappa$, which in general is not true (see section 2). It is important to assess how each of these assumptions affects the accuracy of the ZT.

When cast into spherical co-ordinates, and invoking isotropy, the solution to (20) is given by

$$\rho(r) = c_\rho \exp \left( - \int_{r_{min}}^r \left( S_{\parallel}^P + \lambda_\parallel \right)^{-1} \left( \frac{d}{dr} S_{\parallel}^P + 2 \tau^{-1} \left( S_{\parallel}^L - S_{\perp}^L \right) \right) dr \right), \quad (37)$$

where $c_\rho$ is a constant (chosen to give $\rho(r_{max}) = 1$) and $S_{\parallel}^P$, $S_{\perp}^P$, $\lambda_\parallel$ and $\lambda_\perp$ are the longitudinal and transverse components of the second-order isotropic tensors $S_\parallel^P$ and $\lambda$. In order to evaluate the ZT prediction for $\rho(r)$ independently from its prediction for $S_\parallel^P$, we use $S_\parallel^P$ from DNS data and then generate the solution for $\rho(r)$ from equation (37). Comparing this solution with DNS data for $\rho(r)$ allows us to test the validity of equation (37) separately from the closure approximation for $S_\parallel^P$ (which is investigated in Part II of this paper). Furthermore, in the formula for $\lambda_\parallel$ (see (17)) we used the value for $\tau_\parallel$ taken from the present DNS, which was found to be $\tau_\parallel \approx 2.02 \tau_\parallel$.

Over the range of $r$ accessible by DNS, $\rho(r)$ is a power law. Figure 1 shows a comparison of the power law exponent $c_1(\rho_S)$ obtained from the DNS with that obtained from equation (37). Although the ZT captures the qualitative features of the DNS data for $c_1(\rho_S)$ very well, there is an appreciable quantitative discrepancy. This could be due to the omission of the non-Gaussian cumulants of $\Delta u$ in the ZT or the assumption $\nabla \cdot \lambda \equiv \kappa$. However, another possible source of the discrepancy concerns the closure of $\lambda_\parallel$. The closed form for $\lambda_\parallel$ (obtained from (17)) is derived based on a local closure approximation of (12). Local closures to these dispersion tensors can have significant errors [60], and it is possible that these errors are at least partially responsible for the disagreement observed in figure 1.

As discussed in section 2, the unclosed forms of the diffusion tensors in the ZT and CT are equivalent in the regime $\tau \ll 1$. Indeed, in the regime $\tau \ll 1$ the local closure for $\lambda_{\parallel}$ leads to the same result as the local closure for the diffusion coefficient in the CT, namely $B_{\parallel} = \left(1/15\right) \tau_\parallel^{-1} \tau_S = 0.135$ (note here we are using $\tau_S/\tau_\parallel = 2.02$ from the DNS). The CT developed a theoretical expression for the non-local diffusion that resulted in a modified prefactor $B^{NL} \approx 0.0926$, and their simulations confirmed this value of the coefficient. However, our DNS yields the result $B^{NL} \approx 0.56$, which is consistent with the suggestion in [61]. This implies $B^{NL} \approx 0.42 B_{\parallel}$. Note the superscripts ‘L’ and ‘NL’ refer to the ‘local’ and ‘non-local’ values, respectively.

Based on the equivalence between the ZT and CT diffusion tensors in the regime $\tau \ll 1$, we can substitute the non-local closure from the CT into the ZT, which implies $\lambda_{\parallel}^{NL} \approx 0.42 \times \lambda_{\parallel}^{L}$, where $\lambda_{\parallel}^{L}$ is the ‘local’ expression given in equation (17). Strictly speaking, this non-local correction is only applicable in the regime $\tau \ll 1$; however, it is more realistic than the local expression except possibly in the opposite limit $\tau \gg 1$, but this is not relevant.
since $\lambda_\parallel$ vanishes in this limit. Figure 2 shows the result of the ZT with the non-local closure for $\lambda_\parallel$ in (37). For reference, we also show the prediction for $c_1$ determined from the CT using $B^{NL} \approx 0.42B^L$ and DNS data to specify $\langle S^2 (x^p(t), t) - \mathcal{R}^2(x^p(t), t) \rangle$ in the CT drift velocity expression. There is now excellent agreement among the three curves for $St \lesssim 0.5$. Moreover, the prediction of the ZT with the non-local diffusion correction is now in reasonably good agreement with the DNS over the entire range of Stokes numbers. This supports neglecting the terms associated with the non-Gaussian cumulants of $\Delta u$. Comparing figures 1 and 2 shows that for larger Stokes numbers, the introduction of the non-local closure for $\lambda_\parallel$ does not make much difference. This is not too surprising since $\lim_{St \to 0} S^{2 \parallel} + \lambda_\parallel \to S\tau r_\parallel$, but $\lim_{St \to \infty} S^{2 \parallel} + \lambda_\parallel \to S\tau r_{2 \parallel}$. What is surprising, however, is that the biggest discrepancy between the ZT predictions and the DNS data in figure 2 occurs at higher Stokes numbers. One would expect that the effects of ignoring the non-Gaussian features of $\Delta u$ would be greatest at smaller $St$, where particle motions are more sensitive to the non-Gaussian tails of the PDF for $\Delta u$. Hence the errors at larger Stokes numbers are more likely not due to the Gaussian approximation, but due to the omission of the drift $\nabla_r \cdot \lambda - \kappa$. In appendix C we provide a plausible explanation for why this omission would be negligible in the limit $St \ll 1$, and would grow in importance with increasing Stokes number.

Figure 2 also shows that the CT and ZT predictions for $c_1$ are similar for small $St$ but differ significantly for $St \gtrsim 0.5$. The analysis in section 3.1 provides a good explanation. In the limit $St \ll 1$, the CT captures the leading order contribution to the clustering mechanism in the ZT. As $St$ increases the non-local contribution to the particle relative velocity increases. Beyond the threshold of $St \sim 1$, the non-local contribution to the particle pair dynamics begins to diminish.
the coherence of the inward motion, until at the other extreme limit \( St \gg 1 \), the dynamics are entirely non-local and \( c_1 \rightarrow 0 \). As noted in section 3.2, the CT does not capture this non-local contribution to the dynamics and so does not accurately predict the peak and subsequent decrease of \( c_1 \) at \( St \sim 1 \) (although the CT does correctly predict \( c_1 \rightarrow 0 \) in the limit \( St \rightarrow \infty \), as in this limit \( \langle S^2(x^p(t), t) - R^2(x^p(t), t) \rangle \rightarrow 0 \).

Finally, to show that the non-local contribution the particle relative velocities enhances the inward drift, we compute \( c_1 \) from ZT but using the CT diffusion coefficient in the ZT RDF equation (i.e. replacing \( S_{2\parallel} + \lambda_\parallel^{-1} \) in (37) with \( D = B^{NL} r^{-2} \)). Doing this eliminates the non-local contribution to the diffusion tensor and allows us to isolate its effect upon the drift mechanism. The results are shown in figure 3.

For the results in figure 3, the only difference between the CT and ZT results is that only the ZT captures the non-local contribution to the inward drift. The results clearly demonstrate that this non-local contribution significantly enhances the inward drift. Of course the non-local contribution eventually destroys the inward drift since in the regime \( St \gg 1 \) the particle relative velocities become independent of \( r \). It also demonstrates that the peak and subsequent decrease of \( c_1 \) at \( St \sim 1 \) (shown in figure 2) does not occur because of the effect of the non-local contribution to the inward drift mechanism, but rather because of its enhancement of the diffusion tensor through \( S_{2\parallel}^p \).
5. Relationship to other theories in the literature

5.1. The centrifuge mechanism

The original thinking and analysis of inertial particle clustering goes back to the seminal studies by Maxey and Corrsin [62], and later Maxey [2]. This early work used a cellular flow to demonstrate visually and statistically that an initially homogeneous particle field would segregate, with particles preferring to be in regions of low vorticity. This was followed by DNS by Squires and Eaton [19] who termed the phenomenon ‘preferential concentration’ in recognition of the fact that the particles preferentially accumulated in regions of high strain rate over high rotation rate. Indeed, virtually all of the early literature referred to the centrifuging mechanism and the strong correlation (anti-correlation) of the particle concentration field with the local rate-of-strain (rate-of-rotation) tensor [3, 6, 20, 21, 63]. For binary processes such as collision, the RDF is the precise correction to the collision kernel, and so much of the modern work has focused on the power-law behavior of the RDF at small separations [47]. Certainly, the CT is a continuation of this line of thinking.

Bec and collaborators [64–67] investigated the phenomena of particle clustering in turbulence using tools from dynamical systems theory. In these works, the dynamics of the full phase-space for particle position and velocity are examined, and it is emphasized that the dynamics of inertial particles are dissipative compared to those of fluid particles whose dynamics in incompressible turbulence are conservative. As a consequence, the inertial particles evolve towards a phase-space dynamical attractor. Since particle positions are obtained by the projection of their phase-space positions onto configuration space, it is the evolution of particle phase-space trajectories to the dynamical attractor that gives rise to spatial clustering. Their analysis of the relationship between the particle locations and the local structure of $I$ yielded
the familiar centrifuging argument [65]; however, they emphasized that while the centrifuging mechanism triggers the clustering, it is the dissipative nature of the inertial particle dynamics that is responsible for the strong clustering that develops. In these works, the particle clustering is related to the Hausdorff dimension, which is itself estimated using the Lyapunov dimension, determined through the Lyapunov exponents. Numerical results in [64] showed that the Lyapunov dimension is proportional to $S^2$ for small $S_t$, in agreement with both the CT and ZT.

A conceptual challenge with the intuitive physical argument of particles being centrifuged out of vortices is how such a mechanism could account for clustering at length scales well below the Kolmogorov length scale. That is, it is difficult to imagine centrifugation by eddies on the order of the Kolmogorov scale in size leading to clustering at length scales several orders of magnitude smaller. Indeed, it was this conceptual challenge that provided the motivation for the CT. The theory showed how preferential sampling leads to an inward drift at all separations, allowing point particles to accumulate indefinitely.

5.2. Non-centrifuge mechanisms

Despite the intuitive and physical appeal of the centrifuge mechanism, challenges were raised about its completeness. For example, Bec [64] described simulations of inertial particles in random flows that are white-in-time and unstructured that nevertheless demonstrate significant clustering, suggesting the existence of other clustering mechanisms.

Gustavsson and Mehlig [30] developed a theory for inertial particles in a white-in-time random flow that describes the RDF and relative velocity moments (although not in closed form; they contain unknown functions of $S_t$). In [31] they extended the work to random flows with small, but finite time correlations (the theory cannot yet reach the regime of real turbulence, where the time correlation is on the order of the Kolmogorov time scale), and they identify two distinct mechanisms for clustering, one they call ‘ergodic’ and the other they call ‘non-ergodic.’ The ergodic mechanism is one in which the particles uniformly sample the underlying flow field; this regime applies to $S_t \to \infty$ and $Ku \to 0$. In this regime, they argue that clustering occurs due to ‘multiplicative amplification: small line, area, and volume elements may randomly expand and contract, and depending upon whether the random product of expansion and contraction factor increases or decreases as $t \to \infty$, it is possible to observe clustering.’ This long time expansion and contraction behavior may be described by Lyapunov exponents. The non-ergodic mechanism they argue is essentially the centrifuge mechanism put forward by Maxey [2] (i.e., clustering arises from the fact that inertial particles sample the flow in a non-ergodic manner, in contrast to $S_t \equiv 0$ and $S_t \to \infty$ particles which sample the turbulence in a uniform, ergodic manner). Across the range $0 < S_t < \infty$ the relative importance of the ergodic and non-ergodic mechanisms varies, with the non-ergodic mechanism dominating for small $S_t$ and the ergodic mechanism dominating for large $S_t$. In contrast to [31], the ZT has only a single mechanism that spans all Stokes numbers. Nevertheless, the analysis in section 3.1 suggests that in the regime $S_t \ll 1$, the drift velocity in ZT is to leading order related to $\langle S^2 (x^p(t), t) - R^2 (x^p(t), t) \rangle$. In light of this, it may be considered that the non-ergodic and ergodic mechanisms are similar to the ZT clustering mechanism in the regimes $S_t \ll 1$ and $S_t \gg 1$, respectively.

3 The Kubo number for a turbulent flow is defined as $Ku = u_r \tau \eta$. For real turbulence $Ku \sim 1$, and the theory presented in [31] is only valid for $Ku < 0.2$. 
Reeks and coworkers [43, 68, 69] studied the spatial clustering and relative velocities of inertial particles in homogeneous, isotropic turbulence by considering the evolution of the deformation tensor $J$ defined as

$$J_{ij}(t) = \frac{\partial x^p_i (X, t)}{\partial X_j},$$

(38)

where $X = x^p (t = 0)$. Using the definition $\mathcal{J}(t) = \det [J]$ they are able to consider the compression $C$ of the particle motion $C(t) = \ln [\mathcal{J}(t)]$ (and the net compressibility $\langle \mathcal{C} (t \to \infty) \rangle$) in addition to the spatially averaged moments of the particle number density $n (x, t)$ with $\overline{n^a} = \langle \mathcal{J}^{1-a} \rangle$, where $\langle \cdots \rangle$ denotes a spatial average over the whole system domain.

In these works the authors consider the singularities in the particle concentration field which occur in the limit $\mathcal{J} \to 0$, and which are associated with particle clustering. Through simulations they found that the rate of occurrence of the singularities reaches a maximum for $St \sim 1$, and that the distribution of times between singularities follows a Poisson process. They also showed that above a certain threshold value of $St$, the net compressibility changes sign from being negative to positive, while at the same time their results show that in cases where the net compressibility is positive, segregation of the particles throughout the flow is still observed. They explain this by noting that throughout the flow field there will be regions of both compression and dilution, such that whereas the net compressibility is positive, there may still be regions where the local compressibility is negative, and hence the observation of regions of segregation. In addition they note that the compressibility at a given time is not governed simply by the local topology of the flow (this is only true for $St \ll 1$), but also by the particle’s history of encounters with turbulent eddies. They argue that the traditional centrifuge mechanism invoked to explain clustering might only be appropriate for small $St$; outside of this range other effects (i.e. history effects) could be significant. Note also that in [70] Reeks considers the mechanisms governing the drift and clustering of inertial particles in turbulence. In appendix C we demonstrate that the drift mechanism in this work is the same as that in the ZT and CT in the dissipation regime and for $St \ll 1$. In general the theory in [70] contains an additional drift mechanism to that in ZT, but according to the results in section 4 this is only important for $St > 1$.

Vassilicos and collaborators [35–37] observed that particles tend to cluster near zero-acceleration points in the flow. They argued that the particle equation of motion causes them to tend to ‘stick’ to these zero acceleration points, whereas they tend to move away from non-zero acceleration points. The result is the clustering of inertial particles, which is correlated to the clustering of zero-acceleration points, a quantity that can be computed purely from the flow. Results from their simulations [37] show that spatial clustering may be observed in the inertial range even when the preferential sampling of strain over rotation is absent. The authors caution that the sweep-stick mechanism is primarily intended to describe clustering in the inertial range, and that the centrifuge mechanism is still the dominant mechanism in the dissipation range. Therefore for sub-Kolmogorov scale clustering (the primary topic of this paper), the sweep-stick mechanism does not offer any new physical argument for the clustering mechanism.
6. Relationship to near-wall particle accumulation in a turbulent boundary layer

It has been noted (e.g. [34, 71]) that there is an analogy between particle pair clustering in isotropic turbulence and the near wall accumulation of inertial particles that occurs in turbulent boundary layers. In this section, we explore this in more detail and show in what ways these two systems are similar and in what ways they are different.

Let \( x^p(t), v^p(t) \) denote the single-particle position and velocity vectors. In a fully developed turbulent boundary layer, the statistics are inhomogeneous only in the wall-normal \((x_2)\) direction, and the equation governing the wall-normal steady state particle position distribution \( \rho(x_2) \) is (from the single-particle equivalent of the RDF equation in the ZT)

\[
0 = -\tau_p \left( \left\langle v^p_2(t) v^p_2(t) \right\rangle_{x_2} + \lambda_{22} \right) \frac{d}{dx_2} \rho - \tau_p \rho \frac{d}{dx_2} \left\langle v^p_2(t) v^p_2(t) \right\rangle_{x_2},
\]

where \( \lambda \) is the one-particle equivalent of (12) and the subscript 2 denotes the wall-normal direction of the boundary layer. Note that (39) should, like (20), contain an additional drift velocity \( \nabla \rho \). In appendix C, we argue that in the dissipation range of isotropic turbulence, for \( St \ll 1 \), this drift velocity can be neglected. In the present case of a turbulent boundary layer, where the flow is anisotropic, the same argument cannot be used to show that this drift is negligible in the viscous sublayer. However we conjecture that in this regime \( \nabla \rho \) is much smaller than \( -\tau_p \nabla \rho \left\langle v^p_2(t) v^p_2(t) \right\rangle_{x_2} \). The proof will be left for a future paper.

In the following analysis we consider the particle motion and concentration in the viscous sublayer of the turbulent boundary layer, in which the fluid velocity timescales are independent of \( x_2 \). We denote the Stokes number in wall units as \( \tau_w \), where \( \tau_w \) is the near-wall timescale of the fluid, and consider the limit \( St \ll 1 \). Introducing the standard weak inertia approximation \( v^p(t) \approx u(x^p(t), t) - St \tau_w \rho \left\langle u(x, t) \right\rangle \), where \( \left\langle u(x, t) \right\rangle \) is the fluid acceleration field, yields

\[
-St \tau_w \frac{d}{dx_2} \left\langle v^p_2(t) v^p_2(t) \right\rangle_{x_2} = -St \tau_w \frac{d}{dx_2} \left\langle u'_2(x^p_2(t), t) u'_2(x^p_2(t), t) \right\rangle_{x_2} + O(St^2),
\]

where \( u'(x, t) = u(x, t) - \left\langle u(x, t) \right\rangle \). In the region close to the wall \( u'(x, t) \approx x \cdot \nabla u'(0, t) \) which gives

\[
-St \tau_w \frac{d}{dx_2} \left\langle v^p_2(t) v^p_2(t) \right\rangle_{x_2} = -St \tau_w \frac{d}{dx_2} \left\langle \left( x^p_2(t) \frac{d}{dx_2} u'_2(x^p_2(t) = 0, t) \right)^2 \right\rangle_{x_2}.
\]

By analogy to the analysis in section 3.1, in the limit \( St \ll 1 \), \( \left\langle \cdots \right\rangle_{x_2} \approx \left\langle \cdots \right\rangle \), which implies

\[
-St \tau_w \frac{d}{dx_2} \left\langle v^p_2(t) v^p_2(t) \right\rangle_{x_2} = -2St \tau_w \left\langle \left( \frac{d}{dx_2} u'_2(x^p_2(t = 0, t) \right)^2 \right\rangle_{x_2} = -2St \tau_w \left\langle S_{22}^2(x^p_2(t) = 0, t) \right\rangle,
\]

where \( S_{22} \equiv \frac{d u'_2}{dx_2} \) is the rate-of-strain tensor component. Comparing this to the result in (31), we make several important observations. First, the drift velocity in (42) only contains velocity
contributions in the wall-normal direction and does not contain any contribution from the rate-of-rotation tensor of the turbulence. This reflects the fact that in a turbulent boundary layer the fluid velocity statistics only depend on one direction, the wall normal direction, and so only the velocities in this direction are able to generate a net inward drift leading to clustering. In the case of pair statistics in isotropic turbulence (the main topic of this paper), the inward drift velocity is expressed as \[-\St \nabla \cdot S^p = -\St \nabla r^{-1} (\nabla r S^p_2 + 2 r^{-1} \left[ S^p_2 - S^p_2 \right])\], which contains the centrifugal contribution \[-\St 2 r^{-1} \left[ S^p_2 - S^p_2 \right]\] that is absent from the turbulent boundary layer case because of its lack of spherical symmetry.

A second important observation concerns the dependence of the drift velocities on the inertia. For the isotropic case in the limit \(St \ll 1\), the inward drift is \(\propto St^2\) because the leading order contribution to \(\langle S^2(x^\rho(t), t) - \mathcal{R}^2(x^\rho(t), t) \rangle\) is proportional to \(St\) (since \(\langle S^2(x, t) - \mathcal{R}^2(x, t) \rangle = 0\) for homogeneous isotropic turbulence). As the diffusion tensor in this regime is independent of \(St\), this gives rise to a power-law exponent that is \(\propto St^2\). In contrast, the effect of rotation on the drift in a boundary layer is absent, and \(\langle S^2_{2\perp}(x^\rho(t), t) \rangle \neq 0\) for \(St_w = 0\). Consequently in a boundary layer, the leading order contribution to the inward drift velocity is proportional to \(St_w\) not \(St^2_{w}\). As the diffusion coefficient in the boundary layer too is independent of \(St_w\), the near-wall particle concentration grows as a power law with an exponent \(\propto St_w\), as suggested by [34, 72]. This difference in the scaling arises solely due to the lack of spherical symmetry in the turbulent boundary layer.

The physical interpretation of (42) in the limit \(St \ll 1\) is not as transparent as for particle pairs in isotropic turbulence, where the inward drift vanishes for \(St = 0\); nevertheless, a physical interpretation is possible. The exact equation governing the steady state wall-normal particle distribution \(\rho(x_2)\) is

\[
0 = -\frac{\partial}{\partial x_2} \rho \langle v^p_2(t) v^p_2(t) \rangle_{x_2} + \rho \langle \dot{v}^p_2(t) \rangle_{x_2}. \tag{43}
\]

For \(St_w = 0\) this becomes

\[
0 = -\langle u^2_2(x_2, t) u^2_2(x_2, t) \rangle \frac{\partial}{\partial x_2} \rho - \rho \frac{\partial}{\partial x_2} \langle u^2_2(x_2, t) u^2_2(x_2, t) \rangle + \rho \left\langle \frac{D}{Dt} u_2(x_2, t) \right\rangle. \tag{44}
\]

Using the Navier–Stokes equation we have

\[
\left\langle \frac{D}{Dt} u_2(x_2, t) \right\rangle = -\frac{\partial}{\partial x_2} \langle p^f (x_2, t) \rangle, \tag{45}\n\]

where \(p^f(x, t)\) is the fluid pressure field, and using the definition of the material derivative (noting \(\langle u_2(x_2, t) \rangle = 0\))

\[
\left\langle \frac{D}{Dt} u_2(x_2, t) \right\rangle = \frac{d}{dx_2} \langle u^2_2(x_2, t) u^2_2(x_2, t) \rangle. \tag{46}\n\]

Using these results we can see that the solution to (44) is \(\rho(x_2) = \text{constant}\) because the inward drift associated with the gradient of the wall normal fluid Reynolds stress is precisely canceled by the wall-normal pressure gradient in the fluid.
Inertial particles in the limit $St \ll 1$ also experience a drift towards the wall because of the local gradient of the wall-normal Reynolds stress, however in contrast to fluid particles, this drift is not precisely canceled because the inertial particle acceleration differs from the pressure gradient by $-St \tau \langle a (x^p (t), t) \cdot \nabla_x u (x^p (t), t) \rangle$. This explains the finite drift velocity experienced by inertial particles in a boundary layer that is captured by (42). The same argument can be applied to particle pairs in isotropic turbulence; in that case, the pressure field maintains the incompressibility of the fluid and ensures $\langle S^2 (x^p (t), t) - \mathcal{R}^2 (x^p (t), t) \rangle = 0$ for $St = 0$, whereas for finite $St$, the pressure field is insufficient to constrain their motion and the particles are able to drift away from regions of high streamline curvature causing $\langle S^2 (x^p (t), t) - \mathcal{R}^2 (x^p (t), t) \rangle > 0$.

Outside of the small-Stokes-number limit, the drift velocity $-St \tau \nabla_x \langle v_2^p (t) v_3^p (t) \rangle_x$ has an additional non-local contribution that is analogous to particle pairs in isotropic turbulence. Particles moving towards the wall and arriving at position $x_3$ have come from regions of more energetic turbulence as compared to particles arriving at the same location that are moving away from the wall. This path history effect breaks the symmetry of the particle motions towards and away from the wall, giving rise to a net wall-ward drift that enhances the accumulation of particles near walls.

7. Conclusion

In this paper we have explored in depth the CT and ZT, with particular attention to the physical mechanisms they describe as being responsible for the clustering of inertial particles in isotropic turbulence. Despite appearing to describe the mechanism responsible for the clustering in quite different ways, their predictions for the RDF in the regime $St \ll 1$ are very similar. We have demonstrated that this is not coincidental; the CT captures the leading order effects of the clustering mechanism in the ZT in this regime. The theories differ outside of this regime because only the ZT captures the non-local contribution to the particle velocity dynamics, which gives rise to the formation of caustics and to the peak and subsequent decrease of the RDF power law exponent with increasing $St$ in the dissipation range of the turbulence.

We then showed using DNS data that the clustering mechanism described by the Zaichik et al theory accurately describes the clustering up to $St \approx 1$, and we identified a possible source of error for the small discrepancies at larger $St$.

We then considered how other explanations and theories for clustering presented in the literature compare with the CT and ZT. In agreement with the CT and the ZT, all of the theories identify the ‘centrifuge’ or ‘non-ergodic’ mechanism as the primary mechanism responsible for clustering in the limit of small Stokes numbers. With increasing Stokes number, the ‘non-centrifuge’ mechanisms play an increasingly important role. These mechanisms have different explanations in the different theories, but share the common theme that they are not reliant on the biased sampling of the flow by the primary particle but they arise due to the ‘history’ effect of particle inertia. In our opinion, since the ZT captures the centrifuge and non-centrifuge features of the clustering mechanism well across the range of $St$, it is therefore the theory that we recommend.

Finally, we considered the relationship between clustering in isotropic turbulence and the near-wall accumulation of inertial particles in turbulent boundary layers. We showed that in the
limit of weak inertia the inertial dependence of the clustering in these two systems is different and that this difference arises solely because of the lack of spherical symmetry in the turbulent boundary layer. As a consequence, in the weak inertia limit, the drift velocity in a boundary layer (towards the wall) is proportional to $St_n$, whereas the radial inward drift velocity for particle pairs in isotropic turbulence is proportional to $St^2$.

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**Appendix A. ZT drift velocity in the regime $St \ll 1$**

In this appendix we expand in more detail the proof that in the regime $St \ll 1$ the ZT drift velocity reduces to that of the CT.

Consider the second term on the rhs of (30)

\[
(St_n)^2 \left\{ \Gamma_{ij} \frac{d}{dt} \Gamma_{km}^p \right\} \frac{\partial}{\partial r_j} (r_j r_m) = (St_n)^2 \left\{ \Gamma_{ik} \frac{d}{dt} \Gamma_{km}^p \right\} (r_m \delta_{jk} + r_r \delta_{mk})
\]

\[
= (St_n)^2 r_m \left\{ \Gamma_{ik} \frac{d}{dt} \Gamma_{km}^p \right\} + (St_n)^2 r_j \left\{ \Gamma_{ik} \frac{d}{dt} \Gamma_{km}^p \right\}
\]

\[
= \frac{(St_n)^2}{3} r_m \left\{ \Gamma_{ik} \frac{d}{dt} \Gamma_{km}^p \right\} \delta_{jm}
\]

\[
= \frac{(St_n)^2}{3} r_i \left\{ \frac{\partial u_q}{\partial x_k} \frac{d}{dt} \frac{\partial u_p}{\partial x_q} \right\}
\]

\[
= \frac{(St_n)^2}{3} r_i \left\{ \frac{\partial u_q}{\partial x_k} \left( \frac{\partial}{\partial x_q} \frac{d u_k}{dt} - \frac{\partial u_b}{\partial x_q} \frac{\partial u_k}{\partial x_b} \right) \right\}
\]

\[
= \frac{(St_n)^2}{3} r_i \left\{ \frac{\partial u_q}{\partial x_k} \frac{d u_k}{dt} \right\} - \frac{(St_n)^2}{3} r_i \left\{ \frac{\partial u_q}{\partial x_k} \frac{d u_b}{\partial x_b} \frac{\partial u_k}{\partial x_b} \right\}
\]

\[
= -\frac{(St_n)^2}{3} r_i \left\{ \Gamma_{ik} \Gamma_{bq} \Gamma_{kb}^p \right\},
\]

and similarly for the third term on the rhs of (30) we have

\[
(St_n)^2 \left\{ \Gamma_{km}^p \frac{d}{dt} \Gamma_{ij} \right\} \frac{\partial}{\partial r_k} (r_j r_m) = -\frac{(St_n)^2}{3} r_i \left\{ \Gamma_{ik} \Gamma_{bq} \Gamma_{kb}^p \right\}.
\]
Now consider the fourth term on the rhs of (30)

\[
\left(\Sigma r_\eta^2\right)\left\langle \Gamma^p_{ij}\Gamma^p_{km}\Gamma^p_{mn}\right\rangle \frac{\partial}{\partial r_k} (r_f r_n) = \left(\Sigma r_\eta^2\right)\left\langle \Gamma^p_{ij}\Gamma^p_{km}\Gamma^p_{mn}\right\rangle (r_n \delta_{jk} + r_i \delta_{kn})
\]

\[
= \left(\Sigma r_\eta^2\right)\left\langle \Gamma^p_{ik}\Gamma^p_{km}\Gamma^p_{ml}\right\rangle + \left(\Sigma r_\eta^2\right)\left\langle \Gamma^p_{ij}\Gamma^p_{mn}\Gamma^p_{mn}\right\rangle
\]

\[
= \frac{\left(\Sigma r_\eta^2\right)\left\langle \Gamma^p_{ik}\Gamma^p_{km}\Gamma^p_{ml}\right\rangle}{3} r_i \left(\Gamma^p_{mk} \Gamma^p_{ml}\right) \delta_{im} + \frac{\left(\Sigma r_\eta^2\right)\left\langle \Gamma^p_{ij}\Gamma^p_{mn}\Gamma^p_{mn}\right\rangle}{3} r_j \left(\Gamma^p_{mk} \Gamma^p_{mn}\right) \delta_{ij}
\]

\[
= \frac{\left(\Sigma r_\eta^2\right)\left\langle \Gamma^p_{ik}\Gamma^p_{km}\Gamma^p_{ml}\right\rangle}{3} r_i \left(\Gamma^p_{mk} \Gamma^p_{ml}\right),
\]

(A.3)

and similarly for the fifth term on the rhs of (30) we have

\[
\left(\Sigma r_\eta^2\right)\left\langle \Gamma^p_{ij}\Gamma^p_{jm}\Gamma^p_{kn}\right\rangle \frac{\partial}{\partial r_k} (r_m r_n) = \frac{\left(\Sigma r_\eta^2\right)\left\langle \Gamma^p_{ik}\Gamma^p_{km}\Gamma^p_{ml}\right\rangle}{3} r_i \left(\Gamma^p_{mk} \Gamma^p_{ml}\right).
\]

(A.4)

If we now substitute the results from (A.1), (A.2), (A.3) and (A.4) into (30) we obtain

\[
-\Sigma r_\eta \frac{\partial}{\partial r_k} S_{ik} \approx -\Sigma r_\eta \left\langle \Gamma^p_{ij}\Gamma^p_{km}\right\rangle \frac{\partial}{\partial r_k} (r_f r_m)
\]

\[
+ \frac{2}{3} \left(\Sigma r_\eta^2\right)\left\langle \Gamma^p_{ik}\Gamma^p_{km}\right\rangle \frac{\partial}{\partial r_k} (r_f r_m)
\]

\[
= -\Sigma r_\eta \left\langle \Gamma^p_{ij}\Gamma^p_{km}\right\rangle \frac{\partial}{\partial r_k} (r_f r_m)
\]

\[
= -\Sigma r_\eta \left\langle \Gamma^p_{ij}\Gamma^p_{km}\right\rangle (r_n \delta_{jk} + r_i \delta_{kn})
\]

\[
= -\Sigma r_\eta \left\langle \Gamma^p_{ij}\Gamma^p_{km}\right\rangle - \Sigma r_\eta \left\langle \Gamma^p_{ij}\Gamma^p_{mm}\right\rangle
\]

\[
= \frac{\Sigma r_\eta^2}{3} r_i \left(\Gamma^p_{mk} \Gamma^p_{ml}\right)
\]

\[
= -\frac{1}{3} \Sigma r_\eta r_i \left\{ S^2 (x^p (t), t) - \mathcal{R}^2 (x^p (t), t) \right\}.
\]

(A.5)

which is the result given in (31).

**Appendix B. The RDF transport equation in the Chun et al theory**

In this appendix we consider the RDF transport equation in [32]. The main intention is to highlight certain issues in its formulation as presented in [32] and also to show how these issues can be rectified.

The derivation of the RDF transport equation in [32] begins by defining the following PDFs

\[
\varphi (r, t) = \left\langle \delta (r^p (t) - r) \right\rangle_{r^p}^{r(0)},
\]

(B.1)
\[ \rho(r, t) = \left\langle \delta \left( r^p(t) - r \right) \right\rangle^{r(0)}_{r^p}, \]  
\text{(B.2)}

where
\[ \left\langle \cdots \right\rangle^{r(0)}_{r^p}, \]
means an average over all initial particle pair positions for a given realization of \( I^p \)
\[ \left\langle \cdots \right\rangle^{r^p}, \]
means an average over all realizations of \( I^p \) and
\[ \left\langle \cdots \right\rangle \equiv \left\langle \left\langle \cdots \right\rangle^{r(0)}_{r^p} \right\rangle. \]

The transport equation for \( \phi \) considered in [32] is given by
\[ \frac{\partial}{\partial t} \phi + \frac{\partial}{\partial r} \left[ W \phi \right] = 0, \]  
\text{(B.3)}

where the particle relative velocity field \( W(r, t) \) is defined as
\[ W(r, t) = \left\langle w^p_r(t) \right\rangle^{r(0)}_{r^p}. \]  
\text{(B.4)}

They then make the decomposition \( \phi = \left\langle \phi \right\rangle^{r^p} + \phi' = \rho + \phi' \) and so obtain
\[ \frac{\partial}{\partial t} \rho + \frac{\partial}{\partial r} \left[ \left\langle W \right\rangle^{r^p} \rho + \left\langle W \phi' \right\rangle^{r^p} \right] = 0. \]  
\text{(B.5)}

In [32] the drift velocity \( \langle W \rangle^{r^p} \) is assumed to be zero. This is incorrect and may be demonstrated as follows. Recall that the definition of the field \( W(r, t) \) is
\[ W(r, t) = \left\langle w^p_r(t) \right\rangle^{r(0)}_{r^p}. \]

With this definition, and using the perturbation expansions for \( w^p(t) \) given in [32], we obtain
\[ W(r, t) = \left( \Gamma^p_{ij} \right)^{r(0)}_{r^p} + S \left( \Gamma^p_{ij} \Gamma^p_{kl} - r^p_{ij} \Gamma^p_{kl} - r^p_{ik} \Gamma^p_{jl} - r^p_{il} \Gamma^p_{jk} \right)^{r(0)}_{r^p} \]
\[ = \Gamma^p_{ij} \left( r^p_{ij} \right)^{r(0)}_{r^p} + S \left( \Gamma^p_{ij} \Gamma^p_{kl} - r^p_{ij} \Gamma^p_{kl} - r^p_{ik} \Gamma^p_{jl} - r^p_{il} \Gamma^p_{jk} \right)^{r(0)}_{r^p}. \]  
\text{(B.6)}

Invoking the approximation \( r^p \approx r^0 \) and \( r^{[1]} \approx 0 \) as in [32], and applying the operation \( \left\langle \cdots \right\rangle^{r^p} \) to (B.6) we obtain
\[ \left\langle W(r, t) \right\rangle^{r^p} = -St_{ij} \left\langle \Omega_{ij} \right\rangle^{r^p} = -\frac{St_{ij}}{3} \left\langle \left( S^2 - R^2 \right) \right\rangle. \]  
\text{(B.7)}

Not only is this non-zero for inertial particles, it is in fact equal to their drift velocity expression derived in the absence of diffusion, i.e. (8).

Note from (B.6) that it is the introduction of the approximations \( r^p \approx r^0 \) and \( r^{[1]} = 0 \) that leads to \( W \propto r \) in CT and hence to the negation of caustics.
In order to close the term $\langle W\varphi' \rangle'^{\tau}$ in (B.5) they write down a transport equation for $\varphi'$

$$\frac{\partial}{\partial t} \varphi' + \frac{\partial}{\partial r_i} [W\varphi'] \approx -\frac{\partial}{\partial r_i} [W\rho],$$

(B.8)

and they give the solution

$$\varphi' (r, t) = -\int_{-\infty}^{t'} \frac{\partial}{\partial \xi_i} [W_i (\xi_i (t', r, t'), \xi_i (t', r, t'), \xi_i (t', r, t'))] \, dr',$$

(B.9)

where

$$\frac{d}{dt} \xi_i (t') = W_i (\xi_i (t'), t').$$

(B.10)

However (B.9) is only the correct solution to (B.8) if $W$ is an incompressible field (so that the lhs of (B.8) could be interpreted as a Lagrangian derivative along the trajectory defined by $W$), which of course it is not. Therefore (B.9) can only be considered to be an approximate solution to (B.8). Nevertheless, in [32] (B.9) is used in (B.5) from which a drift diffusion equation governing $\rho (r, t)$ is obtained. Aside from this issue, the main problem is that in the formulation of the RDF transport equation the mean of the field $W$ was assumed to be zero, whereas we have showed above in (B.7) that this is an incorrect assumption. However this issue can be easily rectified as follows.

If we introduce the perturbation expansion

$$\Gamma_{ij} = \Gamma_{ij}^{[0]} + \text{St} \Gamma_{ij}^{[1]} + \cdots,$$

into the perturbation expansion for $w' (t)$, then since the CT only seeks to retain the zeroth and first-order terms in the expansion for $w' (t)$, then the perturbation solution for $w' (t)$ will only involve $\Gamma^{[0]}$ and not the higher order contributions to $\Gamma^{[0]}$. With this modification the resulting transport equation differs from that presented in [32] in two particular ways: first of all, under this modification the mean of $W$ becomes

$$\left\langle W_i (r, t) \right\rangle'^{\tau} = -\text{Str}_N \left\langle \Gamma_{ij}^{[0]} \Gamma_{ji}^{[0]} \right\rangle'^{\tau}\rho.$$ 

(B.11)

Therefore, unlike the original formulation where $\left\langle W_i \right\rangle'^{\tau} \neq 0$, we may now write

$$\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial r_i} \left\langle W_i \varphi' \right\rangle'^{\tau} = 0.$$ 

(B.12)

Secondly, following the same derivation procedure presented in [32] but this time including the perturbation expansion for $\Gamma^{[0]}$, the drift velocity contribution to $\left\langle W_i \varphi' \right\rangle'^{\tau}$ is given by

$$d_i (r, t) = -\frac{\text{Str}_N^2}{3} \int_{-\infty}^{t'} \left\langle \left[ S^2 (x' (t), i) - \mathcal{R}^2 (x' (t), i) \right] \times \left[ S^2 (x' (t'), i') - \mathcal{R}^2 (x' (t'), i') \right] \right\rangle \, dr'.$$ 

(B.13)
Appendix C. Drift in the work of Reeks

In this appendix we consider the form of the drift mechanism in [70]. In this work Reeks derives the following expression for the inertial particle drift velocity (written here in terms of the relative co-ordinates \( \mathbf{r} \) and \( \mathbf{w} \))

\[
\mathbf{d}_r (r, t) = -S \tau_q \frac{\partial}{\partial r_j} S_{2ij}^p - \mathbf{Y},
\]  

(C.1)

with

\[
\mathbf{Y}_r (r, t) = \int_{-\infty}^t \left( \Delta \mathbf{u}_r (r, t) \frac{\partial}{\partial r_j} \mathbf{W}_r (\mathbf{r}^p(s), s) \right) ds.
\]

(C.2)

where the first term on the rhs of (C.1) is the same as the drift velocity in ZT and \( \mathbf{Y} \) is a particle velocity field (see [70] for its definition). The drift \( \mathbf{Y} \) is similar to the CT drift velocity contained within (2.27) of [32] namely (noting that for \( St \ll 1 \), \( \mathbf{W} = \mathbf{W} \))

\[
\mathbf{d}_r (r, t) = - \int_{-\infty}^t \left( \mathbf{W}_r (r, t) \frac{\partial}{\partial r_j} \mathbf{W}_r (\mathbf{r}^p(s), s) \right) ds.
\]

(C.3)

This raises some questions: first of all, how important is \( \mathbf{Y} \) compared to the drift \( \mathbf{d} \) and secondly, given the similarity between \( \mathbf{Y} \) and \( \mathbf{d} \) how can it be that \( -S \tau_q \mathbf{V}_r \cdot S^p_r \neq \mathbf{d} \) for \( St \rightarrow 0 \) (as we have shown in section 3.1) when in (C.1) \( \mathbf{Y} \) is present in addition to \( -S \tau_q \mathbf{V}_r \cdot S^p_r \)? This apparent contradiction is resolved as follows.

Using the CT perturbation solutions we obtain for \( St \ll 1 \)

\[
\frac{\partial}{\partial r_j} \mathbf{W}_r (\mathbf{r}^p(s), s) = -S \tau_q \mathbf{\Gamma}_m^p (s) \mathbf{\Gamma}_m^p (s).
\]

(C.4)

This perturbation solution is obtained in the CT using the approximation \( \mathbf{r}^p \approx \mathbf{r}^{[0]} \) and \( \mathbf{r}^{[1]} \approx \mathbf{0} \) (see appendix B) for which (assuming fully mixed fluid particles)

\[
\langle \cdot \rangle_{\mathbf{r}^{[1]}(t)=\mathbf{r}} \approx \langle \cdot \rangle_{\mathbf{r}^{[0]}(t)=\mathbf{r}} = \langle \cdot \rangle.
\]

(C.5)

Using (C.4) and (C.5) in (C.2) and considering \( \mathbf{r} \) in the dissipation regime (so that \( \Delta \mathbf{u} = \mathbf{\Gamma} \cdot \mathbf{r} \)) we obtain

\[
\mathbf{Y}_r (r, t) = -S \tau_q \int_{-\infty}^t \langle \mathbf{\Gamma}_m^p (s) \mathbf{\Gamma}_m^p (s) \rangle ds
\]

\[
= -S \tau_q \int_{-\infty}^t \langle \mathbf{\Gamma}_m^p (s) \mathbf{\Gamma}_m^p (s) \rangle ds
\]

\[
= 0. \quad \text{(C.6)}
\]

Consequently, although \( \mathbf{d} \) and \( \mathbf{Y} \) appear similar, they are not equivalent even for \( St \ll 1 \). The key point then is that in the regime \( St \ll 1 \) if we apply exactly the same perturbation analysis to both \( S \tau_q \mathbf{V}_r \cdot S^p_r \) and \( \mathbf{Y} \) then to leading order, \( S \tau_q \mathbf{V}_r \cdot S^p_r \neq \mathbf{0} \) (it is equal to the CT drift in this limit, see section 3.1) whereas \( \mathbf{Y} = \mathbf{0} \).
For $St \sim 1$ one cannot invoke the perturbation approximations used above, which lead to $\langle \cdot \rangle_r \approx \langle \cdot \rangle$ to leading order. Consequently for $St \sim 1$, $\Upsilon \neq 0$. In addition, even for $St \ll 1$, $\Upsilon$ would not be zero for anisotropic flows (although it may be small).

Finally, a comment on the relationship between $\Upsilon$ and the drift $\nabla \cdot \lambda - \kappa$ (see section 2.2). Although one cannot formally equate these two drift tensors (they are obtained under subtly different PDF equation closure methods: $\Upsilon$ is derived under the assumption that the process $[W(r^p(t), t), \nabla \cdot W(r^p(t), t), \Delta u(r^p(t), t)]$ is Gaussian whereas $\nabla \cdot \lambda - \kappa$ is derived under the assumption that the field $\Delta u(r, t)$ is Gaussian and such assumptions are not in general equivalent [55]), it is likely that they are quite similar. Assuming this similarity, since $\Upsilon = 0$ in the dissipation regime for $St \ll 1$, then this probably explains why the implicit assumption $\nabla \cdot \lambda - \kappa = 0$ in the ZT does not significantly affect the ability of the theory to accurately describe the clustering in the dissipation regime at small $St$ and even up to $St = 1$. However since $\Upsilon$ is non-zero for larger particles this may also explain some of the discrepancies observed in figure 2 for $St > 1$.

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