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Clustering of randomly advected low-inertia particles: A solvable model

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Measurements and simulations indicate that the particle-pair radial distribution function in isotropic turbulence is a power law in a range of length scales below the Kolmogorov scale for Stokes number $\mathrm{St} \ll 1$. In this range, the exponent is proportional to $\mathrm{St}_1\mathrm{St}_2$ for unlike particles (1 and 2) in a bidispersion, hence St^2 for a monodispersion. Here, this result is derived from a model of particle response to random advection. The analysis generalizes a geometrical interpretation of clustering to polydispersions and suggests an economical Monte Carlo simulation method.

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The number density of inertial particles, unlike the fluid density in incompressible flow, can develop flow-induced fluctuations [1]. The consequent clustering of low-inertia particles in turbulence is sensitive to intermittency properties [2–4] and is believed to enhance droplet coagulation leading to rain formation [5]. Clustering has been the subject of experimental [6], analytical [2,3], computational [4,7,8], and modeling [8,9] studies. One focus has been the flow-property dependencies of the coefficient C in the relation

$$g(r) \sim r^{-C\mathrm{St}^2}, \quad a \ll r \ll \eta \tag{1}$$

that is found to be obeyed to leading order in $\mathrm{St} \ll 1$ by the particle-pair radial distribution function (RDF) $g(r)$ for a monodispersion [8,9]. Here, a is the particle radius, η is the Kolmogorov microscale, and St is the Stokes number, defined as the ratio of the particle response time to the turbulence time scale $(\nu/\epsilon)^{1/2}$, where ϵ is the energy dissipation rate and ν is the kinematic viscosity. Local flow-field linearity is assumed in deriving (1), but for unlike particles (1 and 2) in a bidispersion, a model that invokes departures from linearity gives [8]

$$g(r) \sim r^{-C\mathrm{St}_1\mathrm{St}_2} \quad \frac{a}{\eta} \ll |\mathrm{St}_1 - \mathrm{St}_2| \ll \frac{r}{\eta} \ll 1. \tag{2}$$

(The lower bound on r was previously noted [3], and an analogous regime transition for high-inertia bidispersions has been identified [10].)

Here, a stochastic model that idealizes low-St particle response to turbulence is formulated. For $\mathrm{St}_1 \ll 1$ and $\mathrm{St}_1/\mathrm{St}_2$ of order unity, the leading-order relation (2) is derived without further approximation. This indicates that the idealized model may be useful for Monte Carlo simulation as well as for clarifying the origin of clustering.

Particle motion is idealized as a sequence of instantaneous displacements based on representations of fluid displacements and particle response. A one-dimensional (1D) spatial domain is first assumed, and then the higher-dimensional analysis is outlined.

In 1D, the kth fluid displacement is defined as a transformation $x \to x'(x) = x + d_k(x)$ of the spatial coordinate x. To represent incompressible flow, this transformation must be measure preserving, i.e., $\int_{\sigma'} dx' = \int_{\sigma} dx$ for any subset σ of x, where σ' is the image of the subset σ after displacement k. The displacement rule adopted here,

$$d_k(x) = \begin{cases} \frac{2}{3}(x_k - x) & \text{if } x_k \leqslant x'(x) \leqslant x_k + \frac{1}{3}l, \\ \frac{2}{3}(2x_k - 2x + l) & \text{if } x_k + \frac{l}{3} \leqslant x'(x) \leqslant x_k + \frac{2}{3}l, \\ \frac{2}{3}(x_k - x + l) & \text{if } x_k + \frac{2}{3}l \leqslant x'(x) \leqslant x_k + l, \\ 0 & \text{otherwise}, \end{cases} \tag{3}$$

obeys this property. In Eq. (3), x_k is a random variable that is uniformly sampled within a 1D domain of nominal length $2X$ with periodic boundary conditions applied, yielding a spatially homogeneous displacement sequence. The parameter l is a random variable sampled for given k from a specified probability density function (PDF) $f(l)$. Termed the "triplet map" in other contexts (see [11,12] for a graphical illustration and equivalent mathematical definitions), d_k is a triple-valued function of x in $[x_k, x_k + l]$. Namely, the first three lines of Eq. (3) define "images" $j = 1$, 2, and 3 of $[x_k, x_k + l]$, but the preimage x of fluid displaced to location x' is unique. (In this context, σ' in the incompressibility condition is the union of the images of σ.) Therefore, the inverse $x(x')$ is uniquely defined. It obeys the continuity relation $|x(x_1') - x(x_2')| \leqslant 3|x_1' - x_2'|$. (Here, subscripts denote particular values of x' rather than particular displacements.) This assures that the displacement operation does not introduce spatial discontinuities into a continuous function, i.e., $h(x') \equiv g(x(x'))$ is continuous in x' if $g(x)$ is continuous in x. In addition to their formal connection to multidimensional fluid motion, measure preservation and continuity as defined here have a direct bearing on the particle-clustering properties of present interest, as shown in a more general analysis of clustering induced by d-dimensional maps [13].

To generalize Eq. (3) to three dimensions, choose a line with random orientation (sampled uniformly in solid angle, to enforce isotropy) and define Cartesian coordinates

$\mathbf{x} \equiv (x,y,z)$ with the chosen line as the x axis. Now, Eq. (3) prescribes x-directed displacements, with y and z values unaffected, thus displacing planes rather than points. For general d, the term d-map will denote such displacement of $(d-1)$-dimensional hyperplanes in d-dimensional space.

Particle displacements $\mathbf{D}_k$ are modeled as

$$\mathbf{D}_k(\mathbf{x}) = (1+S)\mathbf{d}_k(\mathbf{x}), \tag{4}$$

where $|S|$ will be interpreted as a particle Stokes number. S is allowed to be different for different particles and for different displacements k of a given particle. Its sign is immaterial provided that it is the same for all particles because Eq. (2) is bilinear in S_1 and S_2. Positive S has intuitive appeal because it gives net particle transfer from the central region of the mapped interval toward the periphery, consistent with particle expulsion from high-vorticity regions and accumulation in high-strain regions [1]. Statistics not considered here, e.g., three-point correlations, may be sensitive to the sign of S and thus indicate a preference.

In Eq. (4), boldface indicates a d-dimensional vector. $d=1$ is now considered.

It is assumed that d_k in Eq. (4) is obtained by randomly sampling, with equal probability, one of the three choices specified by Eq. (3), where the sampling is independent for each particle in $[x_k, x_k+l]$ and each event k. Thus, both the dispersive (extensional) and compressive effects on particle clustering are represented; displacements to a given image are compressive, i.e., they reduce separations, while displacements to different images are primarily dispersive.

The linearization of the particle drag law for small St suggests slip velocities of order St times fluid velocities, hence Eq. (4), but the ultimate justification of Eq. (4) is the resulting clustering behavior. The analog of Eq. (4) for continuous-in-time flow is $\mathbf{V}=(1+S)\mathbf{v}$, implying $\nabla\cdot\mathbf{V}=0$ for fixed S if $\nabla\cdot\mathbf{v}=0$, where $\mathbf{V}$ and $\mathbf{v}$ are the particle-field and fluid velocities, respectively. This is contrary to the exact (for low St) result that $\nabla\cdot\mathbf{V}$ can be nonzero for $\nabla\cdot\mathbf{v}=0$, implying inertia-induced clustering [1]. Thus, Eq. (4) is useful for analyzing clustering only in conjunction with an advection model like Eq. (3).

For $d=1$, consider the two-point probability $p(x,r)$, where $p(x,r)dxdr$ is the probability of finding a particle, labelled 1, in $[x,x+dx]$ and a particle, labelled 2, in $[x+r,x+r+dr]$. S values are denoted S_i for particles $i=1$ and 2. $S_1 \neq S_2$ corresponds to the previously analyzed bidispersion [8]. In homogeneous flow, $p(x,r)$ is independent of x so it is written as $p(r)$. $p(r)$ is proportional to $g(r)$ and therefore is equally suitable for analysis [14]. Fixed l is considered initially [i.e., $f(l)$ is a δ-function]. The finite-particle-size effects indicated by the lower bounds of Eqs. (1) and (2) are omitted for brevity.

$p_k(r)$ denotes $p(r)$ evaluated as an ensemble averaged (or x averaged) property of the system at a given stage of evolution, meaning after some number k of displacements starting from a given initial state. Homogeneity on the periodic domain allows conservation of probability to be expressed as

$$p'(r')|dx'dr'| = (2X)^{-1}\int_{-X}^{X} dx_k \frac{p_{k-1}(r(r',x_k))}{M_1 M_2} \times |dx(r',x_k)dr(r',x_k)|, \tag{5}$$

where x_k controls the x range of event-k fluid displacements (i.e., it is not a particle location), and quantities evaluated after event k are denoted with primes instead of subscript k. Particles 1 and 2 are assumed to reside at $x_1' \equiv x' = 0$ and $x_2' \equiv r' > 0$, respectively, after event k, without loss of generality.

Unprimed quantities expressed as functions of primed quantities are uniquely prescribed by Eqs. (3) and (4). dx and dr are the "particle preimages" of dx' and dr', meaning that they are the x ranges of particles that are mapped into the corresponding primed intervals by event k. (For $S=0$, these correspond to "fluid pre-images". Now S denotes S_1 or S_2 generically; it is assumed that $S \ll 1$ and that S_1/S_2 is of order unity.)

If particle i is in $[x_k, x_k+l]$ before event k, then it is mapped to one of three locations, each with probability 1/3. To conserve probability, this requires p_{k-1} in Eq. (5) to be divided by $M_1 M_2$, where multiplicity M_i is 3 (1) if particle i is inside (outside) $[x_k, x_k+l]$ before event k.

For large enough k, relaxation to statistical stationarity is assumed, implying $p'=p_{k-1}$, so they are both denoted as p. With this assumption, the *ansatz* $p(r)=\beta|r|^{-\epsilon}$ is adopted, and Eq. (5) is used to evaluate $\epsilon \ll 1$ to leading order in S. Equation (5) is now homogeneous in p, so the prefactor β cancels. β is determined by the normalization of p, but the *ansatz* is valid only for $|S_1-S_2|l \ll r \ll l$, so β is not determined here. [In this regard, l is analogous to η in Eq. (2); see below.]

For $1 \leq j \leq 3$, let $d_k^{(j)}$ denote the jth expression for d_k in Eq. (3), and let (j) designate a "P-image" (particle image), i.e., the x_i' range generated by Eq. (4), based on $d_k^{(j)}$ applied to x_i in $[x_k, x_k+l]$. $j=0$ and 4 denote P-images $-X \leq x_i' \leq x_k$ and $x_k+l \leq x_i' \leq X$, respectively (in which $x_i'=x_i$). Writing $d_k^{(j)} = a^{(j)}x + b^{(j)}$, Eq. (3) gives, in ascending order from $j=0$,

$$a^{(j)} = 0, \quad -\frac{2}{3}, \quad -\frac{4}{3}, \quad -\frac{2}{3}, \quad 0,$$

$$b^{(j)} = 0, \quad \frac{2}{3}x_k, \quad \frac{2}{3}(l+2x_k), \quad \frac{2}{3}(l+x_k), \quad 0. \tag{6}$$

For particles $i=1$ and 2, Eq. (4) gives

$$x_i' = [1+(1+S_i)a_i]x_i + (1+S_i)b_i, \tag{7}$$

where a_i denotes "$a^{(j)}$ for the index j of the P-image to which particle i is displaced." Equation (7) allows $r=x_2-x_1$ (which can be negative) to be expressed as

$$r = \frac{r'}{1+(1+S_2)a_2} + \frac{(1+S_1)b_1}{1+(1+S_1)a_1} - \frac{(1+S_2)b_2}{1+(1+S_2)a_2}. \tag{8}$$

Owing to the assumptions $x_1'=0$ [used to obtain Eq. (8)], $x_2' \equiv r' > 0$, $S \ll 1$, and $r' \ll l$, particles 1 and 2 are mapped either to the same P-image or to adjacent P-images in as-

cending order, giving nine possible P-image combinations for the particle pair: (j,j) for $j=0$ through 4 and $(j,j+1)$ for $j=0$ through 3. Based on Eqs. (3) and (4), the boundaries of the five P-images into which particle i may be mapped (depending on the value of x_k) are at x_i' values $-X$, x_k, $x_k+(1-2S_i)(l/3)$, $x_k+(1+S_i)(2l/3)$, x_k+l, and X.

To integrate over dx_k in Eq. (5), the x_k values at which transitions between P-images occur as x_k varies for $x_1'\equiv 0$ and fixed r are expressed in terms of r' and l. For $r'\ll l$, the possible P-image combinations, interleaved with the x_k values of the transitions between the possible combinations, are $-X$, $(4,4)$, $-l$, $(3,4)$, $r'-l$, $(3,3)$, $-(1+S_1)(2l/3)$, $(2,3)$, $r'-(1+S_2)(2l/3)$, $(2,2)$, $-(1-2S_1)(l/3)$, $(1,2)$, $r'-(1-2S_2)(l/3)$, $(1,1)$, 0, $(0,1)$, r', $(0,0)$, X. $\pm X$ are included to fully specify the partitioning of the dx_k integration into one sub-interval $[x_-^{(m,n)},x_+^{(m,n)}]$ per P-image combination (m,n). Note however that the endpoints $\pm X$ are immaterial owing to periodicity, e.g., the case $x_k>X-l$ requires no special treatment.

The integral in Eq. (5) is partitioned accordingly. Invoking stationarity and dividing Eq. (5) by $p(R')|dx'dr'|$,

$$\sum_{\text{cases}} I^{(m,n)}(r')=1 \tag{9}$$

is obtained, where "cases" refers to the x_k sub-intervals $[x_-^{(m,n)},x_+^{(m,n)}]$, and

$$I^{(m,n)}(r')=\frac{J^{(m,n)}}{2X}\int_{x_-^{(m,n)}}^{x_+^{(m,n)}} dx_k\, p[r(r',x_k)]/p(r'), \tag{10}$$

$$J^{(m,n)}=\frac{1}{M_1M_2}\left|\frac{dx}{dx'}\right|\left|\frac{dr}{dr'}\right|, \tag{11}$$

where arguments and some indices are suppressed on the right-hand side of Eq. (11).

$J^{(m,n)}$ is outside the integral in Eq. (10) because the particle-i multiplicities M_i and the dilatation ratios $|dx/dx'|$ and $|dr/dr'|$ depend only on the indices m and n. Namely, $M_i=3$ for images 1, 2, and 3 (i.e., for any displaced particle), otherwise (outside the mapped region) $M_i=1$. According to Eq. (8), $|dr/dr'|=1/|1+(1+S_2)a_2|$, and analogously, $|dx/dx'|=1/|1+(1+S_1)a_1|$. Again, a_i is the $a^{(j)}$ value of Eq. (6) corresponding to the image (j) into which particle i is mapped. These relations apply whether particle i is inside or outside the mapped region; if the latter (image index $j=0$ or 4), then the dilatation ratio is unity.

Assuming $p(r)\sim|r|^{-\epsilon}$, $p(r)/p(r')$ in Eq. (10) becomes $|\hat{r}|^{-\epsilon}\approx 1-\epsilon\ln|\hat{r}|+\ldots$, where $\hat{r}\equiv r/r'$. For $m=n=1$, 2, or 3,

$$I^{(m,m)}(r')\approx\frac{J^{(m,m)}}{2X}\left(x_+^{(m,m)}-x_-^{(m,m)}\right)(1-\epsilon\ln 3). \tag{12}$$

Here, quantities multiplying the order-ϵ term are evaluated to leading order, e.g., $|\hat{r}|\approx 3$ based on Eq. (8), which suffices to evaluate ϵ to leading order. This eliminates x_k dependence in the integrand of Eq. (10), yielding Eq. (12).

The expansion of $|\hat{r}|^{-\epsilon}$ in ϵ is valid only for $\hat{r}\neq 0$. There are two ways to obtain $r'>0$ for $r=0$, hence $\hat{r}=0$. One way requires $S_1\neq S_2$, allowing two initially collocated particles to separate due to their different displacements. Based on Eq. (4), the resulting separation r' cannot exceed order $|S_1-S_2|l$. Here, r' is restricted to the range $|S_1-S_2|l\ll r'\ll l$ because processes at particle separations of order $|S_1-S_2|l$ cause deviations from Eq. (2). Namely, particle relative motion due to $S_1\neq S_2$ causes particle trajectory decorrelation to dominate clustering, so $p(r')$ becomes independent of r' for $r'\ll|S_1-S_2|l$ [8].

The other way to obtain $r'>0$ for $r=0$ does not require $S_1\neq S_2$. It is the mapping of initially collocated particles to different images, i.e., the cases (m,n) for $m\neq n$. However, the consequent singularity is weak enough so that its contribution to the dx_k integral is negligible [13]. In fact, the ϵ dependence is also negligible for $m\neq n$, so to a sufficient approximation,

$$I^{(m,n)}(r')\approx\frac{J^{(m,n)}}{2X}[x_+^{(m,n)}-x_-^{(m,n)}]. \tag{13}$$

Noting that cases $(0,0)$ and $(4,4)$ are trivial, the foregoing reduces Eq. (9) to an algebraic equation, giving the leading-order result [13]

$$\epsilon=(4/\ln 3)[(S_1^2+S_2^2)-(S_1-S_2)^2]=7.3S_1S_2. \tag{14}$$

The two terms inside the square brackets are the contributions of the $m=n$ and $m\neq n$ cases, respectively. The $m\neq n$ contribution is nonzero only if $S_1\neq S_2$. A physical distinction between these two contributions is that the first represents particle response to a linear flow, but the second includes nonlinear effects. The triplet map is piecewise-linear; linearity holds only for displacements to a given image, i.e., for $m=n$. Analogously, [8] shows that a linear mechanism accounts for the scaling of ϵ for $S_1=S_2$, but that nonlinear effects must be invoked for $S_1\neq S_2$.

Several model extensions [13] are summarized. For $d>1$, the ensemble of possible events is generalized to allow averaging over the relative orientation of the map direction x and the postmap particle-separation vector. $\hat{r}$ now includes a contribution orthogonal to x (which is not affected by the map), and hence depends on the orientation angle. This dependence modifies the order-ϵ term in the generalization of Eq. (12). (This term contributes to leading order to the integral over the orientation distribution.) This is the only leading-order modification of the analysis for $d>1$. Instead of the value 7.3 in Eq. (14), the values 11.5 for $d=2$, and 15 for $d=3$, are obtained, i.e., ϵ increases with d.

It might seem that particle relative motion in 1D, being aligned with the particle separation vector, would induce more clustering than for $d>1$. However, dispersion (mapping to different images) and convergence (mapping to a given image) are both more effective for $d=1$. The net clustering is the high-order residual obtained after cancellation of the lower-order effects of convergence and dispersion.

Increase of ϵ with increasing d can be understood using the following approach: Only allow maps aligned with the respective Cartesian coordinate directions. Now, $p(\mathbf{r})$ is anisotropic but the orientation average $\bar{p}(r)$ is isotropic.

Consider the probability $p_1(x_i)$, analogous to $p(r)$ but where x_i is the projection of particle separation in the coor-

dinate direction i. The x_1 separation is unaffected by x_i-directed maps for $i \neq 1$, and the effect of the x_1 maps on $p_1(x_1)$ is the same as in a 1D (x_1-directed) geometry. Therefore, $p_1(x_1)$ obeys the result (14) derived for $d=1$.

Assume that map occurrences in the respective directions x_i are statistically independent. This implies statistical independence of particle motions in the respective coordinate directions. It follows that $p(\mathbf{r}) \sim \Pi_{i=1}^{d} p_1(x_i)$, and accounting for anisotropy, the result $\bar{p}(r) \sim r^{-d\epsilon_1}$ is obtained [13], where ϵ_1 is the 1D exponent value given by Eq. (14).

This shows how the increase of clustering with increasing d can arise within the present framework, although the physical correctness of this trend remains undetermined. In any case, this anisotropic formulation is of practical interest because it can be implemented numerically on a periodic Cartesian domain, as noted shortly.

An ensemble of possible l values governed by the PDF $f(l)$ is accommodated by an averaging procedure much like the treatment of d-dimensional orientation [13], giving $\langle S_1 S_2 l \rangle / \langle l \rangle$ in place of $S_1 S_2$ in Eq. (14), where angle brackets denote averaging over $f(l)$, and l dependence of S_1 and S_2 is allowed, enabling the interpretation of S as a Stokes number. Equation (3) is the model analog of a notional eddy (vortical turnover) in turbulence [11]. If $f(l)$ is assigned the eddy size-versus-frequency scaling of inertial-range turbulence within the range $[\eta, L]$, where L is the turbulence integral scale, then the eddy time scale τ can be estimated using the inertial-range scaling $\tau \sim l^{2/3}$ [15]. For given particle response time t_p, the assignment $S = C_S t_p / \tau$ defines an l-dependent "eddy Stokes number," involving a coefficient C_S that can be assigned empirically by requiring the model exponent ϵ to match known values, e.g., from direct numerical simulations [4,8]. To capture accurately the dependence of clustering on L/η [and thus on turbulence intensity, parameterized by $\mathrm{Re} \sim (L/\eta)^{4/3}$], $f(l)$ and $\tau(l)$ are modified to emulate intermittency [13]. (A more general approach that determines event size and location dynamically based on a representation of the instantaneous flow state is described in [12].)

Thus, the model has practical as well as conceptual implications. It obeys Eqs. (1) and (2), satisfying a key requirement for accurate numerical simulation of particle collisions and (for droplets) coalescence in turbulence [7]. No spatial mesh is required, only a list of particle parameters (including spatial locations) that is updated by displacements. In the absence of processes requiring explicitly defined time evolution (e.g., differential sedimentation), this Lagrangian algorithm is no more costly than the Gillespie algorithm [16], a coalescence simulation that involves weighted sampling of droplet pairs and takes no account of droplet locations. The new method captures spatial evolution, including (as shown here) the clustering mechanism that can increase coalescence rates of initially monodisperse droplets by a factor of 10 or more [7]. Numerical simulation results, and their implications for rain formation, are discussed elsewhere [13].

The present analysis employs a geometrical construction, Eqs. (3) and (4), that does not follow directly from the evolution equations governing particles in turbulent flow, yet reproduces the scaling that governs clustering in bidispersions (including any bidisperse sub-population within a general polydispersion) for $|S_1 - S_2| \eta \ll r \ll \eta$. This geometrical treatment generalizes the geometrical perspective applied to monodispersions in [2].

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