# Clustering, caustics & collisions of particles suspended in turbulent flows

alla la Barbarbar

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-clustering of inertial particles in random & turbulent flows -collision rate of advected particles (small St) -caustics

-collision speeds of inertial particles at large St

## Formulation of the problem

Dynamics of particles suspended in turbulent flows.

Spherical particles of size a move independently.

Force on particles: drag force given by Stokes law  $\ddot{r} = \gamma (u(r,t) - \dot{r})$ .

Flow velocity field  $\boldsymbol{u}(\boldsymbol{r},t)$  random function with appropriate statistics.

**Dimensionless** parameters

$$\operatorname{St} = \frac{1}{\gamma \tau} \qquad \operatorname{Ku} = \frac{u_0 \tau}{\ell}$$

St Stokes number, Ku Kubo number,

 $\ell$ ,  $\tau$ ,  $u_0$  Kolmogorov length, time, velocity.



#### Brownian motion

Scottish botanist R. Brown (1773 - 1858) observed motion of pollen grains in water.

In 1905 Einstein explained that their motion is due to the concerted effect of the small water molecules on the pollen grains. Water molecules (and thus pollen grains) move the faster the higher the temperature. Prediction:

$$\Delta x_t^2 = 2Dt$$
 with  $D = \frac{k_{\rm B}T}{6\pi na}$ 

Experimental verification:



Brownian motion, diffusion, random walk.



# Mixing by random stirring

Computer simulation of  $10^4$  particles (red) in two-dimensional random flow (periodic boundary conditions in space)



**a** initial distribution, **b** particle positions after random stirring.

# Clustering of inertial particles

Computer simulation of  $10^4$  particles (blue) in two-dimensional smooth random incompressible flow u(r, t)





Bec, Phys. Fluids 15 (2003) L81



Wang & Maxey, J. Fluid. Mech. 256 (1993) 27



#### An example: correlated random walks

$$x_i(t_n)$$

Consider N random walks  $x_i(t)$  (i = 1, ..., N), discrete in time ( $t_n = n\delta t$ )

$$x_i(t_{n+1}) = x_i(t_n) + \xi(x_i(t_n), t_n)$$

with Gaussian random displacements  $\xi(x(t), t)$  satisfying

$$\langle \xi(x,t_n) \rangle = 0$$
  
$$\langle \xi(x,t_n)\xi(y,t_m) \rangle = \delta_{nm} \,\xi_0^2 \,\mathrm{e}^{-(x-y)^2/2\ell^2}$$

#### An example: correlated random walks



Consider two particles with small initial separation  $\delta x(0)$ . Does  $\delta x(t)$  typically decrease as  $t \to \infty$ ? Linearise

$$\delta x(t_{n+1}) = \delta x(t_n) \left( 1 + \frac{\partial \xi}{\partial x} (x(t_n), t_n) \right)$$

and determine

$$\lambda = \lim_{t \to \infty} \frac{1}{t} \left\langle \log \left| \frac{\delta x(t)}{\delta x(0)} \right| \right\rangle$$
$$= \frac{1}{\delta t} \left\langle \log \left| 1 + \frac{\partial \xi}{\partial x} \right| \right\rangle$$

#### An example: correlated random walks

$$\lambda = \lim_{t \to \infty} \frac{1}{t} \left\langle \log \left| \frac{\delta x(t)}{\delta x(0)} \right| \right\rangle = \frac{1}{\delta t} \left\langle \log \left| 1 + \frac{\partial \xi}{\partial x} \right| \right\rangle$$

Assume that  $\frac{\partial \xi}{\partial x}$  is small ( $\xi_0 \ll \ell$ ). Neglect  $|\cdots|$ , expand logarithm and average  $\lambda \approx -\frac{1}{2\delta t} \frac{\xi_0^2}{\ell^2} < 0$ 



#### Lyapunov exponents

Exponents  $\lambda_1 > \lambda_2 > \lambda_3$  describe rate of contraction or expansion of small length element  $\delta r_t$ , area element  $\delta \mathcal{A}_t$ , and volume element  $\delta \mathcal{V}_t$ 

$$\lambda_1 = \lim_{t \to \infty} t^{-1} \log_e(\delta r_t)$$
$$\lambda_1 + \lambda_2 = \lim_{t \to \infty} t^{-1} \log_e(\delta \mathcal{A}_t)$$
$$\lambda_1 + \lambda_2 + \lambda_3 = \lim_{t \to \infty} t^{-1} \log_e(\delta \mathcal{V}_t) .$$

J. Sommerer & E. Ott, Science 259 (1993) 351

#### Stochastic differential equation

To calculate  $\lambda_1 > \lambda_2 > \lambda_3$  express spatial separations  $\delta \boldsymbol{r}_{\mu}$  ( $\mu = 1, 2, 3$ ) in terms of a co-moving coordinate system  $\mathbf{n}_{\mu}(t) = \mathbf{O}(t)\mathbf{n}_{\mu}(0)$ , momentum separations  $\delta \boldsymbol{p}_{\mu}$  as  $\delta \boldsymbol{p}_{\mu} = \mathbf{R} \, \delta \boldsymbol{r}_{\mu}$ .

$$\lambda_{\mu} = \langle R'_{\mu\mu} \rangle / m$$

$$\dot{\mathbf{R}}' = -\gamma \mathbf{R}' - {\mathbf{R}'}^2 / m + [\mathbf{R}', \mathbf{O}^{\dagger} \dot{\mathbf{O}}]_{-} + \mathbf{F}'$$
  
 $F_{\mu\nu}(t) = \gamma m \frac{\partial u_{\mu}}{\partial r_{\nu}}$ ,  $\partial u_{\mu} / \partial r_{\nu}$  is the strain tensor,

and  $R'_{\mu\nu}(t) = \mathbf{n}_{\mu}(t) \cdot \mathbf{R}(t)\mathbf{n}_{\nu}(t)$  as well as  $F'_{\mu\nu}(t) = \mathbf{n}_{\mu}(t) \cdot \mathbf{F}(t)\mathbf{n}_{\nu}(t)$ . For rapidly fluctuating forcing (  $\mathrm{Ku} \ll 1$ ) obtain generalised diffusion equation for  $\mathbf{R}'$  which can be mapped onto a quantum problem.

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# Mapping onto quantum problem

Generalised diffusion equation for  $3 \times 3$  matrix  $\mathbf{R}'$  equivalent to perturbation of nine-dimensional isotropic harmonic oscillator

$$\hat{H} = \hat{H}_0 + \mathcal{I}^{1/2} \hat{H}_1 \qquad \qquad \hat{H}_0 = -\sum_{i=1}^{5} \hat{a}_i^{\dagger} \hat{a}_i \\ \hat{H}_1 = -\sum_{ijk} H_{ijk}^{(1)} \hat{a}_i^{\dagger} (\hat{a}_j^{\dagger} + \hat{a}_j) (\hat{a}_k^{\dagger} + \hat{a}_k)$$
  
here  $\mathcal{I} = \frac{1}{2\gamma} \int_{-\infty}^{\infty} \langle \frac{\partial u_1}{\partial x_1} (\mathbf{r}(t), t) \frac{\partial u_1}{\partial x_1} (\mathbf{r}(0), 0) \rangle \propto \mathrm{Ku}^2 \mathrm{St}$  is dimensionless

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measure of strain correlations.

Coefficients  $H_{ijk}^{(1)}$  exactly known. Lyapunov exponents are obtained as matrix elements between ground state of  $\hat{H}_0$  and the state  $|Q\rangle$  given by  $\hat{H}|Q\rangle = 0$ .

#### Perturbation expansion

$$\begin{split} \lambda_1 / \gamma &= 3\mathcal{I} - 29\mathcal{I}^2 + 564\mathcal{I}^3 \\ &- 14977\mathcal{I}^4 + 488784\mathcal{I}^5 - 18670570\mathcal{I}^6 + \cdots \\ \lambda_2 / \gamma &= 8\mathcal{I}^2 - 459/2\mathcal{I}^3 + 14281/2\mathcal{I}^4 \\ &- 757273/3\mathcal{I}^5 + 361653709/36\mathcal{I}^6 + \cdots \\ \lambda_3 / \gamma &= -3\mathcal{I} - 9\mathcal{I}^2 - 789/2\mathcal{I}^3 - 5787/2\mathcal{I}^4 \\ &- 895169/3\mathcal{I}^5 - 101637719/36\mathcal{I}^6 + \cdots . \end{split}$$

Mehlig & Wilkinson, Phys. Rev. Lett. 92 (2004) 250602 Duncan, Mehlig, Östlund & Wilkinson, Phys. Rev. Lett. 95 (2005) 165503

Valid for  $\mathrm{Ku} \ll 1$ . Expansion parameter  $\mathcal{I} \propto \mathrm{Ku}^2 \mathrm{St}$ .

As  $\mathcal{I} \to 0$  obtain known results for advective limit ( $\lambda_1 + \lambda_2 + \lambda_3 = 0$ ) Falkovich, Gawedzki & Vergassola, Rev. Mod. Phys. 73 (2001) 913

#### Perturbation series in one dimension

Obtain series expansion for  $\lambda_1$ 

$$\lambda_1/\gamma = -\sum_{l=1}^{\infty} c_l \mathcal{I}^l$$

Coefficients satisfy recursion ( $c_1 = 1$ )

$$c_{l+1} = (6l-2)c_l + \sum_{j=1}^{l} c_j c_{l+1-j}$$
.

l	$c_l$
1	1
2	5
3	60
4	1105
5	27120
6	828250
7	30220800
8	1282031525
9	61999046400
10	3366961243750

#### Same coefficients appear in

D.Aldous, Brownian excursions, critical random graphs, and the multiplicative coalescent (1996) J. Spencer, Enumerating Graphs and Brownian Motion, Comm. Pure Appl. Math. 1 (1997) 0291 P. Flajolet and P. Poblete and A.Viola, On the analysis of linear probing hashing, Algorithmica 22 (1998) 490 Syclamore, The Wiener index of simply generated random trees (2002)

Sv. Janson, The Wiener index of simply generated random trees (2002)

## Fractal clustering

Fractal dimension of attractor in d-dimensional space

 $d_{\mathrm{f}}=d-\Delta$  (when  $\Delta>0$ ).

Dimension deficit  $\Delta$ . For particles in d = 3 incompressible flow estimate

 $\Delta = -\frac{1}{|\lambda_3|} (\lambda_1 + \lambda_2 + \lambda_3).$ Kaplan & Yorke (1979) J. Sommerer & E. Ott, Science 259 (1993) 351

From Pade-Borel resummation of series for Lyapunov exponents obtain good agreement with direct numerical simulations of particles suspended in turbulent flow ( , from Bec et al. nlin.CD/0606024 ).

Since Ku is not known for turbulent flow, adjusted x-axis by setting  $\mathrm{Ku}=0.25$  .

Wilkinson, Mehlig, Östlund & Duncan, Phys. Fluids 19 (2007) 113303





( $\mathcal{E}$  dissipation,  $\nu$  viscosity, n number density,  $K_d$  constant).

Large St: collisions in gas of randomly moving particles. Random single-scale flow:  $R_{\rm gas} \propto {\rm St}^{-1/2}$ .

### Advective collisions ( $\dot{\boldsymbol{r}} = \boldsymbol{u}(\boldsymbol{r},t)$ )

Consider two spatial dimensions. Collision rate (polar coordinates r,  $\theta$ )

$$R = -2an_0 \int_0^{2\pi} \mathrm{d}\theta \, v_r(2a,\theta,t) \Theta(-v_r(2a,\theta,t)) \chi(2a,\theta,t)$$

measures flux of particles into disc of radius 2a around test particle (radius a).



Characteristic function  $\chi(2a, \theta, t) = 0$  for particles which have already collided, otherwise  $\chi(2a, \theta, t) = 1$ . Initially,  $\chi = 1$  but in general:  $\chi$  depends upon history of flow. Relative velocity  $v_r$ . Number density  $n_0$ .

P. G. Saffman & J. S. Turner, J. Fluid. Mech. 1, 16 (1956)

#### Numerical results

Collision rate

$$R = -2an_0 \int_0^{2\pi} \mathrm{d}\theta \, v_r(2a,\theta,t) \Theta(-v_r(2a,\theta,t)) \chi(2a,\theta,t)$$

Results of numerical simulations (point-particles advected in random flow at small Ku, record collision when separation is for the first time < 2a):



Andersson, Gustavsson, Mehlig & Wilkinson, Europhys. Lett. 80 (2007)

## Theory in the limit of small $\underline{K}\underline{u}$

Problem: in time-dependent flow, the separation  $X_t$  may pass the collision region more than once (whether or not depends upon history of flow).

In the limit of small  $\mathrm{Ku}$ , the separation  $\boldsymbol{X}_t$  diffuses with diffusion constant

$$D_{ij} = \frac{1}{2} \int_{-\infty}^{\infty} dt \left\langle [u_i(\boldsymbol{X}, t) - u_i(\boldsymbol{0}, t)] [u_j(\boldsymbol{X}, 0) - u_j(\boldsymbol{0}, 0)] \right\rangle$$
  
Balkovsky, Falkovich & Fouxon, Phys. Rev. Lett. 86 (2001) 2790

The collision rate can be evaluated exactly in this limit.

In d = 2 dimensions (with X = |X|)

$$R = 16\pi \mathcal{D}n_0 a^2 \quad \text{with } \mathcal{D} = \frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}X} D_{11}(X=0) \sim \frac{u_0^2 \tau}{2\ell^2} \propto \frac{\mathrm{Ku}^2}{\tau}$$

 $(\bigcirc)$  $t = 20 \tau$ 

 $t = 100 \tau$ 

 $t=1000\,\tau$ 

#### Caustics

Falkovich, Fouxon & Stepanov, Nature 419 (2002)151 Wilkinson & Mehlig, Phys. Rev. E 68 (2003) 04010, Europhys. Lett. 71 (2005) 186

One-dimensional model  $\ddot{x} = \gamma(u(x,t) - \dot{x})$ .



This singularity (`catastrophe') is a caustic. Implications for collision rates.





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## Caustic activation

One-dimensional model  $\ddot{x} = \gamma(u(x,t) - \dot{x})$ .

Exact result for rate of caustic formation in the limit of small  $\underline{K}\underline{u}$ 

$$\mathcal{J}/\gamma = -\frac{1}{2\pi} \operatorname{Im} \left[ \frac{1}{\sqrt{z}} \frac{\operatorname{Ai}'(z)}{\operatorname{Ai}(z)} \right]_{z=(i\sqrt{\mathcal{I}})^{-4/3}/4}$$
$$\sim \frac{1}{2\pi} e^{-1/(6\mathcal{I})}$$



where Ai is the Airy function,  $\mathcal{I} \propto {\rm Ku}^2 {\rm St}$  , and `action' 1/6.

Caustic formation is an activated process (compare Arrhenius law  $r = r_0 e^{-T_0/T}$ ). Similar in two and three dimensions, but `action' not known analytically. Duncan, Mehlig, Östlund & Wilkinson, Phys. Rev. Lett. 95 (2005) 165503

### St-dependence of collision rate

Collision rate well approximated by  $R = R_{adv} + exp(-S/\mathcal{I})R_{kin}$ .

Remember  $J/\gamma \sim e^{-S/\mathcal{I}}$  and  $\mathcal{I} \propto \mathrm{Ku}^2 \mathrm{St}$ .



#### Relative speeds in turbulence at largeSt

Inertial range becomes important ( $\langle \Delta u(l,t)\Delta u(l,0)\rangle = (\mathcal{E}l)^{2/3}f(t\mathcal{E}^{1/3}/l^{2/3})$ ( here  $\Delta u$  is component of  $\Delta u(l,t) = u(l,t) - u(0,t)$  and  $\ell \ll l \ll L$ ,  $\ell \sim (\nu^3/\mathcal{E})^{1/4}$  Kolmogorov scale). Grain dynamics in accretion disks.

Model: distribution of collision speeds non-Gaussian:

$$P(\Delta V) = A e^{-C|\Delta V|^{4/3} \gamma^{2/3} \mathcal{E}^{-2/3}}$$

where A and C are constants and  $\mathcal{E}$  is rate of dissipation per unit mass. This result implies

$$\Delta V \sim \sqrt{{\cal E}/\gamma}$$
 (dimensional analysis)

 $R_{\rm gas} \sim {\rm St}^{1/2}$ 

(Epstein damping:  $\mathrm{St} \sim a$ )

Mehlig, Wilkinson & Uski, Phys. Fluids 19 (2007) 098197 Wilkinson, Mehlig & Uski, Astrophys. J. Suppl. Ser. 176 (2008) 484 Gustavsson, Mehlig, Wilkinson & Uski, Phys. Rev. Lett. 101 (2008) 174503





## One-dimensional model

Assume Ku  $\ll 1$ . Dimensionless variables  $t' = \gamma t$ ,  $\Delta x = \Delta X/\ell$ , and  $\Delta v = \Delta V/(\ell \gamma)$ . When  $\Delta u$  fluctuates rapidly, can approximate dynamics by Langevin equation

$$\mathrm{d}\Delta x = \Delta v \,\mathrm{d}t', \quad \mathrm{d}\Delta v = -\Delta v \,\mathrm{d}t' + \delta w$$

with random increments

$$\langle \delta w \rangle = 0 \quad \langle \delta w^2 \rangle = 2 \mathcal{D}(\Delta x) \mathrm{d}t'$$

with diffusion constant  $\mathcal{D}(\Delta x) = \epsilon |\Delta x|^{\alpha}$ .

Parameters  $\epsilon$  and  $\alpha$  . Relevant choice:  $\alpha=2/3$  and  $\epsilon=1$  .

Asymptotically exact WKB solution of corresponding Fokker-Planck equation for  $\rho(\Delta x, \Delta v)$ .

Mehlig, Wilkinson & Uski, Phys. Fluids 19 (2007) 098197 Gustavsson, Mehlig, Wilkinson & Uski, Phys. Rev. Lett. (2008) in press



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# Conclusions

Clustering of inertial particles --exact solution for  $Ku \ll 1$  compared to DNS (Bec et al. nlin.CD/0606024) Parameter  $\mathcal{I}$  from DNS?

#### Caustics

constant  $K_d$ ?

-activated caustic formation  $e^{-C/St}$ 

C determined from DNS Pumir & Falkovich, J. Atm. Sci 64 (2007) Collision rate of advected particles -exact result for Ku  $\ll$  1, influence of clustering -expect  $R = K_d n_0 a^d (\mathcal{E}/\nu)^{1/2}$  in turbulent flows

Collision speeds of inertial particles at large St -exact result at Ku  $\ll 1$ :  $\Delta V = \text{const.} \times \mathcal{E}/\gamma$ -constant from DNS?





 $\rho(0, \Delta v)$ 

10





# Determine universal constants (DNS) Inertial collisions at large St: $R = K_d^{(1)} na^{d-1} \frac{\mathcal{E}^{1/2}}{\gamma^{1/2}}$

Gustavsson, Mehlig, Wilkinson & Uski, Phys. Rev. Lett. 101 (2008) 174503

Advective collisions at small St:  $R = K_d^{(2)} n a^d \frac{\mathcal{E}^{1/2}}{n^{1/2}}$ 

Gustavsson, Mehlig, Wilkinson, New J. Phys. 10 (2008) 075014 Andersson, Gustavsson, Mehlig, Wilkinson, Europhys. Lett. 80 (2007) 69001

Fractal dimension of inertial particles determined by  $\epsilon^2 = \frac{K_d^{(3)}}{\gamma} \frac{\mathcal{E}^{1/2}}{\nu^{1/2}}$ 

Mehlig & Wilkinson, Phys. Rev. Lett. 92 (2004) 250602 Duncan, Mehlig, Östlund & Wilkinson, Phys. Rev. Lett. 95 (2005) 165503

Caustic activation  $e^{-K_d^{(4)}/St}$ 

Falkovich, Fouxon & Stepanov, Nature 419 (2002)151 Wilkinson, Mehlig & Bezuglyy, Phys. Rev. Lett. 97 (2006) 048501 Pumir & Falkovich, J. Atm. Sci. 64 (2007) 4497