

Transport of tracers & particles in fluid flows

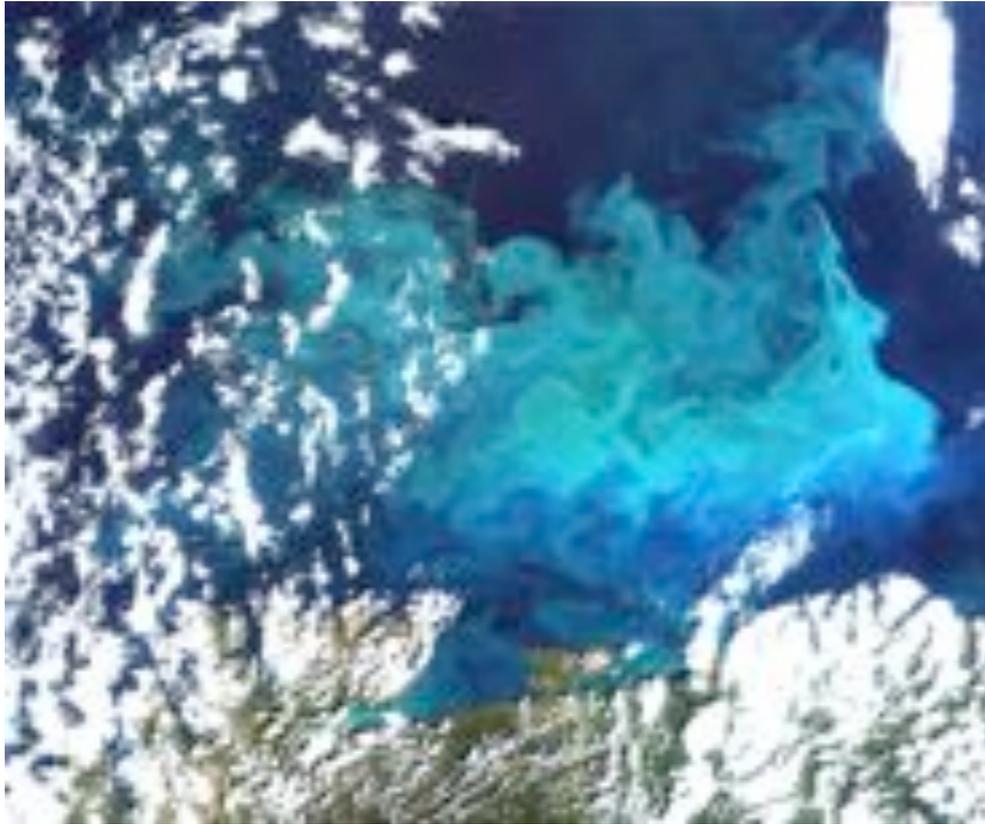
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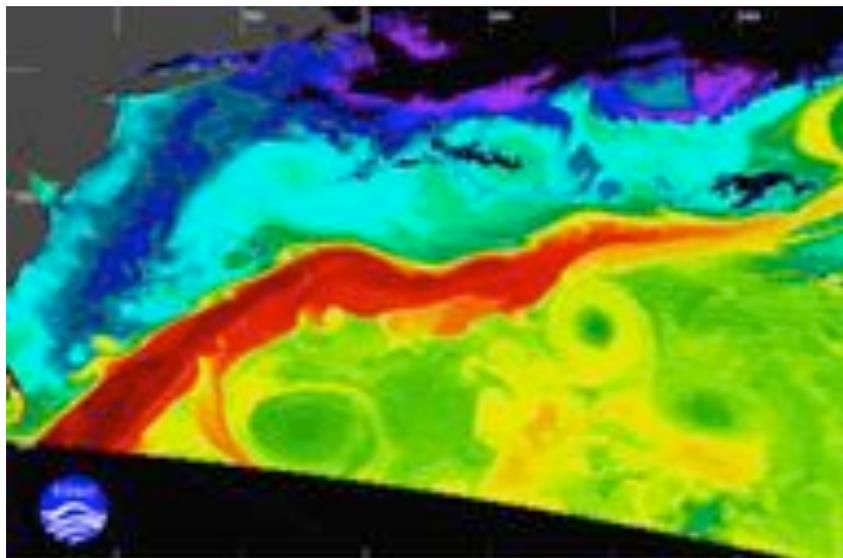
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Conference/School on
Anomalous Transport: from Billiards to Nanosystems
Sperlonga Sept. 2010

transport in fluids flows



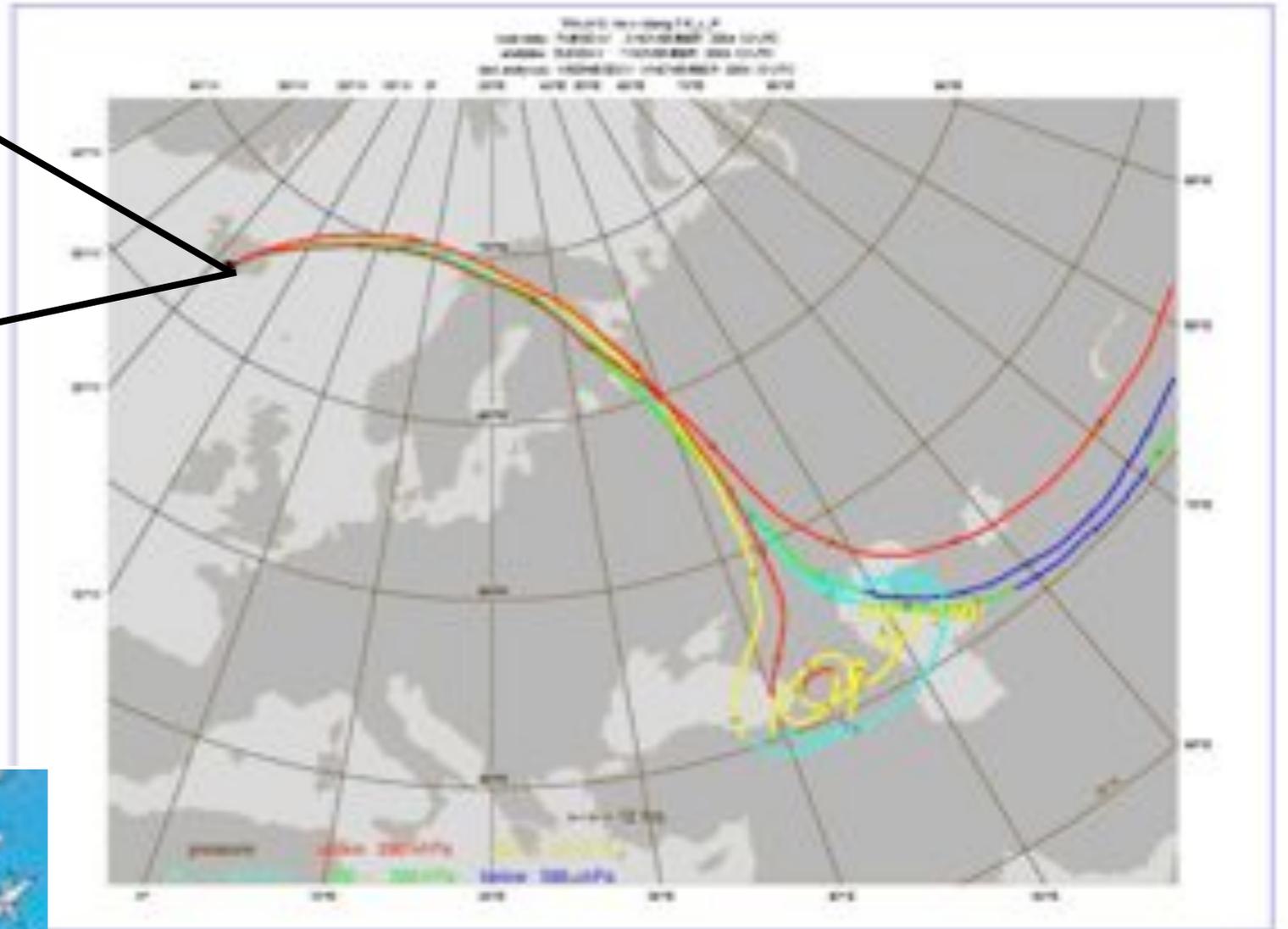
Biology & environment



Pollution

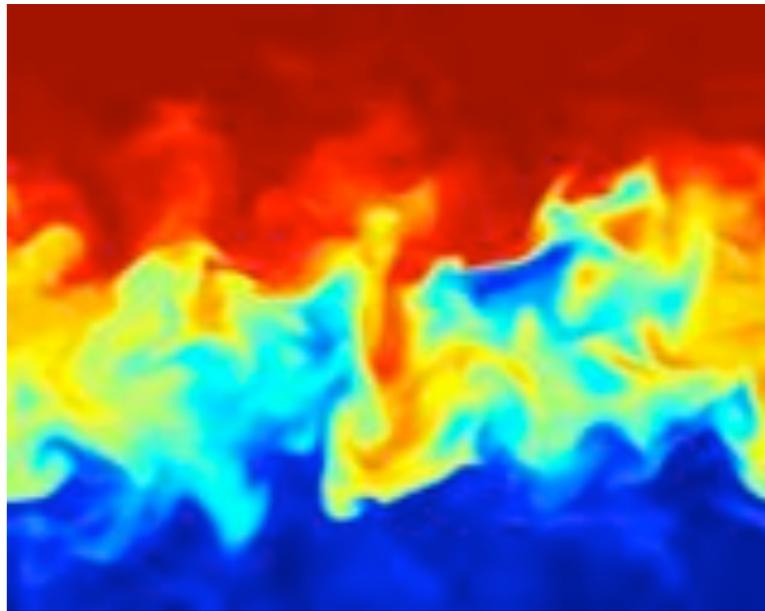


transport in fluids flows

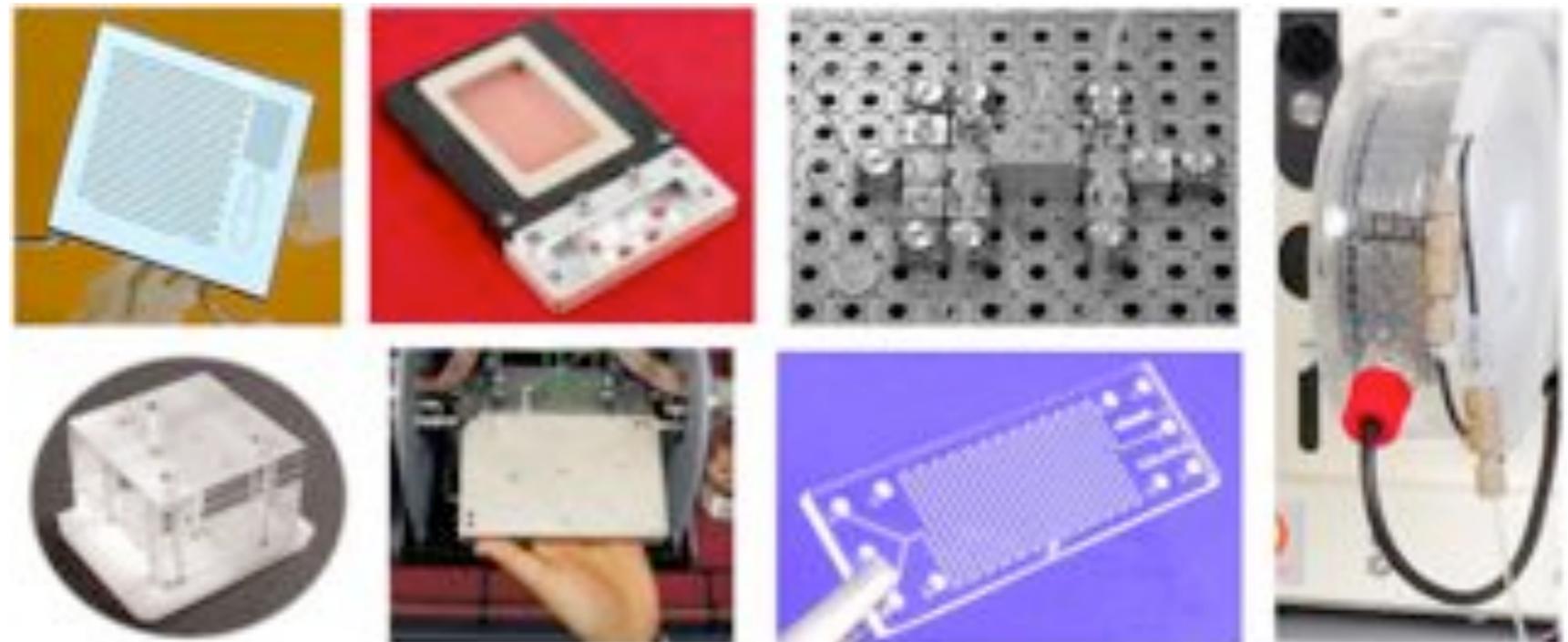
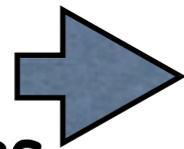


transport in fluids flows

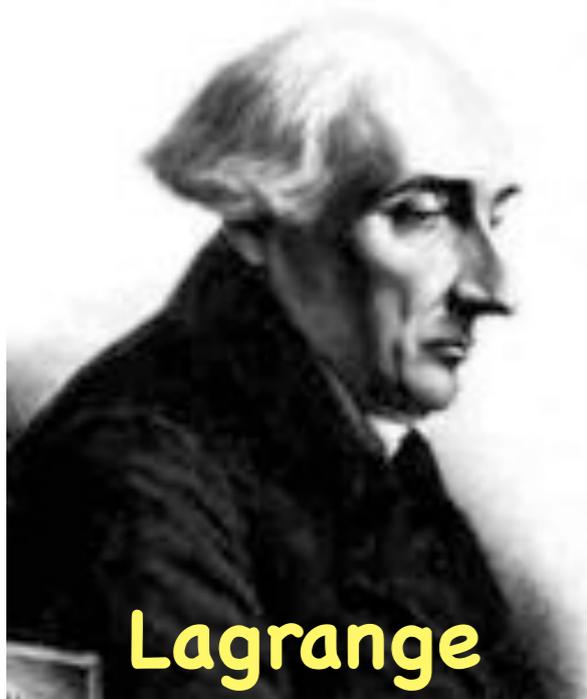
Enhanced Mixing



design
efficient mixers
in microfluids

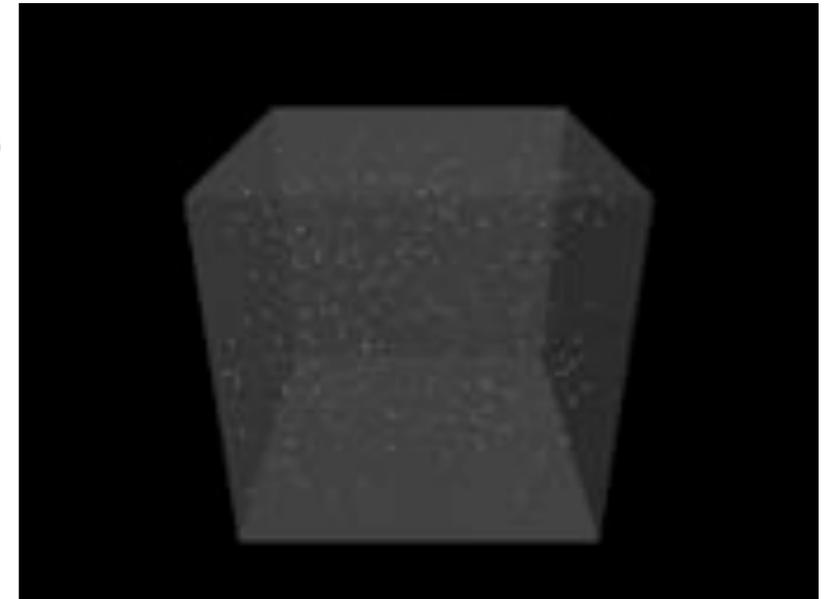


Two points of view



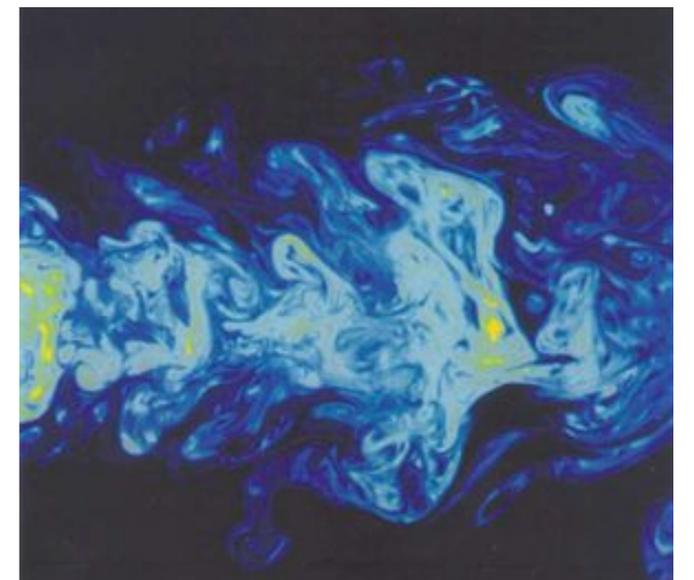
$$\frac{d\mathbf{X}}{dt} = \mathbf{u}(\mathbf{X}(t), t) + \sqrt{2D_0}\boldsymbol{\eta}(t)$$

Aim: understanding properties of trajectories $\mathbf{X}(t)$ given $\mathbf{u}(\mathbf{x}, t)$



$$\partial_t \theta + \mathbf{u} \cdot \nabla \theta = D_0 \Delta \theta$$

Aim: understanding properties of fields $\theta(\mathbf{x}, t)$ given $\mathbf{u}(\mathbf{x}, t)$



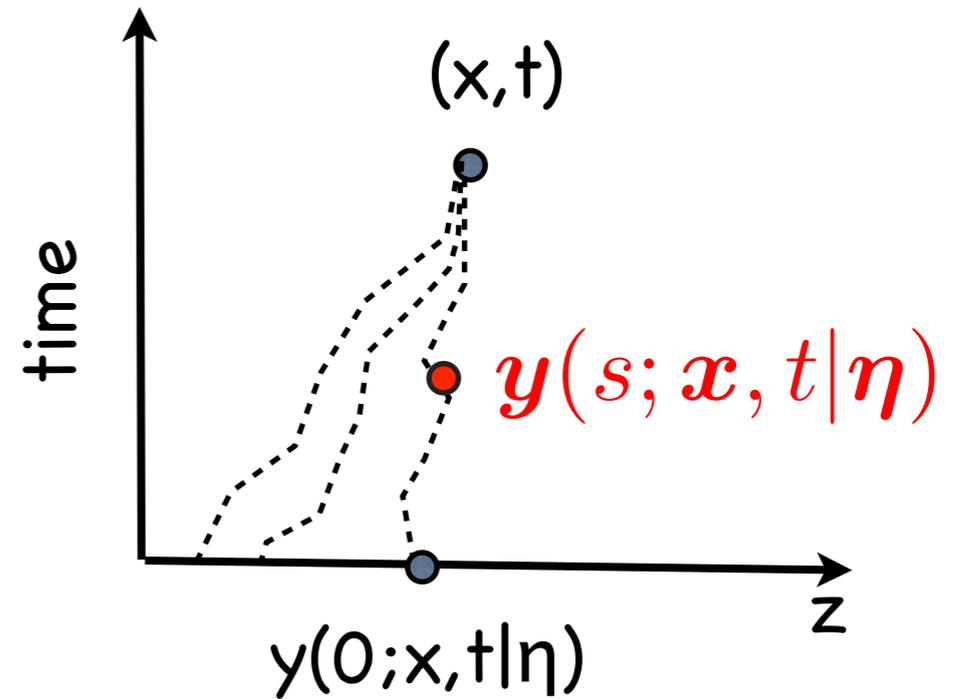
The two descriptions are connected

$$\partial_t \theta + \mathbf{u} \cdot \nabla \theta = D_0 \Delta \theta$$



$$\frac{d\theta}{dt} = 0$$

$$\frac{d\mathbf{y}}{dt} = \mathbf{u}(\mathbf{y}, t) + \sqrt{2D_0} \boldsymbol{\eta}(t)$$



$$p(\mathbf{z}, 0 | \mathbf{x}, t) = \langle \delta(\mathbf{z} - \mathbf{y}(0; \mathbf{x}, t | \boldsymbol{\eta})) \rangle_{\boldsymbol{\eta}}$$

$$\theta(\mathbf{x}, t) = \int d\mathbf{z} \theta(\mathbf{z}, 0) p(\mathbf{z}, 0 | \mathbf{x}, t)$$

Studying particle trajectories is thus relevant also to understand the transport of fields

we will focus on particle motion

Two kind of particles

Tracers

- *same density of the fluid $\rho_p = \rho_f$
- *point-like
- *move with the same velocity of the fluid
- *essentially they move like fluid elements

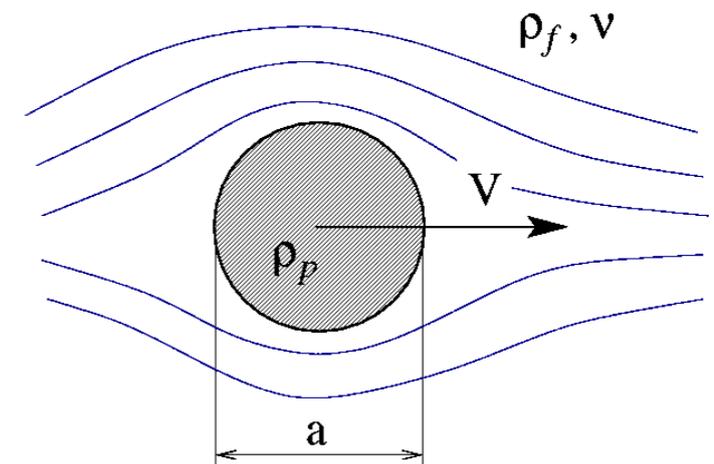
$$\dot{\mathbf{X}} = \mathbf{u}(\mathbf{X}, t) = \mathbf{v}(t)$$

(Inertial) Particles

- *density different from the fluid $\rho_p \neq \rho_f$
 - *finite size
 - *inertia & other forces are acting
- velocity different from the fluid one

$$\dot{\mathbf{X}} = \mathbf{V}$$

$$\dot{\mathbf{V}} = \mathbf{F}(\mathbf{V}, \mathbf{u}(\mathbf{X}, t), \rho_p, a, \nu, \dots)$$



We shall only consider passive particles: i.e. the velocity field is not modified by their presence

Outline

- (I) **Single particle motion** (absolute dispersion)
conditions for standard & anomalous diffusion, examples in simple laminar flows
- (II) **Two particle motion** (relative dispersion)
focus on relative dispersion in laminar & turbulent flows, relative dispersion at changing the scale & characterization of non-asymptotic regimes
- (III) **Clustering of inertial particles** in turbulence
characterization of clustering & preferential concentration for particles which do not follow fluid motion

(I) & (II) focus on tracers

Single particle dynamics

prescribed fluid velocity

thermal noise

$$\langle \eta_i(t) \eta_j(t') \rangle = \delta_{ij} \delta(t - t')$$

$$\dot{\mathbf{X}} = \mathbf{u}(\mathbf{X}(t), t) + \sqrt{2D_0} \boldsymbol{\eta}(t) = \mathbf{V}(t)$$

Lagrangian velocity

We are interested in the long time behavior of $\Delta(t) = |\mathbf{X}(t) - \mathbf{X}(0)|$ and how it depends on the properties of $\mathbf{u}(\mathbf{x}, t)$ $\nabla \cdot \mathbf{u} = 0$

* Typically we expect standard diffusive behaviors $\langle \Delta^2(t) \rangle \sim 2D^E t$

* D^E effective diffusion coefficient, $D^E[\mathbf{u}] \gg D_0$

* Which properties must be present to have non-standard behaviors?

* effective macroscopic description of transport?

Green-Kubo-Taylor relation

$$\dot{\mathbf{X}} = \mathbf{V}(t) \Rightarrow \mathbf{X}(t) = \int_0^t ds \mathbf{V}(s) \quad \mathbf{X}(0) = 0$$

$$\frac{1}{2} \frac{d}{dt} \langle X^2(t) \rangle = \langle X(t) V(t) \rangle = \int_0^t ds \langle V(s) V(t) \rangle \stackrel{\text{Lagrangian velocity correlation function}}{=} \int_0^t d\tau C(\tau)$$

$$\begin{aligned} \frac{d\langle \Delta^2(t) \rangle}{dt} &= 2 \int_0^t ds C(s) \\ \langle \Delta^2(t) \rangle &= 2 \int_0^t ds \int_0^s ds' C(s') \\ &= 2t \int_0^t ds C(s) - 2 \int_0^t ds s C(s) \end{aligned}$$

Everything is written in the Lagrangian velocity correlation function

Green-Kubo-Taylor formula

conditions for standard & anomalous diffusion

$$\frac{d}{dt} \langle (\Delta X(t))^2 \rangle = 2 \int_0^t ds C(s) \quad \langle (\Delta X(t))^2 \rangle = 2 \int_0^t ds \int_0^s ds' C(s') = 2 \int_0^t ds (t-s) C(s)$$

To understand absolute dispersion we just need to know the velocity autocorrelation function $C(t) = \langle V(0)V(t) \rangle$

• Standard diffusion $\int_0^\infty ds C(s) = D < \infty \quad \langle (\Delta X(t))^2 \rangle \propto 2Dt$

• anomalous diffusion

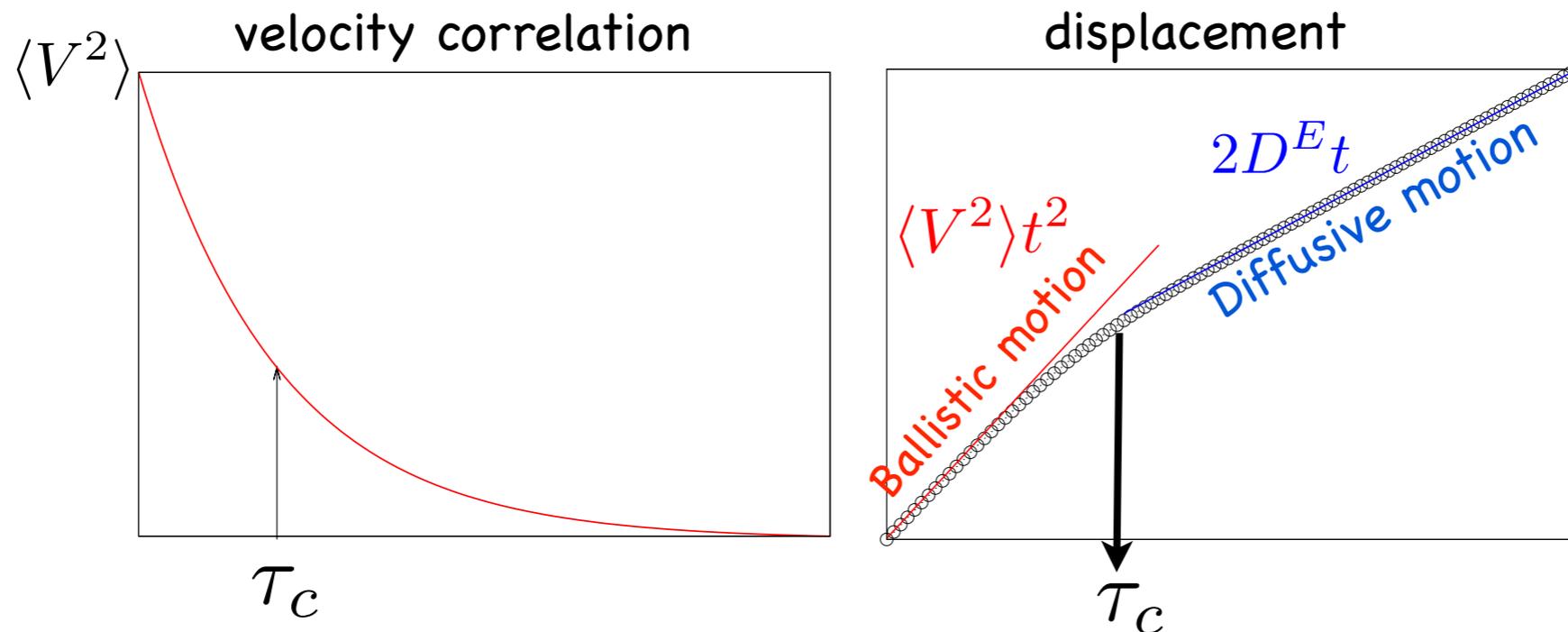
• superdiffusion $\int_0^\infty ds C(s) = \infty \quad \langle (\Delta X(t))^2 \rangle \propto t^\alpha \quad \alpha > 1$

• subdiffusion $\int_0^\infty ds C(s) = 0 \quad \alpha < 1$

Standard diffusion

$$\frac{d}{dt} \langle (\Delta X(t))^2 \rangle = 2 \int_0^t ds C(s) = 2 \int_0^t \langle V(s)V(0) \rangle = \begin{cases} 2t \langle V^2 \rangle & t \ll \tau_c \\ 2 \langle V^2 \rangle \tau_c & t \rightarrow \infty \end{cases}$$

$$\langle (\Delta X(t))^2 \rangle = \begin{cases} t^2 \langle V^2 \rangle & t \ll \tau_c \\ 2 \langle V^2 \rangle \tau_c t = 2D^E t & t \rightarrow \infty \end{cases} \quad \text{essentially CLT holds}$$



$$D^E = \int_0^{t \rightarrow \infty} ds C(s) = \langle V^2 \rangle \tau_c \gg D_0$$

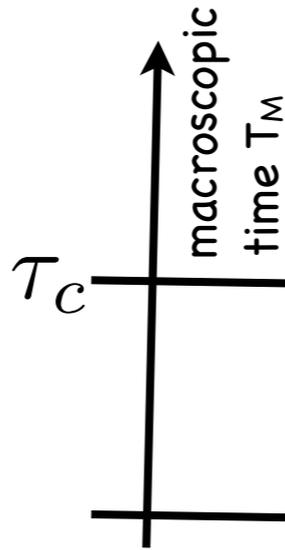
Standard Diffusion

$$\partial_t \theta + \mathbf{u} \cdot \nabla \theta = D_0 \Delta \theta$$

Effective macroscopic description

$$\Theta(\mathbf{X}_M, T_M) = \langle \theta(\mathbf{x}, t) \rangle_{\ell_c, \tau_c}$$

$$\partial_{T_M} \Theta = D^E \Delta_{X_M} \Theta$$



$$\dot{\mathbf{X}} = \mathbf{u}(\mathbf{X}(t), t) + \sqrt{2D_0} \boldsymbol{\eta}(t) = \mathbf{V}(t)$$

if diffusive behavior
at large t & ΔX

$$\langle (\Delta X(t))^2 \rangle \sim 2D^E t$$

$D^E \gg D_0$ will depend non trivially on \mathbf{u} and D_0

Various techniques to derive D^E in periodic or random velocity fields
based on perturbative expansions – **Multiscale methods** –

Idea: slow (X_M, T_M) & fast (\mathbf{x}, t) variables

$$\partial_t = \partial_t + \epsilon \partial_{T_M} \quad \partial_x = \partial_x + \epsilon \partial_{X_M} \quad \theta(x, t; X_M, T_M) = \theta^{(0)} + \epsilon \theta^{(1)} + \dots$$

It comes an effective equation for $\theta^0(x, t; X_M, T_M) = \theta^{(0)}(X_M, T_M) = \Theta(\mathbf{X}_M, T_M)$

Bensoussan, Lions & Papanicolaou, Asymptotic Analysis for Periodic Structures (1978)

Biferale, Crisanti, Vergassola & Vulpiani_PoF 7, 2725 (1995)

Majda & Kramer Phys. Rep. 314, 237 (1999)

Non-Standard diffusion

anomalous superdiffusion

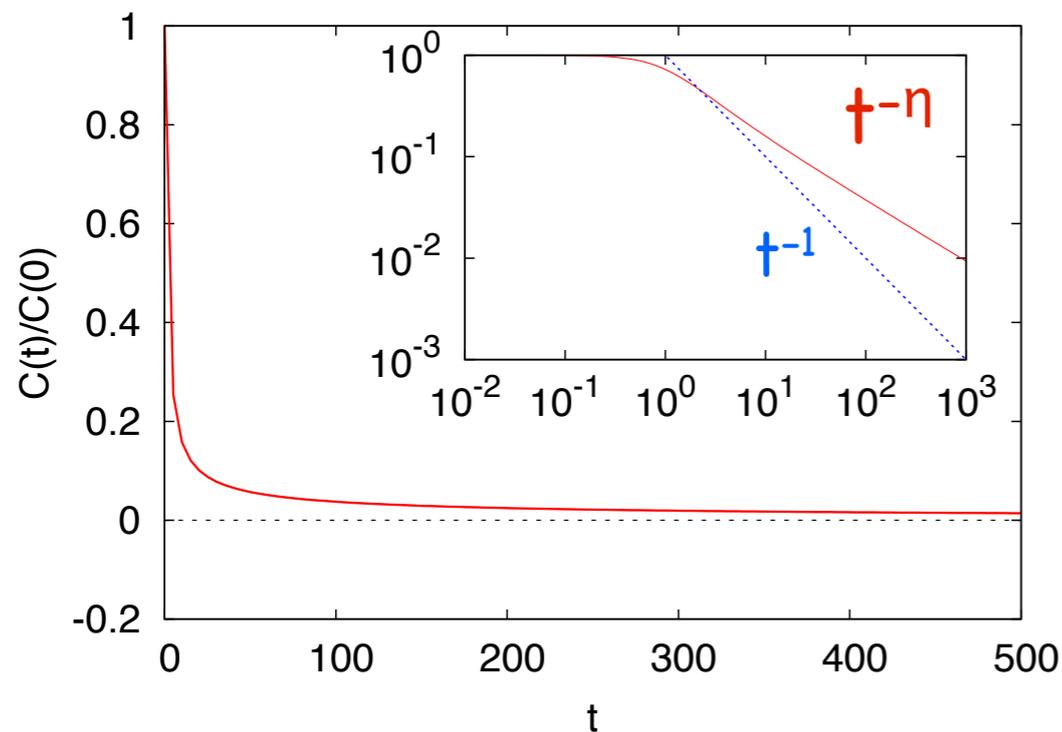
$$\int_0^{t \rightarrow \infty} ds C(s) = \infty$$

long positive tails

$$C(t) \sim t^{-\eta} \quad 0 < \eta < 1$$

$$\langle \Delta^2(t) \rangle = 2 \int_0^t ds \int_0^s ds' C(s') \sim t^\alpha = t^{2-\eta}$$

$$\alpha = 2 - \eta > 1$$



anomalous subdiffusion

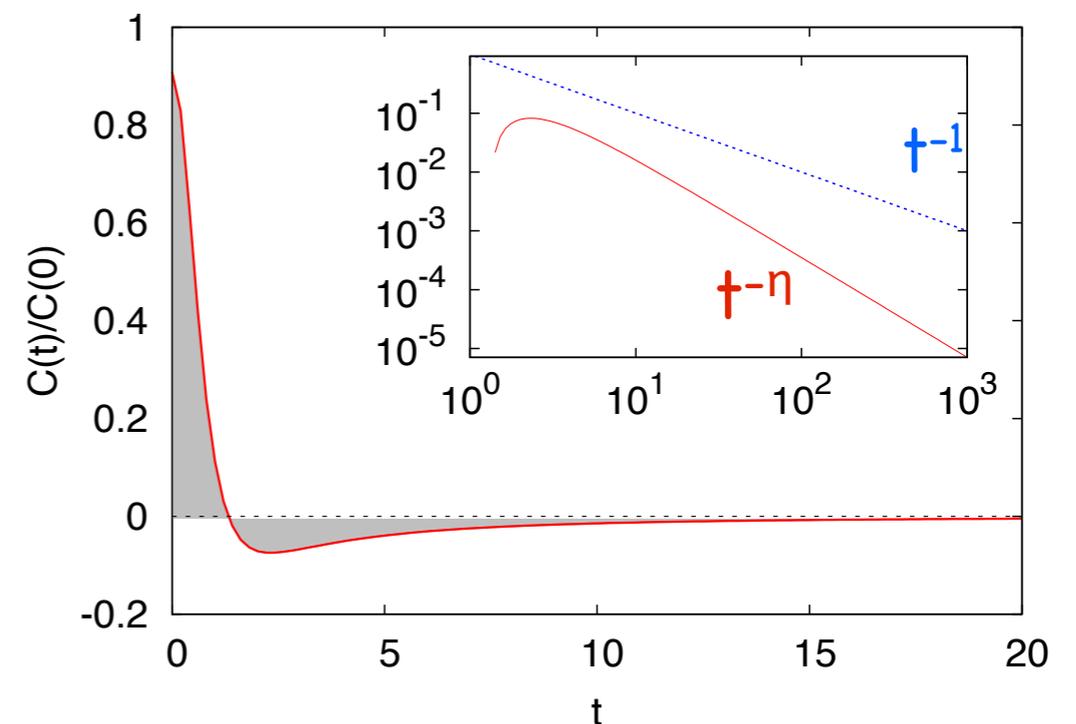
$$\int_0^{t \rightarrow \infty} ds C(s) = 0$$

long negative tails

$$C(t) \sim -t^{-\eta} \quad 1 < \eta < 2$$

$$\langle \Delta^2(t) \rangle = 2t \int_0^t ds C(s) - 2 \int_0^t ds s C(s) \sim t^\alpha = t^{2-\eta}$$

$$\alpha = 2 - \eta < 1$$



if $D_0=0$ impossible in incompressible flows

Physical origin of long correlations?

- ▶ Long spatial correlations of the velocity field

$$\int d\mathbf{k} \frac{\langle |\mathbf{u}(\mathbf{k})|^2 \rangle}{k^2} = \int dk \frac{S(k)}{k^2} \approx \ell_c^2 \langle u^2 \rangle = \begin{cases} < \infty & \text{diffusive} \\ \infty & \text{superdiffusive} \end{cases}$$

time independent flows: Avellaneda & Majda, Commun. Math. Phys. 138, 339 (1991)

time dependent flows: Avellaneda & Vergassola, Phys. Rev. E 52, 3249 (1995)

- ▶ The velocity field has finite correlation length but particle dynamics generate very long Lagrangian velocity correlations

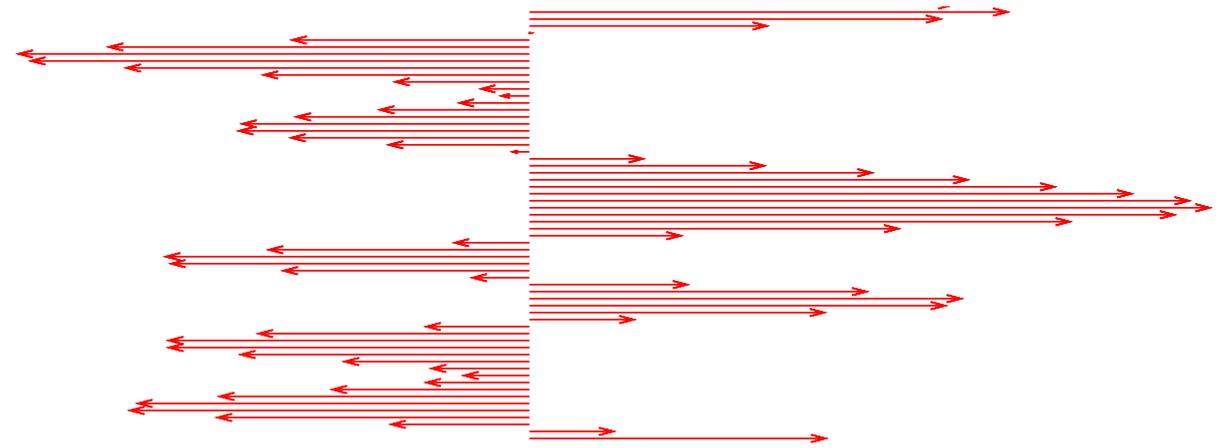
We will see these two mechanisms with some example

Random shear flows

(strong spatial correlations)

$$\dot{\mathbf{X}} = \mathbf{u}(\mathbf{X}(t), t) + \sqrt{2D_0}\boldsymbol{\eta}(t)$$

$$\mathbf{u}(\mathbf{x}, t) = \begin{pmatrix} U(y) \\ V \end{pmatrix}$$



$V = \text{const}$ $U(y)$ random & gaussian

Power spectrum

$$S(k) = \langle |\hat{U}(k)|^2 \rangle$$

spatial correlation function

$$\langle U(y) \rangle = 0 \quad \langle U(y')U(y' + y) \rangle = R(|y|) = \int_{-\infty}^{\infty} dk \cos(ky)S(k)$$

$$S(k) \sim k^\gamma \quad k \ll 1 \implies R(x) \sim x^{-(1+\gamma)} \quad x \gg 1$$

$V=0$ $D_0>0$ G. Matheron & G. de Marsily, Wat. Resour. Res. 16, 901 (1980)

$V \neq 0$ $D_0=0$ F.W. Elliott, D.J. Horntrop & A. Majda, Chaos 7, 39 (1997)

Absolute dispersion in the x-direction?

Random shear: $D_0=0$ $V \neq 0$

$$\dot{V} = V \rightarrow Y(t) = Vt$$

$$\dot{X} = U(Y) \rightarrow X(t) = \int_0^t ds U(Y(s)) = \int_0^t ds U(Vs)$$

to simplify
 $X(0) = Y(0) = 0$

temporal correlation $\langle X^2(t) \rangle = 2 \int_0^t ds \int_0^s ds' \langle U(Y(s))U(Y(s')) \rangle$ spatial correlation

$$C(s - s') = \langle U(Y(s))U(Y(s')) \rangle = R(Y(s) - Y(s')) = R(V(s - s'))$$

At large times

$$C(t) = R(Vt) = R(Y) \sim Y^{-(1+\gamma)} \sim t^{-(1+\gamma)} \rightarrow \langle X^2(t) \rangle \sim t^{1-\gamma}$$

γ	$\langle (\Delta Y(t))^2 \rangle$	behavior
$\gamma \geq 1$	t^0	trapping
$0 < \gamma < 1$	$t^{1-\gamma}$	subdiffusion
$\gamma = 0$	t	diffusion
$\gamma < 0$	$t^{1-\gamma}$	superdiffusion

Elliott, Horntrop & Majda, Chaos 7, 39 (1997)

Random shear: $D_0=0 \quad V \neq 0$

$$\langle X^2(t) \rangle = 2 \int_0^t ds \int_0^s ds' \langle U(Y(s))U(Y(s')) \rangle =$$

$$2 \int_0^t ds \int_0^s ds' R(V|s-s'|) = \frac{4}{V^2} \int_0^\infty (1 - \cos(kVt)) \frac{S(k)}{k^2} dk$$

$$S(k) = |k|^\gamma \exp(-\alpha|k|)$$

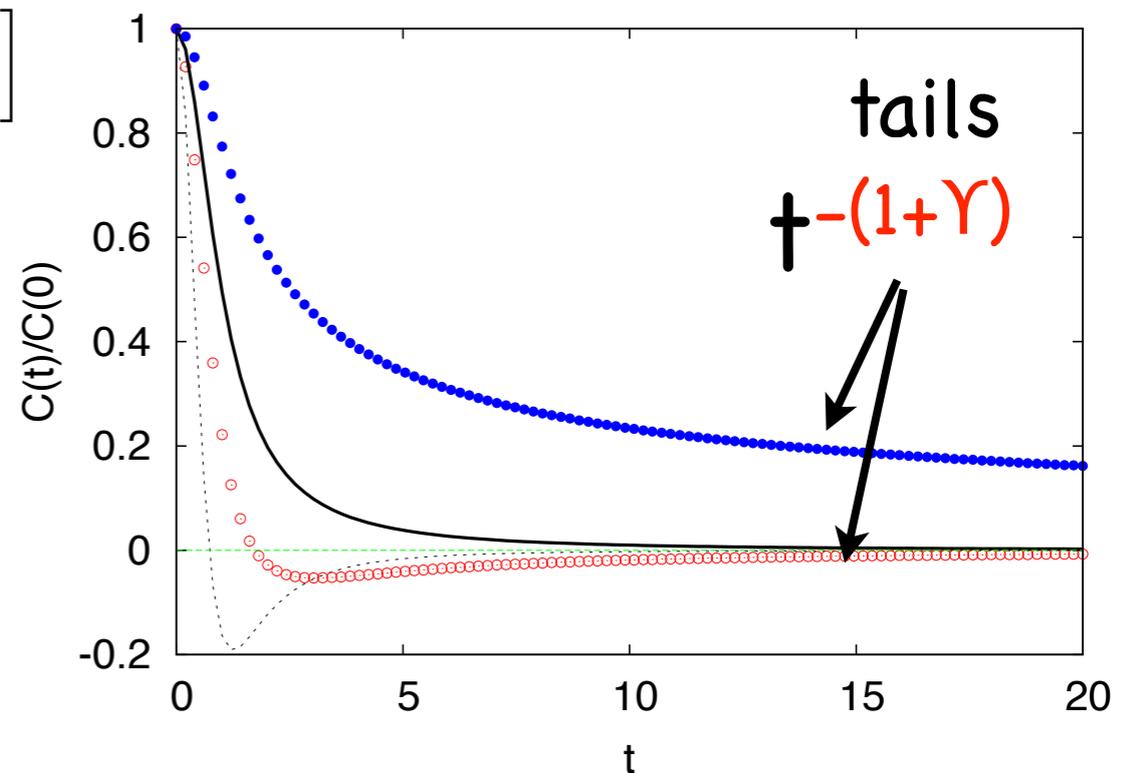
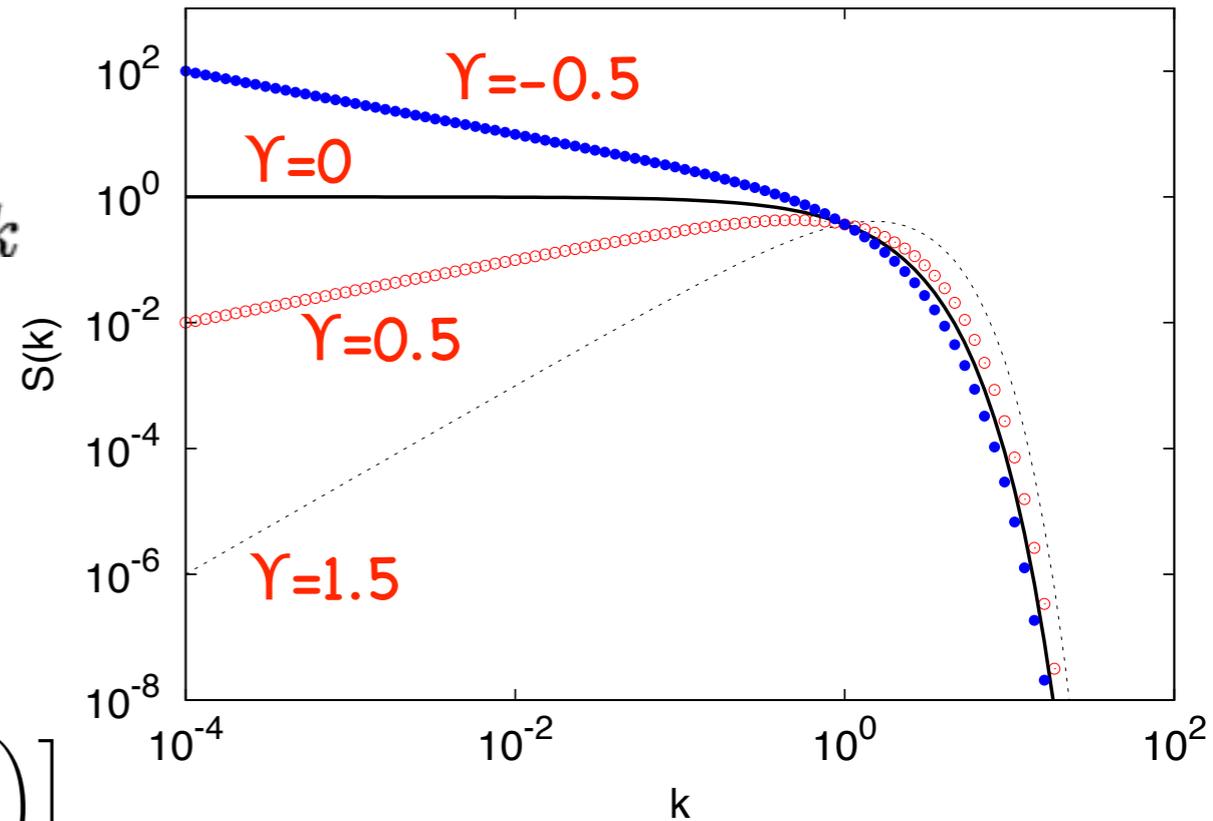
Analytically solvable

$$R(y) = 2\Gamma(1 + \gamma)(\alpha^2 + x^2)^{-(1+\gamma)/2} \cos \left[(1 + \gamma) \arctan \left(\frac{|y|}{\alpha} \right) \right]$$

$$\langle X^2(t) \rangle = 4 \frac{\Gamma(\gamma - 1)}{V^2} \left[\alpha^{1-\gamma} - (\alpha^2 + (Vt)^2)^{(1-\gamma)/2} \cos \left[(1 - \gamma) \arctan \left(\frac{Vt}{\alpha} \right) \right] \right]$$

$\gamma=1$ trapping $\langle X^2(t) \rangle = \frac{2}{V^2} \ln \left(1 + \frac{(Vt)^2}{\alpha^2} \right)$

in incompressible flows trapping & subdiffusion do not happen when $D_0 \neq 0$



Random shear: $D_0 \neq 0$ $V=0$

$$\dot{X} = U(Y(t)) + \sqrt{2D_0}\eta_x(t) \rightarrow X(t) = \int_0^t ds U(Y(s)) + \sqrt{2D_0} \int_0^t ds \eta_x(s)$$

$$\dot{Y} = \sqrt{2D_0}\eta_y(t) \rightarrow Y(t) = \sqrt{2D_0} \int_0^t ds \eta_y(s)$$

$X(t) \approx \int_0^t ds U(Y(s))$
 $Y(t) \approx \sqrt{2D_0}t$

temporal correlation spatial correlation

$$\langle X^2(t) \rangle = 2 \int_0^t ds \int_0^s ds' \langle U(Y(s))U(Y(s')) \rangle$$

$$C(s-s') = \langle U(Y(s) - Y(s')) \rangle = R(Y(s) - Y(s')) \approx R(\sqrt{2D_0}(s-s'))$$

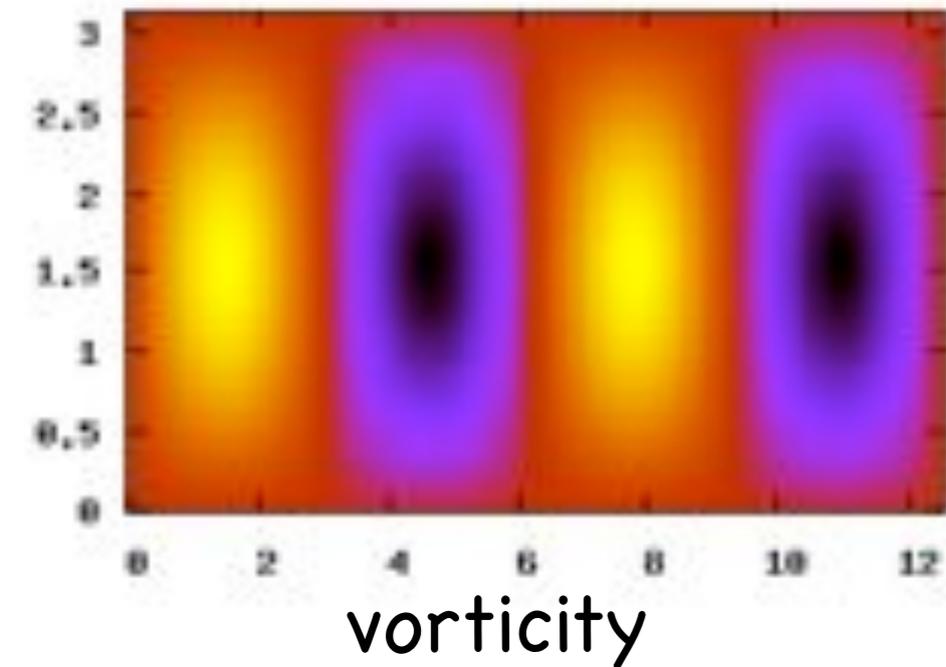
$$S(k) \sim k^\gamma \implies R(y) \sim y^{-(1+\gamma)}$$

$$C(t) \approx R(\sqrt{2D_0}t) \approx (D_0 t)^{-(1+\gamma)/2} \implies \langle X^2(t) \rangle \sim t^{2 - \frac{(1+\gamma)}{2}} = t^{\frac{3-\gamma}{2}}$$

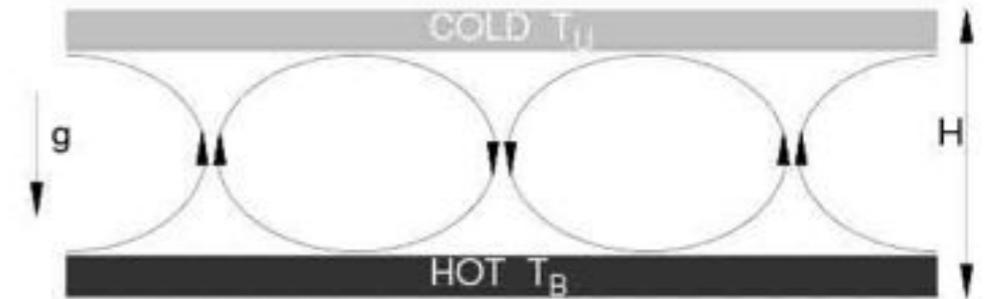
$$D^E = \frac{\langle X^2(t) \rangle}{2t} = D_0 + \frac{1}{D_0} \int dk \frac{S(k)}{k^2} \approx \int dk k^{\gamma-2} \begin{cases} < \infty & \gamma > 1 & \text{standard} \\ = \infty & -1 < \gamma < 1 & \text{anomalous} \end{cases}$$

Time dependent Cellular flows

(Lagrangian persistency)



convection →



2d model (Solomon & Gollub PRA **38**, 6280 (1988))

$$\psi(x, y, t) = \psi_0 \sin(x + B \sin(\omega t)) \sin(y)$$

$$u_x = \partial_y \psi = \psi_0 \sin(x + B \sin(\omega t)) \cos(y)$$

$$u_y = -\partial_x \psi = -\psi_0 \cos(x + B \sin(\omega t)) \sin(y)$$

$$\dot{\mathbf{X}} = \mathbf{u}(\mathbf{X}(t), t) + \sqrt{2D_0} \boldsymbol{\eta}(t)$$

u has a single mode no spatial persistency

Lagrangian chaos

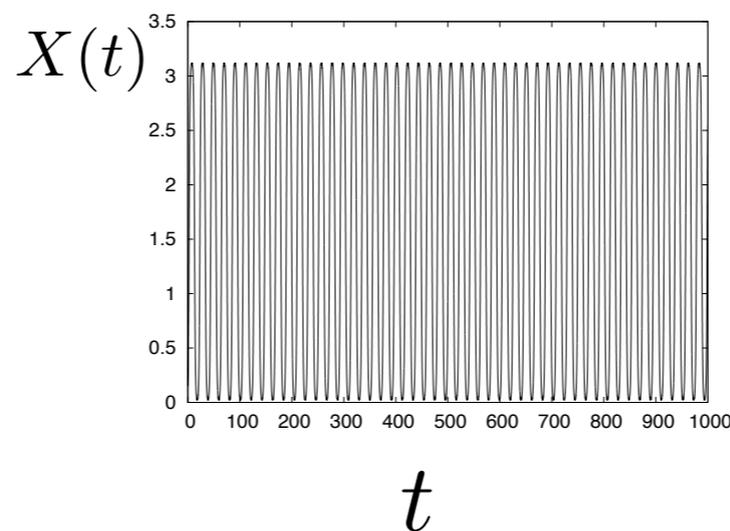
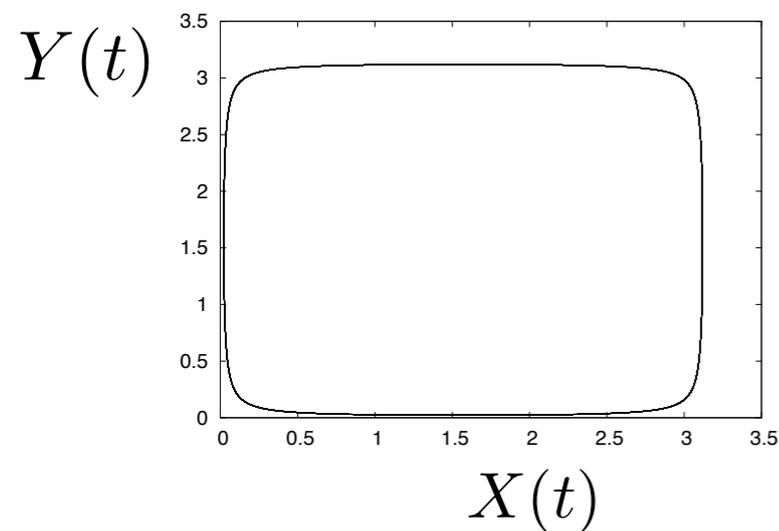
$$u_x = \partial_y \psi = \psi_0 \sin(x + B \sin(\omega t)) \cos(y)$$

$$u_y = -\partial_x \psi = -\psi_0 \cos(x + B \sin(\omega t)) \sin(y)$$

$$\dot{\mathbf{X}}(t) = \mathbf{u}(\mathbf{X}(t), t) = \mathbf{V}(t)$$

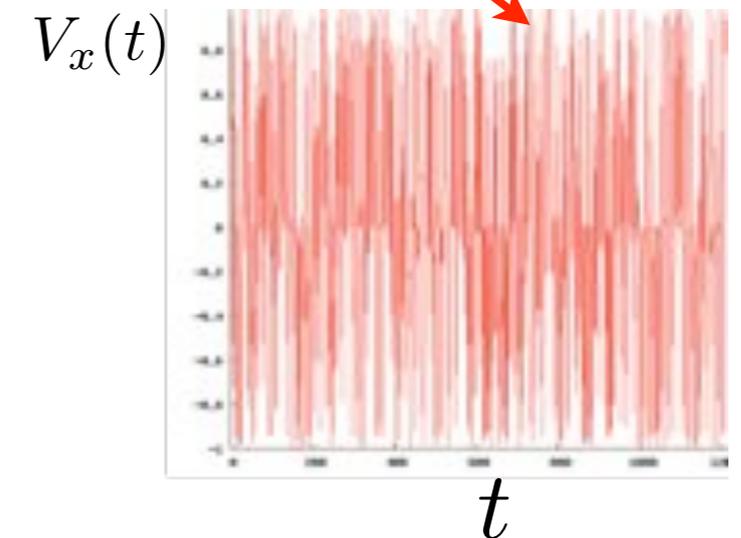
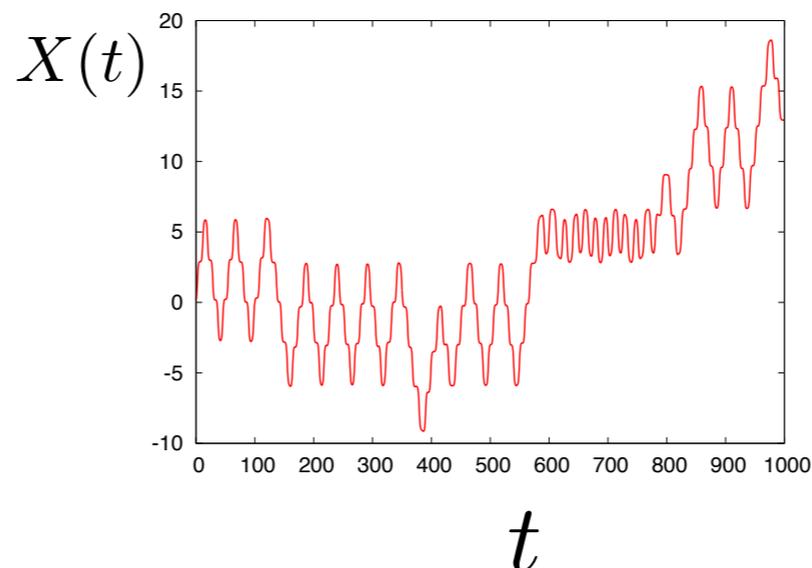
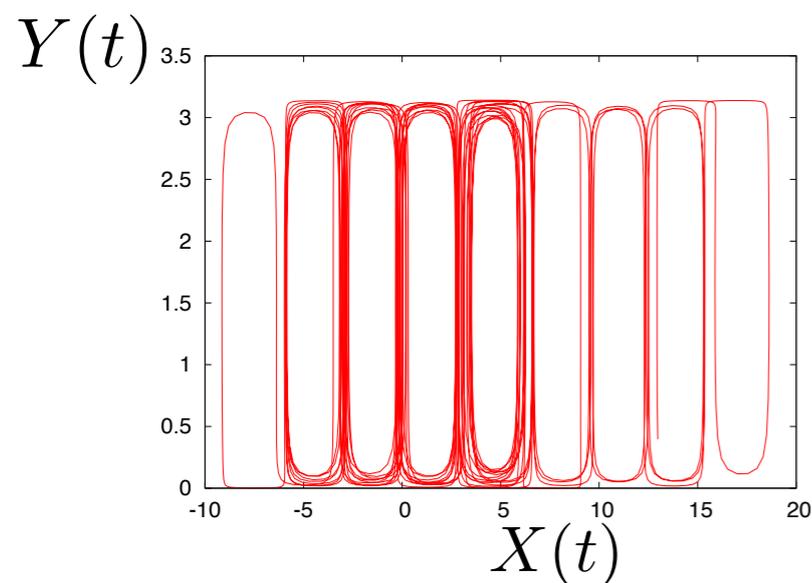
$$D_0 = 0$$

$\omega = 0$ steady flow/ particles cannot escape the vortex



Lagrangian motion is regular

$\omega \neq 0$ time periodic flow: Lagrangian chaos induces motion along x even if $D_0=0$
Lagrangian velocity is irregular even if eulerian velocity is regular

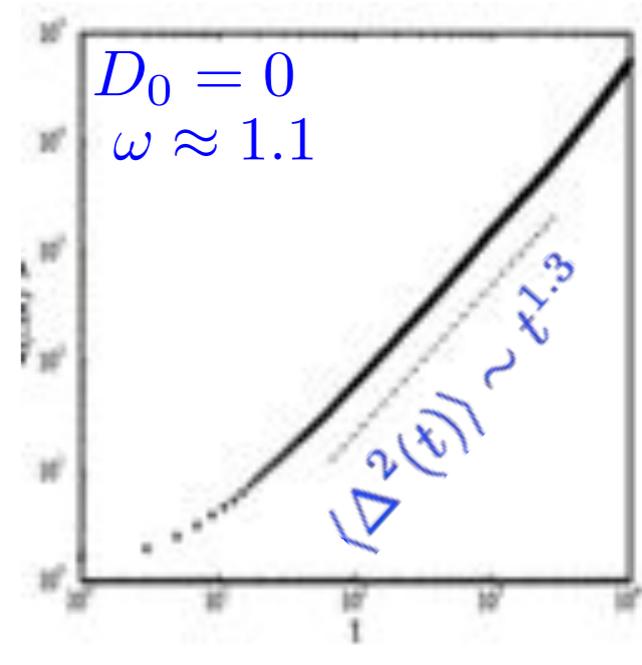
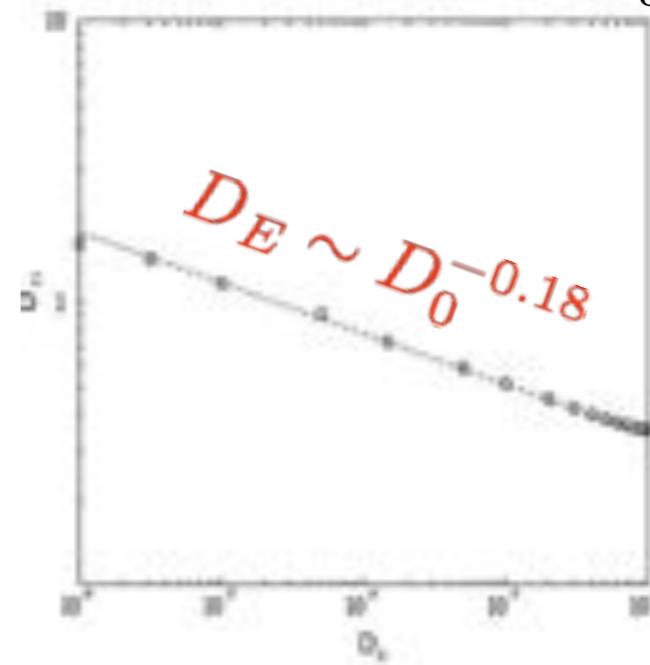
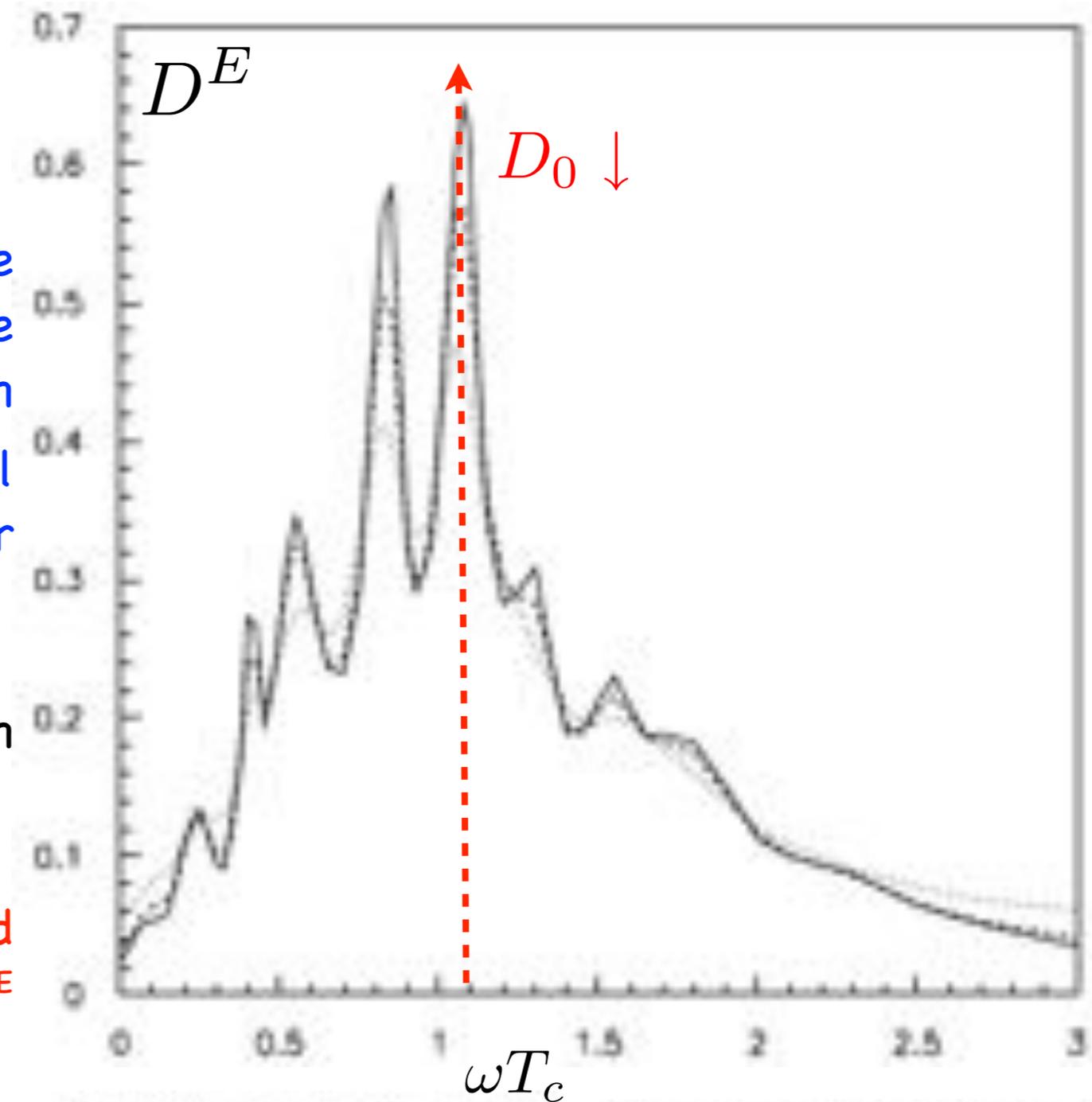


Resonances (**synchronization**) between particle circulation time (T_c) & cell oscillation can cause persistence of the motion in the same direction (**ballistic channel**) for long time causing long tail in the velocity correlation responsible for anomalous diffusion when $D_0=0$

Long tails due to non-trivial Lagrangian motion

For $D_0 \neq 0$ synchronization is imperfect and asymptotically diffusion is standard but D^E depends as a power law on D_0

Castiglione et al J.Phys. A 31, 7197 (1998);
 Castiglione et al. Physica D 134, 75 (1999)
 Solomon et al. Physica D 157, 40 (2001)



"Strong" anomalous diffusion

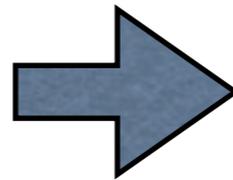
$$\langle \Delta^2(t) \rangle \sim t^\alpha \quad \begin{array}{l} \alpha = 1 \text{ diffusion} \\ \alpha > 1 \text{ superdiffusion} \end{array}$$

What about higher moments?

$$\langle \Delta^q(t) \rangle \sim t^{q\nu(q)}$$

for pure diffusion
or superdiffusion

when "strong"
anomalous diffusion

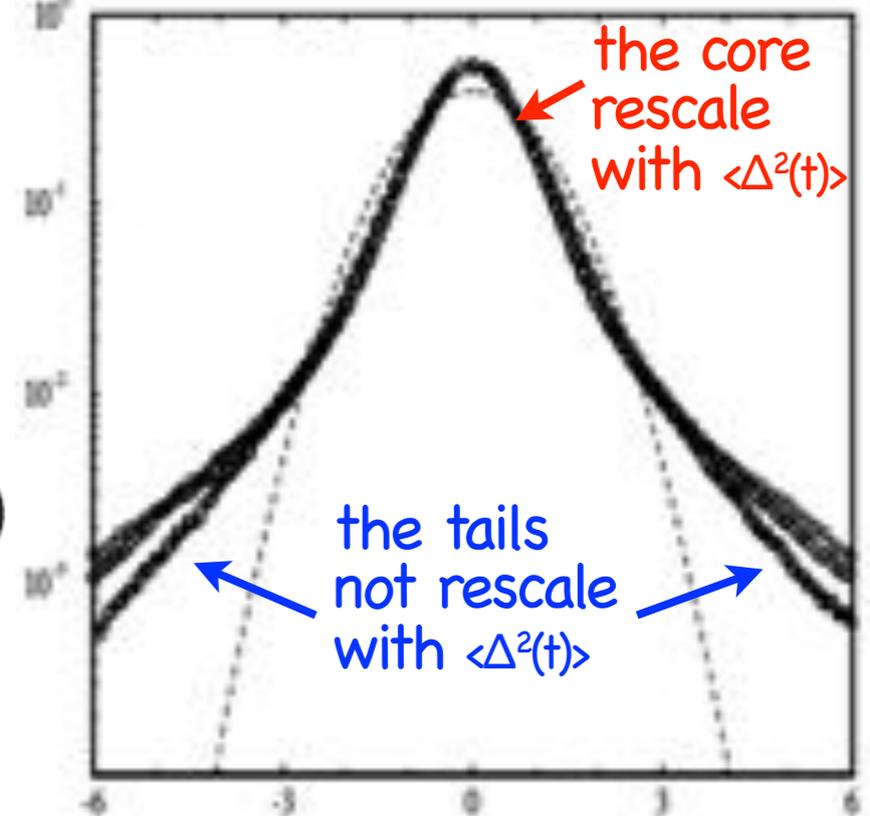
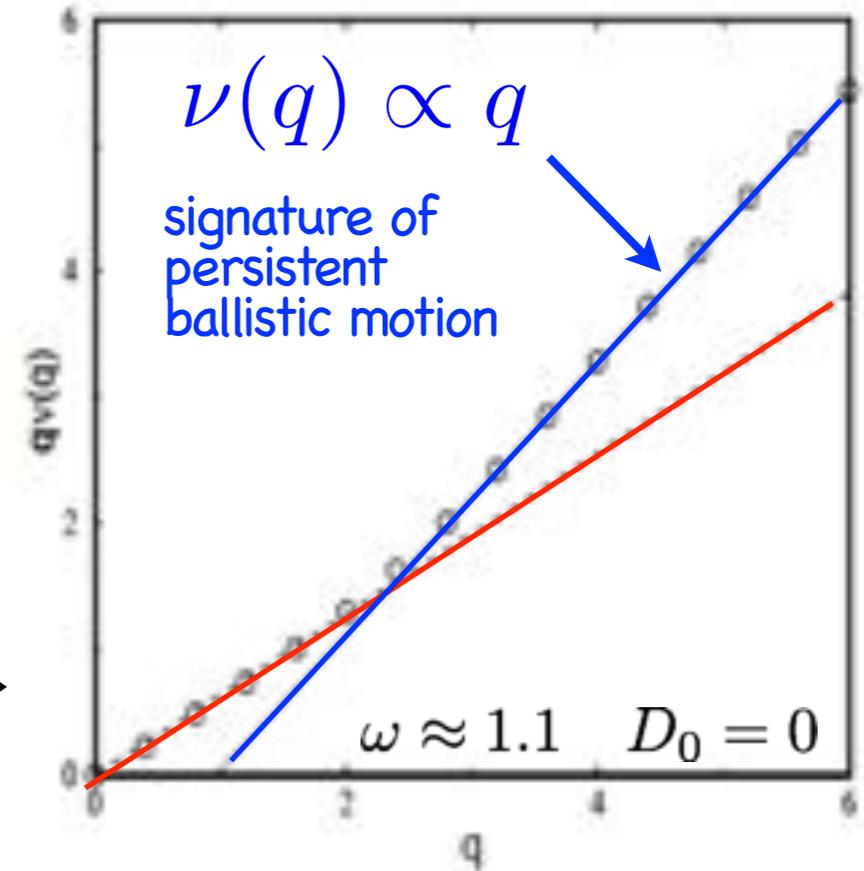


$$q\nu(q) \simeq \begin{cases} \frac{\alpha}{2}q & q < q_c \\ q - c & q > q_c \end{cases}$$

$$\nu(q) = \frac{\alpha}{2}$$



$$P(\Delta, t) = t^{-\frac{\alpha}{2}} F(\Delta t^{-\frac{\alpha}{2}}) \quad P(\Delta, t) \not\sim t^{-\frac{\alpha}{2}} F(\Delta t^{-\frac{\alpha}{2}})$$

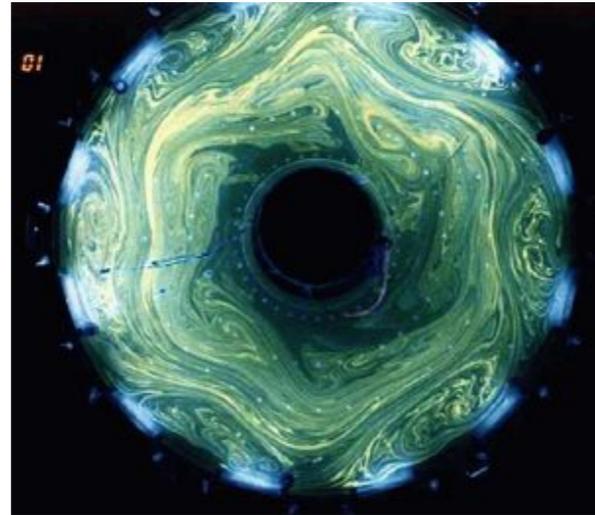
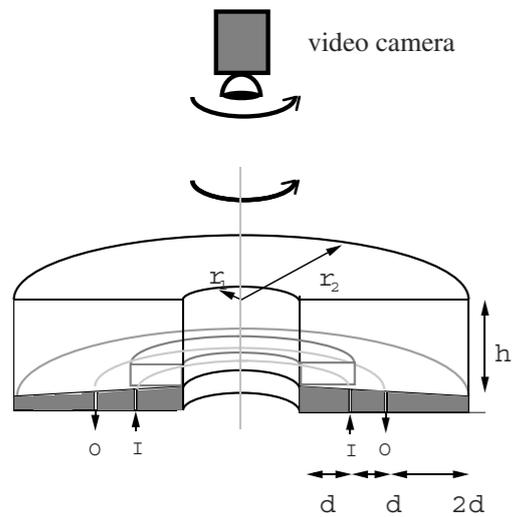


Castiglione et al. Physica D 134, 75 (1999)

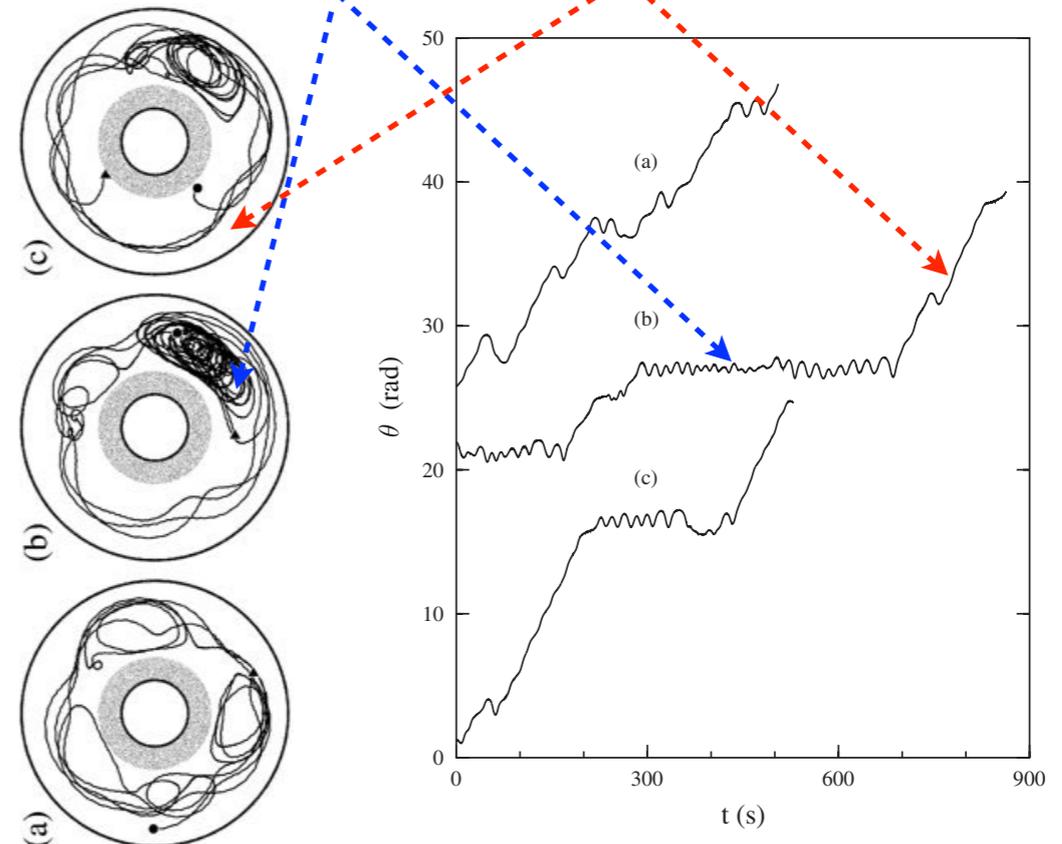
Andersen et al Europ. Phys. J. B 18, 447 (2000)

Anomalous diffusion in experiments

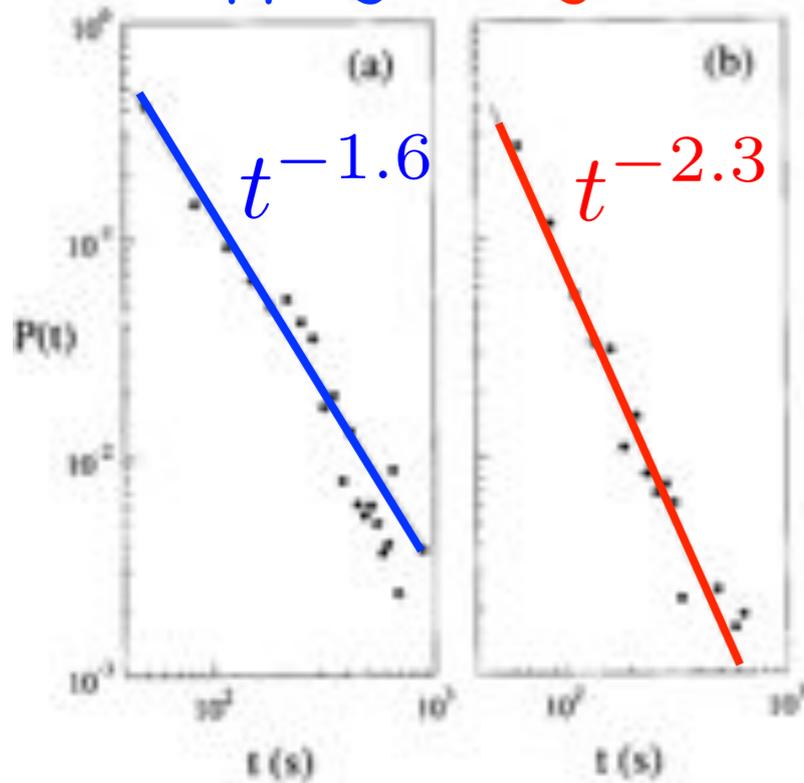
Rotating tank
(water+glycerol)



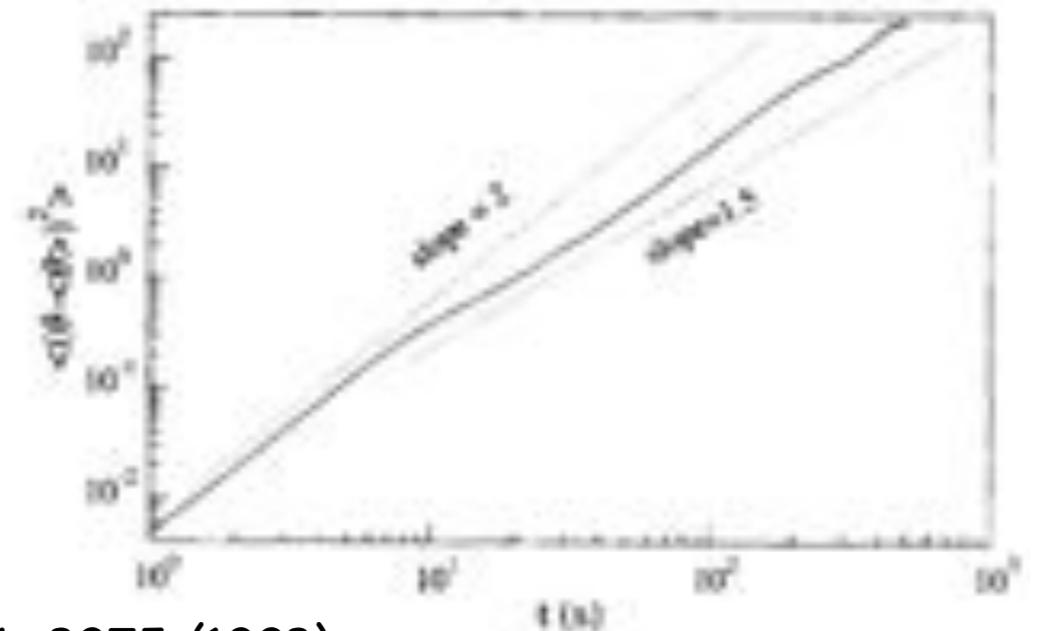
typical trajectories
(trapping+ballistic flights)



Probability duration
trapping & flights



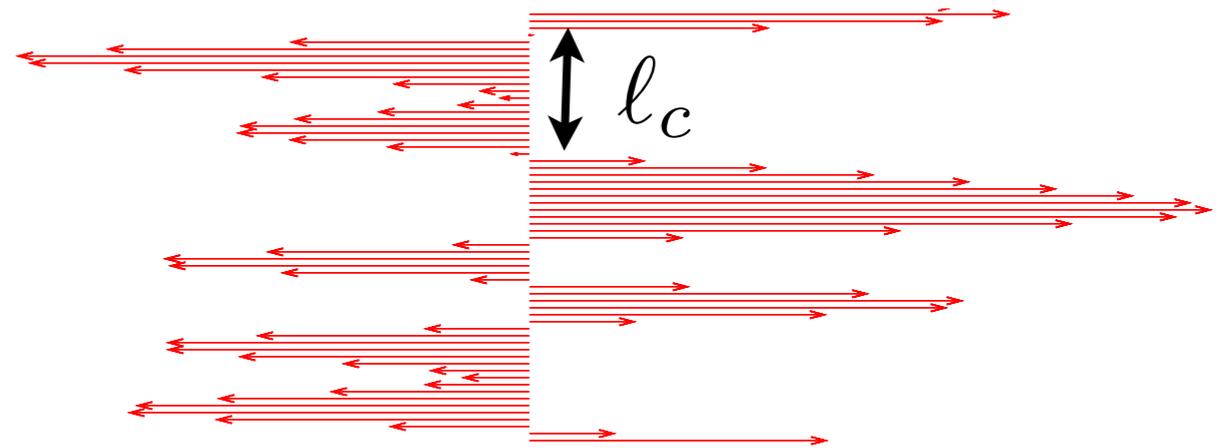
superdiffusion



Modelization of anomalous diffusion

$$\int d\mathbf{k} \frac{\langle |\mathbf{u}(\mathbf{k})|^2 \rangle}{k^2} = \int dk \frac{S(k)}{k^2} \approx \ell_c^2 \langle u^2 \rangle = \infty$$

$$D^E = \langle V^2 \rangle \tau_c = \infty$$



$$\langle u^2 \rangle \rightarrow \infty$$

$$\langle V^2 \rangle \rightarrow \infty$$

can be modeled as a **Levy Flights**
arbitrarily large velocities (**physically unrealistic**)

$$X(t+1) = X(t) + V(t) \quad V \text{ has Levy distribution} \quad P(V) \sim V^{-\gamma}$$

$$\ell_c \rightarrow \infty$$

$$\tau_c \rightarrow \infty$$

Long correlations can be modeled with **Levy Walks**
motion in the same direction for long times

$$X(t) = X(t-T) + VT$$

$$P(V) = \pm V_0 \quad Prob = 1/2$$

$$T \text{ has Levy distribution} \quad P(T) \sim T^{-\gamma}$$



Schlesinger, West & Klafter, PRL 58, 1100 (1987).

Radons, Klages, Sokolov "Anomalous transport & applications (2008)

Macroscopic description

$$\dot{X} = u(X(t), t) + \sqrt{2D_0}\eta(t) = V(t) \quad \partial_t \theta + u \cdot \nabla \theta = D_0 \Delta \theta$$

Time/Space scale separation

$$\int_0^\infty ds C(s) = \langle V^2 \rangle \tau_c = D^E = \text{finite}$$

diffusion

$$\langle (\Delta X(t))^2 \rangle \sim 2D^E t$$

macroscopic description

$$\partial_{T_M} \Theta = D^E \Delta_{X_M} \Theta$$

NO Time/Space scale separation

$$\int_0^\infty ds C(s) = \infty$$

anomalous diffusion

$$\langle (\Delta X(t))^q \rangle \sim t^{q\nu(q)} \quad \nu(q) = \frac{\alpha}{2}$$

macroscopic description

fractional diffusion equation?

“strong” anomalous diffusion

$$\langle (\Delta X(t))^q \rangle \sim t^{q\nu(q)} \quad \nu(q) \neq \frac{\alpha}{2}$$

macroscopic description

???still unclear???

Conclusions

- ▶ In the presence of time scale separation motion in incompressible fluids is diffusive, effective macroscopic description in terms of Fokker-Planck equation with renormalized coefficients
- ▶ Anomalous diffusion is due to long (power law) tails of the Lagrangian velocity correlation function due to:
 - ▶ Strong/persistent spatial correlations
 - ▶ Persistent Lagrangian correlations
- ▶ Models of anomalous behaviors can be obtained in terms of Levy Walks which are more appropriate than Levy Flights
- ▶ Effective macroscopic description of anomalous diffusion is an open issue, especially in the presence of "strong" anomalous behaviors

Some references

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