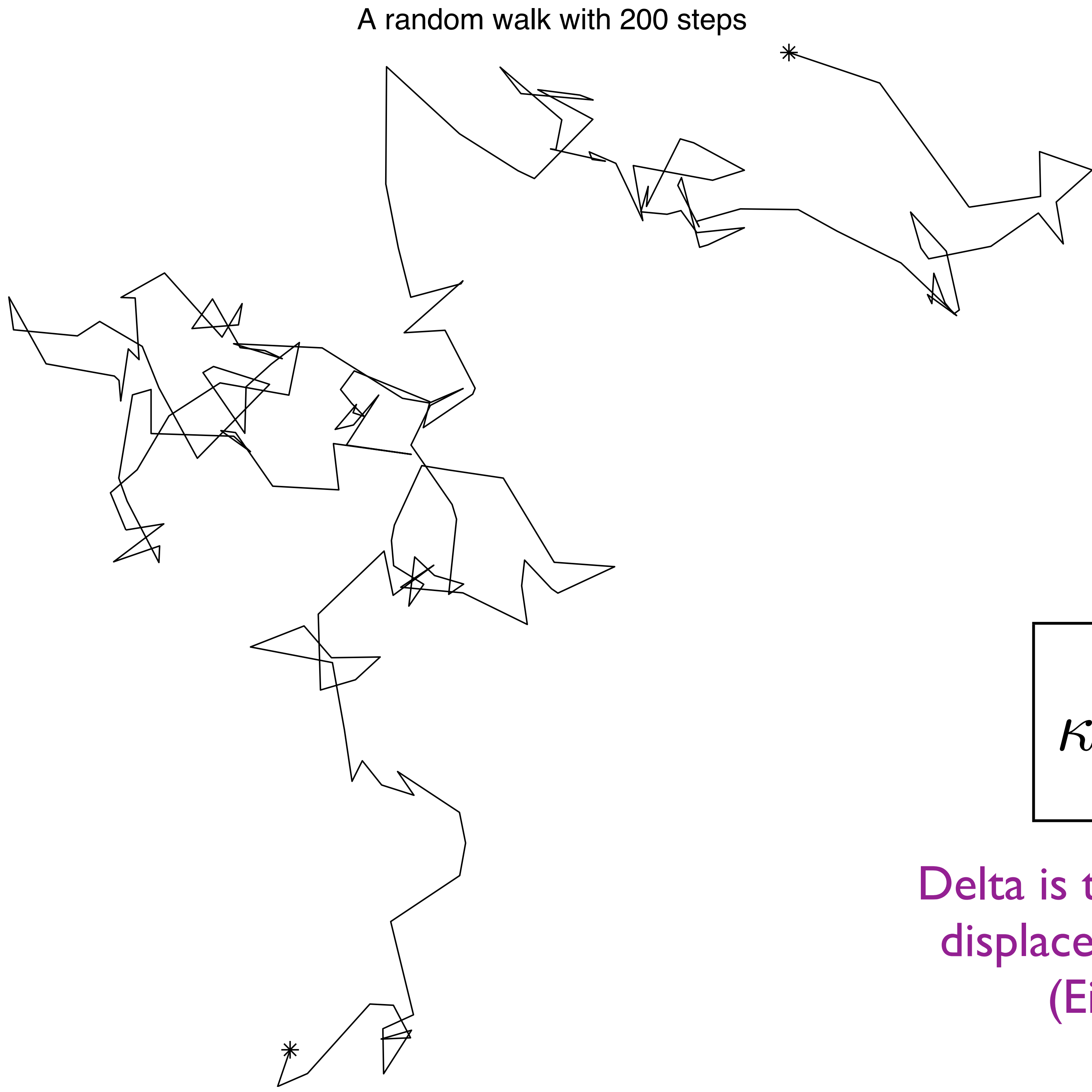
Lecture 2: Diffusion and shear dispersion

Brownian motion, SDE formulation of advection-diffusion, Taylor's formula, some Gaussianology, shear dispersion

Brownian motion

(Brown 1828, Delsaux 1877)



$$\kappa = \frac{\langle \Delta^2 \rangle}{2\tau}$$

Delta is the one-dimensional displacement along an axis (Einstein 1905).

Expansion of the master equation

☛ Observe Brownian particles at intervals: $\tau \gg \tau_c$

☛ Brownian displacements are IID random variables:

$$c(x, t+\tau) = \int_{-\infty}^{\infty} c(x-\Delta, t)\phi(\Delta, \tau)\,\mathrm{d}\Delta$$

project onto the x-axis

$$\mathrm{d}N = N\phi(\Delta, \tau)\,\mathrm{d}\Delta. \qquad \phi(\Delta, \tau) = \phi(-\Delta, \tau)\,, \qquad \int_{-\infty}^{\infty} \phi(\Delta, \tau)\,\mathrm{d}\Delta = 1.$$

☛ Assume scale separation, and expand:

$$c(x,t) + \tau c_t(x,t) \approx \int_{-\infty}^{\infty} \phi(\Delta, \tau)\left[c(x,t) - \Delta c_x(x,t) + \frac{\Delta^2}{2} c_{xx}(x,t) + \cdots\right]\mathrm{d}\Delta.$$

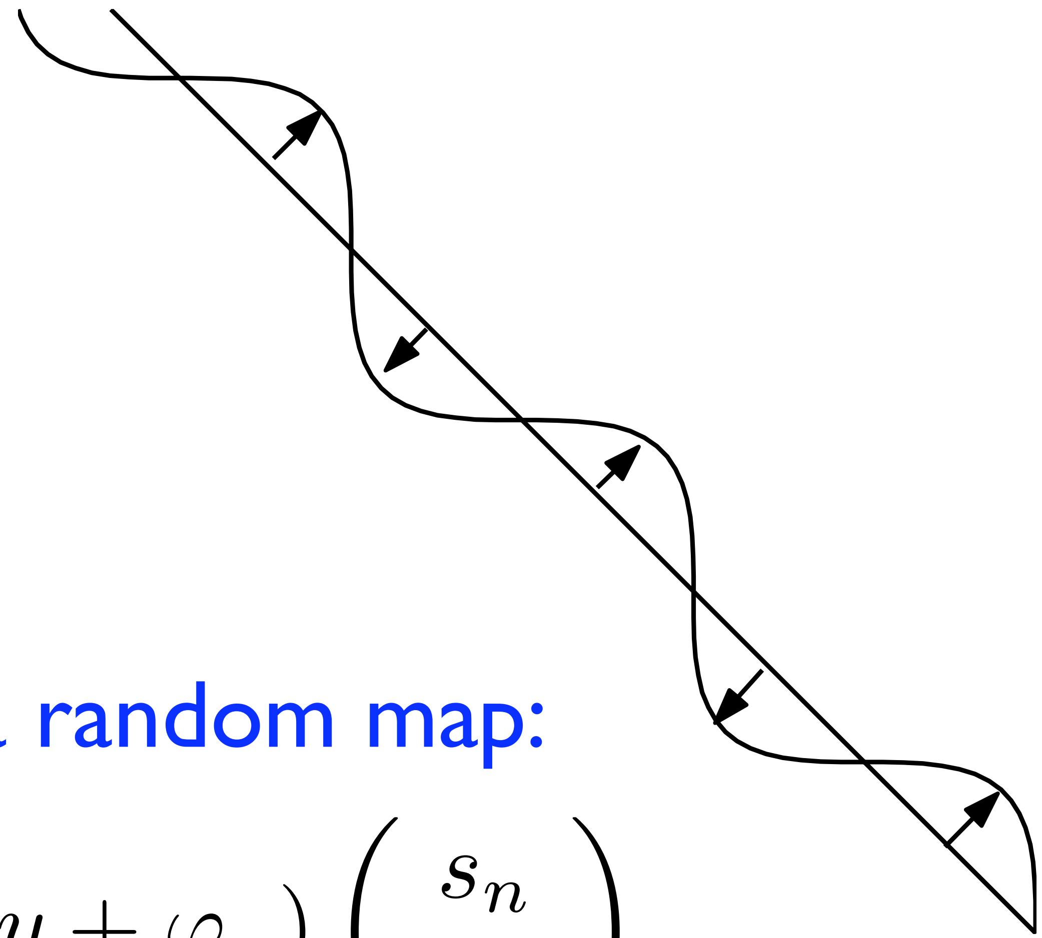
☛ If the concentration changes only a little between observations:

$$c_t(x,t) \approx \kappa c_{xx}(x,t)$$

$$\boxed{\kappa = \frac{\langle \Delta^2 \rangle}{2\tau}}$$

(independent of tau)

Example: the renewing sinusoidal flow



☛ The Cauchy solution is equivalent to a random map:

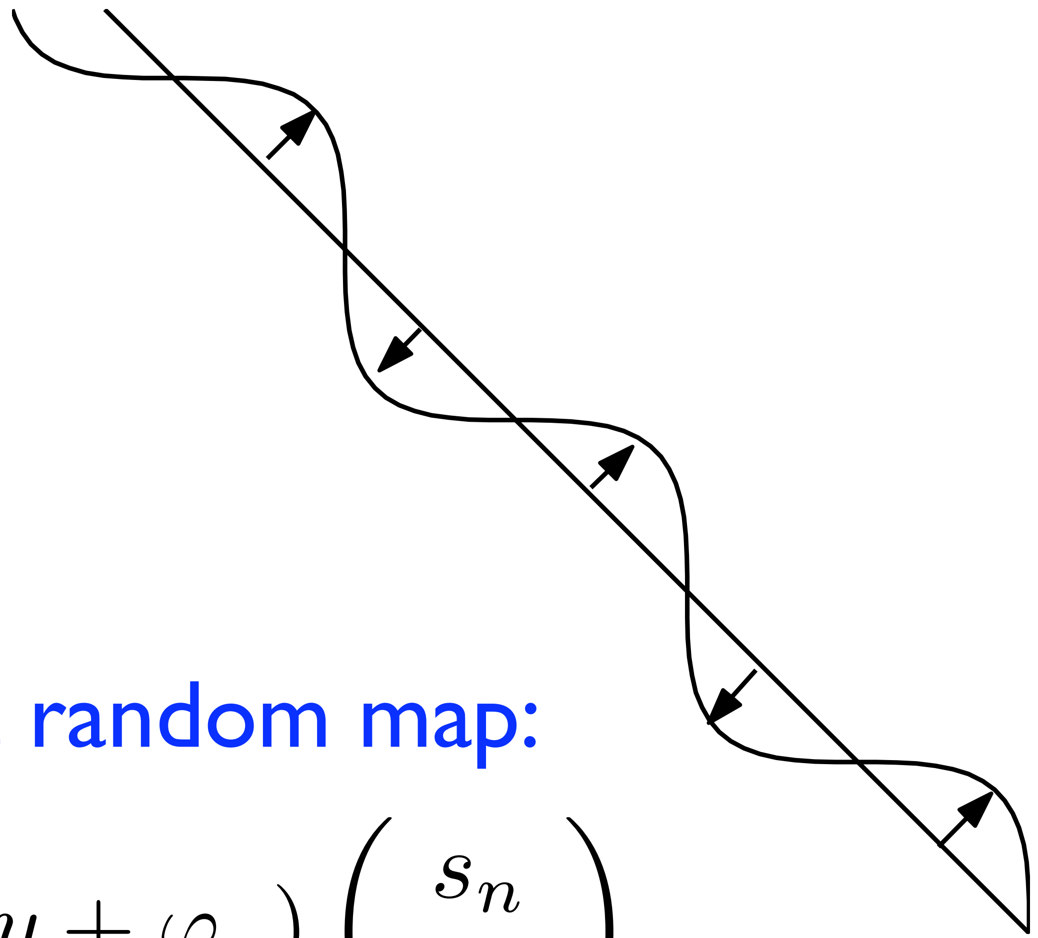
$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} x_n \\ y_n \end{pmatrix} + \tau U \sin\left(k c_n x + k s_n y + \varphi_n\right) \begin{pmatrix} s_n \\ -c_n \end{pmatrix}$$

$$s_n \equiv \sin\theta_n \text{ and } c_n \equiv \cos\theta_n$$

☛ The "eddy diffusivity" of this flow is

☛ Note the "coupling" between particles in this smooth flow.

Example: the renewing sinusoidal flow



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$s_n \equiv \sin\theta_n$ and $c_n \equiv \cos\theta_n$

☛ The "eddy diffusivity" of this flow is $\kappa_e = \dfrac{U^2\tau}{8}$

☛ Note the "coupling" between particles in this smooth flow.

Alternative construction of Brownian Motion

- Use the renewal model,

$$[0 \le t < \tau] \quad [\tau \le t < 2\tau] \quad [2\tau \le t < 3\tau] \quad \text{etc.}$$

the first epoch — the second epoch — the third epoch

- The velocity of a tracer molecule in each epoch is:

$$\tilde{\boldsymbol{u}}(\boldsymbol{x},t) = \boldsymbol{u}(\boldsymbol{x},t) + \sqrt{\frac{2\kappa}{\tau}}\boldsymbol{N}(t)$$

IID normal random variable, with unit variance, renewing at the start of each epoch.

- Monte Carlo recipe:

$$\boxed{\boldsymbol{x}(t+\mathrm{d}t) = \boldsymbol{x}(t) + \boldsymbol{u}(\boldsymbol{x}(t),t)\mathrm{d}t + \sqrt{2\kappa\mathrm{d}t}\boldsymbol{N}}$$

Homework/Discussion

☛Suppose the pdf of the jumps is: $\phi(\Delta, x, \tau)$
Above, x is the position of the particle before the jump. Find the diffusion equation (a.k.a. the Fokker-Planck equation).

$$c_t = (\kappa c)_{xx}$$

Homework

☛ Find a stochastic difference equation equivalent to

$$c_t + \boldsymbol{u}\cdot\boldsymbol{\nabla} c = \boldsymbol{\nabla}\cdot\kappa\boldsymbol{\nabla} c$$

$\kappa(\boldsymbol{x})$

☛ The "obvious" answer,

$$\boldsymbol{x}(t+\mathrm{d}t) = \boldsymbol{x}(t) + \boldsymbol{u}(\boldsymbol{x}(t),t)\mathrm{d}t + \sqrt{2\kappa(\boldsymbol{x}(t))\mathrm{d}t}\boldsymbol{N}$$

is wrong.

☛ Simulate the case: $c_t = [(1-x^2)c_x]_x\,, \qquad -1 < x < 1$

(Make sure that constant concentration is a steady solution!)

Taylor's formula for the "diffusing power" of a turbulent or chaotic flow

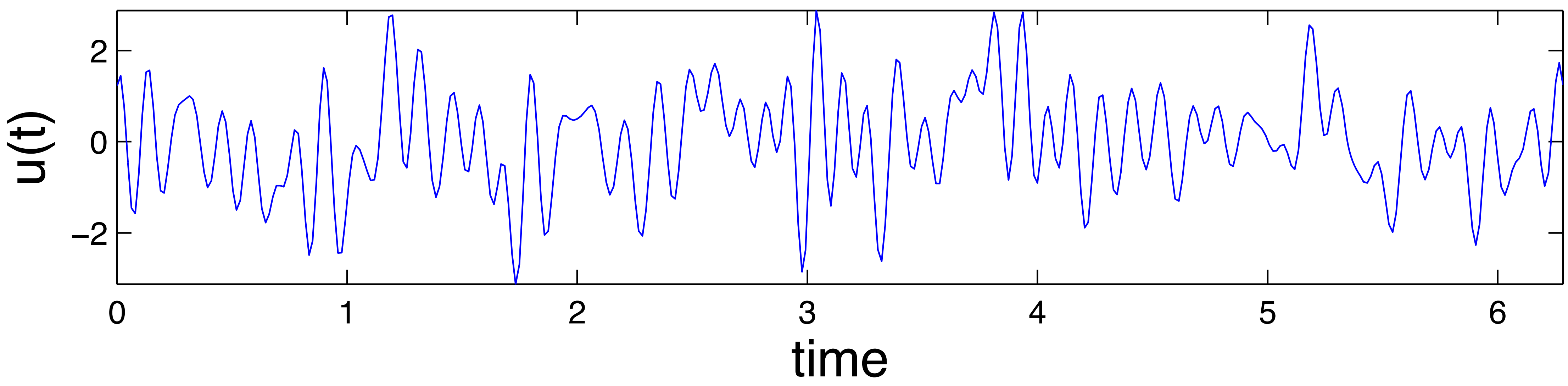
$$C(t_1 - t_2) \equiv \langle u(t_1) u(t_2) \rangle$$

and

$$\boxed{\kappa = \int_0^\infty C(t)\, \mathrm{d}t}$$

Diffusion by continuous movements

(Taylor 1922)



☛ What is the "diffusing power" of a velocity field?

☛ Use the Lagrangian correlation function: $C(t_1 - t_2) \equiv \langle u(t_1) u(t_2) \rangle$

☛ Taylor's formula is:

$$\frac{\mathrm{d}\langle x^2 \rangle}{\mathrm{d}t} = 2 \int_0^t C(t')\,\mathrm{d}t'$$

or

$$\boxed{\kappa = \int_0^\infty C(t)\,\mathrm{d}t}$$

Example 1

- A Markov model: $u(t) = \pm U \,, \qquad \mathrm{prob}(\text{flip in } \mathrm{d}t) = \alpha \mathrm{d}t$

- The correlation function is:

$C(t) = U^2 \mathrm{e}^{-2\alpha t}$ and $\therefore$ $\kappa = \dfrac{U^2}{2\alpha}$

Example 2:

☛ The renewal model again: $\mathrm{pdf}(u) = \frac{\exp\left(-\frac{1}{2}\frac{u^2}{u_{RMS}^2}\right)}{\sqrt{2\pi u_{RMS}^2}}$

$[0 \leq t < \tau]$ — the first epoch

$[\tau \leq t < 2\tau]$ — the second epoch

$[2\tau \leq t < 3\tau]$ — the third epoch

etc.

☛ According to Einstein: $\kappa = \frac{\langle \Delta^2 \rangle}{2\tau} = \frac{1}{2}\tau u_{RMS}^2$

☛ Homework/Discussion: does Taylor agree with Einstein?

$$C(t) = ???$$

Gaussianology: part 1

Recall Townsend's hot-spot

- This advection-diffusion equation $c_t + \sigma x c_x - \sigma y c_y = \kappa \nabla^2 c$
  has a Gaussian solution: $c = c_0(t) \exp\left(-\frac{1}{2}\alpha^2(t) x^2 - \frac{1}{2}\beta^2(t) y^2\right)$

- Substituting the guess, we find

$$\dot{\alpha} + \sigma\alpha = -\kappa\alpha^3\,, \qquad \dot{\beta} - \sigma\beta = -\kappa\beta^3$$

and $\dot{c}_0 = -\kappa(\alpha^2 + \beta^2)c_0$

- Finally $c(x,y,t) = \dfrac{1}{2\pi ab}\exp\left[-\dfrac{x^2}{2a^2} - \dfrac{y^2}{2b^2}\right]$

$$a^2 \equiv \frac{\kappa}{\sigma}\left(e^{2\sigma t} - 1\right)\,, \qquad b^2 \equiv \frac{\kappa}{\sigma}\left(1 - e^{-2\sigma t}\right)$$

- This is the tip of the Gaussian ice-berg.....

The general "hot-spot" problem

☛ The general "local" advection-diffusion equation

$$c_t + (\boldsymbol{W}\boldsymbol{x}) \cdot \boldsymbol{\nabla} c = \kappa \nabla^2 c\,, \qquad \boldsymbol{W}_{ij}(t) \equiv u_{i,j}$$

has a gaussian solution $c = c_0(t)\exp\left(-\tfrac{1}{2}S_{ij}(t)x_i x_j\right)$

☛ The moment matrix $M_{ij} \equiv \dfrac{\int x_i x_j c\,\mathrm{d}V}{\int c\,\mathrm{d}V}$ satisfies

$$\dot{\boldsymbol{M}}(t) = \boldsymbol{W}\boldsymbol{M}^{\intercal} + \boldsymbol{M}\boldsymbol{W}^{\intercal} + 2\kappa\boldsymbol{I}$$

(Lyapunov's equation - which is linear.)

The key to successful Gaussianology

(e.g., van Kampen's textbook)

☛ Possessing the moment matrix, the solution is

$$c(\boldsymbol{x},t) = \frac{\int c\,\mathrm{d}V}{(2\pi)^{d/2}\sqrt{\det \boldsymbol{M}}}\exp\left(-\tfrac{1}{2}\boldsymbol{x}^{\mathsf{T}}\boldsymbol{M}^{-1}\boldsymbol{x}\right)$$

☛ Example (Couette flow)

$$c_t + syc_x = \kappa\nabla^2 c$$

$$c(x,y,0) = \delta(x)\delta(y)$$

☛ We easily find

$$\boldsymbol{M} = \begin{pmatrix} 2\kappa t + \frac{2}{3}\kappa s^2 t^3 & \kappa s t^2 \\ \kappa s t^2 & 2\kappa t \end{pmatrix}$$

Shear dispersion $c_t + syc_x = \kappa \nabla^2 c$

☛ Another Gaussian solution with a "hot-spot" IC

$$c(\boldsymbol{x},t) = \frac{1}{4\pi\kappa\alpha t} \exp\left(- \frac{(x - \frac{1}{2}sty)^2 + \alpha^2 y^2}{4\kappa t \alpha^2} \right)$$

$$\alpha(t) \equiv \sqrt{1 + \tfrac{1}{12}(st)^2}.$$

☛ Algebraic decay $\max_{\forall \boldsymbol{x}} c(\boldsymbol{x},t) \propto t^{-2}$

☛ Super-diffusive (and super-advective) dispersion

$$\Delta x \sim \sqrt{\kappa s^2 t^3}$$

Physical explanation of the power laws

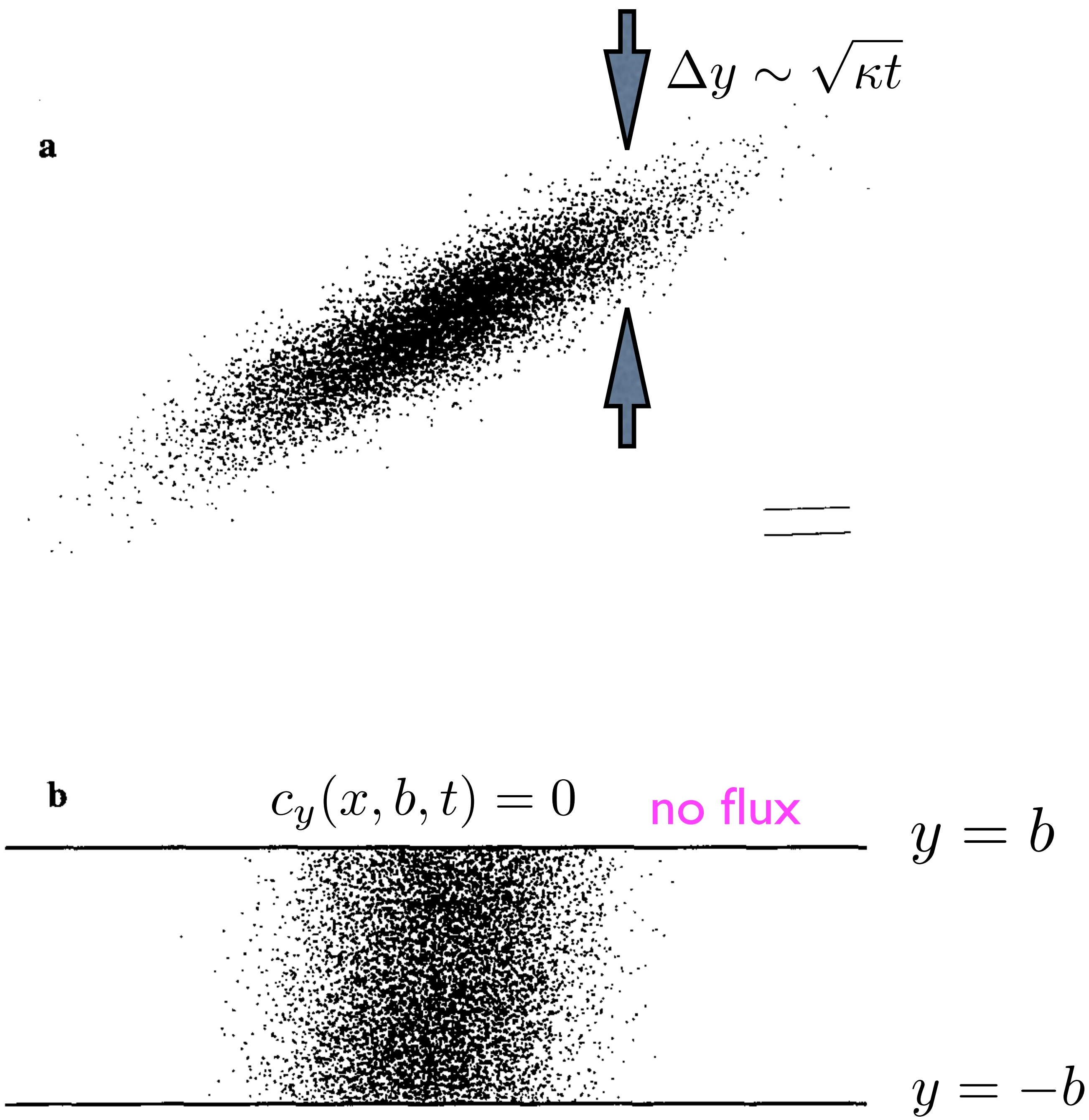


Fig. 1. Dispersion of an ensemble of diffusive particles by the flow $u = 2y$. In an (a) unbounded domain; (b) bounded domain. The channel shown in (b) is reproduced in the lower right-hand corner of (a).

$$\frac{\mathrm{d}\Delta x}{\mathrm{d}t} \sim s\Delta y \qquad \Rightarrow \qquad \Delta x \sim \sqrt{\kappa s^2 t^3}$$

$$\max_{\forall \boldsymbol{x}} c(\boldsymbol{x}, t) \sim \frac{1}{\Delta x \Delta y} \sim t^{-2}$$

☛ In a confined layer, the problem of shear dispersion is more interesting.

(Taylor 1953)

Shear Dispersion

(Taylor 1953)

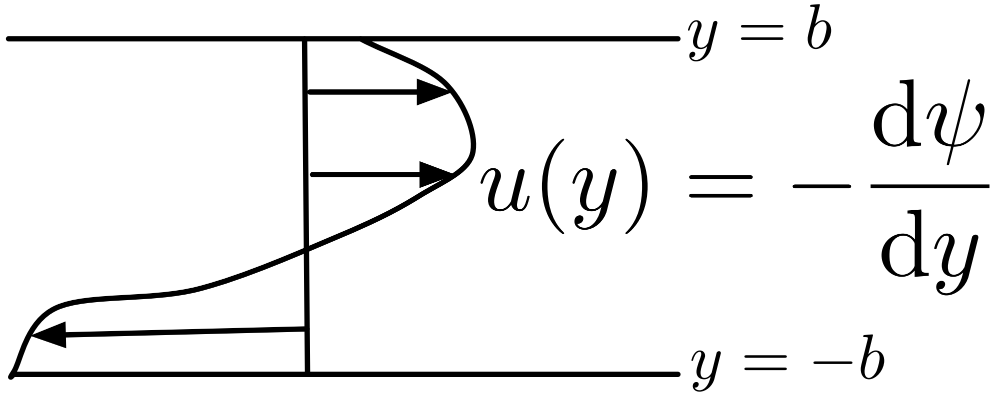
$$\boxed{\kappa_e \propto \frac{1}{\kappa}}$$

Taylor's (1953) derivation

☛ Define a "sectional average" and a "fluctuation":

$$c(x,y,t) = \bar{c}(x,t) + c'(x,y,t) \qquad u(y) = u'(y) = -\psi_y$$

$$\bar{c}(x,t) \equiv \frac{1}{2b}\int_{-b}^{b} c(x,y,t)\,\mathrm{d}y$$



☛ Averaging the equation: $\bar{c}_t + \left(\overline{u'c'}\right)_x = \kappa \bar{c}_{yy}$

So we need the flux: $f(x,t) \equiv \overline{u'c'} = \overline{\psi c'_y}$

The flux $f(x,t) \equiv \overline{u'c'} = \overline{\psi c'_y}$

- The fluctuation equation is:

$$c'_t + \left(u'c' - \overline{u'c'}\right)_x - \kappa \nabla^2 c' = -u'\bar{c}_x$$

The source of "fluctuations"

- In the "homogenization limit", this simplifies to:

$$\boxed{\kappa c'_{yy} \approx u'\bar{c}_x} \quad \Rightarrow \quad c'_y = -\frac{\psi}{\kappa}\bar{c}_x \quad \Rightarrow \quad f = -\frac{\overline{\psi^2}}{\kappa}\bar{c}_x$$

The mean field is large scale, and slowly varying.

BCs✓

- The effective diffusivity is therefore: $\kappa_e = \kappa + \frac{\overline{\psi^2}}{\kappa}$

The Gx trick (a.k.a homogenization)

☛ Look for a steady solution: $c(x, y, t) = Gx + c'(y)$

$$\kappa c'_{yy} = uG \qquad \Rightarrow \qquad c'_y = -\frac{\psi}{\kappa} G$$

(An exact solution.)

☛ Obtain the flux-gradient relation:

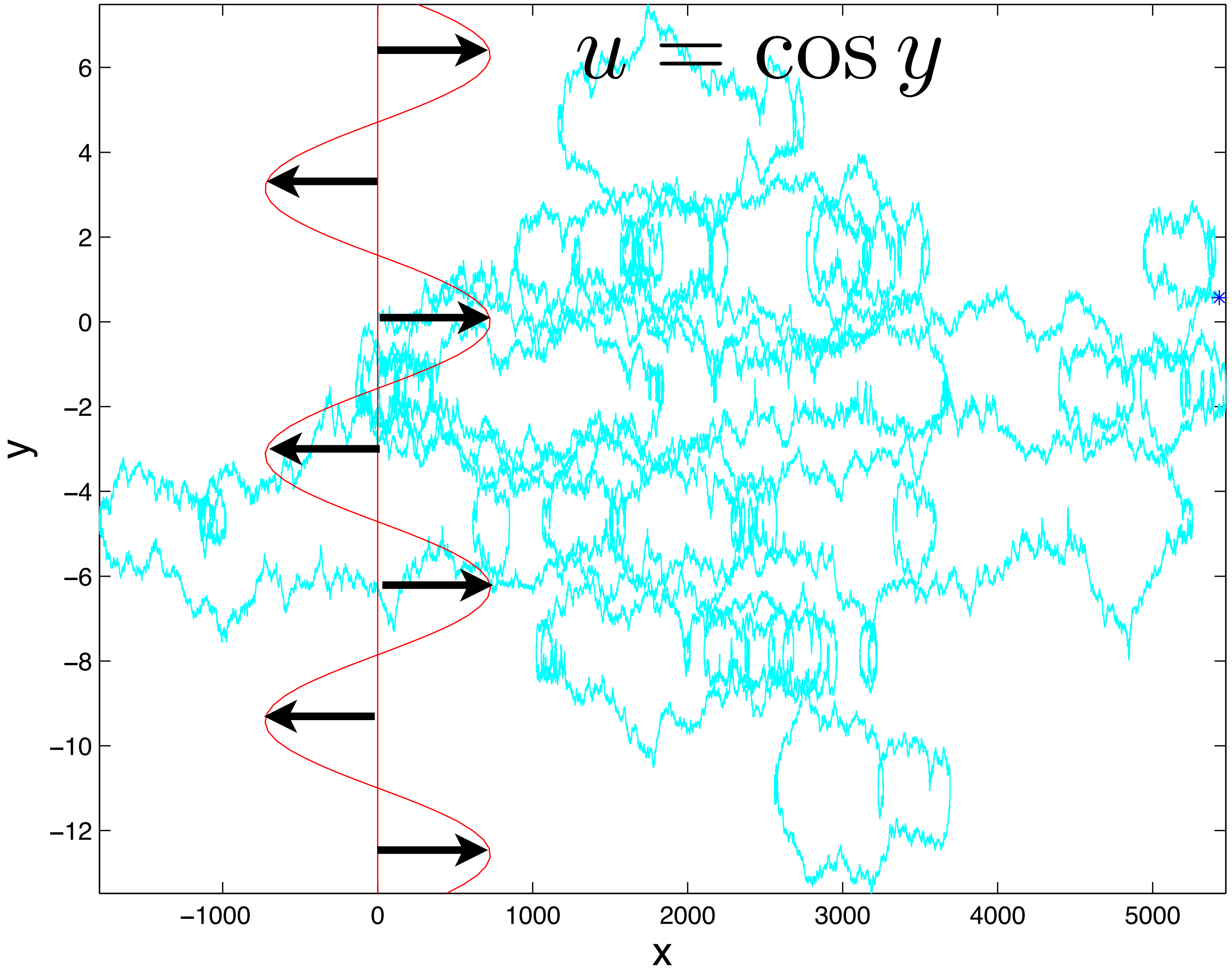
$$\begin{aligned} F &= -\kappa G + \overline{uc} \\ &= -\kappa G + \overline{\psi c'_y} \\ &= -\left(\kappa + \frac{\overline{\psi^2}}{\kappa}\right) G \end{aligned}$$

☛ Identify the effective diffusivity:

$$\kappa_e$$

Taylor's formula also explains $\boxed{\kappa_e \propto \frac{1}{\kappa}}$

$$\kappa_e = \int_0^\infty \mathcal{C}(t)\,\mathrm{d}t \sim u_{\mathrm{RMS}}^2 T_{\mathrm{corr}}$$



$\kappa = 10^{-3}$ and $\Delta t = 10^5$

$$T_{\mathrm{corr}} \sim \frac{b^2}{\kappa} \qquad u_{RMS} = \sqrt{\overline{u^2}}$$

$$\Rightarrow \kappa_e \sim \frac{b^2 u_{RMS}^2}{\kappa}$$

☛ This diffusive regime requires: $t \gg T_{\mathrm{corr}}$

More homework (an easy one)

☛ Calculate the effective diffusivity:

$$c_t + U\cos(\omega t)\cos(my)c_x = \kappa\nabla^2 c$$

☛ Write the solution as

$$\kappa_e = \frac{U^2}{\omega}F\left(\frac{m^2\kappa}{\omega}\right)$$

and explain why F(x) has a maximum at a certain value of m^2 kappa/omega.

Validity of the effective-diffusion approximation

☛ The approximation is valid only at long times (and in a long channel).

$$\sqrt{\kappa t} \gg b \qquad \frac{L}{b} \gg \frac{bu}{\kappa} \equiv Pe$$

☛ The "pre-asymptotic" dispersion problem is non-universal, and therefore more interesting than the final diffusive regime....