Lecture 3: Eddy diffusivity and homogenization

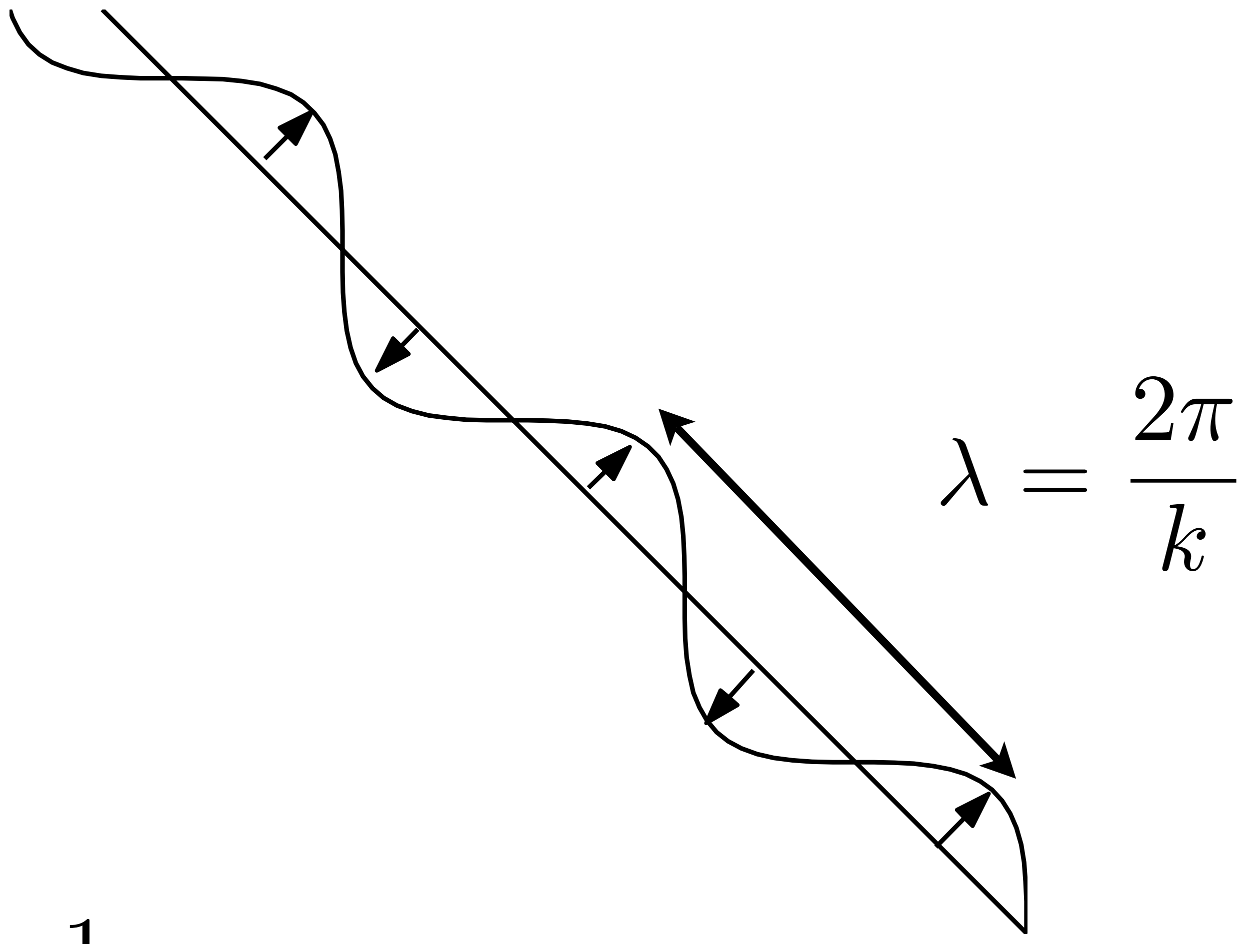
Eddy diffusion, ensemble averages, spatial averages, variance (c^2-stuff) budgets, the Batchelor Spectrum, homogenization

We start with an example.

Example 1: the dispersing front

$$c_t + \boldsymbol{u} \cdot \boldsymbol{\nabla} c = 0\,, \qquad c(\boldsymbol{x}, 0) = \mathrm{sgn}(x)$$

☛ We use the renewing wave flow as an illustration:

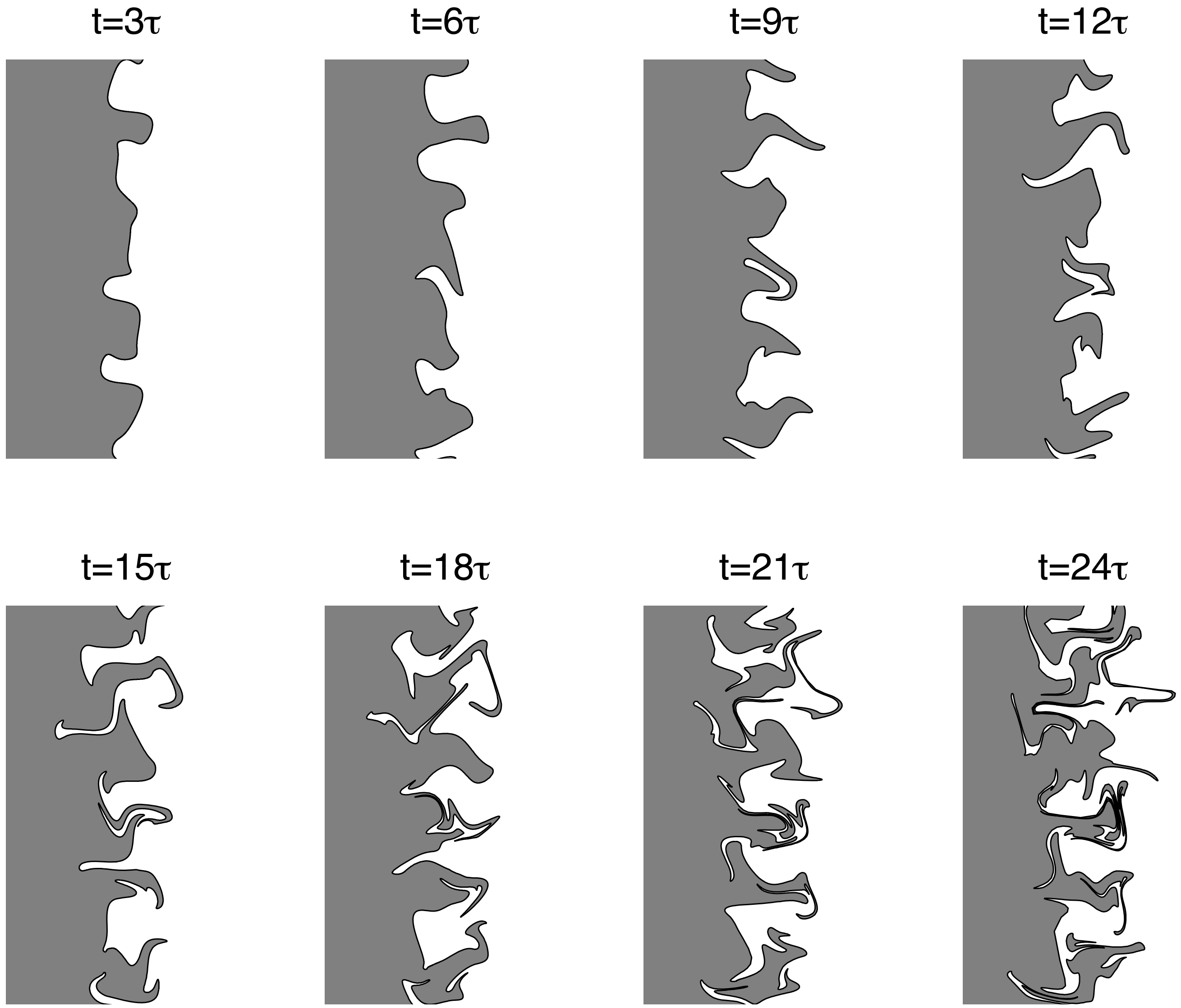


☛ Recall that the eddy diffusivity of this flow is: $\kappa_e = \frac{1}{8}\tau U^2$

(Independent of the flow length scale!)

Dispersion of a front, $c(\boldsymbol{x},0)=\mathrm{sgn}(x)$

$\kappa = 0$



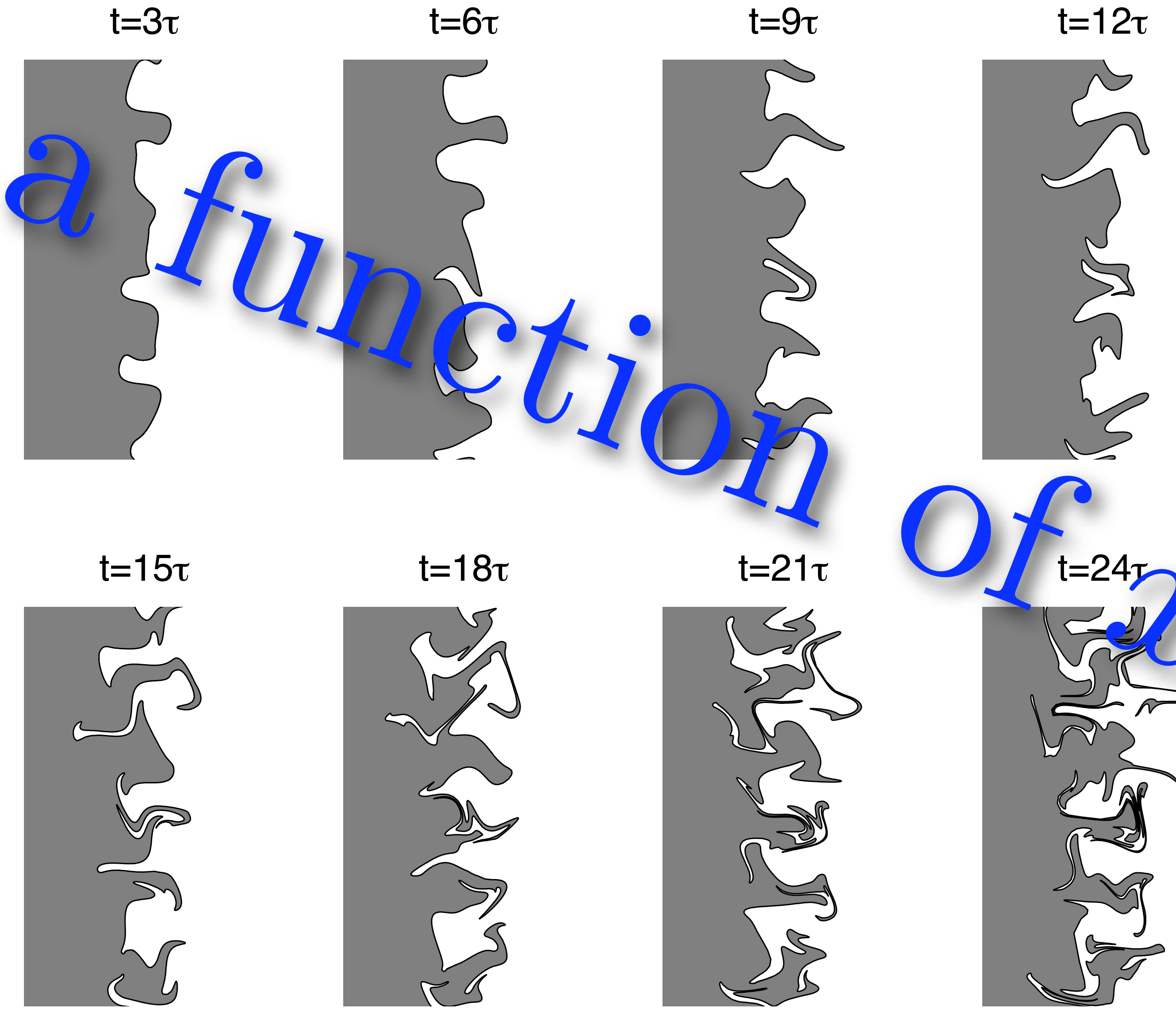
☛ The ensemble average is: $\langle c\rangle_t = \kappa_e \nabla^2 \langle c\rangle$??

or $\langle c\rangle = \mathrm{erf}(\eta)$ with $\eta \equiv \dfrac{x}{2\sqrt{\kappa_e t}}$

Dispersion of a front, $c(\boldsymbol{x},0) = \mathrm{sgn}(x)$

$\langle c \rangle$ is a function of x and t

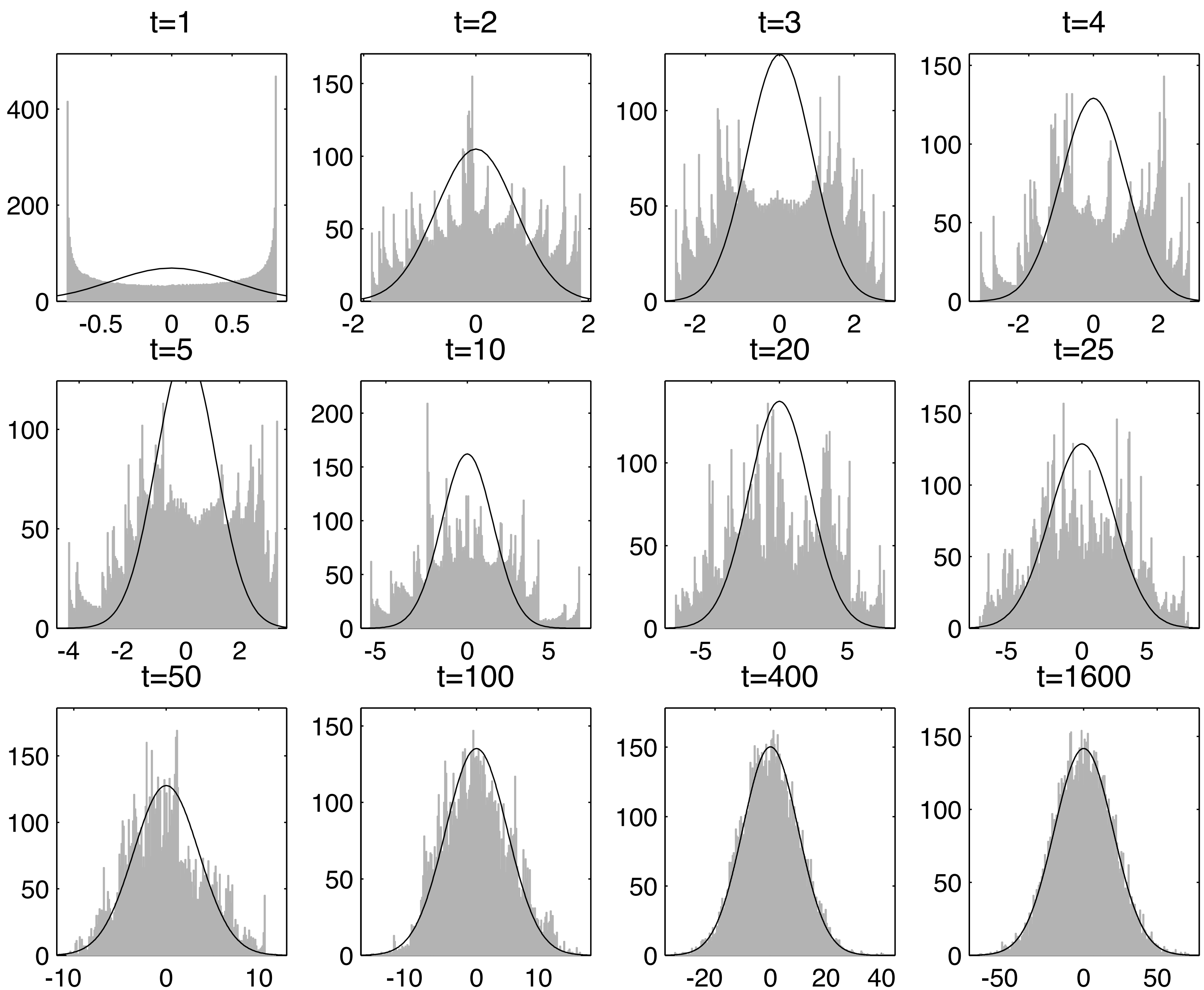
$\kappa = 0$



☛ The ensemble average is: $\langle c \rangle_t = \kappa_e \nabla^2 \langle c \rangle$??

or $\langle c \rangle = \mathrm{erf}(\eta)$ with $\eta \equiv \dfrac{x}{2\sqrt{\kappa_e t}}$

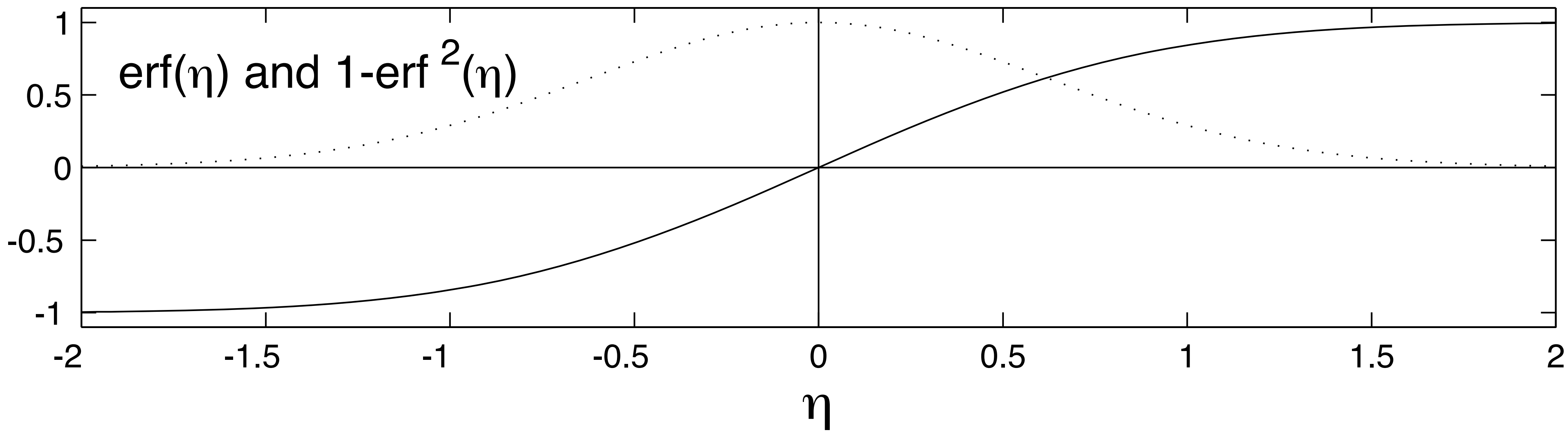
Asymptotic triumph of eddy diffusivity



$Uk\tau = 1$

Histogram of 10^4 particles, all starting on x=0

The concentration variance of the dispersing front



$$c' = \underbrace{c}_{=\pm 1} - \langle c \rangle \quad \Rightarrow \quad \langle c'^2 \rangle = 1 - \mathrm{erf}^2(\eta)$$

☛ Homework/discussion:

$$\mathrm{pdf}(c, \eta) = \frac{1 + \mathrm{erf}(\eta)}{2} \delta(c - 1) + \frac{1 - \mathrm{erf}(\eta)}{2} \delta(c + 1)$$

Now we turn to general principles:
the Reynolds decomposition, scale separation
and variance budgets

The Reynolds decomposition

- In single realization:

$$c_t + \boldsymbol{u}\cdot\boldsymbol{\nabla} c = \kappa\nabla^2 c + s\,,$$

and

$$c = \langle c\rangle + c'\,,$$

- The ensemble average is: $\langle c\rangle_t + \langle\boldsymbol{u}\rangle\cdot\boldsymbol{\nabla}\langle c\rangle + \boldsymbol{\nabla}\cdot\langle\boldsymbol{u}'c'\rangle = \kappa\nabla^2\langle c\rangle + s\,.$

- The fluctuation equation is:

$$c'_t + \langle\boldsymbol{u}\rangle\cdot\boldsymbol{\nabla} c' + \boldsymbol{\nabla}\cdot\left[\boldsymbol{u}'c' - \langle\boldsymbol{u}'c'\rangle\right] - \kappa\nabla^2 c' = -\boldsymbol{u}'\cdot\boldsymbol{\nabla}\langle c\rangle$$

The source of fluctuations

- The fluctuation equation is linear, so with scale separation:

$$\langle\boldsymbol{u}'c'\rangle_i = -\mathcal{D}^{(1)}_{ij} * \langle c\rangle_{,j} - \mathcal{D}^{(2)}_{ijk} * \boldsymbol{\nabla}\langle c\rangle_{,jk} + \cdots$$

where $\mathcal{D}^{(1)}_{ij} * \langle c\rangle_{,j} = \int_0^t \mathcal{D}^{(1)}_{ij}(t')\langle c\rangle_{,j}(t-t')\,\mathrm{d}t'\,.$

The eddy-diffusion equation

☛ With a slowly varying in time mean field:

$$\langle \boldsymbol{u}'c' \rangle \approx -\mathcal{D}^{(1)}_{ij} * \langle c \rangle_{,j} \approx -\int_0^\infty \mathcal{D}^{(1)}_{ij}(t')\,\mathrm{d}t'\,\langle c \rangle_{,j}(t)\,.$$

☛ In the simplest case: $$\int_0^\infty \mathcal{D}^{(1)}_{ij}(t')\,\mathrm{d}t' = \kappa'_e \delta_{ij}$$

(Isotropic, homogeneous and reflexionally invariant flows.)

☛ Finally: $$\langle \boldsymbol{u}'c' \rangle - \kappa \boldsymbol{\nabla} \langle c \rangle = -\kappa_e \boldsymbol{\nabla} \langle c \rangle\,, \qquad \kappa_e = \kappa + \kappa'_e$$

and $$\boxed{\langle c \rangle_t \approx \kappa_e \nabla^2 \langle c \rangle + s}$$

☛ The Gx trick (and an ergodic assumption) provides the eddy diffusivity in simulations.

$$c = Gx + c'(\boldsymbol{x}, t)$$

The variance (c^2-stuff) equation $\mathcal{Z} \equiv \frac{1}{2}\left\langle c'^2 \right\rangle$

- The variance equation is:

$$\mathcal{Z}_t + \langle \boldsymbol{u} \rangle \cdot \boldsymbol{\nabla} \mathcal{Z} + \boldsymbol{\nabla} \cdot \left\langle \frac{1}{2} \boldsymbol{u}' c'^2 \right\rangle - \kappa \nabla^2 \mathcal{Z} = -\kappa \left\langle |\boldsymbol{\nabla} c'|^2 \right\rangle - \left\langle \boldsymbol{u}' c' \right\rangle \cdot \boldsymbol{\nabla} \langle c \rangle$$

SINK SOURCE

- To explicate the source of c^2-stuff:

$$\boxed{\mathcal{Z}_t + \langle \boldsymbol{u} \rangle \cdot \boldsymbol{\nabla} \mathcal{Z} + \boldsymbol{\nabla} \cdot \langle \tfrac{1}{2} \boldsymbol{u}' c'^2 \rangle - \kappa \nabla^2 \mathcal{Z} = \kappa_e' |\boldsymbol{\nabla} \langle c \rangle|^2 - \kappa \langle |\boldsymbol{\nabla} c'|^2 \rangle}$$

SOURCE SINK

- In the kappa =0 dispersing front problem, this monster reduces to:

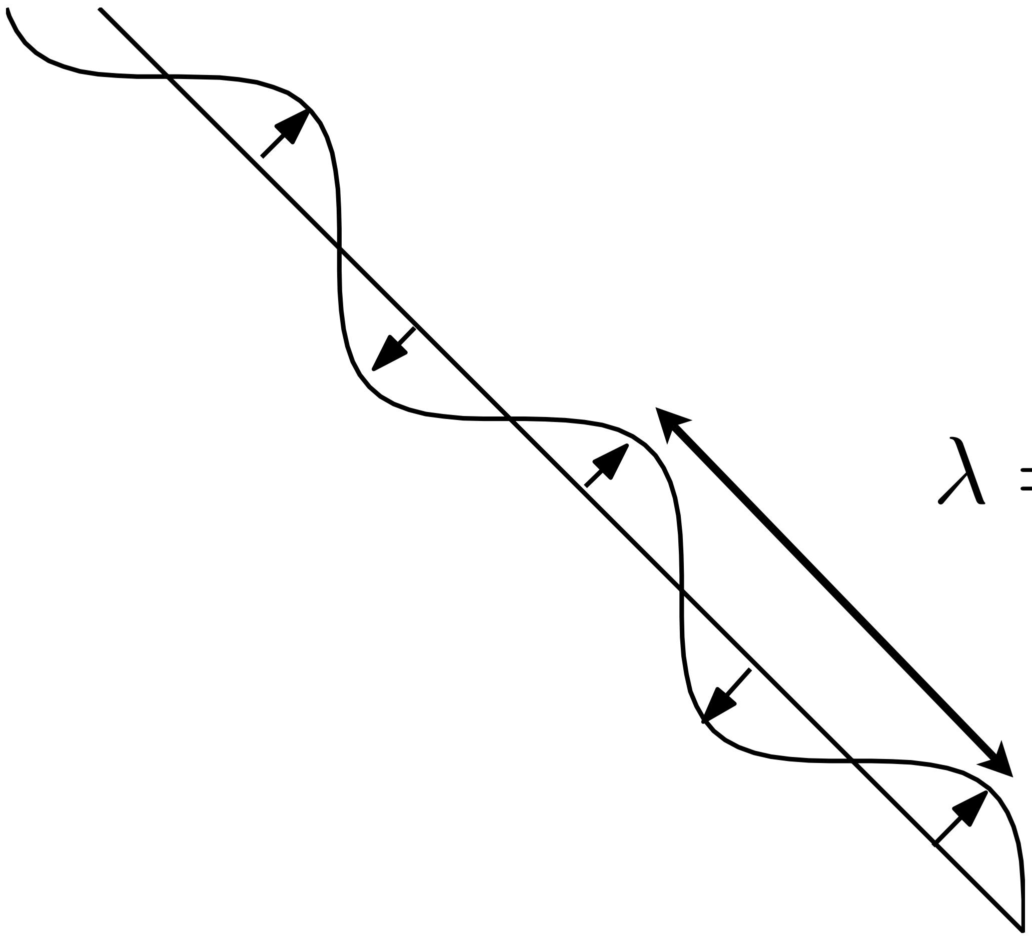
$$\mathcal{Z}_t - \kappa_e' \mathcal{Z}_{xx} = \kappa_e' |\boldsymbol{\nabla} \langle c \rangle|^2$$

and we verify that the solution is indeed: $\mathcal{Z} = \frac{1}{2}\left[1 - \mathrm{erf}^2(\eta)\right]$

Example 2: the source problem

$$c_t + \boldsymbol{u} \cdot \boldsymbol{\nabla} c = \cos qy + \kappa \nabla^2 c$$

☛ Again we use the renewing wave flow as an illustration:



☛ Scale separation is: $\frac{q}{k} \ll 1$

Another renewing wave example

☛ First consider kappa = 0, and look for a statistically steady solution of

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

☛ The ensemble averaged concentration is:

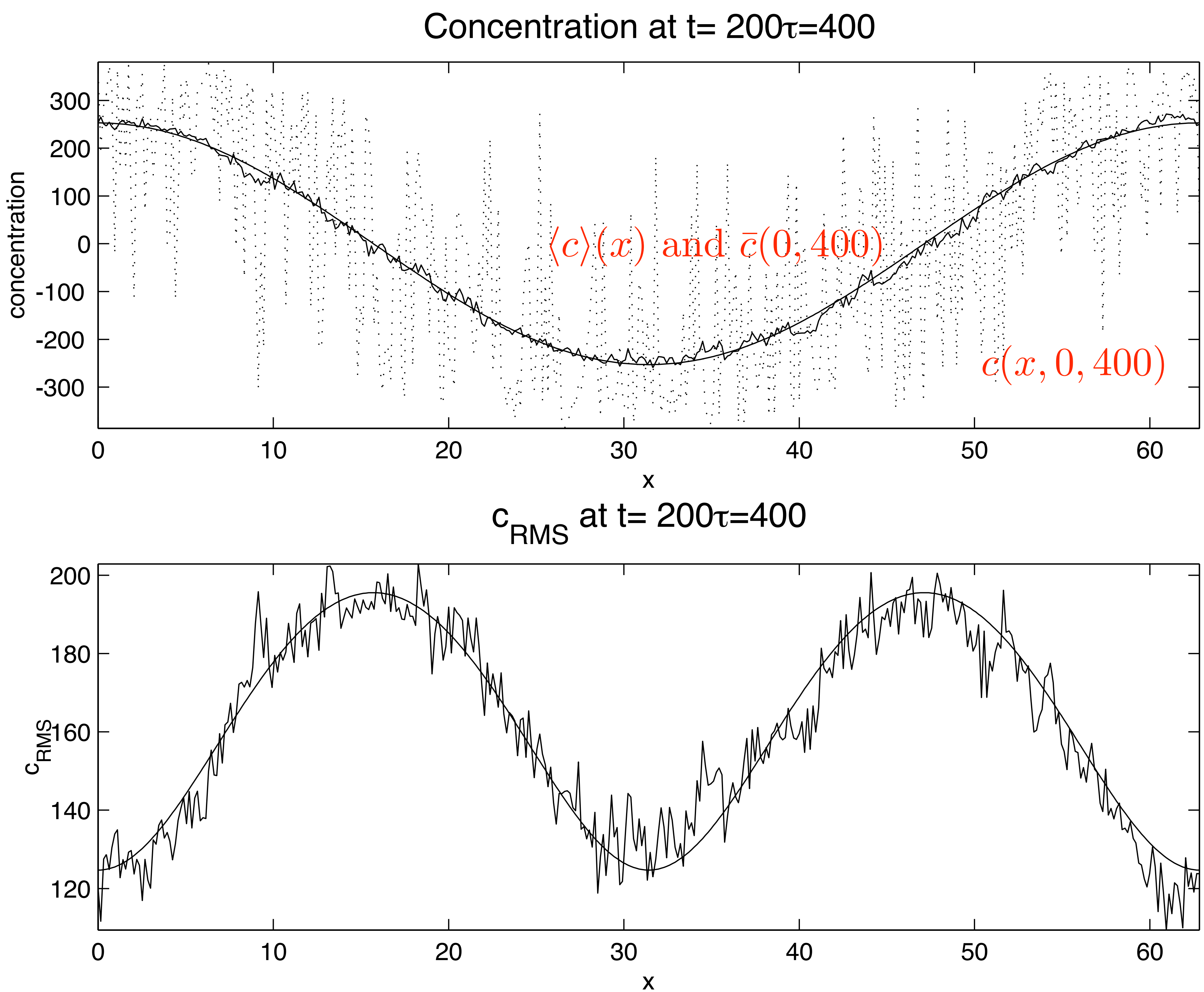
$$\langle c \rangle_t = \kappa_e \langle c \rangle_{xx} + \cos qx \quad \Rightarrow \quad \langle c \rangle(x, \infty) = \frac{\cos qx}{\kappa_e q^2}$$

☛ But the total solution is not statistically steady, because with kappa=0 there is no variance sink.

Runaway variance

$s = \cos\left(\frac{x}{10}\right)$

$Uk\tau = 2$



$$\mathcal{Z}_t - \kappa_e' \mathcal{Z}_{xx} = \kappa_e' |\nabla \langle c \rangle|^2 \quad \Rightarrow \quad \mathcal{Z} \propto \kappa_e q^2 t$$

The sink of c^2-stuff: the Batchelor spectrum

Small-scale variation of convected quantities like temperature in turbulent fluid

Part 1. General discussion and the case of small conductivity

By G. K. BATCHELOR
Cavendish Laboratory, University of Cambridge

JFM vol 5, 1959

$$\mathcal{Z}_t + \langle \boldsymbol{u}\rangle\cdot\boldsymbol{\nabla}\mathcal{Z} + \boldsymbol{\nabla}\cdot\left\langle \tfrac{1}{2}\boldsymbol{u}' c'^2\right\rangle - \kappa\nabla^2\mathcal{Z} = \kappa_e'|\boldsymbol{\nabla}\langle c\rangle|^2 - \kappa\langle|\boldsymbol{\nabla} c'|^2\rangle$$

SOURCE SINK

☛ If the Peclet number is large, then the SOURCE and the SINK are at very different scales.

Flux of c^2-stuff through wavenumber space

$$c_t + \boldsymbol{u}\cdot\boldsymbol{\nabla} c = s + \kappa \nabla^2 c$$

- ☛ Stirring increases gradients exponentially in time.
- ☛ But stirring conserves c^2-stuff.

$$\frac{1}{AT}\int_0^T \iint cs \,\mathrm{d}\boldsymbol{x}\mathrm{d}t = \underbrace{\frac{1}{AT}\int_0^T \iint \kappa |\boldsymbol{\nabla} c|^2 \,\mathrm{d}\boldsymbol{x}\mathrm{d}t}_{\equiv \chi}$$

- ☛ Advection generates new harmonics, and transfers c^2-stuff to larger wavenumbers.

$$c_{RMS}^2 = \frac{1}{AT}\int_0^T \iint c^2(\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{x}\mathrm{d}t = \int_0^\infty \Gamma(k)\,\mathrm{d}k$$

A dimensional argument

☛If stretching by the velocity field is characterized by a single time scale, then we can predict the spectrum with dimensional argument.

$$\Gamma(k) = \frac{\chi}{\gamma k}, \qquad \text{provided} \qquad q \ll k \ll \ell_B^{-1} = \sqrt{\frac{\gamma}{\kappa}}$$

☛In the renewing wave examples, gamma is the Lyapunov exponent

$$k = k_0 \mathrm{e}^{\gamma t}$$

☛B. argues that the the flux through wavenumber space is

$$(\gamma k \Gamma)_k = -\kappa k^2 \Gamma$$

The original problem was high Prandtl number turbulence $\frac{\nu}{\kappa} \gg 1$

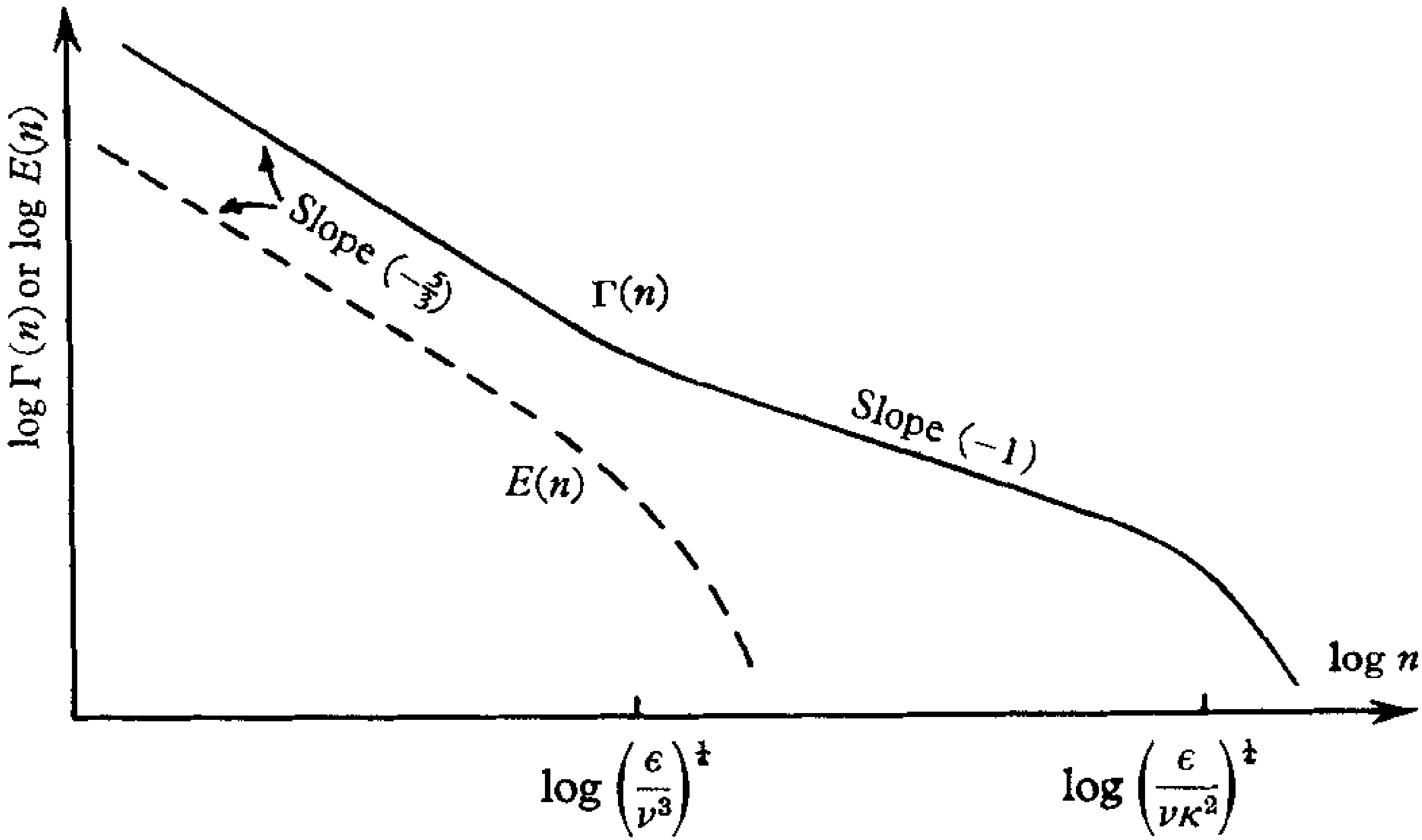


FIGURE 1. Spectra of θ and $\mathbf{u}$ in the equilibrium range of wave-numbers for the case $\nu \gg \kappa$.

☛ But B's argument applies to stirring by any "large-scale" flow.

Numerical simulation of the Batchelor spectrum

- Use the "XY renewal model":

$$\underbrace{[0\ \tau/2]\ [\tau/2\ \tau]}_{\text{The first epoch}}\ \underbrace{[\tau\ 3\tau/2]\ [3\tau/2\ 2\tau]}_{\text{The second epoch}}\ \text{etc.}$$

$$\text{First } (u,v) = (\cos(y+\phi_n), 0)\,,\ \text{and then } (u,v) = (0, \cos(x+\theta_n))$$

- Coerce the displacements onto a grid using shift operations on rows and cols of the c-matrix

Chaos, Vol. 10, No. 1, 2000 Lattice models of advection-diffusion 67

Pierrehumbert (2000)

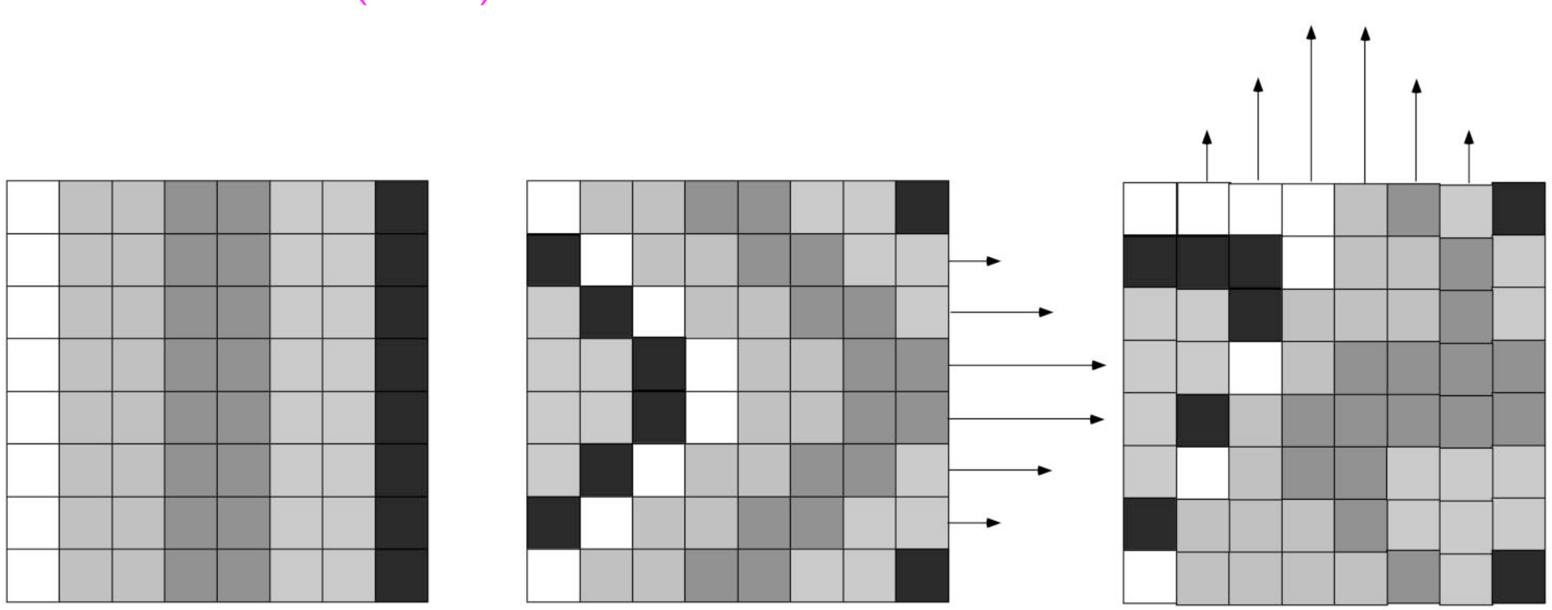


FIG. 2. Schematic of the advection step on a lattice, showing rearrangement by the composition of a shift operation in the x-direction followed by a shift operation in the y-direction.

Homework/Discussion

- ☛ How does

$$\delta_r c \equiv \text{avg}\left(\left|c(\boldsymbol{x}+\boldsymbol{r}) - c(\boldsymbol{x})\right|\right)$$

vary with separation, r, in the Batchelor range?

- ☛ Investigate

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

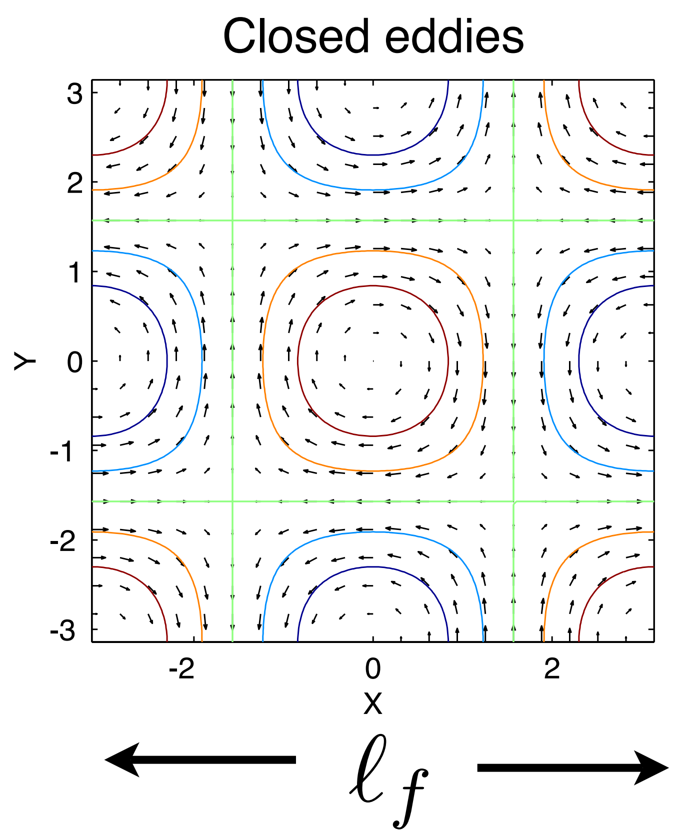
in the Batchelor range. For example, is the spectral slope changed? How about delta_r?

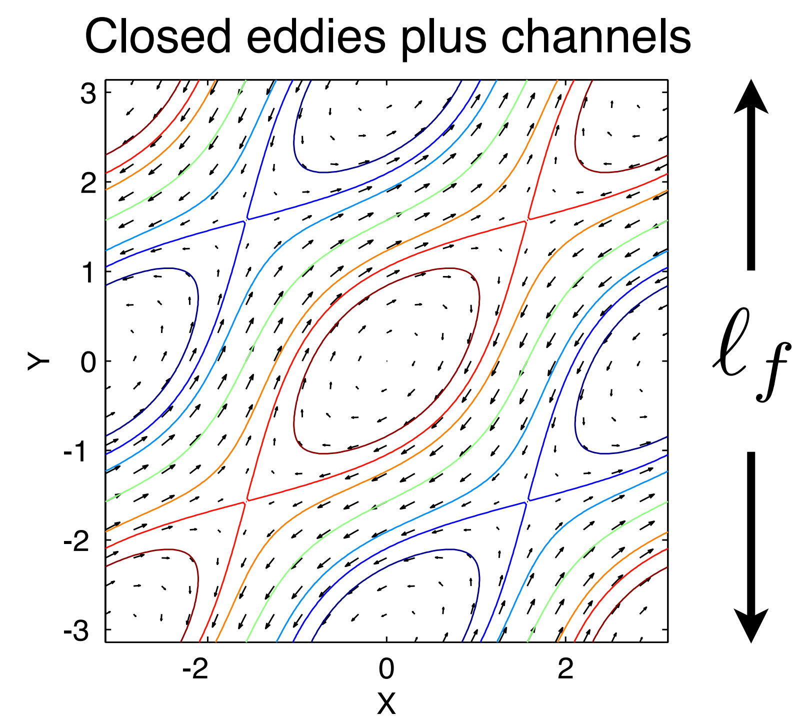
Homogenization: Cellular flows

Homogenization of cellular flows

$$(u, v) = (-\psi_y, \psi_x)$$

$$c_t + J(\psi, c) = \kappa \nabla^2 c$$





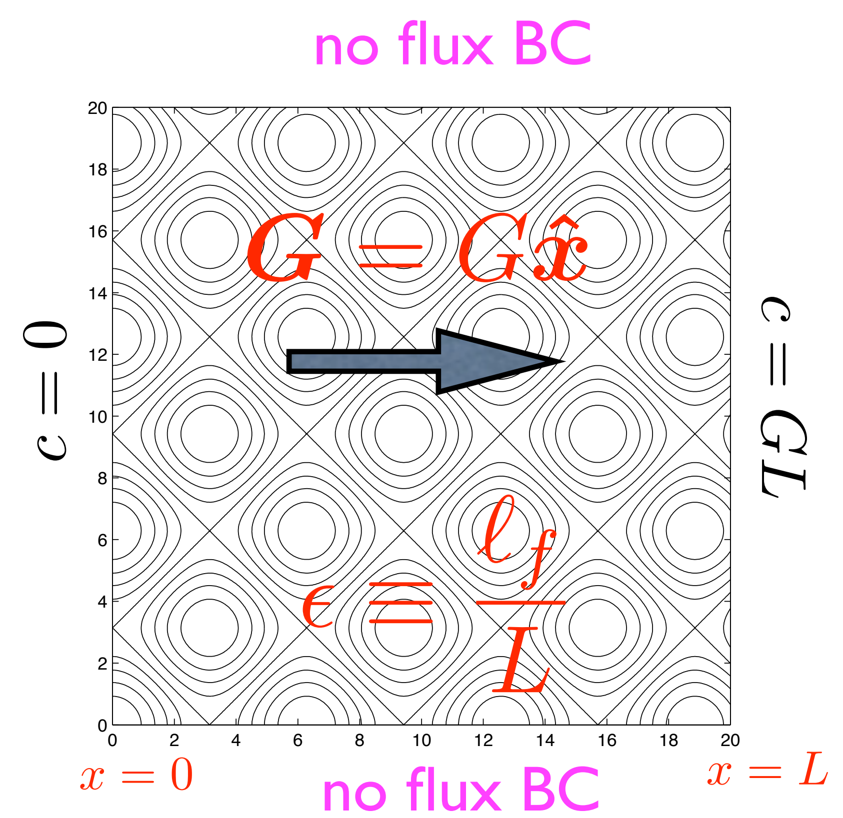
$$\langle \theta \rangle = \ell_f^{-2} \int_{\text{cell}} \theta(x, y)\, \mathrm{d}A$$

☛ Cellular flows provide simple examples of deterministic flows with "effective diffusivities".

The two-scale method

☛ $c(x,y) = \boldsymbol{G}\cdot\boldsymbol{x} + c'(x,y)$

$$\langle c' \rangle = 0$$



☛ The flux is $\boldsymbol{F} = -\kappa\boldsymbol{G} + \langle \boldsymbol{u}c' \rangle$

$$= -\boldsymbol{K}\boldsymbol{G}$$

☛ Linearity $c'(x,y) = -a(x,y)\,\boldsymbol{G}\cdot\hat{\boldsymbol{x}} - b(x,y)\,\boldsymbol{G}\cdot\hat{\boldsymbol{x}}$

The two-scale method (cont'd)

☛ The fundamental cell-problem is:

$$\mathcal{L} \equiv \boldsymbol{u}\cdot\boldsymbol{\nabla} - \kappa\nabla^2, \qquad \mathcal{L}\boldsymbol{a} = \boldsymbol{u}.$$

$$\begin{pmatrix} F_x \\ F_y \end{pmatrix} = -\begin{bmatrix} \kappa + \langle ua \rangle & \langle ub \rangle \\ \langle va \rangle & \kappa + \langle vb \rangle \end{bmatrix} \begin{pmatrix} G_x \\ G_y \end{pmatrix}$$

$$\boldsymbol{K}\left(\frac{\psi_{\max}}{\kappa}\right)$$

☛ The Peclet number is: $p \equiv \dfrac{\psi_{\max}}{\kappa}$

The large-scale evolution

☛ Once we possess the effective diffusion tensor, we dispense with Gx, and assert that:

$$\langle c \rangle_t = \boldsymbol{\nabla} \cdot \boldsymbol{K} \boldsymbol{\nabla} \langle c \rangle$$

☛ This approximation is valid provided that: $L \gg \ell_f$

☛ In fact, homogenization requires that:

$$\frac{L}{\ell_f} \gg p \equiv \frac{\psi_{\max}}{\kappa}$$

Example: $\psi(x,y) = \psi_{\mathrm{max}} \cos kx \cos ky$

(Roberts 1972, Childress 1979)

☛ The Gx cell problem is: $J(\psi, c') - \kappa \nabla^2 c' = G\psi_y$

☛ Symmetry arguments show the diffusion tensor has the form: $\boldsymbol{K} = \kappa_e \boldsymbol{I}$

☛ The small Peclet solution of the cell problem is:

$$c' \approx -\left[\frac{\psi_{\mathrm{max}}}{2k\kappa} \cos kx \sin ky\right] G$$

☛ The flux is then:

$$F \approx -\left[\kappa + \frac{\psi_{\mathrm{max}}^2}{8\kappa}\right] G\,.$$

Pade scenery: $\nabla^2 a = \sin x \cos y + pJ(\sin x \sin y, a)$

The beginning of the small Peclet number expansion is:

$$a_0 = -\frac{1}{2}\sin x \cos y, \qquad a_1 = -\frac{1}{16}\sin 2x, \qquad a_2 = -\frac{1}{16}a_0 - \frac{1}{160}\sin 3x \cos y,$$

and

$$a_3 = \frac{3}{640}\sin 2x - \frac{1}{2560}\sin 4x + \frac{1}{1280}\sin 2x \cos 2y - \frac{1}{6400}\sin 4x \cos 2y.$$

The corresponding expansion of the flux is: $\mathrm{Nu}(p) = 1 + 2q\left[1 - q + \frac{6}{5}q^2 - \frac{381}{250}q^3 + O(p^8)\right]$

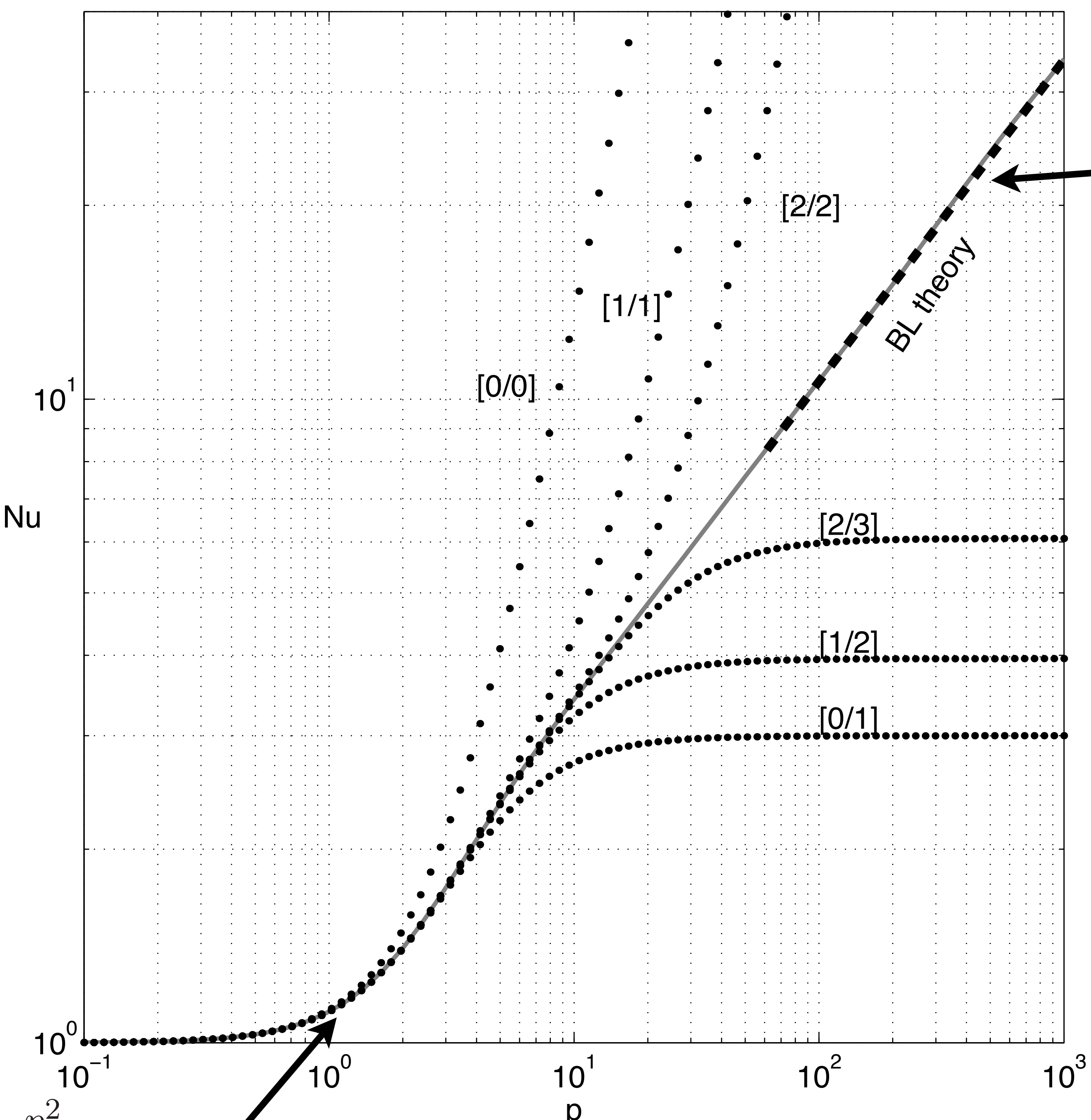
where $q \equiv \left(\frac{p}{4}\right)^2$

Now re-sum, for example $\frac{1}{1+q} = 1 - q + q^2 + \cdots$ suggests $\mathrm{Nu}(p) = 1 + 2q\left[\frac{1}{1+q}\right] + O(p^6)$.

To match ALL the terms we have the [1/2] Pade $\mathrm{Nu}(p) = 1 + 2q\left[\frac{50+31q}{50+81q+21q^2}\right] + O\left(p^{10}\right)$

Summary of the solution

$$\mathrm{Nu} \equiv \frac{F}{(-\kappa G)}$$

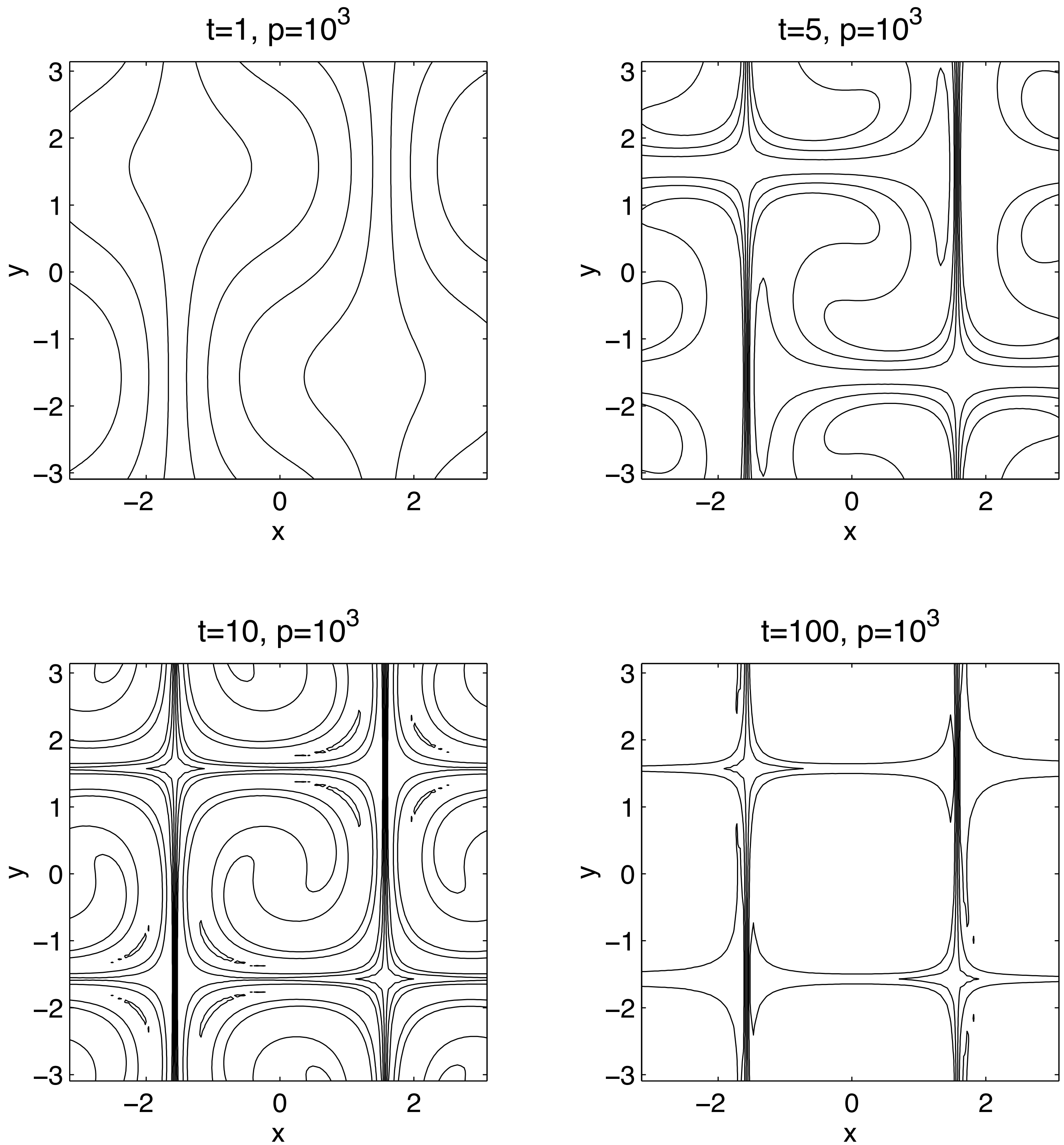


$$\mathrm{Nu} \sim 1.0655 p^{1/2}$$

$$p \equiv \frac{\psi_{\max}}{\kappa}$$

$$\mathrm{Nu} = 1 + \frac{p^2}{8} + O(p^4)$$

Evolution towards the steady-state cell solution large Peclet number



The large Peclet number limit $\kappa_e = 1.0655\sqrt{\psi_{\max}\kappa}$

(Soward 1987)

☛ The gradients are expelled to the cell boundaries (Prandtl-Batchelor).

☛ There is simple scaling for the boundary layers

$$-Xv'(Y)c_X + v(Y)c_Y = C_{XX}$$

with: $X = \dfrac{x}{\delta}$ $\qquad Y = ky \qquad \delta = \dfrac{1}{k}\sqrt{\dfrac{\kappa}{\psi_{\max}}} = \ell_f p^{-1/2}$

☛ The flux through the BLs is therefore $F \sim \kappa\dfrac{\Delta c}{\delta} = \sqrt{\kappa\psi_{\max}}G$

☛ There are problems realizing this large Peclet-number limit...

Now recall the diffusion tensor

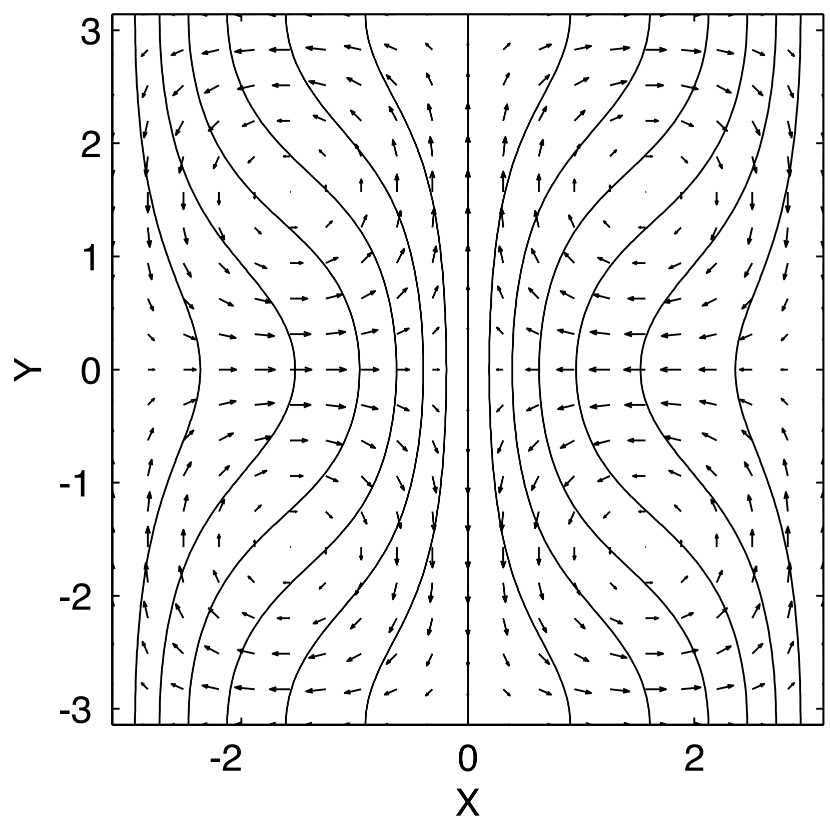
☛ The cell-problem is: $\mathcal{L} \equiv \boldsymbol{u}\cdot\boldsymbol{\nabla} - \kappa\nabla^2, \qquad \mathcal{L}\boldsymbol{a} = \boldsymbol{u}.$

☛ The diffusion tensor is: $\begin{pmatrix} F_x \\ F_y \end{pmatrix} = - \begin{bmatrix} \kappa + \langle ua \rangle & \langle ub \rangle \\ \langle va \rangle & \kappa + \langle vb \rangle \end{bmatrix} \begin{pmatrix} G_x \\ G_y \end{pmatrix}$

☛ For the Roberts cell, the diffusion tensor is simply $\boldsymbol{K} = \kappa_e \boldsymbol{I}$

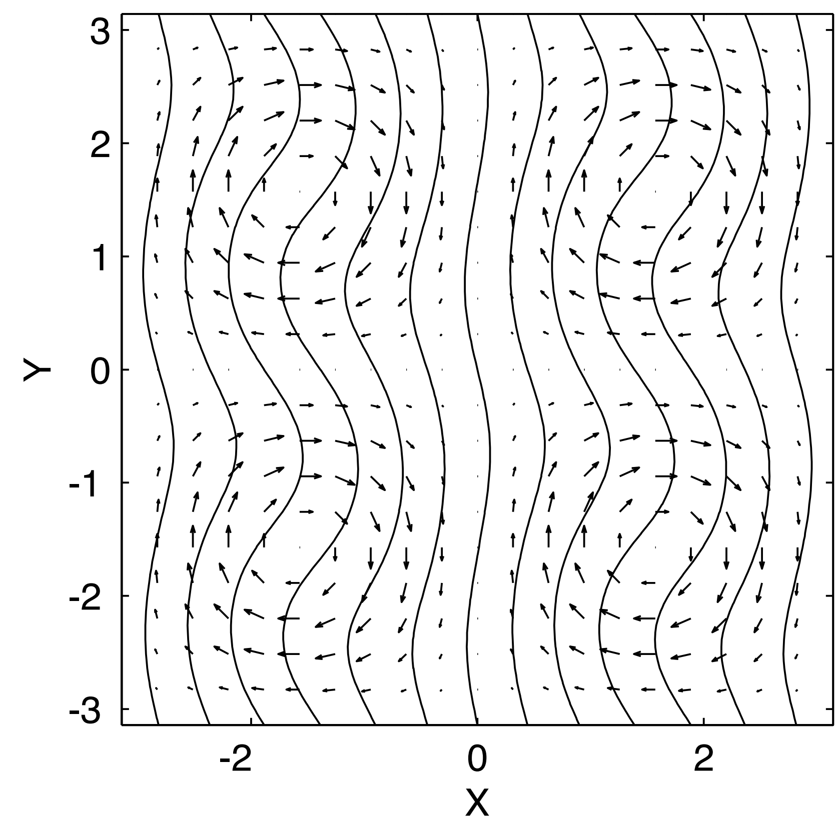
☛ But more complicated flows have more interesting tensors...

The anti-symmetric part



$$\psi = \sin x \sin y$$

$$\phi = 0$$



$$\psi = \sin^2 x \sin^2 y$$

$$\phi \neq 0$$

$p = 2$

(Moffatt 1983)

$$\boldsymbol{K} = \underbrace{\begin{pmatrix} \kappa_e & 0 \\ 0 & \kappa_e \end{pmatrix}}_{\boldsymbol{K}^{(s)}} + \underbrace{\begin{pmatrix} 0 & -\phi \\ \phi & 0 \end{pmatrix}}_{\boldsymbol{K}^{(a)}}$$

The anti-symmetric part is equivalent to advection

☛ A trivial identity

$$\langle c \rangle_t = \nabla \cdot \boldsymbol{K} \nabla \langle c \rangle$$

is equivalent to:

$$\langle c \rangle_t + \boldsymbol{u}_\phi \cdot \nabla \langle c \rangle = \nabla \cdot \boldsymbol{K}^{(s)} \nabla \langle c \rangle$$

where $\boldsymbol{u}_\phi \equiv (-\phi_y, \phi_x).$

☛ We need either BCs or large-scale modulation for this advective transport to be manifest e.g.,

$$\psi = \mathrm{e}^{\epsilon x} \sin^2 x \sin^2 y$$

Homework

- How does the diffusion tensor change if we flip the sign of the velocity?

$$\boldsymbol{u}^{\dagger} \equiv -\boldsymbol{u}.$$

- Hint: the flip generates adjoint differential operator:

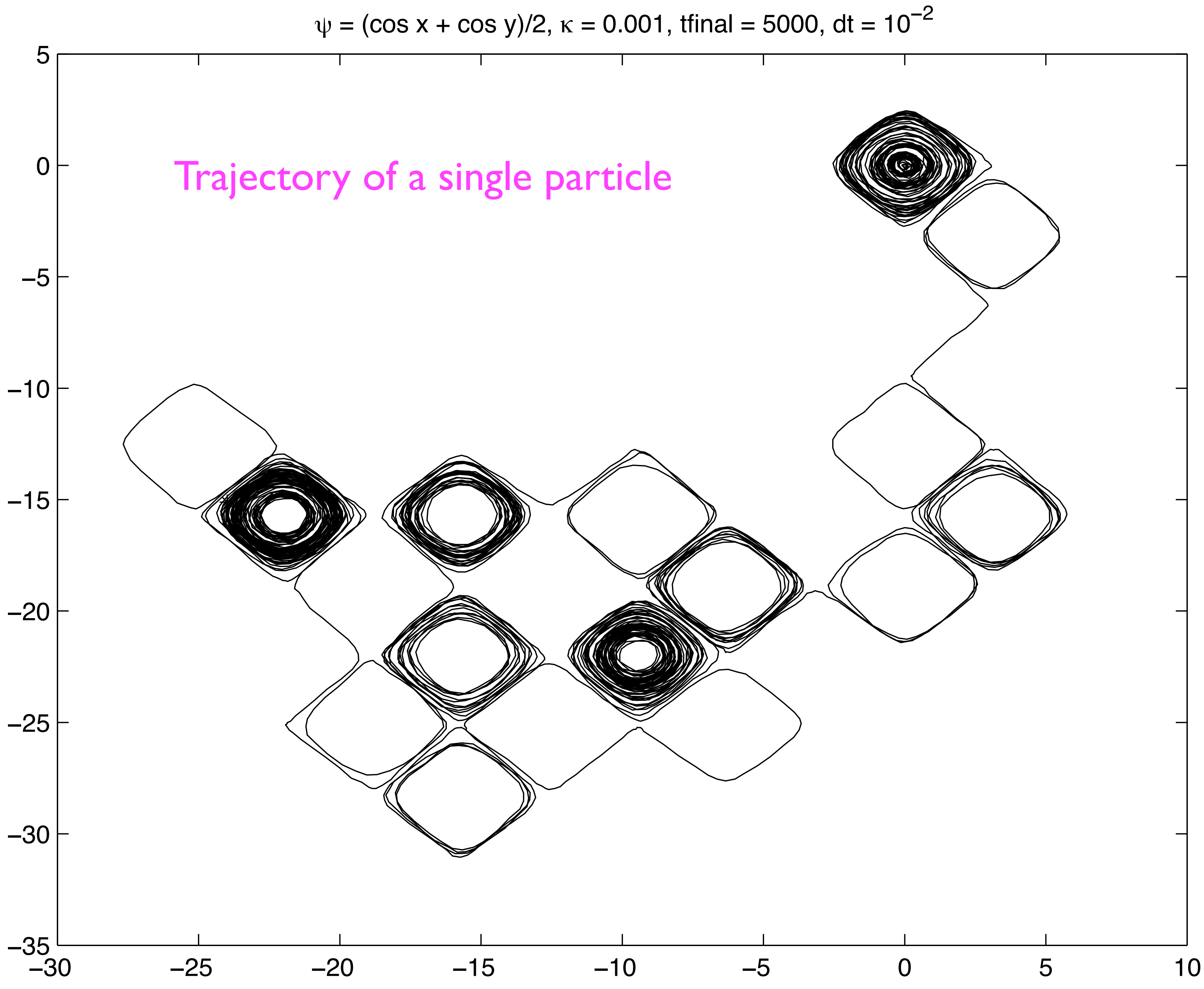
$$\mathcal{L} \equiv \boldsymbol{u}\cdot\boldsymbol{\nabla} - \kappa\nabla^2, \qquad \text{and} \qquad \mathcal{L}^{\dagger} \equiv -\boldsymbol{u}\cdot\boldsymbol{\nabla} - \kappa\nabla^2.$$

and the cell-average satisfies:

$$\langle \theta\mathcal{L}\phi\rangle = \langle \phi\mathcal{L}^{\dagger}\theta\rangle$$

The cellular flow example, with Monte Carlo

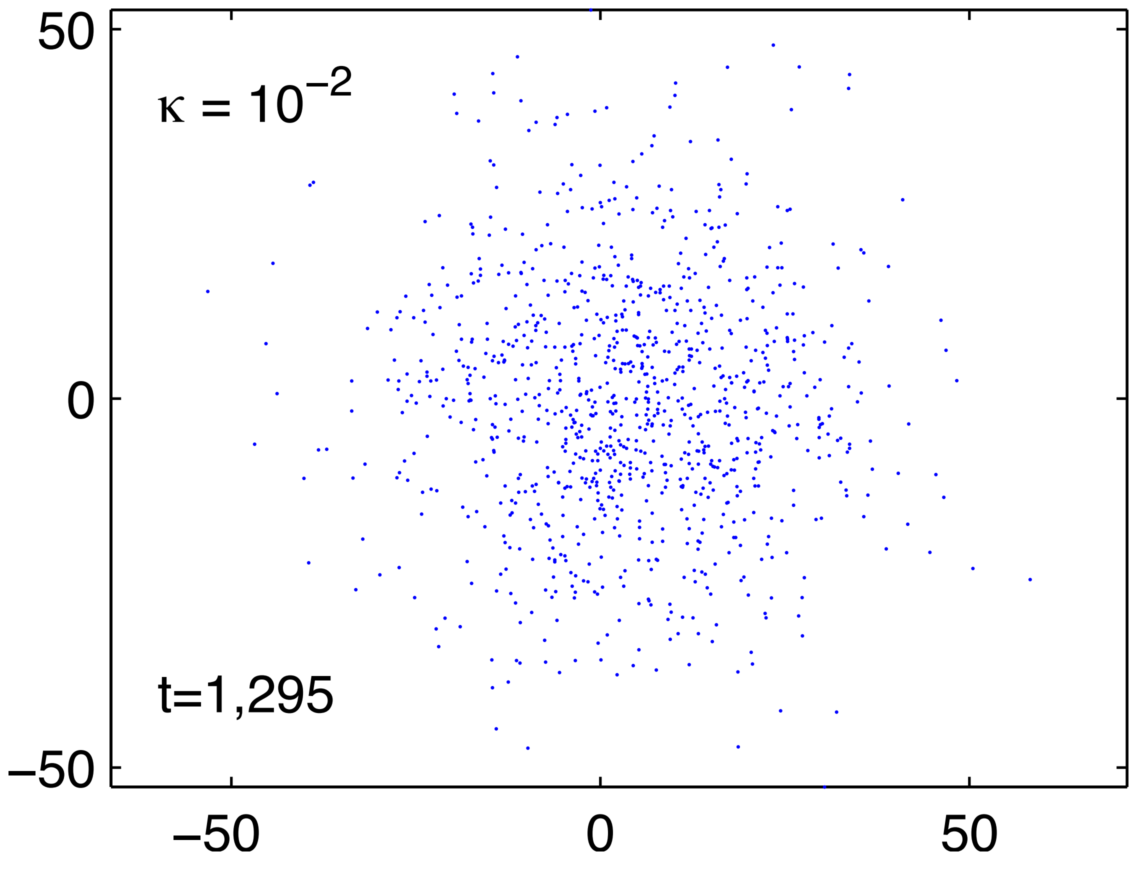
$$\boldsymbol{x}(t+\mathrm{d}t) = \boldsymbol{x}(t) + \boldsymbol{u}(\boldsymbol{x}(t),t)\mathrm{d}t + \sqrt{2\kappa\,\mathrm{d}t}\boldsymbol{N}$$

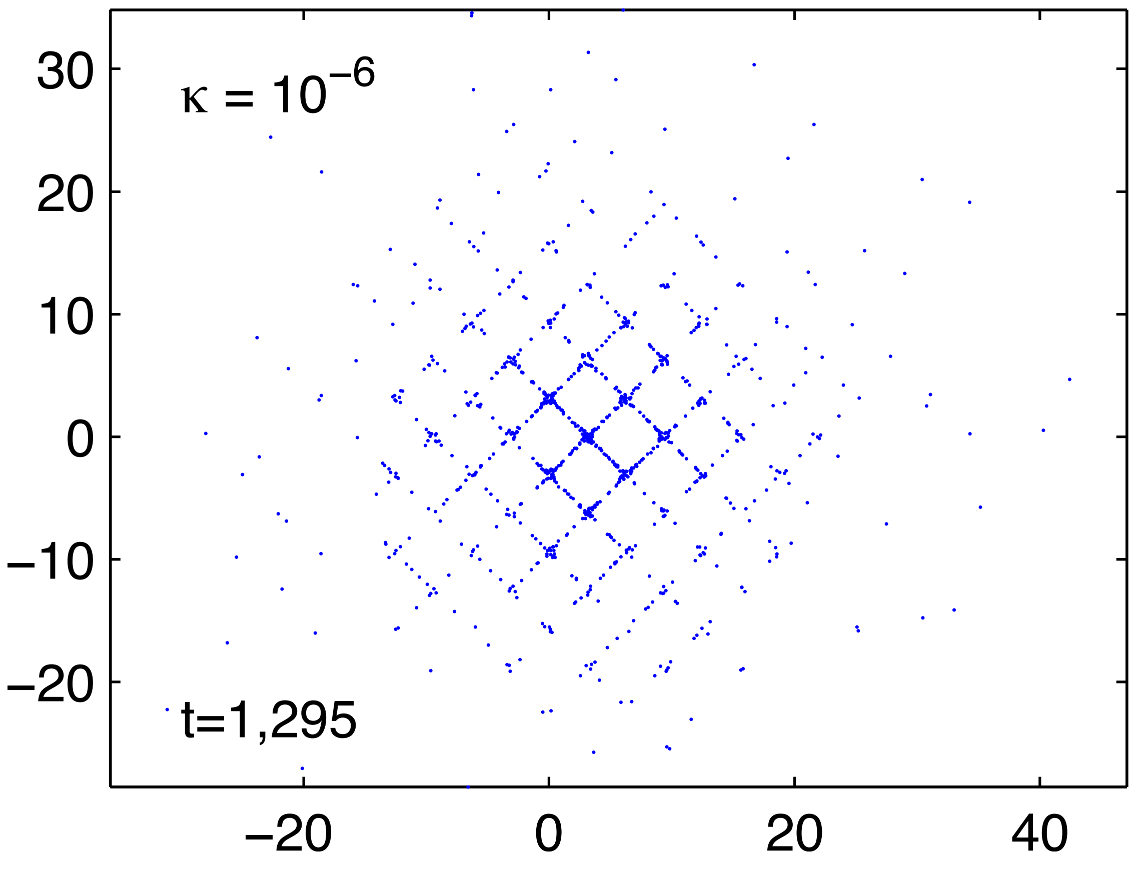


☛ Small diffusion enables motion along the separatrices.

☛ But the particle can also get trapped.

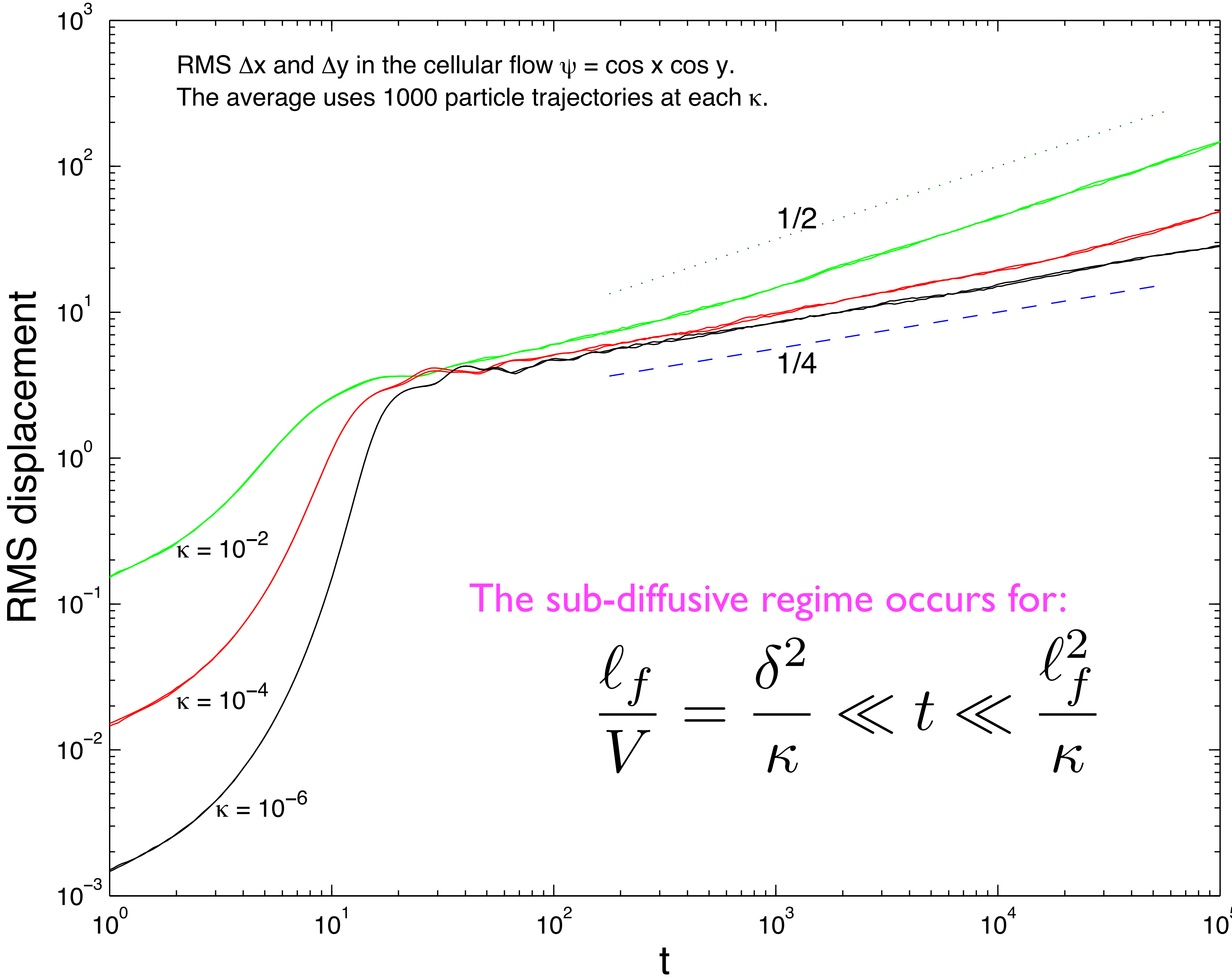
Limitations of homogenization





- ☛ Positions of 10^4 particles (all released at a hyperbolic point).
- ☛ Homogenization requires: $t \gg \dfrac{\ell_f^2}{\kappa}, \qquad \left(\ell_f = \dfrac{1}{k}\right)$

Pre-asymptotic subdiffusion



The sub-diffusive regime occurs for:

$$\frac{\ell_f}{V} = \frac{\delta^2}{\kappa} \ll t \ll \frac{\ell_f^2}{\kappa}$$

$$\ell_f = \frac{1}{k}$$

$$\psi_{\max} = V\ell_f$$

The exponent 1/4

☛ We argue that: $\langle x^2 \rangle \sim V\ell_f \times \dfrac{\delta}{\sqrt{\kappa t}} \times t = V^{1/2}\ell_f^{3/2} t^{1/2}$

The fraction of "active" particles.

☛ There is a cross-over to normal diffusion once: $t \geq \dfrac{\ell_f^2}{\kappa}$

☛ At the cross-over time: $\langle x^2 \rangle \sim \kappa^{-1/2} V^{1/2} \ell_f^{5/2}$

☛ To use the effective diffusivity, the domain must be large enough:

$$L \gg \ell_f^{5/4} V^{1/4} \kappa^{-1/4} = \ell_f p^{1/4}$$