Dispersion in the large-deviation regime

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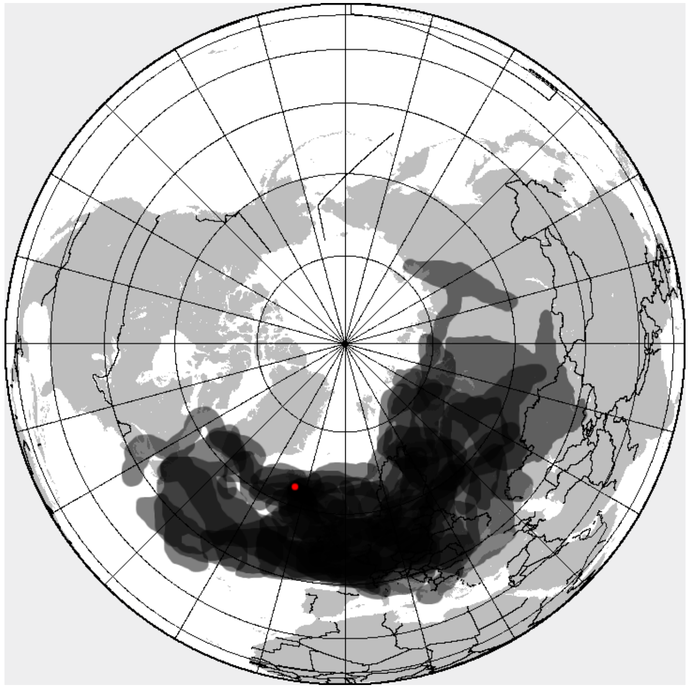
Dispersion

Passive scalar released in a flow: a classical problem with numerous industrial and environmental applications.



Concentration $C(\mathbf{x}, t)$ satisfies the advection-diffusion equation $\partial_t C + \mathbf{u}.\nabla C = \kappa \nabla^2 C$ with given velocity field $\mathbf{u}(\mathbf{x}, t)$ obeying constraint $\nabla.\mathbf{u} = 0$.

Dispersion

With the initial condition $C(\mathbf{x},0)=\delta(\mathbf{x})$, $C(\mathbf{x},t)$ is the pdf of the position of a particle at position $\mathbf{X}$ moving according to

$$d\mathbf{X}=\mathbf{u}(\mathbf{X},t)+\sqrt{2\kappa}\,d\mathbf{W}$$

where $d\mathbf{W}$ is white noise.

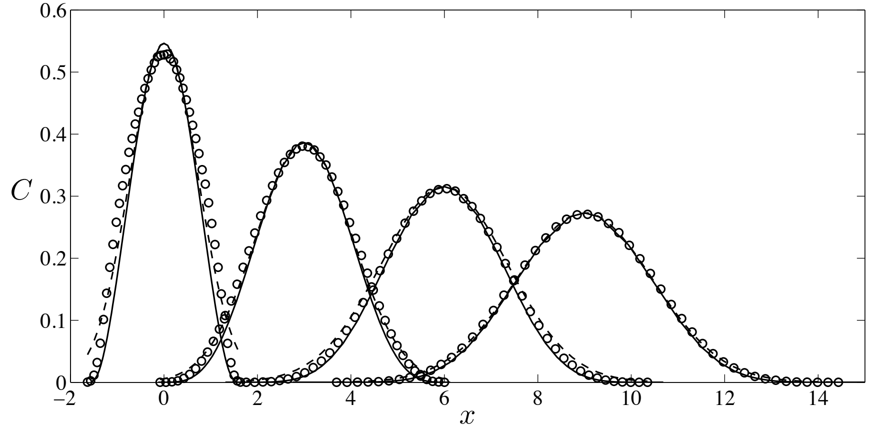
For large times the combined effect of advection and diffusion can often be modelled by *effective diffusivity* κ_{eff}

- $\langle X^2\rangle \sim 2\kappa_{\mathrm{eff}}t$.
- $C \asymp \exp(-x^2/4\kappa_{\mathrm{eff}}t)$: Gaussian distribution

In simple flows κ_{eff} can be calculated explicitly.

Dispersion: Shear Flows

Dye released in a pipe flow spreads along the pipe



Taylor (1953) showed that the dispersion is diffusive, with

$$\kappa_{\text{eff}} \propto \kappa^{-1}$$

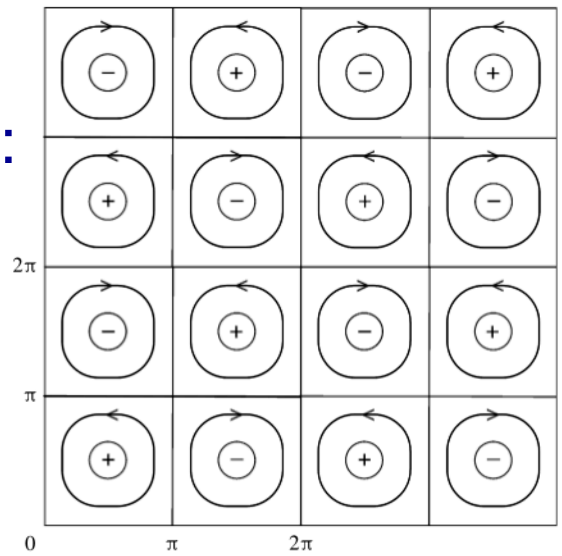
Physically: sampling of velocity profile $U(y)$ with correlation time $\propto \kappa^{-1}$

Several techniques provide κ_{eff} : e.g. homogenisation

$$C(x,y,t) = C_0(\epsilon x, \epsilon^2 t) + \epsilon C_1(\epsilon x, y, \epsilon^2 t) + \ldots$$

Dispersion: Cellular Flows

κ_{eff} can be computed for cellular flows: spatially periodic, time-independent flows.



Simplest example: $\psi = \sin x \, \sin y$

Use homogenisation $C = C_0(\epsilon^2 t, \epsilon \mathbf{x}) + \epsilon C_1(\epsilon^2 t, \epsilon \mathbf{x}, \mathbf{x}) + \ldots$

- C_0 varies on the large scale $\epsilon \mathbf{x}$ only .
- C_1 solves a linear 'cell problem' – a 2D elliptic equation.
- κ_{eff} is deduced from the cell-problem solution.

Main result: (Shraiman, Rosenbluth et al, Childress, Soward, …) for $\kappa \ll 1$ (large Pe), boundary-layer analysis yields $\kappa_{\mathrm{eff}} = 2\nu\kappa^{1/2}$, $\nu = 0.532740705\ldots$.

Large deviations:

Gaussian approximation (and homogenisation) are restricted to $|\mathbf{x}|/t^{1/2} \sim O(1)$ as $t \to \infty$.
More generally $C(\mathbf{x}, t)$ has the large-deviation form

$$\boxed{C(\mathbf{x}, t) \asymp \exp[-tg(\mathbf{x}/t)]}$$

where $g(.)$ is the *rate function* or *Cramer function*.
This holds for $|\mathbf{x}|/t \sim O(1)$ as $t \to \infty$.

(The Gaussian approximation typically fails to predict the tails of the distribution. Information on the tails is provided by $g(.)$.)

Large deviations: this talk

- general approach to compute $g(.)$.
- explicit form of $g(.)$ for cellular flows for $\kappa \ll 1$.

Motivation

- Small concentrations are important: e.g. highly toxic chemicals,
- Unification of previous 'improvements' to homogenisation for Taylor dispersion (Mercer & Roberts, Young & Jones),
- Novel application of extreme-event statistics.

(For application to chemical reactions see Tzella talk.)

Large deviations: analysis

Start with the advection-diffusion equation
$\partial_t C + Pe\,\mathbf{u}.\nabla C = \nabla^2 C$ with $Pe = UL/\kappa$.

Introduce $C(\mathbf{x},t) \sim \phi(\mathbf{x},t)\exp[-tg(\boldsymbol{\xi})]$, with $\boldsymbol{\xi} = \mathbf{x}/t$ and neglect $O(1/t)$ terms to obtain

$$(\boldsymbol{\xi}.\nabla_{\boldsymbol{\xi}} g - g)\phi = \nabla^2\phi - (Pe\,\mathbf{u} + 2\nabla_{\boldsymbol{\xi}}).\nabla\phi + (Pe\,\boldsymbol{u}.\nabla_{\boldsymbol{\xi}} g + |\nabla_{\boldsymbol{\xi}}|^2)\phi$$

Let $\mathbf{q} = \nabla_{\boldsymbol{\xi}} g$ and $f(\mathbf{q}) = \mathbf{q}.\boldsymbol{\xi} - g(\boldsymbol{\xi})$ to give

$$\boxed{\nabla^2\phi - (Pe\,\mathbf{u} + 2\mathbf{q}).\nabla\phi + (Pe\,\mathbf{u}.\mathbf{q} + |\mathbf{q}|^2)\phi = f(\mathbf{q})\phi}$$

Eigenvalue problem: solve to find $f(\mathbf{q})$ for a range of $\mathbf{q}$.
Deduce $g(.)$ by Legendre transform.

Large deviations:

- Interpretation of $f(\mathbf{q})$: cumulant generating function

$$\langle e^{\mathbf{q}.\mathbf{X}} \rangle \asymp e^{tf(\mathbf{q})}$$

(Gartner-Ellis theorem). $f(\mathbf{q})$ can be estimated directly by Monte Carlo (with pruning/cloning importance sampling).

- Small- $|\mathbf{q}|$ limit: $f(\mathbf{q}) = \frac{1}{2}\mathbf{q}.H_f.\mathbf{q} + O(|\mathbf{q}|^3)$

$$g(\boldsymbol{\xi}) \sim \tfrac{1}{2}\boldsymbol{\xi}.H_f^{-1}.\boldsymbol{\xi}$$

corresponding to the effective diffusivity $\kappa_{\mathrm{eff}} = H_f/2$

- Cell problem of homogenisation is recovered when solving the eigenvalue for $f(\mathbf{q})$ in the limit $\mathbf{q} \to 0$.

Shear flows

In shear flow $\mathbf{u} = (U(y), 0)$, $-1 \leq y \leq 1$ 1-D eigenvalue problem with form for $Pe \gg 1$

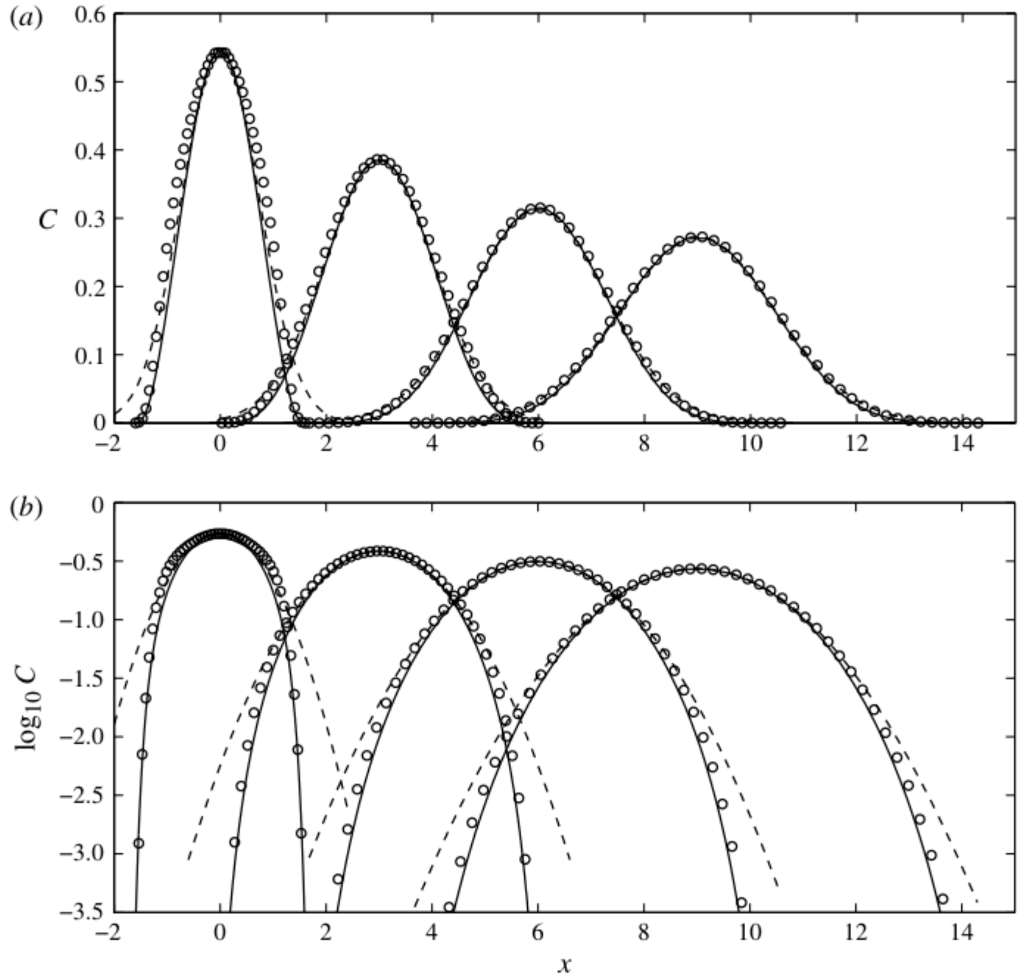
$$\phi'' + qU(y)\phi = f(q)\phi \;,\; \phi'(\pm 1) = 0 \;.$$

- solve numerically
- for $|q| \ll 1$, recover Taylor dispersion
- for $|q| \gg 1$, $f(q) \sim U_{\pm} q$, equivalently $g(\xi) \to \infty$ as $\xi = x/t \to U_{\pm}$

Shear flows

Plane Couette Flow

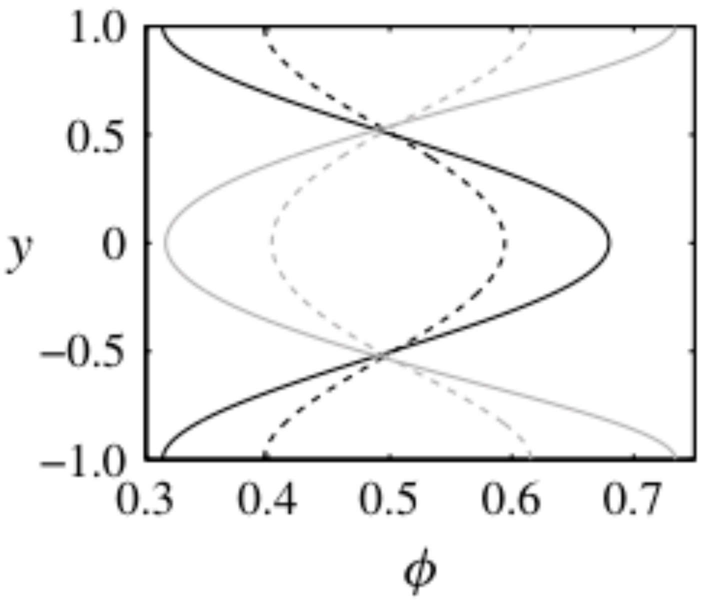
(comparison of diffusive approximation, large deviation prediction and Monte Carlo)



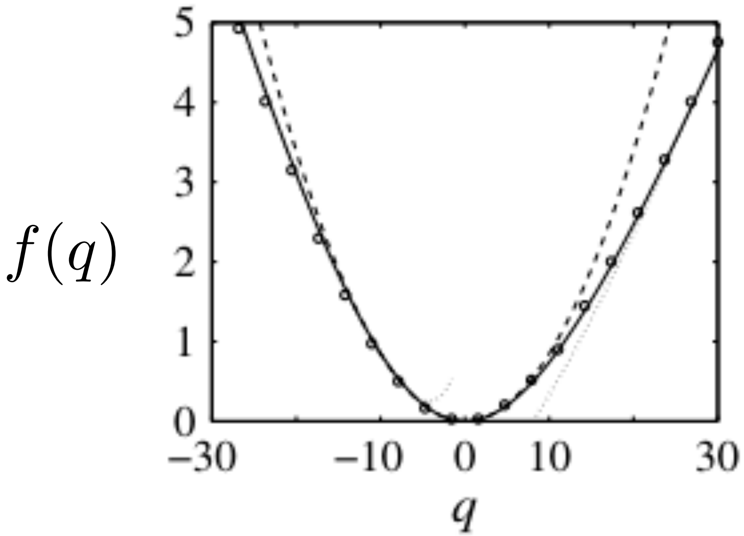
Shear flows

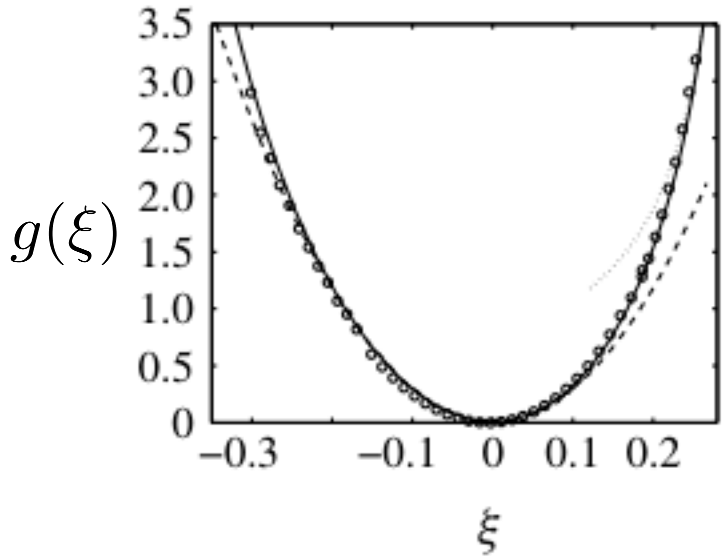
Plane Poiseuille flow

$$U(y) = \tfrac{1}{3} - y^2$$



$$q = -10, -5, 5, 10$$



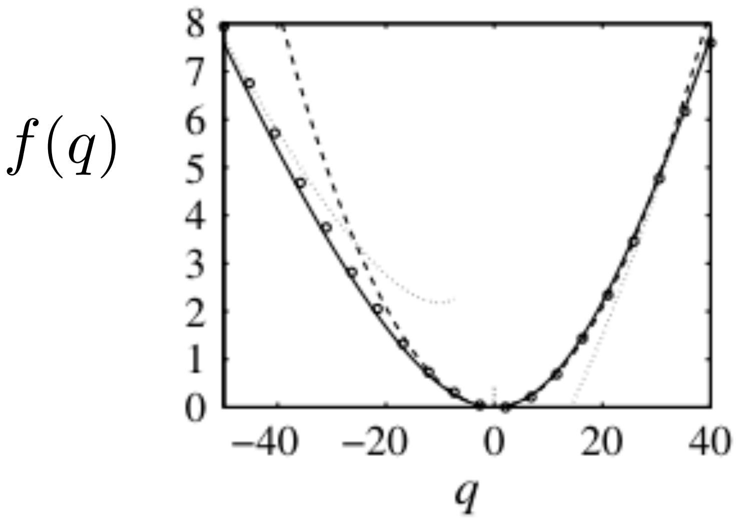


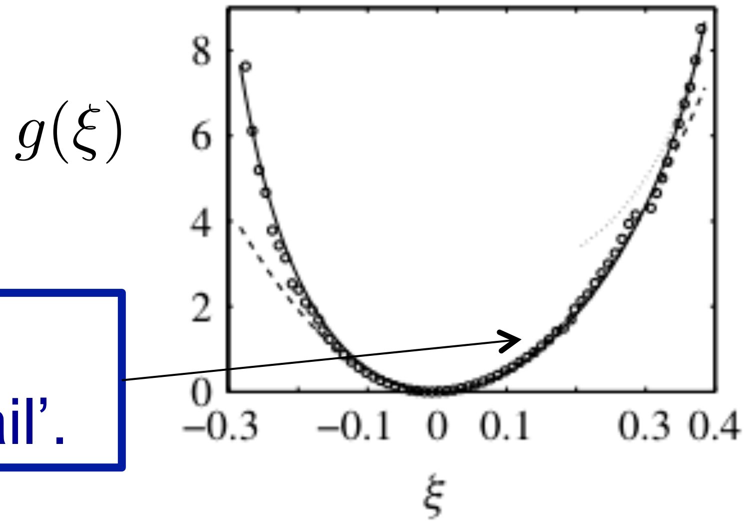
Monte Carlo requires importance sampling (e.g. Vanneste 2010)

Shear flows

Pipe Poiseuille flow

$$U(r) = \tfrac{1}{2} - r^2$$





Gaussian solution underpredicts 'near tail'.

Cellular flow

Consider the flow $\psi = \sin x \sin y$ for arbitrary Pe including $Pe \gg 1$.

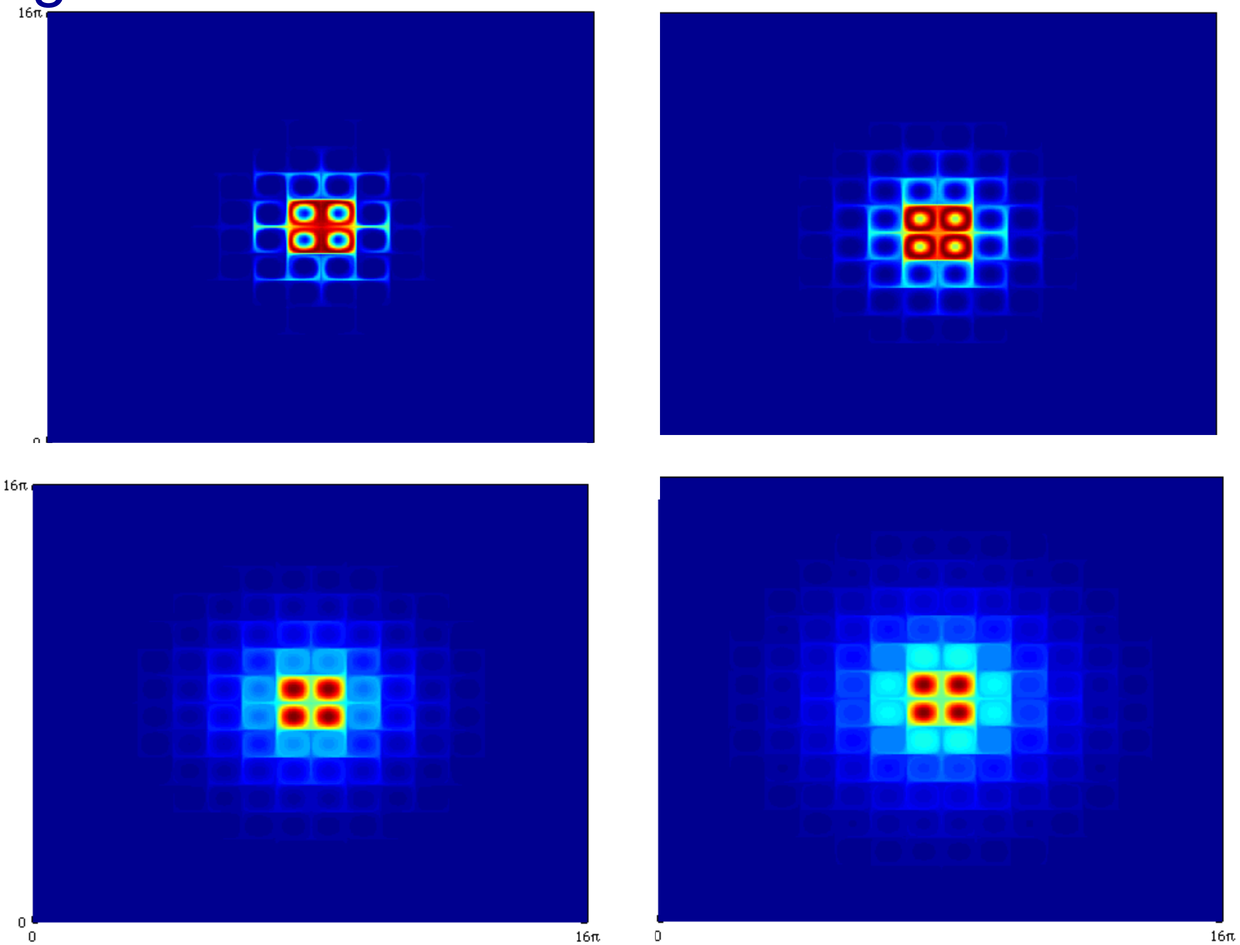
$t = 0.5$

$t = 1$

$\boxed{Pe = 10^3}$

$t = 3$

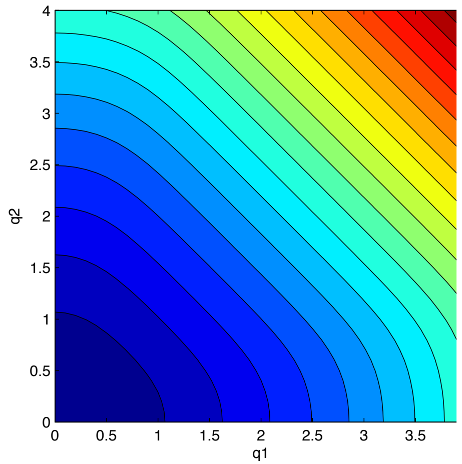
$t = 5$

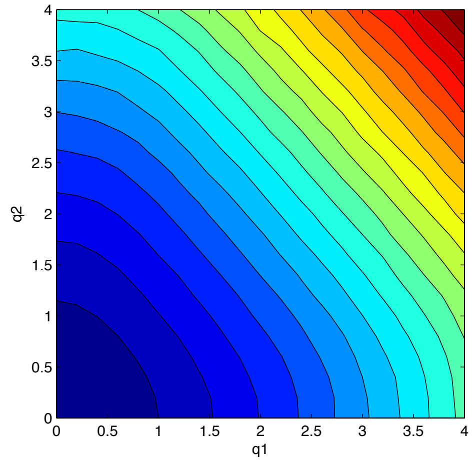


[movie]

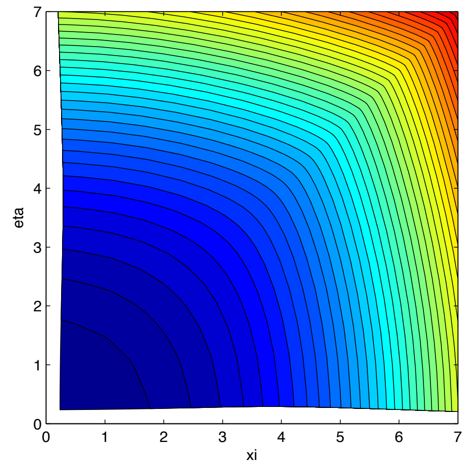
Cellular flow $Pe = 1$

Numerical solution of eigenvalue problem vs
Monte Carlo estimation of $f(\mathbf{q})$





$g(\boldsymbol{\xi})$

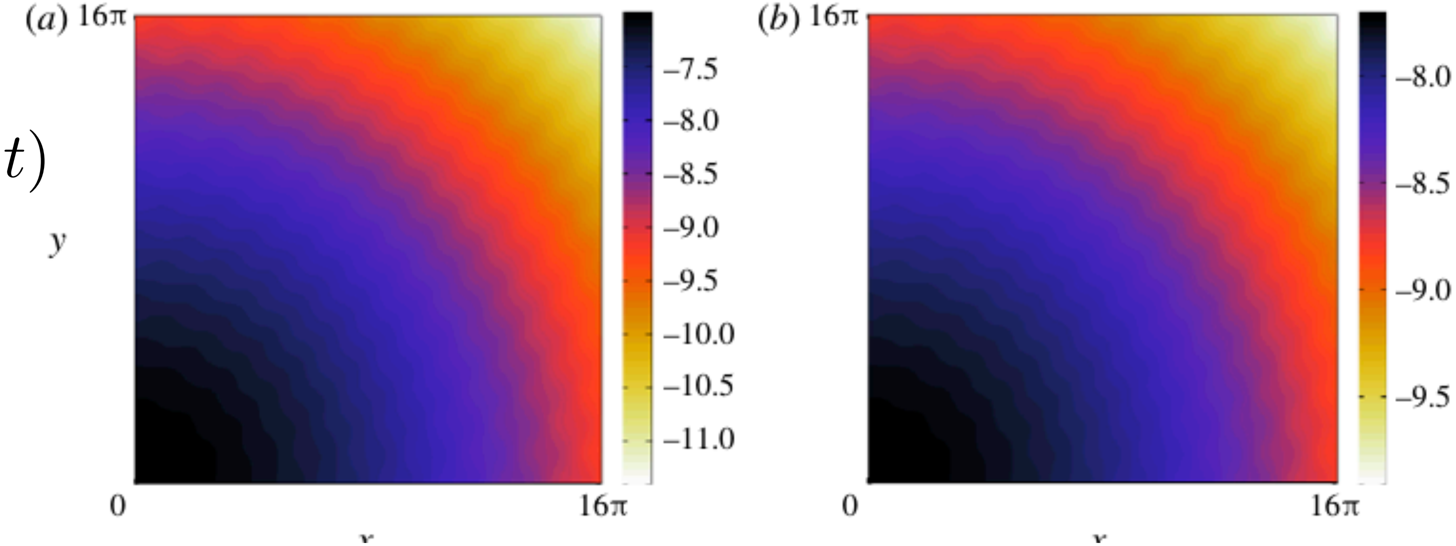


No axisymmetry for $\mathbf{q} = O(1)$.
Faster transport along diagonal.

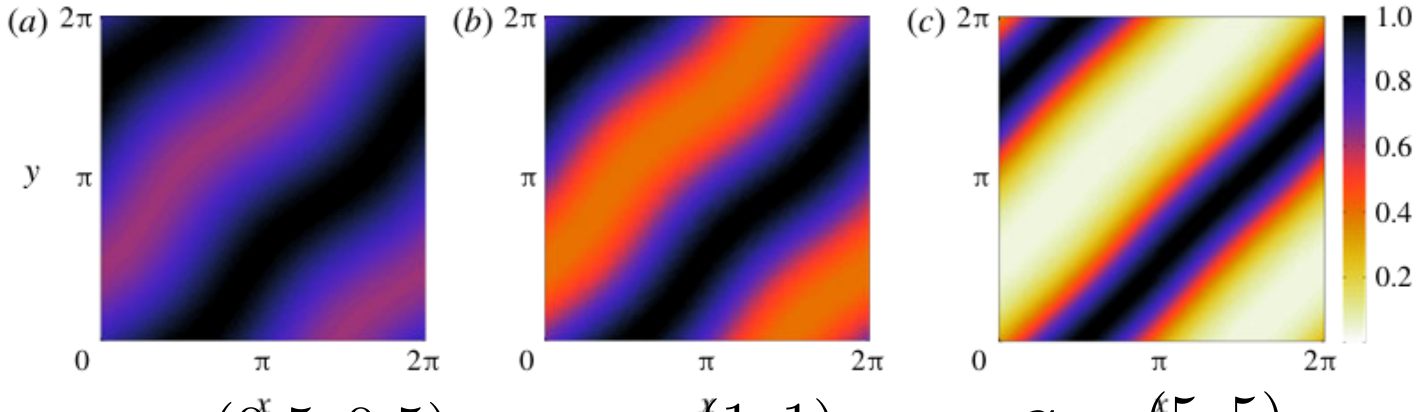
Cellular flow $Pe = 1$

$t = 250$ $\quad$ $t = 500$

$\log \chi(\mathbf{x}, t)$



$\phi(\mathbf{x}; \mathbf{q})$



$\mathbf{q} = (0.5, 0.5)$ $\quad$ $\mathbf{q} = (1, 1)$ $\quad$ $\mathbf{q} = (5, 5)$

Cellular flow: $Pe \gg 1$

Solve eigenvalue problem asymptotically:
non uniformity in $\mathbf{q}$ with 3 regimes.

1. $|\mathbf{q}| = O(Pe^{-1/4})$: non-trivial concentration field in cell interior + matching across boundary layers.

   $$f(\mathbf{q}) = F(Pe^{1/2}|\mathbf{q}^2|)$$

2. $|\mathbf{q}| = O(1)$: concentration confined to boundary layers with corner interactions crucial.

   $$f(\mathbf{q}) = O(Pe/\log Pe)$$

3. $|\mathbf{q}| = O(Pe)$: see Tzella and Vanneste. $f(\mathbf{q}) = O(Pe^2)$

Cellular flow: 1. $|\mathbf{q}| = O(Pe^{-1/4})$, $|\boldsymbol{\xi}| = O(Pe^{1/4})$

•Cell interior: average eigenvalue equation along streamlines,
$$\frac{d}{d\psi}(a(\psi)\frac{d\phi}{d\psi}) = f(\mathbf{q})b(\psi)\phi$$

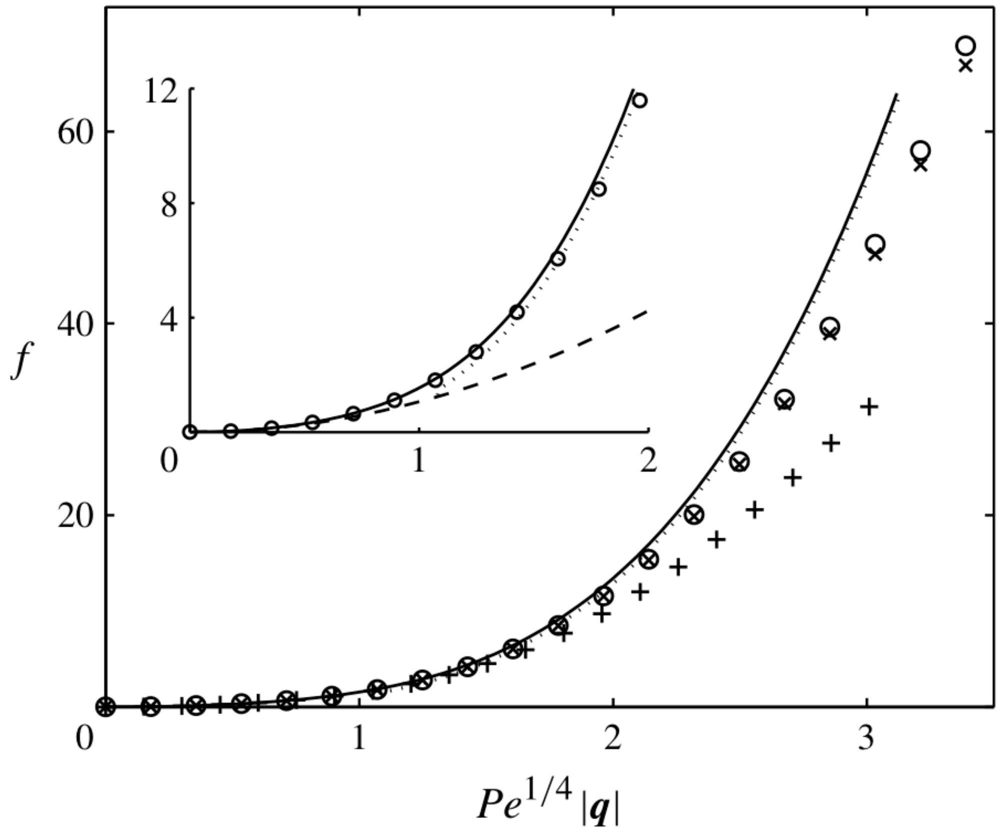
which determines ϕ'/ϕ on separatrices in terms of $f(\mathbf{q})$.

•Boundary layers: Soward (1987) W-H solution of Childress (1979) problem gives $\phi'/\phi = -\pi^2\nu Pe^{1/2}|\mathbf{q}|^2/4$.

•Combining two gives $f(\mathbf{q}) = F(Pe^{1/4}|\mathbf{q}|)$.

•Recover homogenisation for $Pe^{1/4}|\mathbf{q}| \ll 1$.

Cellular flow: 1. $|\mathbf{q}| = O(Pe^{-1/4}), |\boldsymbol{\xi}| = O(Pe^{1/4})$



$Pe = 500$ +

$Pe = 5000$ x o

Cellular flow: 2. $|\mathbf{q}| = O(1)$, $|\boldsymbol{\xi}| = O(Pe/\log Pe)$

- $\phi = 0$ in cell interior
- ϕ satisfies heat equation in boundary layer
- use Childress (1979) coordinates

$$\zeta = \mp Pe^{1/2}\psi \,, \quad \sigma = \int_0^l |\nabla\psi|\, dl \quad \text{(corners at } \sigma = 0, 2, 4, 6\text{)}.$$

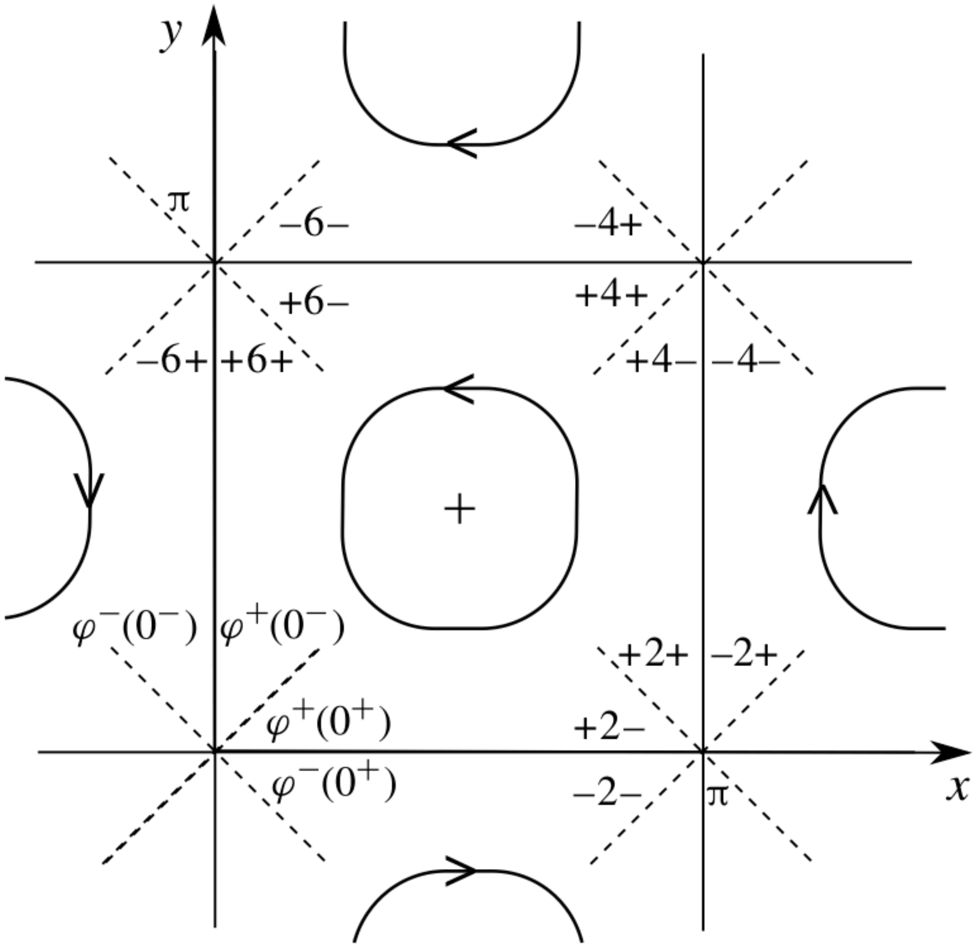
$$\partial^2_{\zeta\zeta}\phi - \partial_\sigma\phi + \frac{\mathbf{u}.\mathbf{q}}{|\mathbf{u}|^2}\phi = \frac{\mathfrak{f}}{|\mathbf{u}|^2}\phi \quad \text{(with } f = Pe\,\mathfrak{f}\text{)}.$$

- $\phi = e^{\mathbf{q}.\mathbf{x}+\mathfrak{f}H(\sigma)}\varphi$ gives $\partial^2_{\zeta\zeta}\varphi - \partial_\sigma\varphi = 0$.

- analysis of corner regions, for $k = 0, 2, 4, 6$,

$$\lim_{\sigma\to k^+}\varphi(\sigma,\zeta) = (16Pe)^{-\mathfrak{f}/2}\zeta^{\mathfrak{f}}\lim_{\sigma\to k^-}\varphi(\sigma,\zeta) \;.$$

Cellular flow: 2. $|\mathbf{q}| = O(1)$, $|\boldsymbol{\xi}| = O(Pe/\log Pe)$



Eigenvalue problem

$$(16Pe)^{\mathfrak{f}/2}\boldsymbol{\varphi} = \mathcal{L}(\mathbf{q},\mathfrak{f})\boldsymbol{\varphi}$$

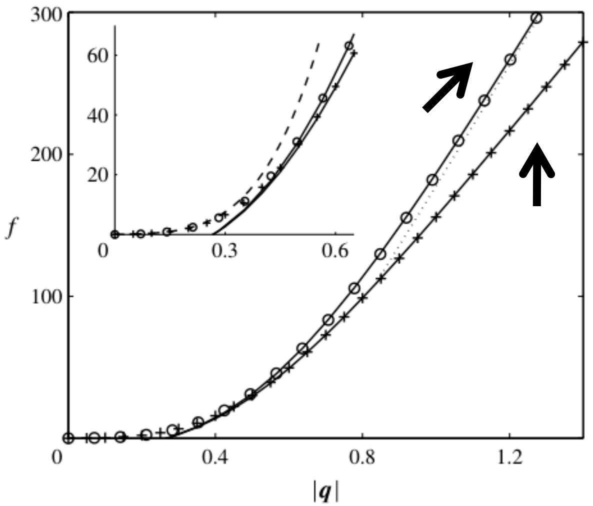
$\mathcal{L}(\mathbf{q},\mathfrak{f})$ is 8x8 matrix of linear integral operators with principal eigenvalue $\mu(\mathbf{q},\mathfrak{f})$.

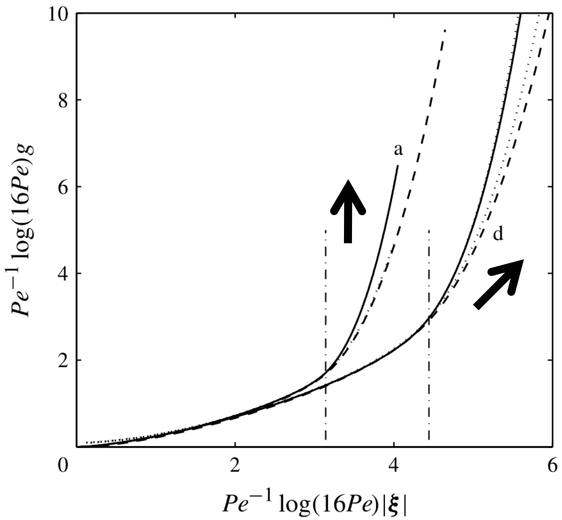
Cellular flow: 2. $|\mathbf{q}| = O(1)$, $|\boldsymbol{\xi}| = O(Pe/\log Pe)$

- Heuristic solution $f(\mathbf{q}) = Pe\mathfrak{f}(\mathbf{q}) \sim \dfrac{2Pe}{\log(16Pe)} \log \mu(\mathbf{q}, 0)$.

- For $|\mathbf{q}| \gg 1$, $f \sim \dfrac{\pi Pe}{\log(16Pe)}(|q_1| + |q_2|)$ corresponding to discrete-time random walk on lattice of stagnation points.

$f(\mathbf{q})$



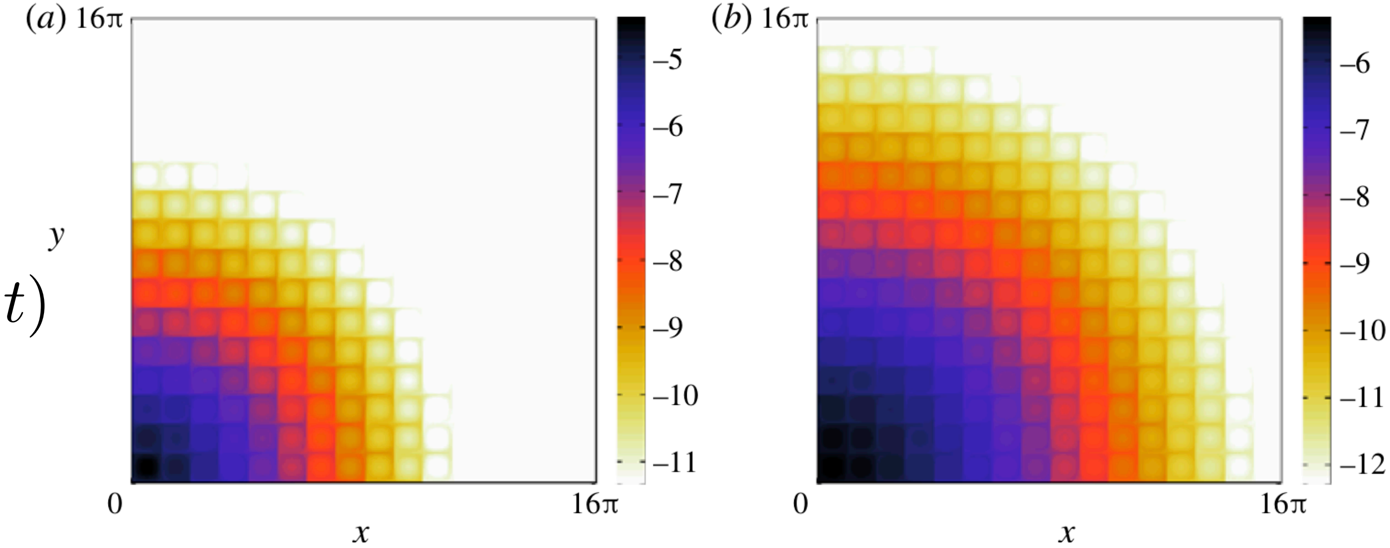


$g(\boldsymbol{\xi})$

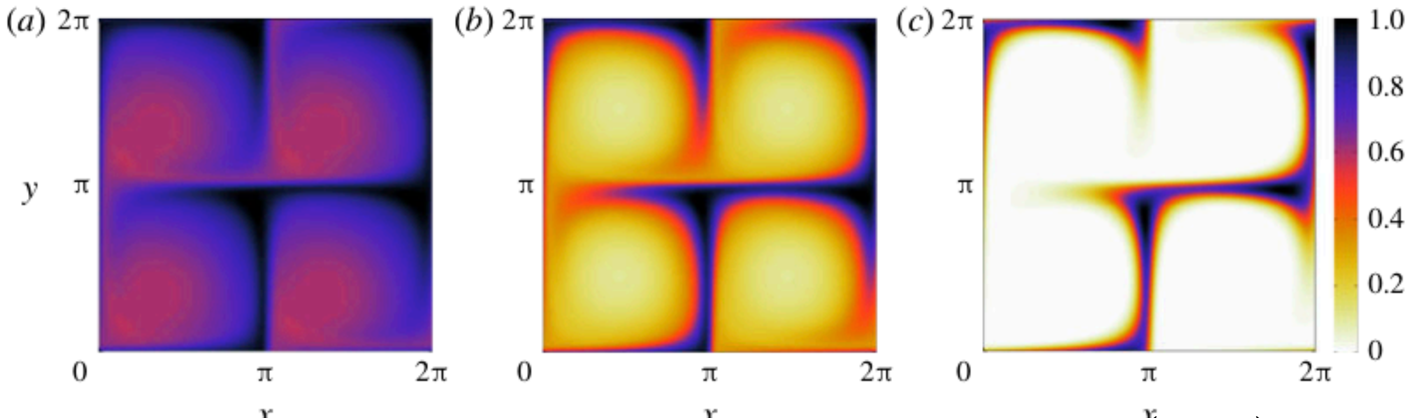
Cellular flow $Pe = 250$

$t = 2$ $\qquad$ $t = 4$

$\log \chi(\mathbf{x}, t)$



$\phi(\mathbf{x}; \mathbf{q})$



$\mathbf{q} = (0.1, 0.1)$ $\quad$ $\mathbf{q} = (0.25, 0.25)$ $\quad$ $\mathbf{q} = (1, 1)$

Summary

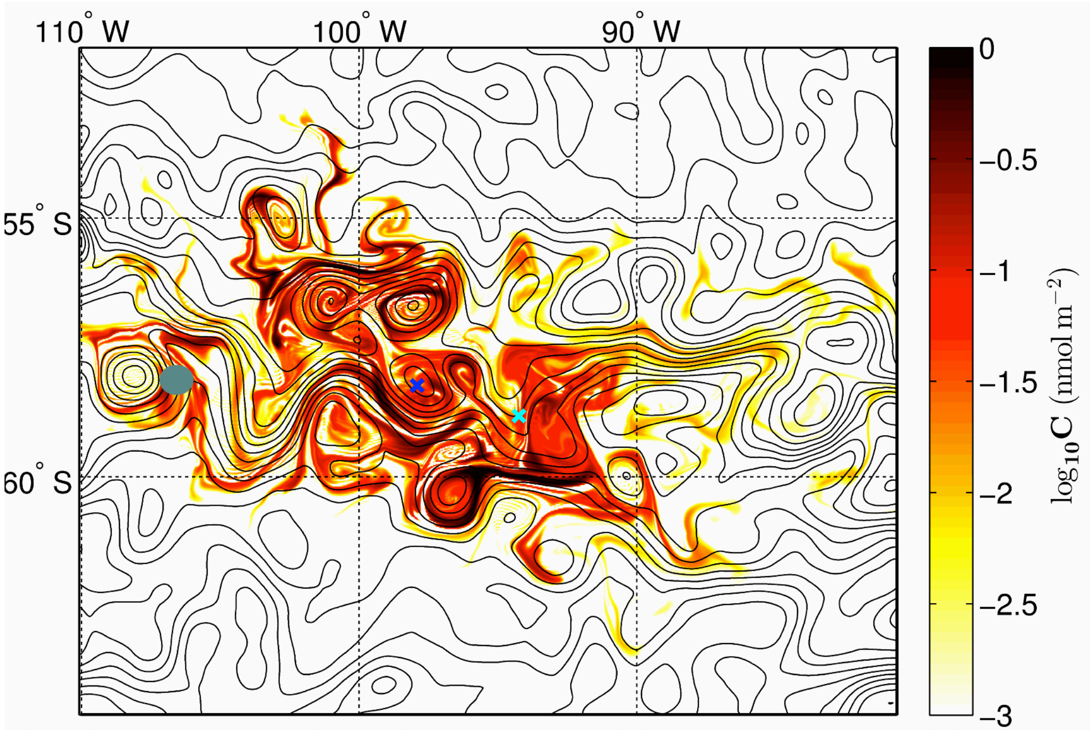
- Large deviation theory for dispersion: beyond central limit theorem, $\exp(-x^2/4\kappa_{\text{eff}}t)$ generalises to $\exp(-tg(x/t))$. $g(\xi)$ describes tails of distribution.
- Rate function $g(\xi)$ found by solving eigenvalue problem for Legendre transform $f(q)$. ('generalised cell problem').

$$\nabla^2\phi - (Pe\,\mathbf{u} + 2\mathbf{q}).\nabla\phi + (Pe\,\mathbf{u}.\mathbf{q} + |\mathbf{q}|^2)\phi = f(\mathbf{q})\phi$$

ϕ gives spatial structure at given $\boldsymbol{\xi}$.

- Shear flows: large deviation generalises Taylor dispersion.
- Cellular flow: complete theory for $\kappa \ll 1$, explicit analytical results for different $|\mathbf{q}|$ regimes.
- ?Random (in time and space) flows.?

Extension to wider class of flows?



Emma Boland PhD thesis 2012: numerical simulation of DIMES tracer release

Long-range dispersion clear in individual realisations – can *statistics* of long-range dispersion be deduced from *statistics* of velocity field?