Dispersion in the large-deviation regime

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Advection-diffusion

Concentration $C(x, t)$ obeys the advection–diffusion equation:

$$\partial_t C + u \cdot \nabla C = \kappa \nabla^2 C,$$

with a flow $u(x, t)$ that is given and satisfies $\nabla \cdot u = 0$.

Pdf of particles positions:

$$\dot{X} = u(X, t) + \sqrt{2\kappa} \dot{W}.$$
Advection-diffusion

For $t \gg 1$, the combined effect of advection and diffusion can often be modelled by an effective diffusivity $\kappa_{\text{eff}}$:

- $\mathbb{E} X \otimes X \sim 2\kappa_{\text{eff}} t$,
- $C \approx \exp(-x \cdot \kappa_{\text{eff}}^{-1} \cdot x/(4t))$: Gaussian distribution,
- effective equation

$$\partial_t C = \nabla \cdot (\kappa_{\text{eff}} \cdot \nabla C).$$

In simple flows: $\kappa_{\text{eff}}$ can be computed explicitly.

- shear flows (Taylor dispersion),
- periodic flows.

e.g. Majda & Kramer 1999
Effective diffusivity

Shear dispersion: dye in pipe flows spreads along the pipe.

\[ \kappa_{\text{eff}} = \kappa^{-1} \left( \left( \int_{-1}^{y} U(y') \, dy' \right)^2 \right) + \kappa \propto \kappa^{-1}. \] \quad \text{Taylor 1953}

Cellular flow: \( \psi = \sin x \sin y \)

\[ \kappa_{\text{eff}} = 2\nu \kappa^{1/2} \quad \text{for } \kappa \ll 1, \]

with \( \nu \sim 0.5327407 \cdots \) Shraiman, Rosenbluth et al, Childress, Soward…
Limitations of effective diffusivity

Diffusive approximation assumes $x/t^{1/2} = O(1)$ as $t \to \infty$. It cannot describes the tails of $C(x, t)$ which are non-Gaussian.

Large deviations:
- obtain $C(x, t)$ for $x/t = O(1)$,
- recover homogenisation as a limiting case.

Interest:
- Low concentrations can be important:
  - anecdotaly: highly toxic chemicals,
  - exactly: FKPP fronts.
- Unifies ‘improvements’ to homogenisation.
- Example of extreme-event statistics.
Large deviations
For $t \gg 1$, the concentration takes the large-deviation form

$$C(x, t) \asymp \exp(-tg(\xi))$$
for $\xi = x/t = O(1)$,

with $g$ the rate function, convex with $g(0) = g'(0) = 0$.

Computing $g$: define $f(q)$ by

$$e^{tf(q)} \asymp \mathbb{E} e^{q \cdot X},$$

$f$ and $g$ are a Legendre transform pair.

$f$ can be estimated
- by Monte Carlo (incl importance sampling),
- by solving eigenvalue problems (for $\partial_t u = 0$).

Effective equation: $\partial_t C = f(-\nabla)C$.

Haynes & Vanneste 2014a
Large deviations: cellular flow

For $\text{Pe} \gg 1$, particles are trapped inside cells, with rare exits across separatrices.

$log \ C$ at $t = 2, 4$ for $\text{Pe} = 250$.

Three regimes: (I) $|x|/t = O(\text{Pe}^{-3/4})$; (II) $|x|/t = O(\log \text{Pe})$ and (III) $|x|/t = O(\text{Pe})$. Haynes & Vanneste 2014b
FKPP fronts

Advection–diffusion–reaction equation:

\[
\partial_t C + u \cdot \nabla C = \text{Pe}^{-1} \nabla^2 C + \text{Da} C(C - 1),
\]

logistic reaction, with \( \text{Da} = L/(U\tau) \), Damköhler number.
FKPP fronts

Front speed is related to large deviations:

\[ c = g^{-1}(Da) . \]

Gartner & Freidlin (1979)
**FKPP fronts**

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Tzella & Vanneste 2014, 2015
Rectangular network

Non-Gaussian behaviour induced by geometry.
Applications: urban pollution, porous media...

Rate function $g$:
- For $U = V = 0$: from $g \sim |\xi|^2/2$ to $g \sim (|\xi_1| + |\xi_2|)^2/4$
  (diffusion with $\kappa/2$ in $L_2$-norm vs. $\kappa$ in $L_1$-norm),
- For $U, V \gg 1$: $g$ independent of $\kappa$, topological dispersion.
Rectangular network

‘Real Manhattan’
Conclusions

- Large-deviation theory to obtain
  - scalar concentrations $C \approx \exp(-tg(x/t))$ for $x/t = O(1)$,
  - speed of FKPP fronts: $c = g^{-1}(Da)$,
- Assumes $t \gg 1$ but works well for $t = O(1)$.
- Rate function $g$ is calculated by solving an e’value problem.
- Extensions: towards turbulent flows,
  - time-periodic flows,
  - random flows (with A. Renaud),
  - simulation data.
- Complex geometries.

References: