Dispersion in the large-deviation regime

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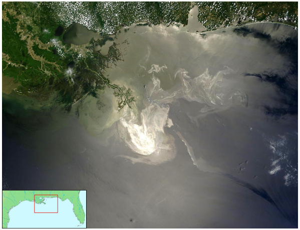
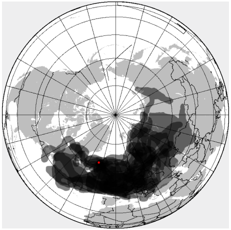
and Peter Haynes (Cambridge)

Advection-diffusion

Passive scalar released in a flow: a classical problem.





Concentration $C(\boldsymbol{x}, t)$ obeys the advection–diffusion equation:

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

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

Pdf of particles positions:

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

Advection-diffusion

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

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

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

In simple flows: κ_{eff} can be computed explicitly.

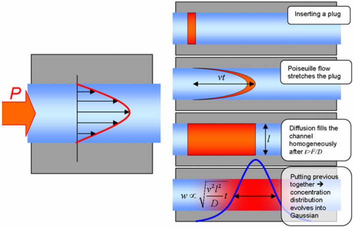
- shear flows (Taylor dispersion),
- periodic flows.

e.g. Majda & Kramer 1999

Effective diffusivity

Shear dispersion:

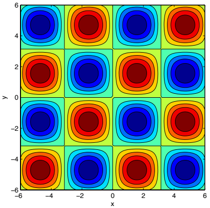
dye in pipe flows spreads along the pipe.



$$\kappa_{\rm eff} = \kappa^{-1}\left\langle \left(\int_{-1}^{y} U(y')\,\mathrm{d}y'\right)^2 \right\rangle + \kappa \propto \kappa^{-1}.$$

Taylor 1953

Cellular flow: $\psi = \sin x \sin y$



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

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:
  - anecdotally: 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

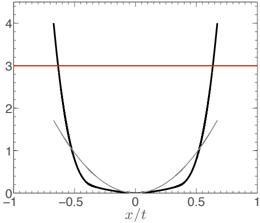
$$C(x,t) \asymp \exp(-tg(\boldsymbol{\xi})) \quad \text{for} \quad \boldsymbol{\xi} = \boldsymbol{x}/t = O(1),$$

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

Computing g: define $f(\boldsymbol{q})$ by

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

f and g are a Legendre transform pair.



f can be estimated

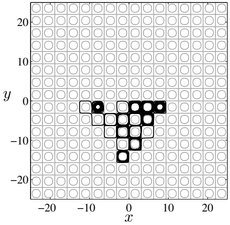
- by Monte Carlo (incl importance sampling),
- by solving eigenvalue problems (for $\partial_t \boldsymbol{u} = 0$).

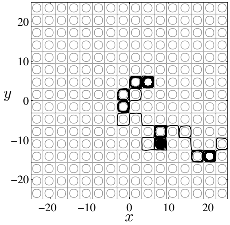
Effective equation: $\partial_t C = f(-\nabla)C$.

Haynes & Vanneste 2014a

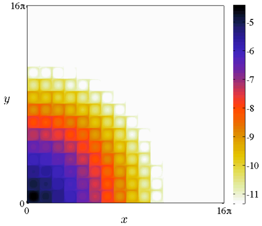
Large deviations: cellular flow

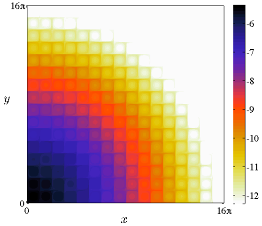
For Pe $\gg 1$, particles are trapped inside cells, with rare exits across separatrices.





log C at $t = 2, 4$ for Pe $= 250$.





Three regimes: (I) $|\boldsymbol{x}|/t = O(\mathrm{Pe}^{-3/4})$; (II) $|\boldsymbol{x}|/t = O(\log \mathrm{Pe})$ and (III) $|\boldsymbol{x}|/t = O(\mathrm{Pe})$.

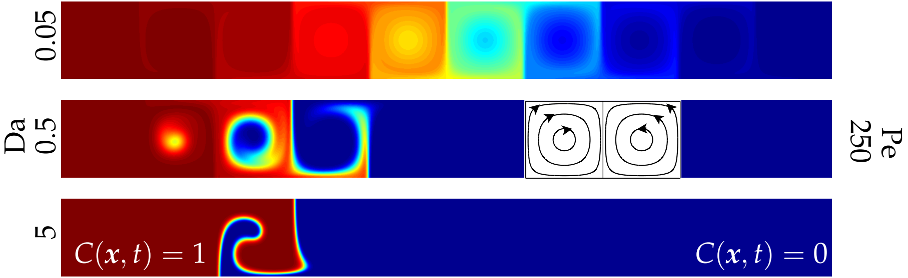
Haynes & Vanneste 2014b

FKPP fronts

Advection–diffusion–reaction equation:

$$\partial_t C + \boldsymbol{u} \cdot \nabla C = \mathrm{Pe}^{-1} \nabla^2 C + \mathrm{Da}\, C(C-1),$$

logistic reaction, with $\mathrm{Da} = L/(U\tau)$, Damköhler number.

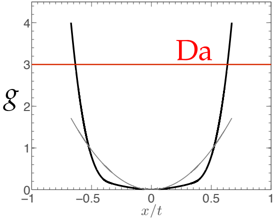


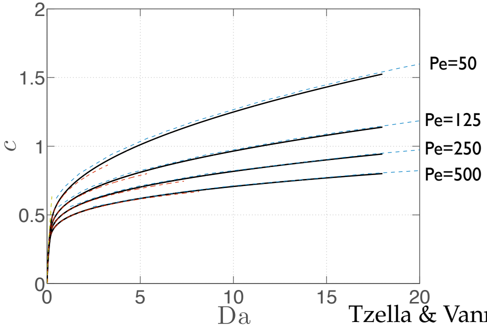
FKPP fronts

Front speed is related to large deviations:

$$c = g^{-1}(\mathrm{Da}).$$

Gartner & Freidlin (1979)





Tzella & Vanneste 2014, 2015

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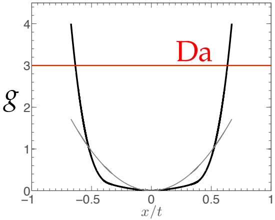
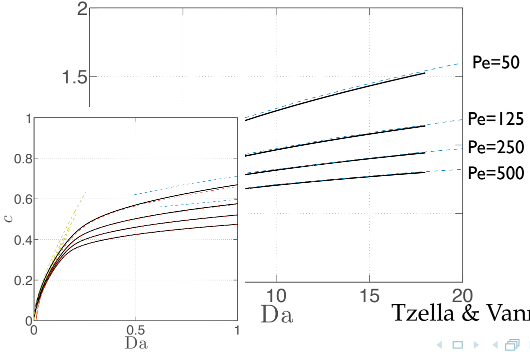
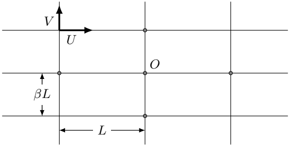




Tzella & Vanneste 2014, 2015

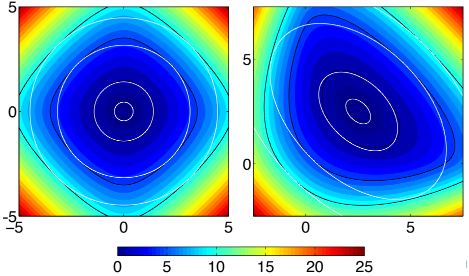
Rectangular network



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

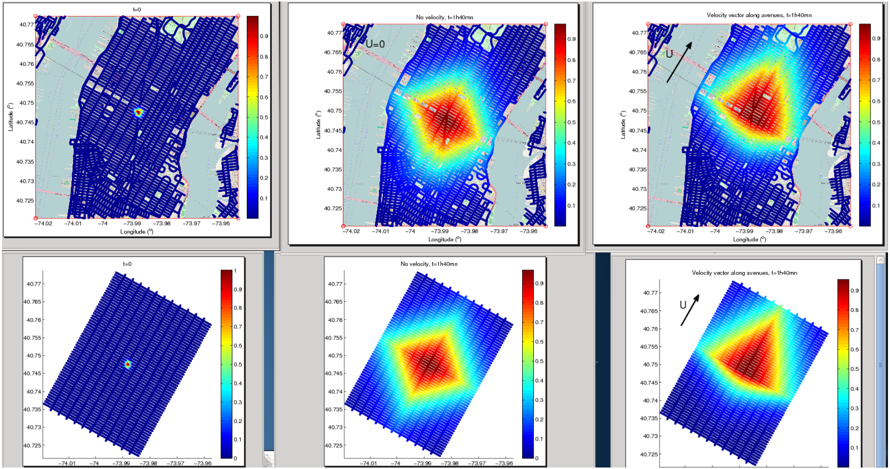
Rate function g:

- for $U = V = 0$: from $g \sim |\boldsymbol{\xi}|^2/2$ to $g \sim (|\xi_1| + |\xi_2|)^2/4$ (diffusion with $\kappa/2$ in L_2-norm vs. κ in L_1-norm),
- for $U,\ V \gg 1$: g independent of κ, topological dispersion.



Rectangular network

'Real Manhattan'



Conclusions

- Large-deviation theory to obtain
  - scalar concentrations $C \asymp \exp(-tg(x/t))$ for $x/t = O(1)$,
  - speed of FKPP fronts: $c = g^{-1}(\mathrm{Da})$,
- 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:

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