Chemical front propagation in cellular flows

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with A Tzella (Birmingham) and P H Haynes (Cambridge)

FKPP equation

Concentration $\theta(\boldsymbol{x}, t)$ of chemicals or biological species is governed by the advection–diffusion–reaction equation

$$\partial_t \theta + \boldsymbol{u} \cdot \nabla \theta = \kappa \Delta \theta + r(\theta) \,,$$

with diffusivity κ.

A common type of reaction (autocatalytic reactions, population dynamics) is logistic:

$$r(\theta) = \tau^{-1} \theta(\theta - 1) \,,$$

leading to the Fisher-Kolmogorov-Petrovsky-Piskunov eqn.

For $\kappa = \boldsymbol{u} = 0$, $\theta \to 1$ as $t \to \infty$.
For $\boldsymbol{u} = 0$, travelling front:

$$\theta = f(x - c_0 t), \quad f \to \begin{cases} 1 & \text{as } x \to -\infty \\ 0 & \text{as } x \to \infty \end{cases}, \quad \text{with } c_0 = 2\sqrt{\kappa/\gamma}.$$

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FKPP equation

For $\kappa \neq 0$, $\boldsymbol{u} \neq 0$,

$$\partial_t \theta + \boldsymbol{u} \cdot \nabla \theta = \mathrm{Pe}^{-1} \Delta \theta(\boldsymbol{x}, t) + \mathrm{Da}\, \theta(1 - \theta),$$

where $\mathrm{Pe} \equiv U\ell/\kappa$ flow strength

$\mathrm{Da} \equiv \ell/U\tau$ reaction strength

For $\boldsymbol{u}$ time-independent, spatially periodic: pulsating front.

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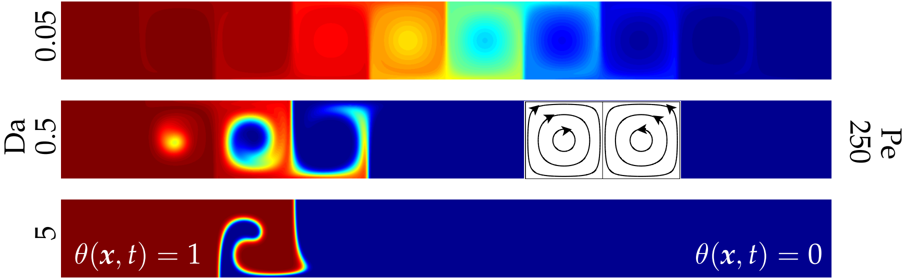

Theory: Constantin *et al.* (2000), Audoly *et al.* (2000), Berestycki & Hamel (2002), Novikov and Ryzhik (2007);

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Question:
What is the front speed $c > c_0$ as a function of Pe and Da?
(when $\mathrm{Pe} \gg 1$)

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Front and large deviations

Derive the front speed from the linearised FKPP (pulled front).

Without flow, $\boldsymbol{u} = 0$:

linearise around the tip of the front, $\theta \approx 0$,

$$\partial_t \theta(\boldsymbol{x}, t) = \mathrm{Pe}^{-1} \Delta \theta(\boldsymbol{x}, t) + \mathrm{Da}\, \theta \cancel{(1 - \theta)}.$$

For $t \gg 1$, Gaussian solution gives

$$\theta(x,t) \asymp \mathrm{e}^{-t\left(\mathrm{Pe}\, x^2/(4t)^2 - \mathrm{Da}\right)}$$
$$= \begin{cases} \infty, & \text{for } \frac{x}{t} < 2\sqrt{\mathrm{Da}/\mathrm{Pe}} \\ 0, & \text{for } \frac{x}{t} > 2\sqrt{\mathrm{Da}/\mathrm{Pe}}. \end{cases}$$

Front speed controlled by transition between exponential growth and decay:

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For $t \gg 1$, use large-deviation form of the passive scalar:

$$\theta(x,t) \asymp \mathrm{e}^{-tg(x/t)}, \qquad \text{with rate function } g.$$

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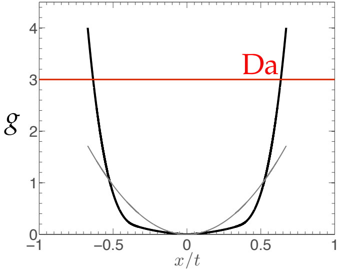
Large deviations

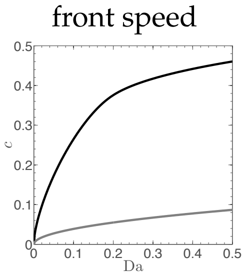
The rare function $g(\xi)$, $\xi = x/t$, can be obtained by solving an eigenvalue equation for its Legendre transform $f(q)$:

$$\mathrm{Pe}^{-1}\Delta\phi - (\boldsymbol{u} + 2\mathrm{Pe}^{-1}q\hat{\boldsymbol{x}}) \cdot \nabla\phi + (uq + \mathrm{Pe}^{-1}q^2)\phi = f(q)\phi. \quad (1)$$

Gartner & Freidlin (1979), Xin (2000)

Example: $\mathrm{Pe} = 250$





For $\mathrm{Da} \ll 1$, i.e. $x/t \ll 1$, homogenization gives $g \propto \sqrt{\mathrm{Pe}}\,(x/t)^2$.

Childress (1979), Shraiman (1987), Soward (1987)

Large deviations

Solve e'value problem for $\mathrm{Pe} \ll 1$. Haynes & Vanneste (2014)

Non-uniformity in q, equivalent to x/t or Da.

3 distinguished regimes:

I. $q = O(\mathrm{Pe}^{-1/4})$: non-trivial concentration in cells + boundary layers,

$$f(q) = \mathrm{Pe}^{-1} F(\mathrm{Pe}^{1/4} |\boldsymbol{q}|^2).$$

II. $|q| = O(1)$: empty cells, boundary layers with crucial corners,

$$f(q) = O(1/\log \mathrm{Pe}).$$

III. $|q| = O(\mathrm{Pe})$: f and g controlled by a single trajectory (Friedlin–Wentzell),

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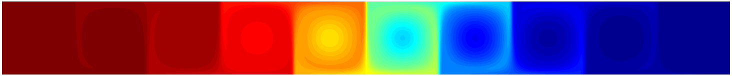
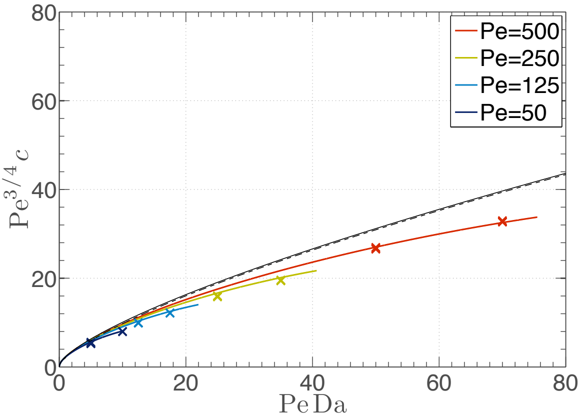
Regime I

$$\mathrm{Da} = O(\mathrm{Pe}^{-1}),\, c = \mathrm{Pe}^{-\frac{3}{4}}\mathcal{C}_1(\mathrm{PeDa})$$





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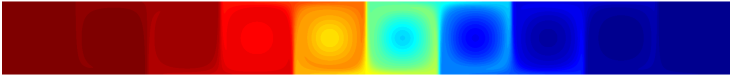
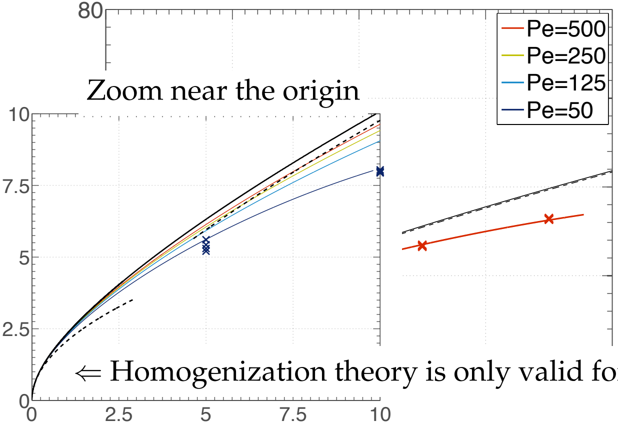
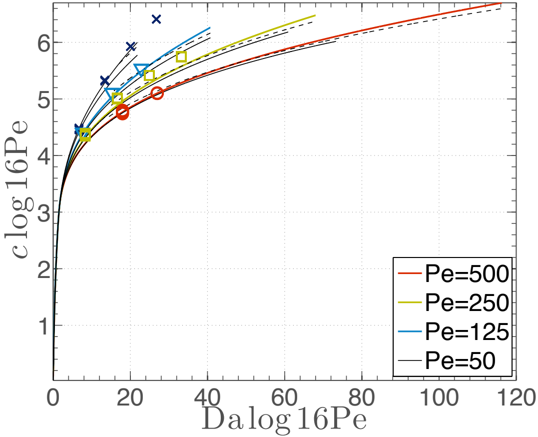




$\Leftarrow$ Homogenization theory is only valid for $\mathrm{Da} \ll \mathrm{Pe}^{-1}$!

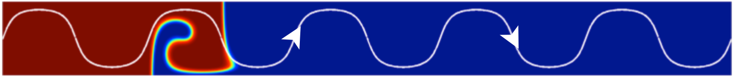
Regime II

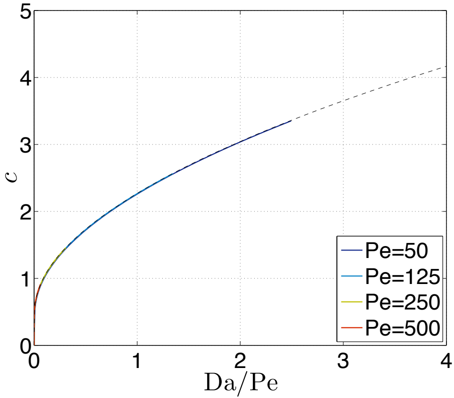
$$\mathrm{Da} = O((\log \mathrm{Pe})^{-1}),\ c = (\log \mathrm{Pe})^{-1}\mathcal{C}_2(\mathrm{Da}\log \mathrm{Pe})$$



Regime III

$$\mathrm{Da} = O(\mathrm{Pe}),\, c = \mathcal{C}_3(\mathrm{Da}/\mathrm{Pe})$$





Freidlin–Wentzell theory: control by action-minimizing instantons

Regime III

Large deviation for $t \gg 1$ meets large deviation for $\mathrm{Pe} \gg 1$.

Freidlin–Wentzel small noise theory:

$$g(x/t) = \lim_{t\to\infty} \frac{\mathrm{Pe}}{4t} \inf_{X(t)=x} \int_0^t |\dot{X} - u(X)|^2 \mathrm{d}s,$$

can be periodised to

$$g(c) = \frac{\mathrm{Pe}}{8\pi} \inf_{X(t)=2\pi} \int_0^{2\pi} |c\dot{X} - u(X)|^2 \mathrm{d}s = \mathrm{Da}\,.$$

This is easily solved (i) numerically, using an optimisation routine; (ii) asymptotically to obtain

$$c = \mathcal{C}_3(\mathrm{Da}/\mathrm{Pe}).$$

Tzella and Vanneste 2014

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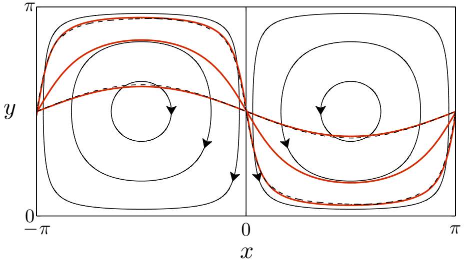

Instantons for $c = 0.5,\ 1,\ 5$

Explicit asymptotics results:

$$c \sim c_0\left(1 + \frac{3\mathrm{Pe}}{16\mathrm{Da}} + \cdots\right) \quad \text{for } \mathrm{Da} \gg \mathrm{Pe},$$

$$c \sim \frac{\pi}{W(8\mathrm{Pe}/\mathrm{Da})} \sim \frac{\pi}{\log \mathrm{Pe}} \quad \text{for } \mathrm{Da} \ll \mathrm{Pe}.$$

Regime III

In this regime, c can alternatively be written as

$$c = 2\pi / T_*,$$

with T_* shortest time to join $x = 0$ to $x = 2\pi$ subject to

$$T_*^{-1} \int_0^{T_*} |\dot{\boldsymbol{X}} - \boldsymbol{u}(\boldsymbol{X})|^2 \mathrm{d}s = c_0^2 .$$

Cf. G-equation, giving front as level set of solution of the eikonal equation

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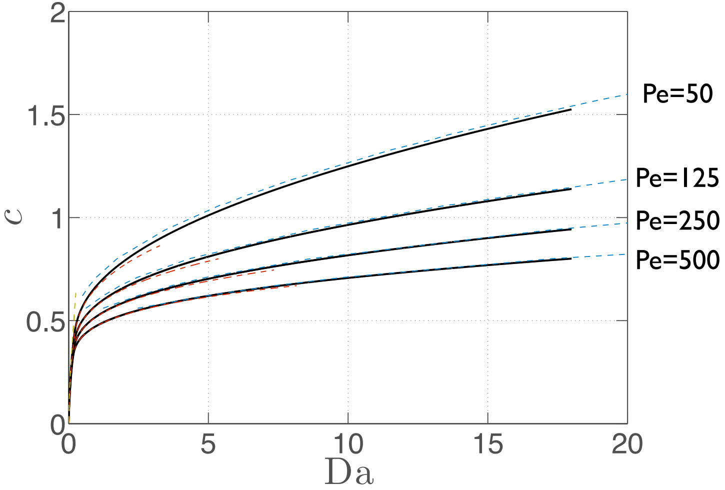
The three regimes together



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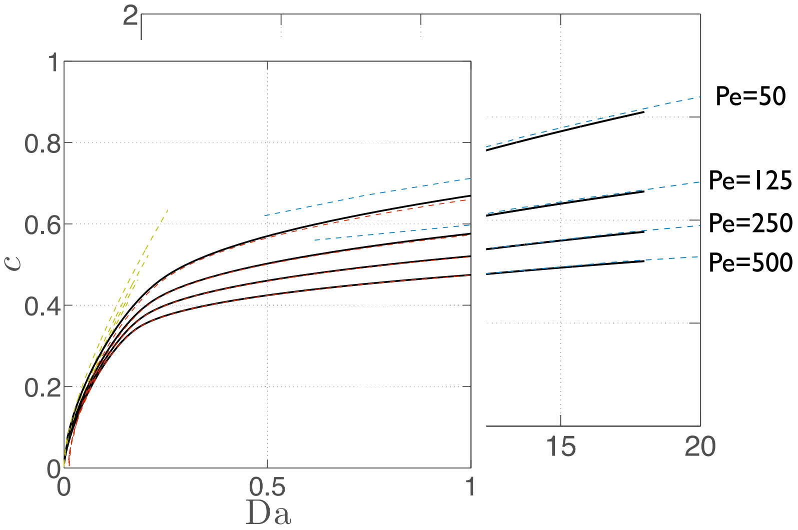

Conclusions

- Large-deviation theory to obtain the front speed: $\theta \asymp \exp[-t(g(x/t) - \mathrm{Da})]$ gives:

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where the rate function g is calculated by solving an eigenvalue problem.

- For cellular flow, we have identified three regimes for $\mathrm{Pe} \gg 1$.
- Extensions: towards turbulent flows,
  - time-periodic flows,
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