Diffusion in arrays of obstacles: beyond homogenisation

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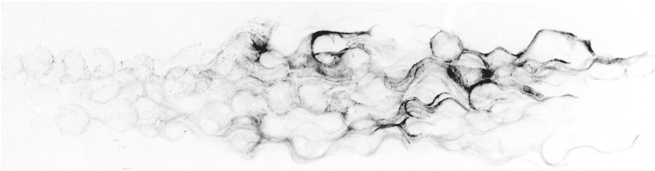

with
Yahya Farah, Daniel Loghin (Birmingham) and Jacques Vanneste (Edinburgh)

International Centre for Mathematical Sciences

Dispersion and mixing in media with obstacles

A multiscale problem with many science and engineering applications

- contaminant transport in soils and aquifers
- drug delivery and nutrient transport in biological tissues
- filtration devices ...

Challenge due to advection+diffusion+geometry.

Souzy et al. 2020

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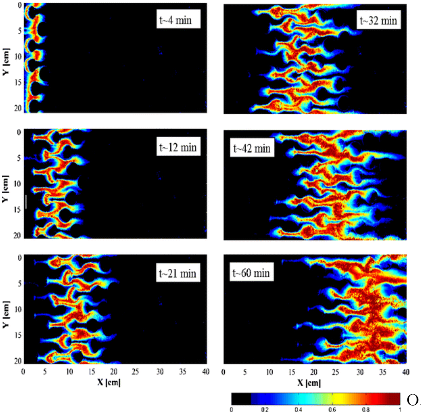


Oates and Harvey 2006

Dispersion and mixing in media with obstacles

For $t \gg 1$, a Gaussian approximation is used to describe how a blob evolves:

$$\theta(\boldsymbol{x}, t) \approx \frac{1}{\sqrt{2\pi}\mathsf{K}_{\mathrm{eff}} t} \exp\left(-\frac{1}{4t}(\boldsymbol{x} - \boldsymbol{\xi}_{\mathrm{eff}} t)^T \mathsf{K}_{\mathrm{eff}}^{-1} (\boldsymbol{x} - \boldsymbol{\xi}_{\mathrm{eff}} t)\right)$$

where $\theta(\boldsymbol{x}, t)$ is the concentration and $\boldsymbol{\xi}_{\mathrm{eff}}$ and $\mathsf{K}_{\mathrm{eff}}$ are the mean velocity and the effective diffusivity tensor.

MAXWELL 1873, RAYLEIGH 1892, TAYLOR 1953, ARIS 1956, BRENNER 1981

- captures dispersion for $\|\boldsymbol{x} - \boldsymbol{\xi}_{\mathrm{eff}} t\| = O(t^{1/2})$.

PAVLIOTIS AND STUART 2007

- do better, with large deviations e.g. TOUCHETTE 2009:

$$\theta(\boldsymbol{x}, t) \asymp \exp(-t g(\boldsymbol{x}/t)).$$

HAYNES & VANNESTE 2014

The basic problem: diffusion in the presence of obstacles

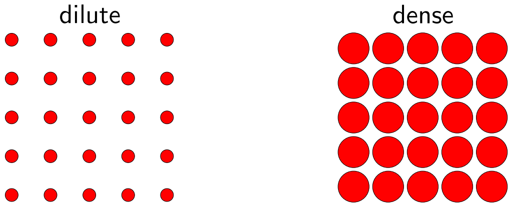


Figure: An example of a medium with circular obstacles arranged in square arrays (red).

$$\frac{\partial \theta}{\partial t} = \nabla^2 \theta,$$
$$0 = \boldsymbol{n} \cdot \nabla \theta, \quad \boldsymbol{x} \text{ on } \mathcal{B},$$

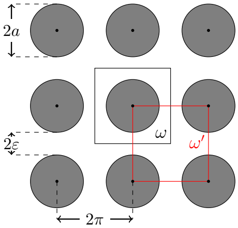
where $\boldsymbol{n}$ is the unit normal to the boundaries of the obstacle $\mathcal{B}$.

Macroscopic behaviour: large deviations

To capture both the Gaussian core and the tales, take the two-scale form

$$\theta(\boldsymbol{x}, t) \sim t^{-1}\phi(\boldsymbol{x})e^{-tg(\boldsymbol{\xi})}, \quad \text{where } \boldsymbol{\xi} = \frac{\boldsymbol{x}}{t} \in \mathbb{R}^2 \text{ and } \boldsymbol{x} \in \omega$$

Haynes and Vanneste 2014



- rate function g captures dispersion for $|\boldsymbol{x}| = O(t)$
- find g by solving a family of cell eigenvalue problems

Cell eigenvalue problem

Leading-order problem satisfies

$$\begin{aligned} \nabla^2_{\boldsymbol{x}}\phi - 2\boldsymbol{q}\cdot\nabla_{\boldsymbol{x}}\phi + |\boldsymbol{q}|^2\phi &= f(\boldsymbol{q})\phi, \\ \boldsymbol{n}\cdot[\nabla_{\boldsymbol{x}}\phi - \phi\boldsymbol{q}] &= 0, \qquad \boldsymbol{x} \text{ on } \mathcal{B} \\ \phi \quad \text{periodic in} \quad \boldsymbol{x}&. \end{aligned}$$

where

$$\boldsymbol{q} = \nabla_{\boldsymbol{\xi}} g(\boldsymbol{\xi}) \quad \text{and} \quad f(\boldsymbol{q}) = \sup_{\boldsymbol{\xi}} (\boldsymbol{\xi}\cdot\boldsymbol{q} - g(\boldsymbol{\xi})).$$

- Principal eigenvalue determines the rate function $g(\boldsymbol{x}/t)$ by taking a Legendre transform.

Macroscopic behaviour: effective diffusion

- For $|\boldsymbol{x}| \ll t$,

$$g(\boldsymbol{x}/t) \sim \frac{1}{2}(\boldsymbol{x}/t)^T \nabla_{\boldsymbol{x}/t} \nabla_{\boldsymbol{x}/t} g(0)(\boldsymbol{x}/t) = \frac{1}{4}\kappa_{\text{eff}}^{-1}(|\boldsymbol{x}|/t)^2, \quad (1)$$

  where κ_{eff} is the effective diffusivity.
- Introducing (1) inside

$$\theta(\boldsymbol{x}, t) \asymp \exp(-tg(\boldsymbol{x}/t))$$

  recovers Gaussian approximation for θ obtained via homogenisation.

Effective diffusivity in the dilute limit

In periodic arrays κ_{eff} was first computed using Rayleigh's multipole method:

$$\kappa_{\text{eff}} \sim 1 - \sigma, \quad \text{as } \sigma \to 0$$

where σ is the solid area fraction.

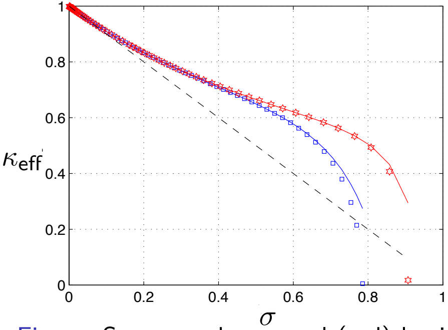
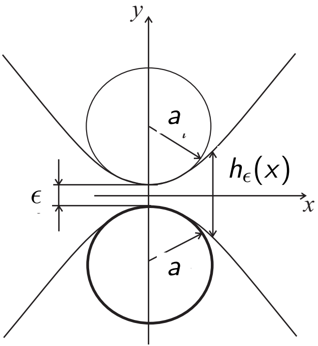


Figure: Square vs hexagonal (red) lattice.

Bruna and Chapman 2015

Effective diffusivity in the dense limit



Keller's total flux inside the narrow gaps between obstacles:

$$F = h_\epsilon(x)\frac{\partial \theta}{\partial x},$$

where the gap width

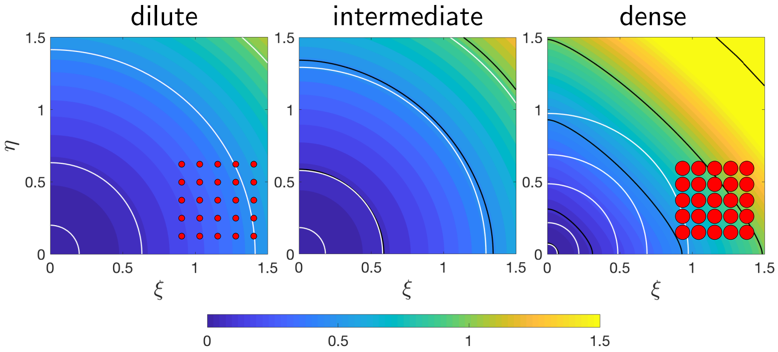
$$h_\epsilon(x) \approx \frac{1}{\pi}x^2 + \epsilon \quad \text{for} \quad \epsilon \ll 1.$$

Divide by h_ϵ and integrate:

$$F = \alpha \Delta\theta, \quad \text{where } \alpha = \sqrt{2\epsilon/\pi^3}.$$

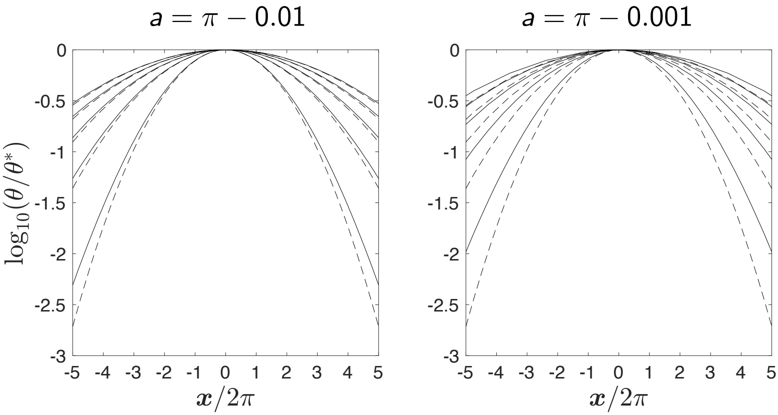
$$\kappa_{\text{eff}} \sim \frac{2\sqrt{2}\pi^2}{\mathscr{A}}\alpha = \frac{2}{\pi^{3/2}}\frac{(\pi/4-\sigma)^{1/2}}{1-\sigma}, \quad \text{as } \sigma \to \pi/4.$$

Circular obstacles in square lattices: rate function $g(\boldsymbol{x}/t)$



- dilute case: quadratic (Gaussian) approximation (white lines) excellent for $|\boldsymbol{x}| = O(t)$
- more generally: does not capture the anisotropic behaviour for $|\boldsymbol{x}| = O(t)$

Circular obstacles in square lattices: concentration $\theta(\boldsymbol{x}/t)$



- tail concentrations much fatter than predicted by the effective diffusion approximation
- discrepancy largest at earlier times and bigger radii

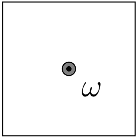
Asymptotic analysis of the cell eigenvalue problem.

Let $\boxed{\psi = e^{-\boldsymbol{q}\cdot\boldsymbol{y}}\phi}$. The eigenvalue problem becomes the modified Helmholtz equation

$$\nabla^2_{\boldsymbol{y}}\psi = f(\boldsymbol{q})\psi, \quad (2a)$$

$$0 = \frac{\partial \psi}{\partial r} \quad \text{on } r = a \quad (2b)$$

$$\psi e^{\boldsymbol{q}\cdot\boldsymbol{y}} \quad 2\pi\text{-periodic} \quad (2c)$$



Dilute limit

- *outer region*: $r = O(1)$, $\psi \sim e^{-\boldsymbol{q}\cdot\boldsymbol{y}}$
- *inner region*: $R = r/a = O(1)$,

$$\Psi \sim 1 - a|\boldsymbol{q}|((R + \boxed{R^{-1}})\cos(\theta - \alpha),$$

where $\boldsymbol{q} = |\boldsymbol{q}|(\cos\alpha, \sin\alpha)$.

Multiply (1a) by $e^{\boldsymbol{q}\cdot\boldsymbol{y}}$ and integrate:

$$f(\boldsymbol{q}) \sim \kappa_{\text{eff}}|\boldsymbol{q}|^2 \Rightarrow g(\boldsymbol{x}/t) \sim |\boldsymbol{x}|^2/(4\kappa_{\text{eff}}t)$$

$\Rightarrow$ effective diffusion accurate for $|\boldsymbol{x}| \sim O(t)$

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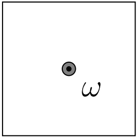

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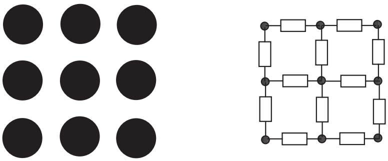
Dense limit: discrete network model

Use Keller's flux to build a discrete network model:

$$\mathscr{A}\frac{d\theta_{m,n}}{dt} = \alpha(\theta_{m+1,n} + \theta_{m,n+1} + \theta_{m-1,n} + \theta_{m,n-1} - 4\theta_{m,n}).$$



Taking $\theta_{m,n} \sim t^{-1}\exp(-t g_{\mathrm{d}}(\boldsymbol{r}_{m,n}/t))$ yields

$$g_{\mathrm{d}}(\boldsymbol{\xi}) = \frac{2\alpha}{\mathscr{A}}\left(\mathsf{S}(\beta\xi) + \mathsf{S}(\beta\eta)\right),$$

where $\mathsf{S}(x) = 1 + x\sinh^{-1}x - \sqrt{1+x^2}$ and $\beta = \mathscr{A}/(4\pi\alpha)$.

Dense limit: discrete network model

Rate function g

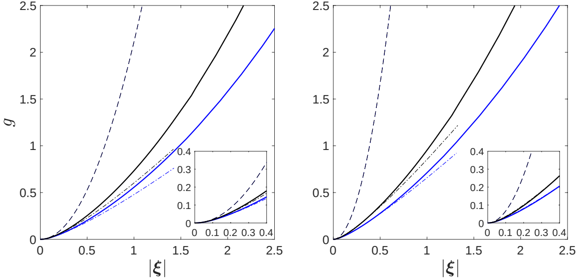
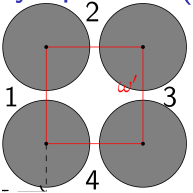


Figure: Rate function g against $|\boldsymbol{\xi}| = |\boldsymbol{x}|/t$ for (left) $\epsilon = 0.01$ and (right) 0.001 in the directions $(1,1)$ (black) and $(1,0)$ (blue). Numerical results (thick solid lines), quadratic (Gaussian) approximation (dashed lines) and the network approximation (dashed-dotted).

- Captures part of the rate function and thus the tails

Dense limit: matched asymptotics (1)



Inner gap regions: $X = x/\sqrt{\epsilon} = O(1)$, $Y = (y+\pi)/\epsilon \sim \pm H(X)$

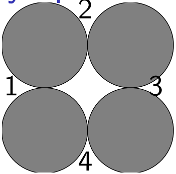
Leading-order inner solution satisfies $\boxed{\partial_X(H(X)\Psi_0) = 0} \Rightarrow$

$$\Psi_0 = \alpha_1 \int_0^X \frac{dX}{\underbrace{X^2/(2\pi)+1}_{H(X)}} + \beta_1 = \alpha_1 \tan^{-1}(X/\sqrt{2\pi}) + \beta_1,$$

and similarly for the solution in the other 3 gaps.
+ "tilted" periodicity:

$$(\alpha_3, \beta_3) = e^{-2\pi p}(\alpha_1, \beta_1) \quad \text{and} \quad (\alpha_4, \beta_4) = e^{-2\pi q}(\alpha_2, \beta_2)$$

Dense limit: matched asymptotics (2)



Outer region: $x = O(1)$, $y = \pm h(x)$ where $h(x) = x^2/(2\pi)$

Leading-order outer solution satisfies $\boxed{\partial_x(h(x)\psi_0) = 0} \Rightarrow$

$$\psi_0 \sim \gamma_1 x^{-1} + \delta_1 \quad \text{as } \boldsymbol{x} \to \boldsymbol{x}_1$$

and similarly for the other 3 gaps.

$\boxed{\text{Canonical problem: } \nabla^2\psi^* = f\psi^*, \quad x^2\partial_x\psi^* \to 1 \quad \text{as} \quad \boldsymbol{x} \to \boldsymbol{x}_1}$

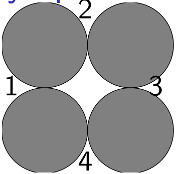
$$\psi^* \sim -x^{-1} - D_1(f) \quad \text{as } \boldsymbol{x} \to \boldsymbol{x}_1$$

$$\psi^* \sim -D_i(f) \quad \text{as } \boldsymbol{x} \to \boldsymbol{x}_i \text{ for } i = 2, 3, 4$$

$$\boxed{\psi_0 = \gamma_1\psi^* + \gamma_2\mathcal{R}_{\pi/2}\psi^* + \gamma_3\mathcal{R}_{\pi}\psi^* + \gamma_4\mathcal{R}_{3\pi/2}\psi^*}$$

Matching: Linear system, 12 unknowns $\Rightarrow$ trans. equation $\Rightarrow f(\boldsymbol{q})$

Dense limit: matched asymptotics (2)



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Dense limit: matched asymptotics

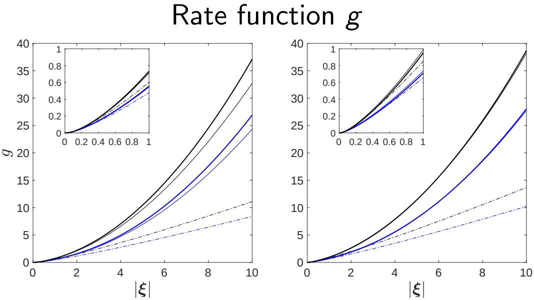

Figure: Numerical results (thick solid lines), matched asymptotic approximation (thin solid lines) and discrete-network approximation (dashed-dotted).

- discrete network approximation as a limit of the matched asymptotic prediction
- analysis breaks down for $|\boldsymbol{x}| \gg t$ when

$$\theta \propto \exp(-d^2(\boldsymbol{x})/4t)$$

where $d(\boldsymbol{x})$ is the distance along the shortest path $\approx L^1$.

Conclusions

- large deviations generalise scalar dispersion in arrays of obstacles.
- effective diffusion underestimates concentrations at large distances/short times from the point/time of release
- effect is strongest in the dense limit, when obstacles are nearly touching.
- explicit results capture anisotropic shape of the scalar patch.
- results relevant for chemical reactions e.g. FKPP.

$$\frac{\partial\theta}{\partial t} = \nabla^2\theta + \alpha\theta(1-\theta),$$
$$0 = \boldsymbol{n}\cdot\nabla\theta, \quad \boldsymbol{x} \text{ on } \mathcal{B},$$

The front speed is deduced from $\boxed{g(c(\boldsymbol{e})\boldsymbol{e}) = \alpha}$.

Farah, Loghin, Tzella & Vanneste, Proc. Royal Soc., 2020

Thank you for your attention!

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