Lecture 32: Homogenization for a perforated domain

I. THE HOMOGENIZED HEAT EQUATION

Consider a domain consisting of periodic cells Ω of characteristic size ℓ, each containing a reflecting perforation D. The diffusion equation for the concentration $\varphi(t,\boldsymbol{r})$ is then

$$\partial_t\varphi(t,\boldsymbol{r}) = \Delta_{\boldsymbol{r}}\varphi(t,\boldsymbol{r}), \qquad \boldsymbol{r}\in\Omega\setminus D; \tag{1a}$$

$$\hat{\boldsymbol{n}}\cdot\nabla_{\boldsymbol{r}}\varphi(t,\boldsymbol{r}) = 0, \qquad \boldsymbol{r}\in\partial D. \tag{1b}$$

Assume the initial condition for φ varies on a scale L that is large with respect to ℓ. Define $\varepsilon = \ell/L \ll 1$. We write $\varphi(0,\boldsymbol{r}) = \varphi_0(\varepsilon\,\boldsymbol{r})$.

Now introduce the large scale and slow time, whose magnitudes are related to the fast variables by

$$\boldsymbol{R}\sim\varepsilon\,\boldsymbol{r}, \qquad T\sim\varepsilon^2 t\,, \tag{2}$$

and assume that the concentration depends on these scales,

$$\varphi(t,\boldsymbol{r}) = \varphi^\varepsilon(T,\boldsymbol{r},\boldsymbol{R}). \tag{3}$$

Using $\partial_t\to\varepsilon^2\,\partial_T$, $\nabla_{\boldsymbol{r}}\to\nabla_{\boldsymbol{r}}+\varepsilon\,\nabla_{\boldsymbol{R}}$, Eq. (1a) becomes

$$-\Delta_{\boldsymbol{r}}\varphi^\varepsilon + \varepsilon^2\,\partial_T\varphi^\varepsilon = 2\varepsilon\,\nabla_{\boldsymbol{r}}\cdot\nabla_{\boldsymbol{R}}\varphi^\varepsilon + \varepsilon^2\Delta_{\boldsymbol{R}}\varphi^\varepsilon, \qquad \boldsymbol{r}\in\Omega\setminus D; \tag{4a}$$

$$\hat{\boldsymbol{n}}\cdot\nabla_{\boldsymbol{r}}\varphi^\varepsilon + \varepsilon\hat{\boldsymbol{n}}\cdot\nabla_{\boldsymbol{R}}\varphi^\varepsilon = 0, \qquad \boldsymbol{r}\in\partial D. \tag{4b}$$

We expand the concentration in a power series in ε,

$$\varphi^\varepsilon(T,\boldsymbol{r},\boldsymbol{R}) = \varphi^{(0)}(T,\boldsymbol{r},\boldsymbol{R}) + \varepsilon\,\varphi^{(1)}(T,\boldsymbol{r},\boldsymbol{R}) + \dots \tag{5}$$

and at order ε^0 obtain from Eq. (4),

$$\Delta_{\boldsymbol{r}}\varphi^{(0)} = 0, \qquad \hat{\boldsymbol{n}}\cdot\nabla_{\boldsymbol{r}}\varphi^{(0)} = 0. \tag{6}$$

We take φ^ε is periodic in $\boldsymbol{r}$. The only solution to Eq. (6) is a constant in $\boldsymbol{r}$, that is

$$\varphi^{(0)}(T,\boldsymbol{r},\boldsymbol{R}) = \Phi(T,\boldsymbol{R}). \tag{7}$$

At order ε^1, Eq. (4) with the expansion (5) gives

$$\Delta_{\boldsymbol{r}}\varphi^{(1)} = 0, \qquad \hat{\boldsymbol{n}}\cdot\nabla_{\boldsymbol{r}}\varphi^{(1)} = -\hat{\boldsymbol{n}}\cdot\nabla_{\boldsymbol{R}}\Phi. \tag{8}$$

We can solve this by letting

$$\varphi^{(1)}(T,\boldsymbol{r},\boldsymbol{R}) = \boldsymbol{\chi}(\boldsymbol{r})\cdot\nabla_{\boldsymbol{R}}\Phi(T,\boldsymbol{R}) \tag{9}$$

where the periodic vector field $\boldsymbol{\chi}(\boldsymbol{r})$ solves the *cell problem* [2, p. 15],

$$\Delta_{\boldsymbol{r}}\boldsymbol{\chi} = 0, \qquad \boldsymbol{r}\in\Omega\setminus D; \tag{10a}$$

$$\hat{\boldsymbol{n}}\cdot\nabla_{\boldsymbol{r}}\boldsymbol{\chi} = -\hat{\boldsymbol{n}}, \qquad \boldsymbol{r}\in\partial D. \tag{10b}$$

Note that Eq. (10) does not have a unique solution for $\boldsymbol{\chi}$, since an arbitrary constant can be added. This constant doesn't affect the final result (see discussion after Eq. (16)), so we can force the solution to be unique by requiring $\langle \boldsymbol{\chi} \rangle = 0$.

Assuming the cell problem (10) has been solved, we can proceed to order ε^2 in Eq. (4),

$$-\Delta_{\boldsymbol{r}}\varphi^{(2)} + \partial_T \Phi = 2\nabla_{\boldsymbol{r}} \cdot \nabla_{\boldsymbol{R}}\varphi^{(1)} + \Delta_{\boldsymbol{R}}\Phi\,; \tag{11a}$$

$$\hat{\boldsymbol{n}} \cdot \nabla_{\boldsymbol{r}}\varphi^{(2)} = -\hat{\boldsymbol{n}} \cdot \nabla_{\boldsymbol{R}}\varphi^{(1)}. \tag{11b}$$

Define integration over the cell as

$$\langle f \rangle := \int_{\Omega \setminus D} f \,\mathrm{d}V_{\boldsymbol{r}}. \tag{12}$$

Integrating Eq. (11a) over $\Omega \setminus D$, we find the first term becomes

$$\left\langle \Delta_{\boldsymbol{r}}\varphi^{(2)} \right\rangle = \int_{\Omega \setminus D} \Delta_{\boldsymbol{r}}\varphi^{(2)} \,\mathrm{d}V_{\boldsymbol{r}} = \int_{\partial D} \nabla_{\boldsymbol{r}}\varphi^{(2)} \cdot \hat{\boldsymbol{n}} \,\mathrm{d}A_{\boldsymbol{r}} = -\int_{\partial D} \nabla_{\boldsymbol{R}}\varphi^{(1)} \cdot \hat{\boldsymbol{n}} \,\mathrm{d}A_{\boldsymbol{r}}\,, \tag{13}$$

where we used the boundary condition (11b), and the fact that boundary terms vanish at the surface of the periodic cell Ω. So far the choice of normal was immaterial, but in using the divergence theorem we must ensure that $\hat{\boldsymbol{n}}$ points towards the *interior* of D, since it must point towards the exterior of $\Omega \setminus D$.

The first term on the right of Eq. (11a) is

$$\left\langle 2\nabla_{\boldsymbol{r}} \cdot \nabla_{\boldsymbol{R}}\varphi^{(1)} \right\rangle = 2\int_{\Omega \setminus D} \nabla_{\boldsymbol{r}} \cdot \nabla_{\boldsymbol{R}}\varphi^{(1)} \,\mathrm{d}V_{\boldsymbol{r}} = 2\int_{\partial D} \nabla_{\boldsymbol{R}}\varphi^{(1)} \cdot \hat{\boldsymbol{n}} \,\mathrm{d}A_{\boldsymbol{r}}\,. \tag{14}$$

Both (13) and (14) are of the same form, and can be combined and rewritten using Eq. (9) as

$$\begin{aligned}\int_{\partial D} \nabla_{\boldsymbol{R}}\varphi^{(1)} \cdot \hat{\boldsymbol{n}} \,\mathrm{d}A_{\boldsymbol{r}} &= \nabla_{\boldsymbol{R}} \cdot \int_{\partial D} \boldsymbol{\chi} \cdot \nabla_{\boldsymbol{R}}\Phi \,\hat{\boldsymbol{n}} \,\mathrm{d}A_{\boldsymbol{r}} \\ &= \nabla_{\boldsymbol{R}} \cdot \left\{ \int_{\partial D} \boldsymbol{\chi}\,\hat{\boldsymbol{n}} \,\mathrm{d}A_{\boldsymbol{r}} \cdot \nabla_{\boldsymbol{R}}\Phi \right\}.\end{aligned}$$

We also have $\langle \partial_T \Phi \rangle = |\Omega \setminus D|\,\partial_T\Phi$ and $\langle \Delta_{\boldsymbol{R}}\Phi \rangle = |\Omega \setminus D|\,\Delta_{\boldsymbol{R}}\Phi$, since neither quantity depends on $\boldsymbol{r}$, where $|\Omega \setminus D|$ is the available cell volume. We thus finally obtain the homogenized diffusion equation

$$\partial_T \Phi = \nabla_{\boldsymbol{R}} \cdot (\mathbb{D}_{\text{eff}} \cdot \nabla_{\boldsymbol{R}}\Phi) \tag{15}$$

where the *effective diffusivity tensor* is

$$\mathbb{D}_{\text{eff}} := \mathbb{I} + \frac{1}{|\Omega \setminus D|} \int_{\partial D} \boldsymbol{\chi}\,\hat{\boldsymbol{n}} \,\mathrm{d}A_{\boldsymbol{r}}. \tag{16}$$

Note that adding a constant to $\boldsymbol{\chi}$ doesn't change the integral, since $\int_{\partial D} \hat{\boldsymbol{n}} \,\mathrm{d}A_{\boldsymbol{r}} = 0$; the lack of uniqueness of solutions to Eq. (10) is thus inconsequential. We prove some useful identities for $\mathbb{D}_{\text{eff}}$ in Appendix A.

II. A SMALL PERFORATION

To make the cell problem tractable, consider a d-dimensional periodic cell Ω with a small perforation D_δ of size δ in the center of the cell, enclosing the origin. Near the perforation, define a fine scale $\boldsymbol{\eta} = \boldsymbol{r}/\delta$; with $\boldsymbol{\chi}^\delta_{\text{inner}}(\boldsymbol{\eta}) = \boldsymbol{\chi}^\delta(\delta\boldsymbol{\eta})$, the cell problem (10) is

$$\Delta_{\boldsymbol{\eta}}\boldsymbol{\chi}^\delta_{\text{inner}} = 0, \qquad \boldsymbol{\eta} \in \mathbb{R}^3 \backslash D_1; \tag{17a}$$
$$\hat{\boldsymbol{n}}_{\boldsymbol{\eta}} \cdot \nabla_{\boldsymbol{\eta}}\boldsymbol{\chi}^\delta_{\text{inner}} = -\delta\hat{\boldsymbol{n}}_{\boldsymbol{\eta}}, \qquad \boldsymbol{\eta} \in \partial D_1. \tag{17b}$$

The inhomogeneous boundary condition (17b) implies that $\boldsymbol{\chi}^\delta_{\text{inner}}(\boldsymbol{\eta})$ is of order δ at leading order. We can thus expand

$$\boldsymbol{\chi}^\delta_{\text{inner}}(\boldsymbol{\eta}) = \delta\,\boldsymbol{\chi}^{(1)}_{\text{inner}}(\boldsymbol{\eta}) + \delta^2\,\boldsymbol{\chi}^{(2)}_{\text{inner}}(\boldsymbol{\eta}) + \dots. \tag{18}$$

At leading order in δ for the inner problem we thus solve

$$\Delta_{\boldsymbol{\eta}}\boldsymbol{\chi}^{(1)}_{\text{inner}} = 0, \qquad \boldsymbol{\eta} \in \mathbb{R}^3 \backslash D_1; \tag{19a}$$
$$\hat{\boldsymbol{n}}_{\boldsymbol{\eta}} \cdot \nabla_{\boldsymbol{\eta}}\boldsymbol{\chi}^{(1)}_{\text{inner}} = -\hat{\boldsymbol{n}}_{\boldsymbol{\eta}}, \qquad \boldsymbol{\eta} \in \partial D_1 \tag{19b}$$

with $\boldsymbol{\chi}^{(1)}_{\text{inner}}$ decaying at infinity. Note that there is no need to solve the outer problem to get the leading-order effective diffusivity: it is the inhomogeneity that sets the amplitude of the outer solution. For the higher orders we have for $k > 0$:

$$\Delta_{\boldsymbol{\eta}}\boldsymbol{\chi}^{(k)}_{\text{inner}} = 0, \qquad \boldsymbol{\eta} \in \mathbb{R}^3 \backslash D_1; \tag{20a}$$
$$\hat{\boldsymbol{n}}_{\boldsymbol{\eta}} \cdot \nabla_{\boldsymbol{\eta}}\boldsymbol{\chi}^{(k)}_{\text{inner}} = 0, \qquad \boldsymbol{\eta} \in \partial D_1. \tag{20b}$$

These must be matched at each order to the outer Green's function solution.

$$\Delta_{\boldsymbol{r}}\boldsymbol{\chi}^\delta_{\text{outer}} = 0, \tag{21}$$

$$\boldsymbol{\chi}^\delta_{\text{outer}}(\boldsymbol{r}) = \delta\,\boldsymbol{\chi}^{(1)}_{\text{outer}}(\boldsymbol{r}) + \delta^2\,\boldsymbol{\chi}^{(2)}_{\text{outer}}(\boldsymbol{r}) + \dots \tag{22}$$

As mentioned above, in pratice we won't need to actually find the outer solution in order to get the leading-order effective diffusivity.

A. Spherical perforation

As a first attempt, let's solve this for an perforation shaped like a ball of radius δ. Exploiting the spherical symmetry, take $\boldsymbol{\chi}^{(1)}_{\text{inner}}(\boldsymbol{\eta}) = f(\eta)\,\hat{\boldsymbol{\eta}}$, where $\eta = |\boldsymbol{\eta}|$ and $\hat{\boldsymbol{\eta}} = \boldsymbol{\eta}/\eta$. Then the vector Laplacian takes the simple form [3]

$$\Delta_{\boldsymbol{\eta}}\boldsymbol{\chi}^{(1)}_{\text{inner}} = \left(\frac{1}{\eta^{d-1}}\frac{d}{d\eta}\left(\eta^{d-1}\frac{df}{d\eta}\right) - \frac{(d-1)}{\eta^2}f\right)\hat{\boldsymbol{\eta}} = 0. \tag{23}$$

This is solved by $f(\eta) = C/\eta^{d-1}$. The boundary condition Eq. (19b) then gives $f'(1) = -(d-1)C = -1$, so $C = 1/(d-1)$.

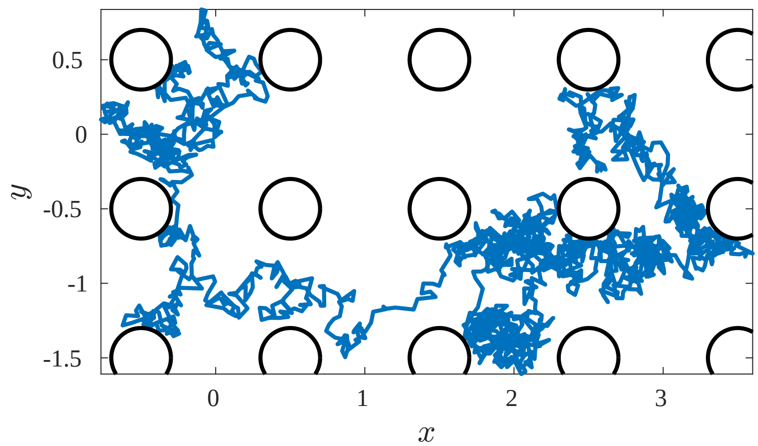

FIG. 1. Trajectory of a Brownian particle in an array of reflecting disks. The cells have size $\ell = 1$ and the disks have radius $\delta = .2\ell$.

We can immediately do the integral in Eq. (16) using only the inner solution:

$$\int_{\partial D} \boldsymbol{\chi}\, \hat{\boldsymbol{n}}_{\boldsymbol{r}}\, \mathrm{d}A_{\boldsymbol{r}} = \delta^d \int_{\partial D_1} \boldsymbol{\chi}^{(1)}_{\text{inner}}(\boldsymbol{\eta})\, \hat{\boldsymbol{n}}_{\boldsymbol{\eta}}\, \mathrm{d}A_{\boldsymbol{\eta}} = -C\delta^d \int_{\partial D_1} \hat{\boldsymbol{\eta}}\hat{\boldsymbol{\eta}}\, \mathrm{d}\Omega \tag{24}$$

where we used $\hat{\boldsymbol{n}}_{\boldsymbol{\eta}} = -\hat{\boldsymbol{\eta}}$ to ensure the normal is outward to $\Omega \setminus D$. By isotropy, the last integral must be proportional to $\mathbb{I}$, and its trace must be σ_d, the area of the unit sphere in d dimensions: $\sigma_1 = 2$, $\sigma_2 = 2\pi$, $\sigma_3 = 4\pi$, $\sigma_d = 2\pi^{d/2}/\Gamma(d/2)$. Hence,

$$\int_{\partial D} \boldsymbol{\chi}\, \hat{\boldsymbol{n}}_{\boldsymbol{r}}\, \mathrm{d}A_{\boldsymbol{r}} = -C\delta^d(\sigma_d/d)\, \mathbb{I} = -C\delta^d \nu_d\, \mathbb{I} = -C|D|\, \mathbb{I}, \qquad \nu_d = \pi^{d/2}/\Gamma(1 + d/2), \tag{25}$$

where $\nu_d = \sigma_d/d$ is the volume of the unit ball. The effective diffusivity from Eq. (16) is thus

$$\mathbb{D}_{\text{eff}} = \mathbb{I} - \frac{C}{|\Omega|/|D| - 1}\, \mathbb{I} \approx \mathbb{I} - \frac{|D|}{|\Omega|}\, C\, \mathbb{I}, \qquad |D| = \nu_d\, \delta^d. \tag{26}$$

The diffusivity *decreases*, due to reflection against the perforation. The tensor $\mathbb{D}_{\text{eff}}$ remains isotropic even when we take a rectangular cell; anisotropic diffusion only manifests itself at the next order in δ.

Appendix A: Properties of the effective diffusivity

It isn't obvious that the integral in Eq. (16) gives a symmetric tensor. Rewrite the integral as

$$\begin{aligned} \int_{\partial D} \boldsymbol{\chi}\, \hat{\boldsymbol{n}}\, \mathrm{d}A_{\boldsymbol{r}} &= -\int_{\partial D} \boldsymbol{\chi}\, \hat{\boldsymbol{n}} \cdot \nabla_{\boldsymbol{r}} \boldsymbol{\chi}\, \mathrm{d}A_{\boldsymbol{r}} \\ &= -\int_{\Omega \setminus D} \partial_{r_i}(\boldsymbol{\chi}\, \partial_{r_i} \boldsymbol{\chi})\, \mathrm{d}V_{\boldsymbol{r}} \\ &= -\int_{\Omega \setminus D} \boldsymbol{\chi}\, \Delta_{\boldsymbol{r}} \boldsymbol{\chi}\, \mathrm{d}V_{\boldsymbol{r}} - \int_{\Omega \setminus D} \partial_{r_i} \boldsymbol{\chi}\, \partial_{r_i} \boldsymbol{\chi}\, \mathrm{d}V_{\boldsymbol{r}}\, . \end{aligned} \tag{A1}$$

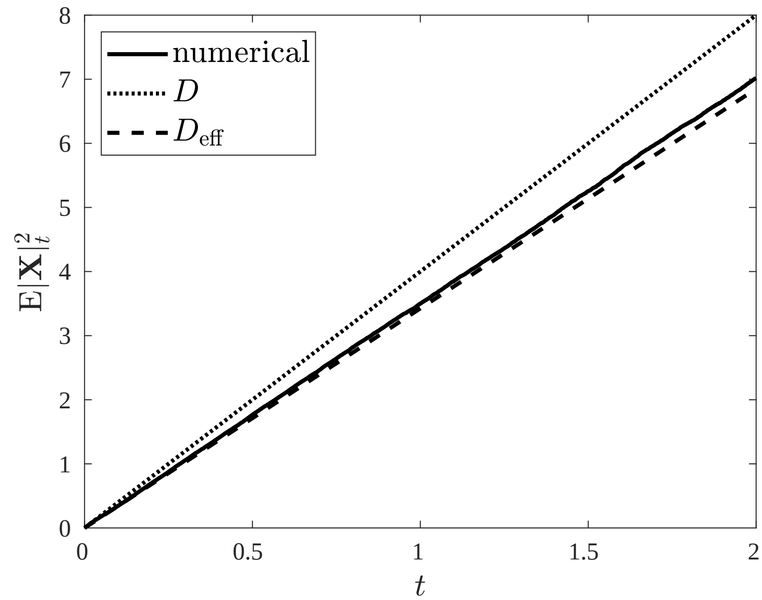

FIG. 2. For the array in Fig. 1: the solid line is the mean-squared displacement averaged over 20000 Brownian particles. The dotted line gives the molecular diffusivity, and the dashed line is the reduced effective diffusivity Eq. (26).

(Here and elsewhere we use and the fact integrals on $\partial\Omega$ vanish, by periodicity.) The term $\Delta_{\boldsymbol{r}}\boldsymbol{\chi}$ vanishes, and we are left with

$$\int_{\partial D} \boldsymbol{\chi}\, \hat{\boldsymbol{n}}\, \mathrm{d}A_{\boldsymbol{r}} = -\int_{\Omega\setminus D} \partial_{r_i}\boldsymbol{\chi}\, \partial_{r_i}\boldsymbol{\chi}\, \mathrm{d}V_{\boldsymbol{r}}\,. \tag{A2}$$

Since the right-hand dyadic is manifestly symmetric, so is the left. Moreover, this also shows that the integral is a *negative*-definite matrix, so that diffusion is always hindered by the perforation.

[1] M. Bruna and S. J. Chapman, 'Diffusion in spatially varying porous media,' *SIAM J. Appl. Math.* **75** (4), 1648–1674 (2015).

[2] U. Hornung, ed., *Homogenization and porous media* (Springer, New York, 1997).

[3] P. Moon and D. E. Spencer, 'The meaning of the vector Laplacian,' *J. Franklin Inst.* **256** (6), 551–558 (1953).

[4] L. Rayleigh, 'On the influence of obstacles arranged in rectangular order upon the properties of a medium,' *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science* **34** (211), 481–502 (1892).