Effective diffusivity: a dynamical systems approach

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Abstract

A dynamical systems approach to the effective parameter problem for advection-diffusion is presented.

1 The cell problem as a dynamical system

Consider the cell problem associated with the advection-diffusion equation

$$(\partial_t + \mathbf{u}\cdot\boldsymbol{\nabla} - \varepsilon\Delta)\chi_j(t,\mathbf{x}) = u_j(t,\mathbf{x}) \tag{1}$$

with velocity field

$$\mathbf{u}(t,\mathbf{x}) = (\cos y, \cos x) + \theta\cos t\,(\sin y, \sin x). \tag{2}$$

The components D^*_{jk}, $j,k = 1,\ldots,d$, of the effective diffusivity tensor D^* are given by

$$\mathsf{D}^*_{jk} = \varepsilon\delta_{jk} + \langle u_j, \chi_k\rangle_2, \tag{3}$$

where $\langle f,h\rangle = \langle f\,\overline{h}\rangle$ denotes the $L^2(\mathcal{T}\times\mathcal{V})$ inner-product over the period cell $\mathcal{T}\times\mathcal{V}$, $\langle\cdot\rangle$ denotes space-time average over $\mathcal{T}\times\mathcal{V}$, and $\overline{h}$ denotes complex conjugation of the function h. We stress that u_j and χ_k are *real-valued*. Inserting the formula for u_j in (1) into equation (3) yields

$$\mathsf{S}^*_{jk} = \varepsilon(\delta_{jk} + \langle\chi_j,\chi_k\rangle_1), \qquad \mathsf{A}^*_{jk} = \langle A\chi_j,\chi_k\rangle_1, \quad A = (-\Delta)^{-1}(\partial_t + \mathbf{u}\cdot\boldsymbol{\nabla}). \tag{4}$$

Here S^*_{jk} and A^*_{jk} are the components of the symmetric S^* and antisymmetric A^* parts of D^* and $\langle f,h\rangle_1 = \langle\boldsymbol{\nabla}f\cdot\boldsymbol{\nabla}h\rangle$.

Since $\chi(t,\cdot)\in\mathcal{H}^1_{\mathcal{V}}$ for each $t\in\mathcal{T}$ and the orthogonal set $\{\mathrm{e}^{\imath(mx+ny)}\}_{m,n\in\mathbb{Z}}$, is complete in $L^2(\mathcal{V})\supset\mathcal{H}^1_{\mathcal{V}}$, we can represent $\chi_j(t,\mathbf{x})$ by

$$\chi_j(t,\mathbf{x}) = \sum_{m,n} a^j_{m,n}(t)\,\mathrm{e}^{\imath(mx+ny)}, \quad a^j_{m,n}(t) = \langle\chi_j(t,\mathbf{x}),\mathrm{e}^{\imath(mx+ny)}\rangle_{\mathcal{V}}, \quad a^j_{m,n}(0) = a^j_{m,n}(2\pi), \tag{5}$$

where $\langle\cdot\rangle_{\mathcal{V}}$ denotes spatial averaging over the spatial period $\mathcal{V}$. Inserting the formula for χ_j in (5) into equation (1) yields

$$\sum_{m,n}\mathrm{e}^{\imath(mx+ny)}[\partial_t + \imath m u_1 + \imath n u_2 + \varepsilon(m^2+n^2)]a^j_{m,n} = u_j, \tag{6}$$

where we have written $\mathbf{u} = (u_1,u_2)$. Writing $\cos x = (\mathrm{e}^{\imath x}+\mathrm{e}^{-\imath x})/2$ and $\sin x = (\mathrm{e}^{\imath x}-\mathrm{e}^{-\imath x})/(2\imath)$, for example, equation (6) can be written, for $j=1$, as

$$\begin{aligned}\sum_{m,n}\mathrm{e}^{\imath(mx+ny)}[\partial_t a^1_{m,n} &+ \frac{\imath}{2}(m(a^1_{m,n-1}+a^1_{m,n+1}) + n(a^1_{m-1,n}+a^1_{m+1,n})) \\ &+\frac{\theta\cos t}{2}(m(a^1_{m,n-1}-a^1_{m,n+1}) + n(a^1_{m-1,n}-a^1_{m+1,n})) + \varepsilon(m^2+n^2)a^1_{m,n} \\ &-\frac{1}{2}\delta_{0,m}(\delta_{1,n}+\delta_{-1,n}) - \frac{\theta\cos t}{2\imath}\delta_{0,m}(\delta_{1,n}-\delta_{-1,n})] = 0,\end{aligned} \tag{7}$$

where $\delta_{l,m}$ is the Kronecker delta. Since $u_2(t,x,y) = u_1(t,y,x)$, the formula for $a^2_{m,n}$ follows from interchanging $\delta_{l,m}$ with $\delta_{l,n}$ in (7), $l = -1, 0, 1$. By the completeness of the orthogonal set $\{\mathrm{e}^{\imath(mx+ny)}\}$, equation (7) and its analogue for $a^2_{m,n}$ can be written as the following two (infinite) linear, coupled dynamical systems

$$\begin{aligned}
\partial_t a^1_{m,n} &+ \frac{\imath}{2}(m(a^1_{m,n-1} + a^1_{m,n+1}) + n(a^1_{m-1,n} + a^1_{m+1,n})) \\
&+ \frac{\theta \cos t}{2}(m(a^1_{m,n-1} - a^1_{m,n+1}) + n(a^1_{m-1,n} - a^1_{m+1,n})) + \varepsilon(m^2+n^2)a^1_{m,n}, \\
&= \frac{1}{2}\delta_{0,m}(\delta_{1,n} + \delta_{-1,n}) + \frac{\theta \cos t}{2\imath}\delta_{0,m}(\delta_{1,n} - \delta_{-1,n}), \\
\partial_t a^2_{m,n} &+ \frac{\imath}{2}(m(a^2_{m,n-1} + a^2_{m,n+1}) + n(a^2_{m-1,n} + a^2_{m+1,n})) \\
&+ \frac{\theta \cos t}{2}(m(a^2_{m,n-1} - a^2_{m,n+1}) + n(a^2_{m-1,n} - a^2_{m+1,n})) + \varepsilon(m^2+n^2)a^2_{m,n} \\
&= \frac{1}{2}\delta_{0,n}(\delta_{1,m} + \delta_{-1,m}) + \frac{\theta \cos t}{2\imath}\delta_{0,n}(\delta_{1,m} - \delta_{-1,m}),
\end{aligned} \tag{8}$$

with boundary condition $a^j_{m,n}(0) = a^j_{m,n}(2\pi)$, $j = 1, 2$, $m, n \in \mathbb{Z}$. When $\theta = 0$, the velocity field in (2) is time-independent. In this case the function χ_j, hence the Fourier coefficients $a^j_{m,n}$ are also time-independent, and equation (8) reduces to the following algebraic system of equations

$$\begin{aligned}
\frac{\imath}{2}(m(a^1_{m,n-1} + a^1_{m,n+1}) + n(a^1_{m-1,n} + a^1_{m+1,n})) + \varepsilon(m^2+n^2)a^1_{m,n} &= \frac{1}{2}\delta_{0,m}(\delta_{1,n} + \delta_{-1,n}) \\
\frac{\imath}{2}(m(a^2_{m,n-1} + a^2_{m,n+1}) + n(a^2_{m-1,n} + a^2_{m+1,n})) + \varepsilon(m^2+n^2)a^2_{m,n} &= \frac{1}{2}\delta_{0,n}(\delta_{1,m} + \delta_{-1,m}).
\end{aligned} \tag{9}$$

By restricting the indices, $-M \le \ell, m, n \le M$, and imposing the boundary conditions

$$a^l_{m,n} = 0 \quad \text{if} \quad \max(|m|,|n|) > M, \tag{10}$$

the infinite systems of equations in (8) and (9) become finite sets of equations. The bijective mapping

$$\Theta_s(m,n) = (M+m+1) + (M+n)(2M+1), \tag{11}$$

maps the finite sets of equations to matrix equations

$$\partial_t \mathbf{a}^j(t) = (A + \theta\cos t\, B + \varepsilon C)\mathbf{a}^j(t) + \boldsymbol{\xi}^j_1 + \theta \cos t\, \boldsymbol{\xi}^j_2, \quad \mathbf{a}^j(0) = \mathbf{a}^j(2\pi) \tag{12}$$

$$(A + \varepsilon C)\mathbf{a}^j = \boldsymbol{\xi}^j_1 \tag{13}$$

Equation (12) is a linear, inhomogeneous dynamical system of equations, while equation (13) is a linear system of algebraic equations. In equation (13), the rows and columns of the matrices A and C corresponding to the $a^j_{0,0}$ component of the unknown vector $\mathbf{a}^j$, consist entirely of zero elements, and can be removed without loss of generality. Consequently, for each $0 < \varepsilon < \infty$, this algebraic system in (13) can be directly solved using techniques of linear algebra, to determine the Fourier coefficients of χ_j in $\mathbf{a}^j$. Moreover, the matrix $(A + \varepsilon C)$ is *sparse*, so that iterative methods are applicable.

We now discuss how the symmetric S^* and antisymmetric A^* parts of the effective diffusivity tensor D^* are determined from the Fourier coefficients $a^j_{m,n}$ of χ_j. Inserting the formula for χ_j in (5) into the formula for S^*_{jk} in equation (4) and using the orthogonality of the set $\{\mathrm{e}^{\imath(mx+ny)}\}$ yields

$$\mathsf{S}^*_{jk}/\varepsilon - \delta_{jk} = \langle \chi_j, \chi_k \rangle_1 = \mathrm{Re} \sum_{m,n} (m^2+n^2)\, \langle a^j_{m,n}\, \overline{a^k_{m,n}} \rangle_{\mathcal{T}}. \tag{14}$$

Here, $\langle \cdot \rangle_{\mathcal{T}}$ denotes time averaging over the temporal period $\mathcal{T}$ and, since χ_j is real-valued, we have $\langle \chi_j, \chi_k \rangle_1 = \mathrm{Re}\, \langle \chi_j, \chi_k \rangle_1$. As discussed above, when $\theta = 0$, the Fourier coefficients $a^j_{m,n}$ are time-independent, so that $\langle a^j_{m,n}\, \overline{a^k_{m,n}} \rangle_{\mathcal{T}} = a^j_{m,n}\, \overline{a^k_{m,n}}$. Note that $\langle A\chi_j, \chi_k \rangle_1 = \langle \nabla(-\Delta)^{-1}(\partial_t + \boldsymbol{\nabla}\cdot\mathbf{u})\chi_j \cdot \nabla \chi_k \rangle = \langle (\partial_t + \boldsymbol{\nabla}\cdot\mathbf{u})\chi_j, \chi_k \rangle_2$.

Consequently, inserting the formula for χ_j in (5) into the formula for A^*_{jk} in equation (4) and using the orthogonality of the set $\{\mathrm{e}^{\imath(mx+ny)}\}$ yields

$$\begin{aligned}\langle A\chi_j, \chi_k\rangle_1 = \sum_{m,n} \langle \overline{\gamma^{\theta,j}_{m,n}}\, a^k_{m,n}\rangle_{\mathcal{T}}, \quad \gamma^{\theta,j}_{m,n} &= \partial_t a^j_{m,n} + \frac{\imath}{2}(m(a^j_{m,n-1} + a^j_{m,n+1}) + n(a^j_{m-1,n} + a^j_{m+1,n})) \\ &+ \frac{\theta \cos t}{2}(m(a^j_{m,n-1} - a^j_{m,n+1}) + n(a^j_{m-1,n} - a^j_{m+1,n})).\end{aligned} \tag{15}$$

When $\theta = 0$, the Fourier coefficients $a^j_{m,n}$ are time-independent, so that $\langle \overline{\gamma^{\theta,j}_{m,n}}\, a^k_{m,n}\rangle_t = \overline{\gamma^{\theta,j}_{m,n}}\, a^k_{m,n}$ and $\gamma^{\theta,j}_{m,n} = (m(a^j_{m,n-1} + a^j_{m,n+1}) + n(a^j_{m-1,n} + a^j_{m+1,n}))/(-2\imath)$.