Supplementary material to *Simulating Diffusion Processes in Discontinuous Media: Benchmark Tests*

Antoine Lejay[*†‡§] Géraldine Pichot[¶‖]

February 19, 2016

Abstract

In this short note, we give explicit derivations for the eigenfunctions and eigenvalues in a composite one-dimensional medium with two different diffusivities.

In the article [2], we use the spectral representation of the density $p(t,x,y)$ which solves the parabolic partial differential equation

$$\begin{cases} \dfrac{\partial p(t,x,y)}{t} = \nabla(D(y)\nabla p(t,x,y)),\ t>0,\ x,y\in[0,L], \\ p(t,x,y) \xrightarrow[t\to 0]{} \delta_x(y), \\ p(t,x,\cdot) \text{ satisfies prescribed boundary conditions at 0 and } L \end{cases}$$

to get a tractable expression to which we may compare Monte Carlo simulations. Indeed, if the $\{\lambda_k\}_{k\geq 0}$ are the eigenvalues with eigenfunctions ϕ_k defined by

$$\begin{cases} \nabla(D\nabla\phi_k) = -\lambda_k^2\phi_k, \\ \phi_k \text{ satisfies prescribed boundary conditions at 0 and } L, \\ \int_0^L \phi_k(x)^2\,\mathrm{d}x = 1 \end{cases}$$

then

$$p(t,x,y) = \sum_{k\geq 0} e^{-\lambda_k^2}\phi_k(x)\phi_k(y). \tag{1}$$

*Université de Lorraine, IECL, UMR 7502, Vandœuvre-lès-Nancy, F-54500, France

†CNRS, IECL, UMR 7502, Vandœuvre-lès-Nancy, F-54500, France

‡Inria, Villers-lès-Nancy, F-54600, France

§Contact: IECL, BP 70238, F-54506 Vandœuvre-lès-Nancy CEDEX, France. Email: Antoine.Lejay@univ-lorraine.fr

¶Inria, Rennes, France

‖Contact: Inria de Paris, Inria, 2 rue Simone Iff, CS 42112, 75589 Paris Cedex 12, France. Email: Geraldine.Pichot@inria.fr

Assuming that $\lambda_0 \leq \lambda_1 \leq \cdots$, then truncating (1) up to the first few terms is numerically sufficient.

Here, we consider the case where D takes only two values. This leads to rather simple computations this note aims at keeping track of. A large literature is devoted to deal with more general cases (See *e.g.* [1,3], ...).

1 Computing eigenvalues and eigenfunctions for the bimaterial problem

Consider a diffusivity

$$D(x) = \begin{cases} D^- \text{ if } x \in [0, L/2], \\ D^+ \text{ if } x \in [L/2, L]. \end{cases}$$

We are interested in solving the eigenvalue problem

$$\begin{cases} \nabla(D\nabla\phi(x)) = -\lambda^2\phi(x), \ x \in (0, L), \\ \phi'(L) = \phi'(0) = 0. \end{cases} \tag{2}$$

Formally, this eigenvalue problem shall be solved in the Sobolev space $\mathrm{H}^1([0, L])$. Since the problem is one-dimensional, there exists a continuous version of any eigenvalue, which we consider.

Fix $\lambda > 0$ and write $\alpha^\pm = \lambda/\sqrt{D^\pm}$.

The (non-normalized) eigenfunctions of (2) have the form

$$\phi(x, \lambda) = \begin{cases} \cos(\alpha^- x) & \text{if } x \in [0, L/2], \\ \gamma\cos(\alpha^+(L - x)) & \text{if } x \in [L/2, L], \end{cases}$$

with the conditions

$$\phi\left(\frac{L}{2}-, \lambda\right) = \phi\left(\frac{L}{2}+, \lambda\right) \text{ and } D^-\phi'\left(\frac{L}{2}-, \lambda\right) = D^+\phi'\left(\frac{L}{2}+, \lambda\right).$$

With $\beta = \sqrt{D^+}/\sqrt{D^-}$, the eigenvalues $-\lambda^2$ are given by

$$\lambda^2 = \frac{4z^2D^+}{L^2} \tag{3}$$

with

$$\beta\tan(z) + \tan(\beta z) = 0. \tag{4}$$

If z is solution to (4), then $-z$ is also solution to (4). Besides, $z = 0$ is solution to (4).

We plot in Figure 2 the map $f : z \mapsto \beta\tan(z)+\tan(\beta z)$. Let $J = \left\{(2k + 1)\frac{\pi}{2}; k \in \mathbb{N}\right\} \cup \left\{(2k + 1)\frac{\pi}{2\beta}; k \in \mathbb{N}\right\}$. Write $\mathbb{R}_+ \setminus J = \cup_{k\in\mathbb{N}}(\alpha_k, \alpha'_k)$ with $\alpha_0 = 0 < \alpha_0 < \alpha_1 < \alpha'_1 < \dots$.

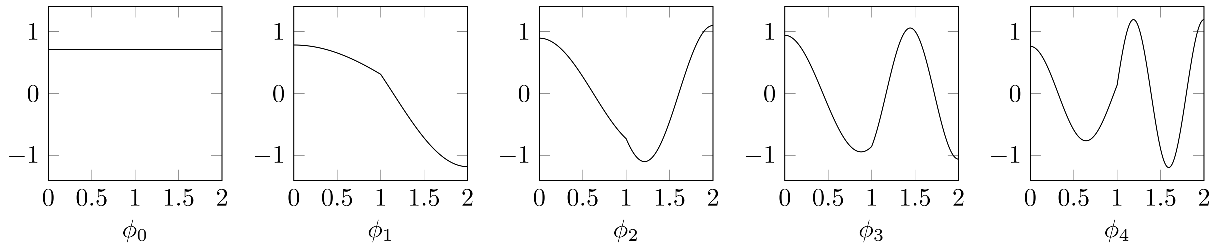

Figure 1: Eigenfunctions solution to (2) with a reflecting boundary conditions at $x = 0$ and $x = 2$ when $D^-/D^+ = 2.5$ corresponding to the smallest unsigned eigenvalues $0 = \lambda_0^2 < \lambda_1^2 < \lambda_2^2 < \lambda_3^2 < \lambda_4^2$.

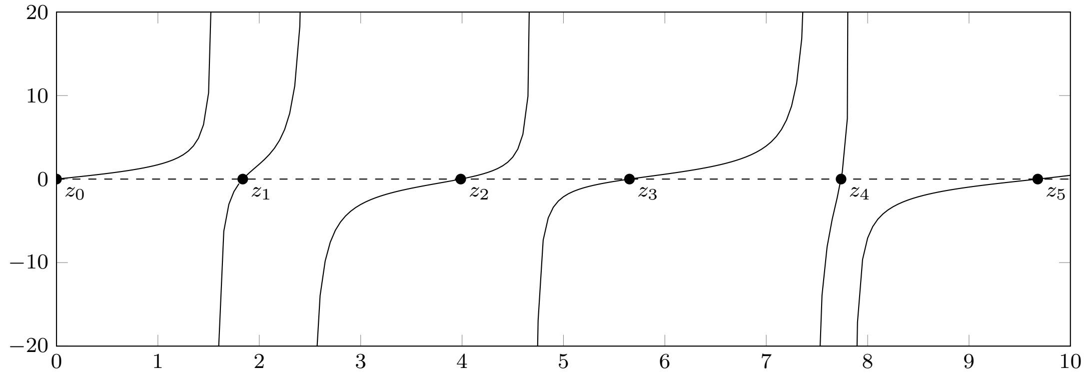

Figure 2: Plot of $z \mapsto \beta \tan(z) + \tan(\beta z)$ with $\beta = 1/\sqrt{2.5}$.

Then f restricted to (α_k, α'_k) is continuous and strictly increasing from $-\infty$ to $+\infty$ so that there exists only one root on each of these intervals.

Let z_k, $k = 0, 1, 2, \dots$ be the solutions to (4) with $z_0 = 0 < z_1 < z_2 < \cdots$. Let λ_k be the corresponding eigenvalues given by (3).

For an eigenvalue $-\lambda^2$, the eigenfunctions are continuous at $L/2$ so that

$$\gamma = \frac{\cos(\alpha^- L/2)}{\cos(\alpha^+ L/2)}$$

and

$$D^-\phi'(L/2-, \lambda) = -\lambda\sqrt{D^-}\sin(\alpha^- L/2),$$
$$D^+\phi'(L/2+, \lambda) = \lambda\sqrt{D^+}\sin(\alpha^+ L/2)\frac{\cos(\alpha^- L/2)}{\cos(\alpha^+ L/2)}.$$

Besides,

$$\kappa^2(\lambda) = \int_0^L \phi(x)^2\,\mathrm{d}x = \frac{L}{4}(1+\gamma^2) + \frac{\sin(\alpha^- L/2)\cos(\alpha^- L/2)}{2\alpha^-} + \gamma^2\frac{\sin(\alpha^+ L/2)\cos(\alpha^+ L/2)}{2\alpha^+}.$$

Set $\psi_k = \phi(\cdot, \lambda_k)/\kappa(\lambda_k)$. Hence, $\{\psi_k\}$ is an orthonormal basis with respect to the scalar product $\int_0^L f(x)g(x)\,\mathrm{d}x$. The density is the expressed as

$$p(t,x,y) = \frac{1}{L} + \sum_{k\geq 1} e^{-\lambda_k t}\psi_k(x)\psi_k(y).$$

Let X be the stochastic process generated by the operator $\nabla(D\nabla\cdot)$ with reflecting boundary conditions at 0 and L. It follows that

$$\mathbb{P}_x[X_t \geq L/2] = \int_{L/2}^{L} p(t,x,y)\,\mathrm{d}y = \frac{1}{2} + \sum_{k\geq 1} e^{-\lambda_k^2 t}\psi_k(x)\int_{L/2}^{L}\psi_k(y)\,\mathrm{d}y$$
$$\mathbb{P}_x[X_t \leq L/2] = \int_{L/2}^{L} p(t,x,y)\,\mathrm{d}y = \frac{1}{2} + \sum_{k\geq 1} e^{-\lambda_k^2 t}\psi_k(x)\int_{0}^{L/2}\psi_k(y)\,\mathrm{d}y.$$

A simple analytic expression holds for the constants, since

$$\int_0^{L/2}\psi(x)\,\mathrm{d}x = \frac{1}{\kappa}\frac{\sin(\alpha^- L/2)}{\alpha^-},$$
$$\text{and } \int_{L/2}^{L}\psi(x)\,\mathrm{d}x = \frac{\gamma}{\kappa}\frac{\sin(\alpha^+ L/2)}{\alpha^+}.$$

One could check that

$$\begin{aligned}\int_0^L \psi(x)\,\mathrm{d}x &= \frac{\sin(\alpha^- L/2)}{\alpha^-} + \frac{\cos(\alpha^- L/2)}{\cos(\alpha^+ L/2)}\frac{\sin(\alpha^+ L/2)}{\alpha^+}\\ &= \frac{\cos(\alpha^- L/2)}{\alpha^-}(\tan(\alpha^- L/2) + \frac{\alpha^-}{\alpha_+}\tan(\alpha^+ L/2))\\ &= \frac{\cos(\alpha^- L/2)}{\alpha^-}(\tan(\beta z) + \beta\tan(z)) = 0\end{aligned}$$

with $z = \lambda L/2\sqrt{D^+} = \alpha^+ L/2$.

2 Computing eigenvalues and eigenfunctions for the bimaterial problem with an absorbing condition

Let us consider now the eigenvalue problem with a reflecting condition at 0 and an absorbing condition at L:

$$\begin{cases}\nabla(D\nabla\phi(x)) = -\lambda^2\phi(x),\ x\in(0,L),\\ \phi(L) = 0,\\ \phi'(0) = 0.\end{cases} \tag{5}$$

As above, the (non-normalized) eigenfunctions of (5) have the form

$$\phi(x,\lambda) = \begin{cases} \cos(\alpha^- x) & \text{if } x \in [0, L/2], \\ \gamma \sin(\alpha^+(L-x)) & \text{if } x \in [L/2, L] \end{cases}$$

with the conditions

$$\phi\left(\frac{L}{2}-,\lambda\right) = \phi\left(\frac{L}{2}+,\lambda\right) \text{ and } D^-\phi'\left(\frac{L}{2}-,\lambda\right) = D^+\phi'\left(\frac{L}{2}+,\lambda\right).$$

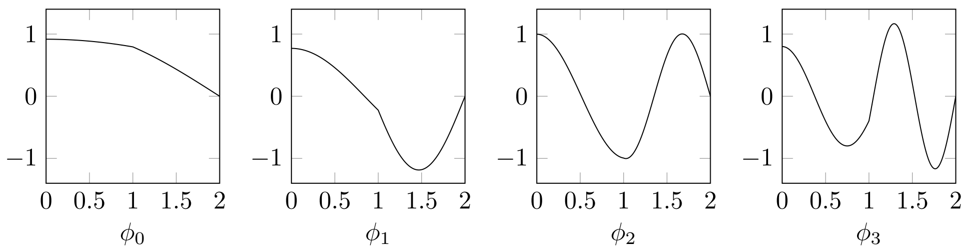

Figure 3: Eigenfunctions solution to (5) with a reflecting boundary conditions at $x = 0$ and an absorbing boundary condition at $x = 2$ when $D^-/D^+ = 2.5$ corresponding to the smallest unsigned eigenvalues $\lambda_0^2 < \lambda_1^2 < \lambda_2^2 < \lambda_3^2$.

With $\beta = \sqrt{D^+}/\sqrt{D^-}$ and z given by (3),

$$\cos\left(\frac{\lambda}{\sqrt{D^-}}\frac{L}{2}\right) = \cos\left(\frac{\beta\lambda}{\sqrt{D^+}}\frac{L}{2}\right) = \cos(\beta z) = \gamma \sin\left(\frac{\lambda}{\sqrt{D^+}}\frac{L}{2}\right) = \gamma \sin(z) \tag{6}$$

and

$$\sqrt{D^-}\sin(\beta z) = \sqrt{D^+}\gamma\cos(z). \tag{7}$$

Dividing (6) by (7) when possible,

$$\frac{1}{\tan(\beta z)} - \frac{\tan(z)}{\beta} = 0. \tag{8}$$

If z is solution to (8), $-z$ is also solution to (8). However, z is not a solution because $f : z \mapsto 1/\tan(\beta z) - \tan(z)/\beta$ converges to $+\infty$ as $z \to 0$.

Set $J = \cup_{k\geq 0}\{k\pi/\beta\} \cup \{(2k+1)\pi/2\}$, then $\mathbb{R}_+ \setminus J = \cup_{k\geq 0}(\alpha_k, \alpha'_k)$ with $\alpha_0 < \alpha'_0 < \alpha_1 < \alpha'_1 < \cdots$ and f is defined on each interval (α_k, α'_k) and is strictly decreasing (See Figure 4).

From (6),

$$\gamma = \frac{\cos(\beta z)}{\sin(z)}.$$

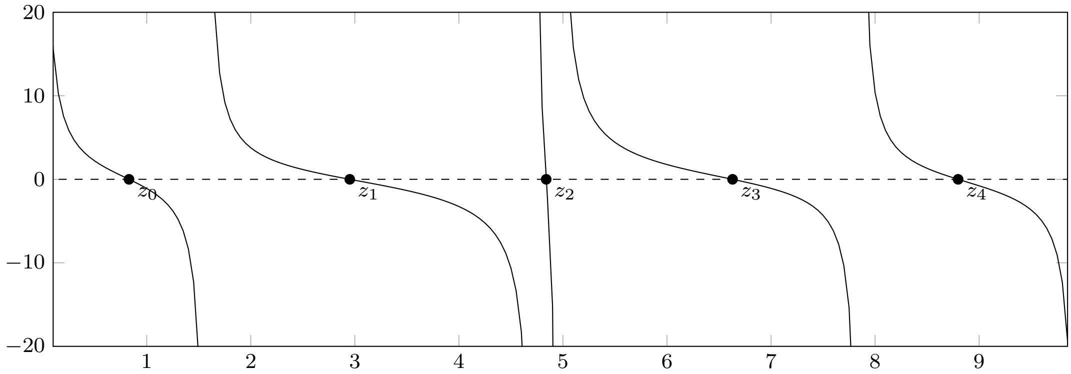

Figure 4: Plot of $z \mapsto 1/\tan(\beta z) - \tan(z)/\beta$ with $\beta = 1/\sqrt{2.5}$.

For an eigenvalue $-\lambda^2$,

$$\int_0^{L/2} \cos^2(\alpha^- x)\,\mathrm{d}x = \frac{L}{4} + \frac{\sin(\alpha^- L)}{4\alpha^-}$$
$$\text{and } \int_{L/2}^{L} \sin^2(\alpha^+(L-x))\,\mathrm{d}x = \frac{L}{4} - \frac{\sin(\alpha^+ L)}{4\alpha^+}.$$

Thus,

$$\kappa(\lambda)^2 = \int_0^L \phi(x,\lambda)^2\,\mathrm{d}x = \frac{L}{4}(1+\gamma^2) + \frac{\sin(\alpha^- L)}{4\alpha^-} - \gamma^2\frac{\sin(\alpha^+ L)}{4\alpha^+}.$$

Since $z = \alpha^+ L/2$ and $\beta z = \alpha^- L/2$,

$$\kappa(\lambda)^2 = \frac{L}{4}(1+\gamma^2) + \sqrt{D^-}\frac{\sin(2\beta z)}{4\lambda} - \gamma^2\sqrt{D^+}\frac{\sin(2z)}{4\lambda}.$$

We have also that

$$\int_0^L \phi(x,\lambda)\,\mathrm{d}x = \frac{\sin(\alpha^- L/2)}{\alpha^-} + \frac{\gamma}{\alpha^+} - \gamma\frac{\cos(\alpha^+ L/2)}{\alpha^+} = \frac{\sin(\beta z)}{2\alpha^-} + \frac{\gamma}{\alpha^+} - \gamma\frac{\cos(z)}{\alpha^+}.$$

Let $z_0 < z_1 < \cdots$ be the solutions to (8) and λ_k^2, $k \geq 0$ be the corresponding eigenvalues through (3). Let ψ_k be the orthonormal eigenvalues associated with $\psi_k = \phi(\cdot, \lambda_k)/\kappa(\lambda)$.

The density of the process X generated by $\nabla(D\nabla\cdot)$ with a reflecting boundary condition at 0 and an absorbing boundary condition at L is

$$p(t,x,y) = \sum_{k\geq 0} e^{-\lambda_k^2 t}\psi_k(x)\psi_k(y).$$

Let $\tau = \inf\{t > 0; X_t = L\}$. Then

$$\mathbb{P}[t < \tau] = \int_0^L p(t,x,y)\,\mathrm{d}y = \sum_{k\geq 0} e^{-\lambda_k^2 t}\psi_k(x)\int_0^L \psi_k(y)\,\mathrm{d}y.$$

The distribution function G of τ is $G(t) = \mathbb{P}[\tau < t] = 1 - \mathbb{P}[t < \tau]$ so that an analytic expression for G may be given.

Bibliography

[1] B. Gaveau, M. Okada, and T. Okada, *Second order differential operators and Dirichlet integrals with singular coefficients. I. Functional calculus of one-dimensional operators*, Tohoku Math. J. (2) **39** (1987), no. 4, 465–504.

[2] A. Lejay and G. Pichot, *Simulating Diffusion Processes in Discontinuous Media: Benchmark Tests* (2014).

[3] J. D. Pryce, *Numerical solution of Sturm-Liouville problems*, Monographs on Numerical Analysis, The Clarendon Press Oxford University Press, 1993. Oxford Science Publications.