

Semi-analytic solution of the 1D multilayer diffusion problem with an application to macroscopic modelling

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Elliot Carr
(elliot.carr@qut.edu.au)



School of Mathematical Sciences
Queensland University of Technology

Joint work with...



Prof. Ian Turner
(Mathematical Sciences, QUT)

Diffusion (Homogeneous medium)

- ▶ Diffusion in a homogeneous medium:



- ▶ Diffusion problem:

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2} \quad l_0 < x < l_m$$

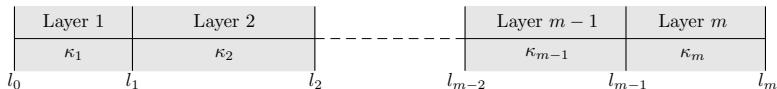
Initial condition $u(x, 0) = f(x)$ and external boundary conditions:

$$a_L u(l_0, t) + b_L \frac{\partial u}{\partial x}(l_0, t) = c_L \quad a_R u(l_m, t) + b_R \frac{\partial u}{\partial x}(l_m, t) = c_R$$

- ▶ **Multilayer diffusion:** What if the diffusivity is piecewise constant?

Multilayer diffusion (Heterogeneous medium)

- ▶ Diffusion in a heterogeneous medium consisting of m layers:



- ▶ Multilayer diffusion problem:

$$\frac{\partial u_i}{\partial t} = \kappa_i \frac{\partial^2 u_i}{\partial x^2} \quad l_{i-1} < x < l_i$$

Initial condition $u_i(x, 0) = f(x)$ and external boundary conditions:

$$a_L u_1(l_0, t) + b_L \frac{\partial u_1}{\partial x}(l_0, t) = c_L \quad a_R u_m(l_m, t) + b_R \frac{\partial u_m}{\partial x}(l_m, t) = c_R$$

Suitable internal boundary conditions at the interfaces ($i = 1, \dots, m-1$), e.g.,

$$u_i(l_i, t) = u_{i+1}(l_i, t) \quad \kappa_i \frac{\partial u_i}{\partial x}(l_i, t) = \kappa_{i+1} \frac{\partial u_{i+1}}{\partial x}(l_i, t)$$

Why are we interested in this problem?

- ▶ Many authors have been interested in this problem:
 - [de Monte \(2000, 2002\)](#)
 - [Sun and Wichman \(2004\)](#)
 - [Hickson et al. \(2009a,b, 2011\)](#)
 - [Deconinck et al. \(2014\)](#)
 - [Asvestas et al. \(2014\)](#)
 - [Mantzavinos et al. \(2014\)](#)
 - [Rodrigo and Worthy \(2016\)](#)
- ▶ ARC DECRA Project (2015–2018):
Two-scale modelling of transport processes in heterogeneous materials exhibiting small-scale heterogeneities in material properties
- ▶ Multilayer diffusion provides a good prototype problem for developing and testing macroscopic and two-scale approaches

Analytic solution for single layer diffusion

- ▶ Exact solution can be expressed as:

$$u(x, t) = w(x) + \sum_{n=0}^{\infty} c_n e^{-t\lambda_n^2} \phi_n(x)$$

- ▶ Eigenvalues and eigenfunctions satisfy:

$$\begin{aligned} -\kappa \frac{d^2 \phi_n}{dx^2} &= \lambda_n^2 \phi_n & l_0 < x < l_m \\ a_L \phi_n + b_L \frac{d\phi_n}{dx} &= 0 & x = l_0 \\ a_R \phi_n + b_R \frac{d\phi_n}{dx} &= 0 & x = l_m \end{aligned}$$

- ▶ The eigenfunctions take the form:

$$\phi_n(x) = \alpha_n \sin\left(\frac{\lambda_n}{\sqrt{\kappa}}(x - l_0)\right) + \beta_n \cos\left(\frac{\lambda_n}{\sqrt{\kappa}}(x - l_0)\right)$$

Analytic solution for single layer diffusion

- ▶ Substituting into the boundary conditions we obtain a system of two linear equations in two unknowns. For example, assuming $a_L = a_R = 1$ and $b_L = b_R = 0$, for simplicity, we obtain:

$$\begin{bmatrix} 0 & 1 \\ \sin\left(\frac{\lambda_n}{\sqrt{\kappa}}(l_m - l_0)\right) & \cos\left(\frac{\lambda_n}{\sqrt{\kappa}}(l_m - l_0)\right) \end{bmatrix} \begin{bmatrix} \alpha_n \\ \beta_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Leftrightarrow \mathbf{Ax} = \mathbf{0}$$

- ▶ We want non-trivial solutions (i.e., at least one of α_n or β_n nonzero) to this linear system. Hence, eigenvalues λ_n ($n = 0, 1, \dots$) are the roots of the transcendental equation:

$$\det(\mathbf{A}) = 0 \Rightarrow \sin\left(\frac{\lambda_n}{\sqrt{\kappa}}(l_m - l_0)\right) = 0 \Rightarrow \lambda_n = \frac{(n+1)\pi\sqrt{\kappa}}{l_m - l_0}$$

Analytic solution for multilayer diffusion

- ▶ **Hickson et al. (2009a)**: Exact solution in each layer can be expressed as:

$$u_i(x, t) = w_i(x) + \sum_{n=0}^{\infty} c_n e^{-t\lambda_n^2} \phi_{i,n}(x)$$

- ▶ Eigenvalues and eigenfunctions satisfy:

$$-\kappa_i \frac{d^2 \phi_{i,n}}{dx^2} = \lambda_n^2 \phi_{i,n} \quad l_{i-1} < x < l_i, \quad i = 1, \dots, m$$

$$a_L \phi_{1,n} + b_L \frac{d\phi_{1,n}}{dx} = 0 \quad x = l_0$$

$$a_R \phi_{m,n} + b_R \frac{d\phi_{m,n}}{dx} = 0 \quad x = l_m$$

$$\phi_{i,n} = \phi_{i+1,n}, \quad \kappa_i \frac{d\phi_{i,n}}{dx} = \kappa_{i+1} \frac{d\phi_{i+1,n}}{dx} \quad x = l_i, \quad i = 1, \dots, m-1$$

- ▶ The eigenfunctions take the form:

$$\phi_{i,n}(x) = \alpha_{i,n} \sin\left(\frac{\lambda_n}{\sqrt{\kappa_i}}(x - l_{i-1})\right) + \beta_{i,n} \cos\left(\frac{\lambda_n}{\sqrt{\kappa_i}}(x - l_{i-1})\right)$$

Analytic solution for multilayer diffusion

- ▶ Substituting into the boundary conditions we obtain a system of $2m$ linear equations in $2m$ unknowns:

$$\mathbf{A}\mathbf{x} = \mathbf{0}$$

where $\mathbf{A} \in \mathbb{R}^{2m \times 2m}$ and $\mathbf{x} = (\alpha_{1,n}, \beta_{1,n}, \dots, \alpha_{m,n}, \beta_{m,n})^T \in \mathbb{R}^{2m}$.

- ▶ We want non-trivial solutions to this linear system. Hence, eigenvalues λ_n ($n = 0, 1, \dots$) are the roots of the transcendental equation:

$$\det(\mathbf{A}) = 0 \quad \Rightarrow \quad f(\lambda_n) = 0$$

where, if m is large, f is a very complex function of λ_n .

- ▶ For a large number of layers (large m):
 - ✗ computing $\det(\mathbf{A})$ is numerically unstable
- ▶ I couldn't get it working beyond 10 layers

Semi-analytic solution for multilayer diffusion

Carr and Turner (2015): The solution is split into two parts:

$$u_i(x, t) = w_i(x) + v_i(x, t)$$

where $w_i(x)$ is the steady state solution and $v_i(x, t)$ satisfies:

$$\frac{\partial v_i}{\partial t} = \kappa_i \frac{\partial^2 v_i}{\partial x^2} \quad l_{i-1} < x < l_i$$

subject to the initial, internal and external boundary conditions:

$$v_i(x, 0) = f(x) - w_i(x) \quad i = 1, \dots, m$$

$$a_L v_1(l_0, t) + b_L \frac{\partial v_1}{\partial x}(l_0, t) = 0$$

$$a_R v_m(l_m, t) + b_R \frac{\partial v_m}{\partial x}(l_m, t) = 0$$

$$v_i(l_i, t) = v_{i+1}(l_i, t) \quad i = 1, \dots, m - 1$$

$$\kappa_i \frac{\partial v_i}{\partial x}(l_i, t) = \kappa_{i+1} \frac{\partial v_{i+1}}{\partial x}(l_i, t) \equiv g_i(t) \quad i = 1, \dots, m - 1$$

Semi-analytic solution for multilayer diffusion

- ▶ Take Laplace transforms, the transformed solution can be expressed as an orthogonal eigenfunction expansion:

$$\bar{v}_i(x, s) = \sum_{n=0}^{\infty} \langle \bar{v}_i, \phi_{i,n} \rangle_i \phi_{i,n}(x) \quad \langle f, g \rangle_i = \int_{l_{i-1}}^{l_i} f(x)g(x) dx$$

- ▶ Eigenvalues and eigenfunctions satisfy:

$$-\frac{d^2 \phi_{i,n}}{dx^2} = \lambda_{i,n}^2 \phi_{i,n}$$

subject to boundary conditions local to each layer:

$$\boxed{\text{Layer } i = 1:} \quad a_L \phi_{1,n}(l_0) + b_L \frac{d\phi_{1,n}}{dx}(l_0) = 0 \text{ and } \frac{d\phi_{1,n}}{dx}(l_1) = 0$$

$$\boxed{\text{Layer } i = 2, \dots, m-1:} \quad \frac{d\phi_{i,n}}{dx}(l_{i-1}) = 0 \text{ and } \frac{d\phi_{i,n}}{dx}(l_i) = 0$$

$$\boxed{\text{Layer } i = m:} \quad \frac{d\phi_{m,n}}{dx}(l_{m-1}) = 0 \text{ and } a_R \phi_{m,n}(l_m) + b_R \frac{d\phi_{m,n}}{dx}(l_m) = 0$$

Semi-analytic solution for multilayer diffusion

- ▶ Eigenvalues are roots of simple transcendental equations:

Layer $i = 1$: $\lambda_{1,n}$ are positive roots of

$$a_L \lambda \tan(\lambda(l_1 - l_0)) = -b_L$$

Layer $i = 2, \dots, m - 1$: $\lambda_{i,n}$ are non-negative roots of

$$\sin(\lambda(l_i - l_{i-1})) = 0 \quad \Rightarrow \quad \lambda_{i,n} = \frac{n\pi}{l_i - l_{i-1}}$$

Layer $i = m$: $\lambda_{m,n}$ are positive roots of

$$a_R \lambda \tan(\lambda(l_m - l_{m-1})) = -b_R$$

- ▶ Inverting the Laplace transformed solution, the solution within each layer is expressed in terms of inverse Laplace transforms $\bar{g}_i(s) = \mathcal{L}\{g_i(t)\}$. For example, in the first layer:

$$u_1(x, t) = w_1(x) + \sum_{n=0}^{\infty} \left[c_{1,n} e^{-t\kappa_1 \lambda_{1,n}^2} + \mathcal{L}^{-1} \left\{ \frac{\bar{g}_1(s)}{s + \kappa_1 \lambda_{1,n}^2} \right\} \phi_{1,n}(l_1) \right] \phi_{1,n}(x)$$

Semi-analytic solution for multilayer diffusion

- ▶ Inverse Laplace transforms are computed numerically:

$$\mathcal{L}^{-1} \left\{ \frac{\bar{g}_i(s)}{s + \kappa_i \lambda_n^2} \right\} \approx -2\Re \left\{ \sum_{k=1}^{N/2} c_k \frac{\bar{g}_i(z_k/t)}{z_k + \kappa_i \lambda_n^2 t} \right\},$$

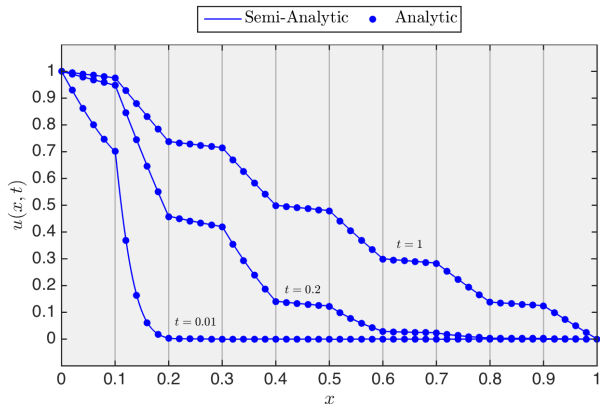
where c_k and z_k are the residues and poles of the best (N, N) rational approximation to e^z on the negative real line computed using the Carathéodory-Fejér method [[Trefethen et al. \(2006\)](#)].

- ▶ To compute $\bar{g}_i(z_k/t)$ ($i = 1, \dots, m-1$) we solve an $(m-1) \times (m-1)$ tridiagonal linear system:

$$\begin{aligned} \bar{v}_1(l_1, z_k/t) &= \bar{v}_2(l_1, z_k/t) \\ \bar{v}_2(l_2, z_k/t) &= \bar{v}_3(l_2, z_k/t) \\ &\vdots \\ \bar{v}_{m-1}(l_{m-1}, z_k/t) &= \bar{v}_m(l_{m-1}, z_k/t) \end{aligned}$$

which come from the interface conditions: $\bar{v}_i(l_i, s) = \bar{v}_{i+1}(l_i, s)$.

Example

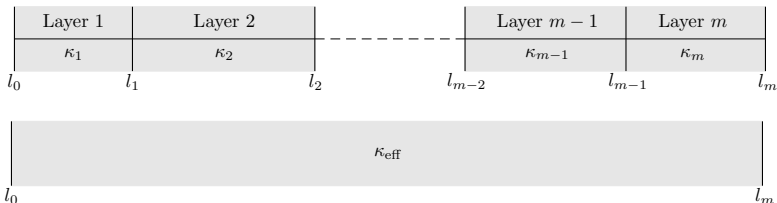


$$\text{Diffusivities } \kappa_i = \begin{cases} 1.0 & \text{if } i \text{ is odd} \\ 0.1 & \text{if } i \text{ is even} \end{cases} \quad (i = 1, \dots, 10)$$

Problem originally appeared in [Hickson et al. \(2009b\)](#).

Application to macroscopic modelling

- ▶ Replace heterogeneous medium with an effective homogeneous medium:



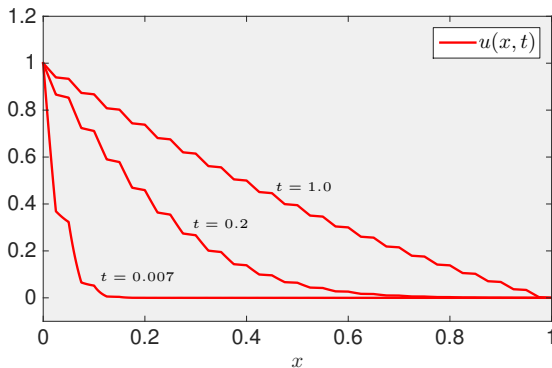
- ▶ Macroscopic equation:

$$\frac{\partial U}{\partial t} = \kappa_{\text{eff}} \frac{\partial^2 U}{\partial x^2} \quad l_0 < x < l_m$$

where $u_i(x, t) \simeq U(x, t)$ for all $x \in (l_{i-1}, l_i)$ and $i = 1, \dots, m$, and

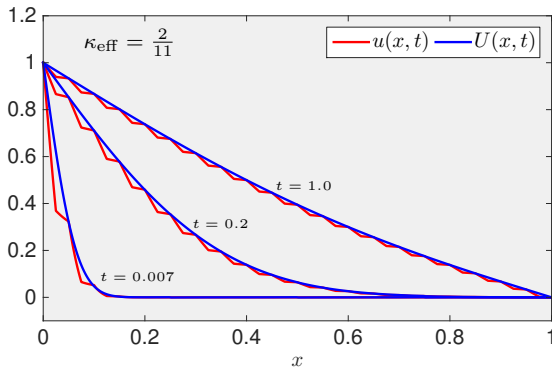
$$\kappa_{\text{eff}} = \left(\frac{1}{l_m - l_0} \sum_{i=1}^m \frac{l_i - l_{i-1}}{\kappa_i} \right)^{-1}$$

Application to macroscopic modelling



$$\text{Diffusivities } \kappa_i = \begin{cases} 0.1 & \text{if } i \text{ is odd} \\ 1.0 & \text{if } i \text{ is even} \end{cases} \quad (i = 1, \dots, 40)$$

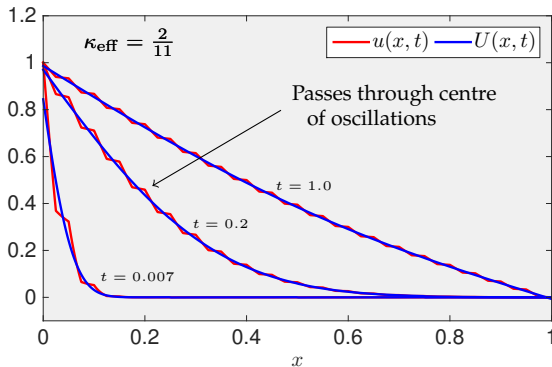
Application to macroscopic modelling



Macroscopic BCs: $U(0, t) = 1$ and $U(1, t) = 0$

$$\frac{\|U(x, t) - u(x, t)\|_2}{\|u(x, t)\|_2} = 4.94 \times 10^{-2} \text{ at } t = 0.2$$

Application to macroscopic modelling



Macroscopic BCs ($\sigma = -9/880$): $U(0, t) + \sigma \frac{\partial U}{\partial x}(0, t) = 1$ and $U(1, t) + \sigma \frac{\partial U}{\partial x}(1, t) = 0$

$$\frac{\|U(x, t) - u(x, t)\|_2}{\|u(x, t)\|_2} = 2.39 \times 10^{-2} \text{ at } t = 0.2$$

Summary

- ▶ Presented a new semi-analytic method for solving the transient diffusion equation in a one-dimensional composite medium consisting of m layers
- ▶ Method is based on the Laplace transform and an orthogonal eigenfunction expansion using simple or classical Sturm-Liouville problems that are local to each layer and not coupled across layers
- ▶ Method is valid for both perfect and imperfect contact at the interfaces and Dirichlet, Neumann or Robin conditions at the boundaries
- ▶ Advantages of semi-analytic method:
 - ✓ Avoids solving a complex transcendental equation for the eigenvalues involving the matrix determinant
 - ✓ Eigenvalues are roots of simple transcendental equations
 - ✓ Works well for a large number of layers (tested up to 10,000 layers with no problems)
- ▶ MATLAB code is available at: <http://github.com/elliottcarr/MultDiff>

Thank you!

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