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

QANZIAM Meeting, University of Queensland, 25 November 2015

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

QUT

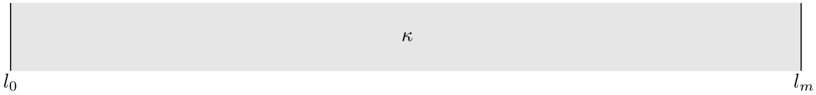
School of Mathematical Sciences
Queensland University of Technology

Joint work with...

Prof. Ian Turner
(Mathematical Sciences, QUT)

Diffusion (Homogeneous medium)

- Diffusion in a homogeneous medium:



- Diffusion problem:

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

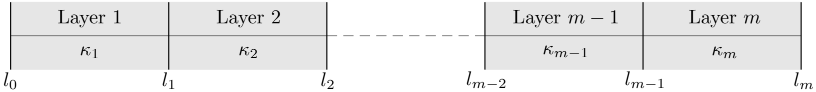
Initial condition $u(x, 0) = f(x)$ and external boundary conditions:

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

- **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:

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

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

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

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

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

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 (2015)**
- ARC DECRA Project (2015–2018):
  Two-scale modelling of transport/fluid flow in heterogeneous materials exhibiting small-scale heterogeneities in material properties
- Multilayer diffusion provides a good prototype problem for developing and testing 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:

$$-\kappa \frac{d^2\phi_n}{dx^2} = \lambda_n^2 \phi_n \qquad l_0 < x < l_m$$

$$a_L \phi_n + b_L \frac{d\phi_n}{dx} = 0 \qquad x = l_0$$

$$a_R \phi_n + b_R \frac{d\phi_n}{dx} = 0 \qquad x = l_m$$

- 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:

$$\begin{bmatrix} 0 & 1 \\ \sin\left(\frac{\lambda_n}{\sqrt{\kappa}}(l_1 - l_0)\right) & \cos\left(\frac{\lambda_n}{\sqrt{\kappa}}(l_1 - l_0)\right) \end{bmatrix} \begin{bmatrix} \alpha_n \\ \beta_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Leftrightarrow \quad \mathbf{A}\mathbf{x} = \mathbf{0}$$

- 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 $(n = 0, 1, \ldots)$ are the roots of the transcendental equation:

$$\det(\mathbf{A}) = 0 \quad \Rightarrow \quad \sin\left(\frac{\lambda_n}{\sqrt{\kappa}}(l_1 - l_0)\right) = 0 \quad \Rightarrow \quad \lambda_n = \frac{(n+1)\pi\sqrt{\kappa}}{l_1 - l_0}$$

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:

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

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

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

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

- 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 $\mathbf{x} = (\alpha_{1,n}, \beta_{1,n}, \ldots, \alpha_{m,n}, \beta_{m,n})^T \in \mathbb{R}^{2m}$.

- We want non-trivial solutions to this linear system. Hence, eigenvalues λ_n ($n = 0, 1, \ldots$) 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!) complicated function of λ_n.

- For a large number of layers (large m):
  - ✗ computing $\det(\mathbf{A})$ is numerically unstable
  - ✗ risk of missing eigenvalues

- 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:

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

subject to the initial, internal and external boundary conditions:

$$\begin{aligned}
v_i(x,0) &= f(x) - w_i(x) \qquad && i = 1,\ldots,m \\
a_L v_1(l_0,t) + b_L \frac{\partial v_1}{\partial x}(l_0,t) &= 0 && \\
a_R v_m(l_m,t) + b_R \frac{\partial v_m}{\partial x}(l_m,t) &= 0 && \\
v_i(l_i,t) &= v_{i+1}(l_i,t) && i = 1,\ldots,m-1 \\
\kappa_i \frac{\partial v_i}{\partial x}(l_i,t) = \kappa_{i+1} \frac{\partial v_{i+1}}{\partial x}(l_i,t) &\equiv g_i(t) && i = 1,\ldots,m-1
\end{aligned}$$

Semi-analytic solution for multilayer diffusion

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

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

- 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:

Layer $i = 1$:	$a_L \phi_{1,n}(l_0) + b_L \frac{d\phi_{1,n}}{dx}(l_0) = 0$ and $\frac{d\phi_{1,n}}{dx}(l_1) = 0$
Layer $i = 2, \ldots, m-1$:	$\frac{d\phi_{i,n}}{dx}(l_{i-1}) = 0$ and $\frac{d\phi_{i,n}}{dx}(l_i) = 0$
Layer $i = m$:	$\frac{d\phi_{m,n}}{dx}(l_{m-1}) = 0$ 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 $i = 2, \ldots, m-1$: $\lambda_{i,n}$ are non-negative roots of
  $$\sin(\lambda(l_i - l_{i-1})) = 0 \quad \Rightarrow \quad \lambda_n = \frac{n\pi}{l_i - l_{i-1}}$$

  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 involving the interface functions: $\overline{g}_i(s) = \mathcal{L}^{-1}\{g_i(t)\}$. For example, in the first layer:

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

Semi-analytic solution for multilayer diffusion

- Inverse Laplace transforms are computed numerically:

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

  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 $\overline{g}_i(z_{2k-1}/t)$ $(i = 1, \ldots, m)$ we solve an $(m-1)\times(m-1)$ tridiagonal linear system:

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

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

Solution verification

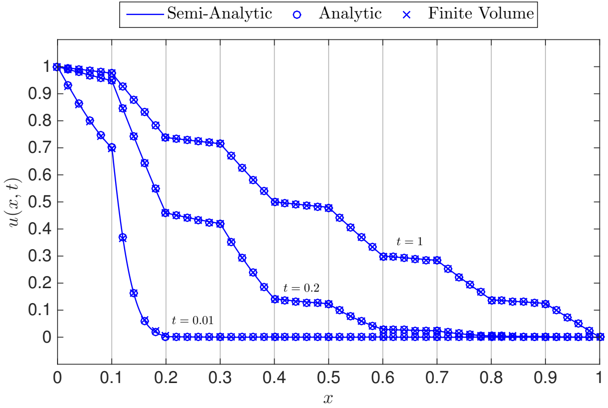
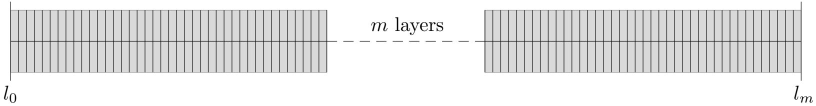


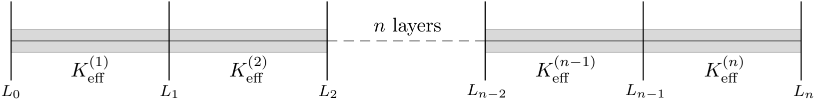
Figure: Diffusivities $\kappa = [1.0, 0.1, 1.0, 0.1, 1.0, 0.1, 1.0, 0.1, 1.0, 0.1]$.
Problem originally appeared in **Hickson et al. (2009b)**.

Application to macroscopic modelling

- **Fine-scale model**: composite medium consisting of m layers



- **Macroscopic model**: composite medium consisting of n layers ($n \ll m$)



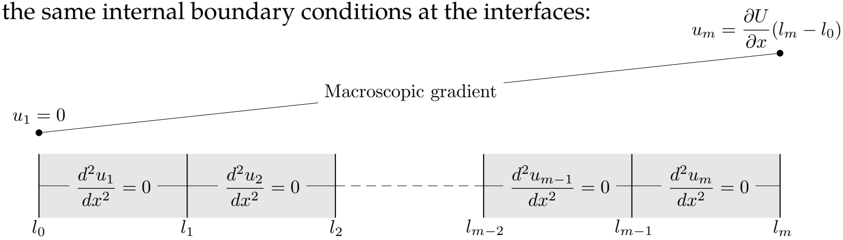
Macroscopic equation:

$$\frac{\partial U_k}{\partial t} = K_{\text{eff}}^{(k)} \frac{\partial^2 U_k}{\partial x^2} \qquad L_{k-1} < x < L_k$$

where $K_{\text{eff}}^{(k)}$ is the *effective (macroscopic) diffusivity* in the kth macro-layer defined as the harmonic average of the fine-layer diffusivities comprising the kth macro-layer.

Application to macroscopic modelling

- Apply a macroscopic gradient $\dfrac{\partial U}{\partial x}$ and solve the steady state problem with the same internal boundary conditions at the interfaces:



- One can show that the effective (macroscopic) flux is given by:

$$q_{\text{eff}} = \frac{1}{l_m - l_0}\sum_{i=1}^{m}\left(\int_{l_{i-1}}^{l_i} -\kappa_i \frac{du_i}{dx}\,dx\right) = -\underbrace{\left(\frac{1}{l_m - l_0}\sum_{i=1}^{m}\frac{l_i - l_{i-1}}{\kappa_i}\right)^{-1}}_{K_{\text{eff}}}\frac{\partial U}{\partial x}$$

Application to macroscopic modelling

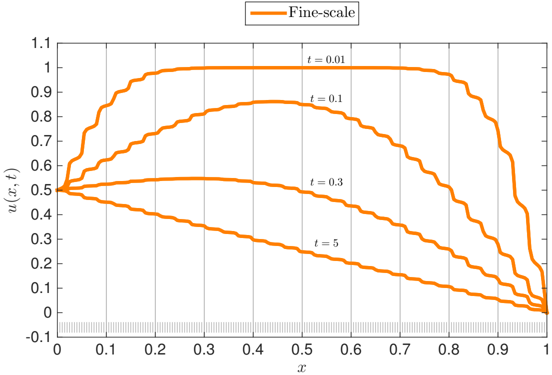


Figure: Fine-layer diffusivities $\kappa_i = 1.1 + \sin(i)$ $(i = 1, \ldots, 200)$

Application to macroscopic modelling

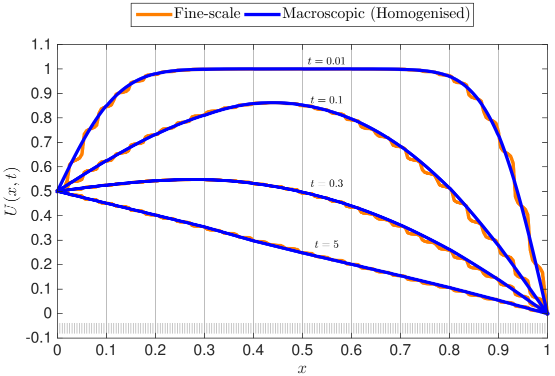


Figure: Fine-layer diffusivities $\kappa_i = 1.1 + \sin(i)$ $(i = 1, \ldots, 200)$
Computation time: 15 secs (Fine-scale), 1 sec (Macroscopic) in MATLAB

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 Sturm-Liouville problems that are local to each layer and not coupled across layers
- Solution is valid for both perfect and imperfect contact at the interfaces and Dirichlet, Neumann or Robin boundary conditions at either end of the medium
- Advantages of the new approach:
  - ✓ Avoids solving a complex transcendental equation for the eigenvalues involving the matrix determinant
  - ✓ Eigenvalues are roots of simple transcendental equations
  - ✓ Scales well to a large number of layers (tested up to 10,000 layers with no problems)
- MATLAB code is available at: http://github.com/elliotcarr/MultDiff

Thank you!

References

M. Asvestas, A. G. Sifalakis, E. P. Papadopoulou, and Y. G. Saridakis. Fokas method for a multi-domain linear reaction-diffusion equation with discontinuous diffusivity. *Journal of Physics: Conference Series*, 490:012143, 2014.

E. J. Carr and I. W. Turner. A semi-analytic solution for multilayer diffusion in a composite medium consisting of a large number of layers. *Submitted to Appl. Math. Model.*, 2015.

F. de Monte. Transient heat conduction in one-dimensional composite slab. A 'natural' analytic approach. *Int. J. Heat Mass Tran.*, 43:3607–3619, 2000.

F. de Monte. An analytic approach to the unsteady heat conduction process in one-dimensional composite media. *Int. J. Heat Mass Tran.*, 45:1333–1343, 2002.

B. Deconinck, B. Pelloni, and N. Sheils. Non-steady state heat conduction in composite walls. *P. Roy. Soc. A-Math. Phy.*, 470(2165):Article No. 20130605, 2014.

R. I. Hickson, S. I. Barry, and G. N. Mercer. Critical times in multilayer diffusion. Part 1: Exact solutions. *Int. J. Heat Mass Tran.*, 52:5776–5783, 2009a.

R. I. Hickson, S. I. Barry, and G. N. Mercer. Critical times in multilayer diffusion. Part 2: Approximate solutions. *Int. J. Heat Mass Tran.*, 52:5784–5791, 2009b.

R. I. Hickson, S. I. Barry, G. N. Mercer, and H. S. Sidhu. Finite difference schemes for multilayer diffusion. *Math. Comput. Model.*, 54:210–220, 2011.

D. Mantzavinos, M. G. Papadomanolaki, Y. G. Saridakis, and A. G. Sifalakis. Fokas transform method for a brain tumor invasion model with heterogeneous diffusion in 1+1 dimensions. *Applied Numerical Mathematics*, page http://dx.doi.org/10.1016/j.apnum.2014.09.006, 2014.

M. R. Rodrigo and A. L. Worthy. Solution of multilayer diffusion problems via the Laplace transform. *Preprint*, 2015.

Y. Sun and I. S. Wichman. On transient heat conduction in a one-dimensional composite slab. *Int. J. Heat Mass Tran.*, 47:1555–1559, 2004.

L. N. Trefethen, J. A. C. Weideman, and T. Schmelzer. Talbot quadratures and rational approximations. *BIT Numer. Math.*, 46:653–670, 2006.