The boundary conditions for diffusion in a material with microscale varying diffusivities

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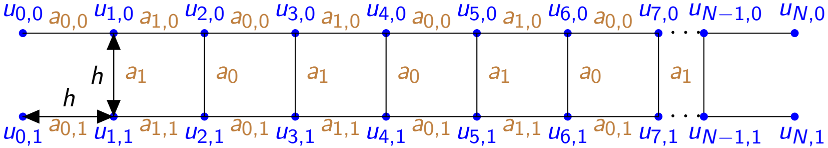
Acknowledge

- CSIRO
- ANZIAM

Diffusion in a material with fine structure



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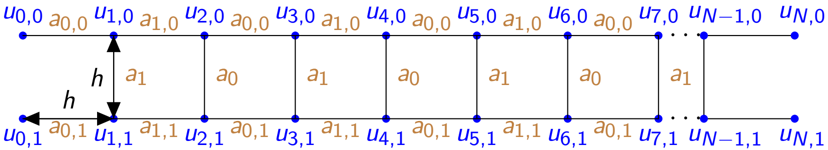
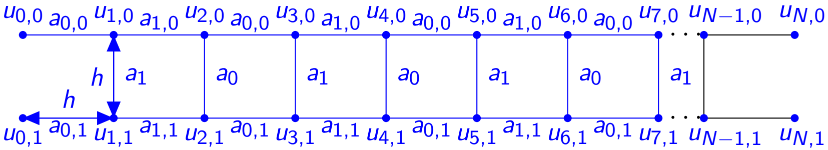


$$h^2 \frac{\partial u_{n,0}}{\partial t} = a_{n-1,0}(u_{n-1,0} - u_{n,0}) + a_{n,0}(u_{n+1,0} - u_{n,0}) + a_n(u_{n,1} - u_{n,0}),$$
$$h^2 \frac{\partial u_{n,1}}{\partial t} = a_{n-1,1}(u_{n-1,1} - u_{n,1}) + a_{n,1}(u_{n+1,1} - u_{n,1}) + a_n(u_{n,0} - u_{n,1}),$$

with Dirichlet boundary condition $u_{0,0}$, $u_{0,1}$, $u_{N,0}$ and $u_{N,1}$.

Analysis delivers macroscale model and boundary conditions



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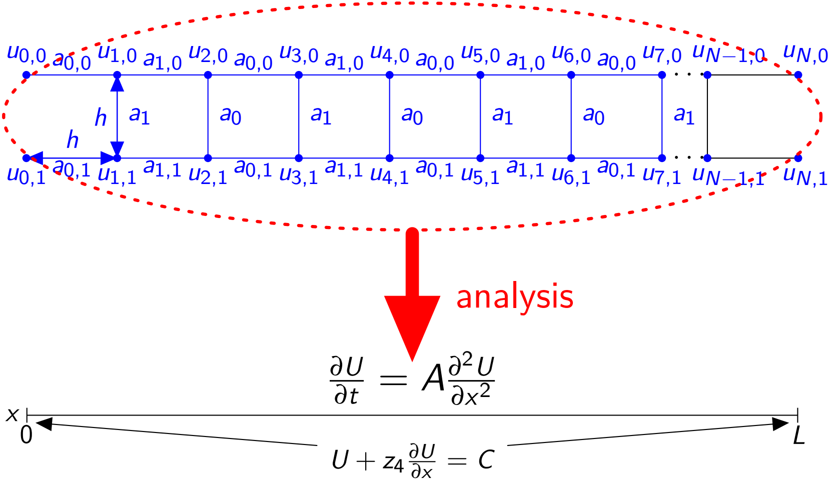
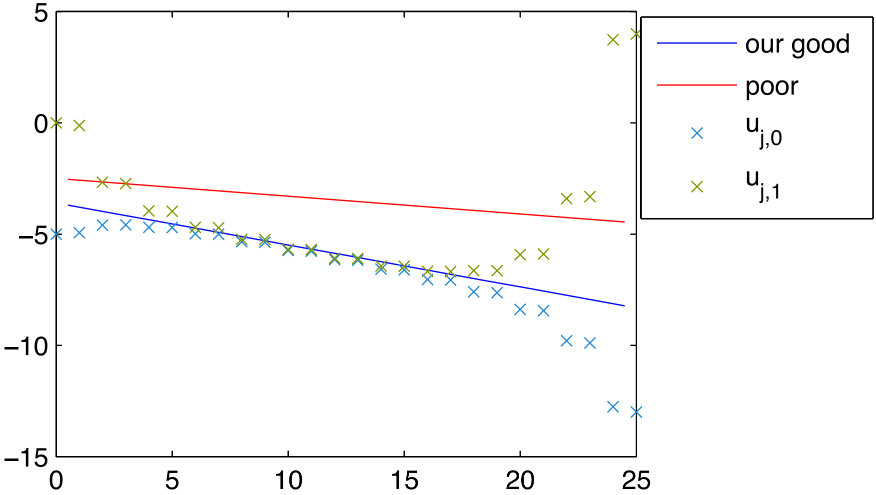


Macroscale boundary condition with coarse grid

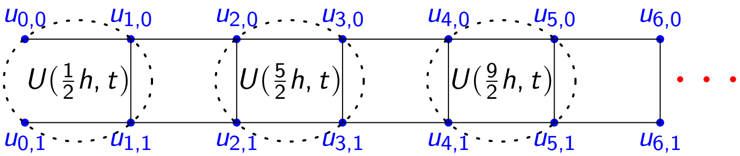


Definition of macroscopic field

- Aim:

$$\frac{\partial U}{\partial t} = A\frac{\partial^2 U}{\partial x^2}$$

for 'mean' $U(x, t)$.



Microscale eigenvalue analysis

- Seek solution $u_{j,l} \propto e^{ikx+\lambda t}$.

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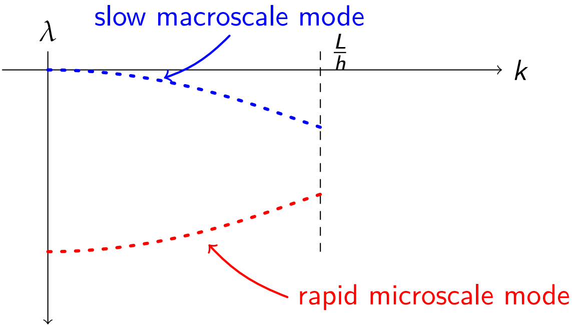

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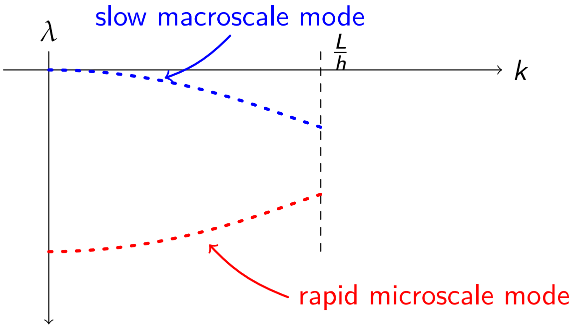


- The slow eigenvalues to errors $\mathcal{O}(k^4)$ are

$$-k^2 \frac{a_0 a_1 (a_{01} + a_{00})(a_{11} + a_{10}) + (a_0 + a_1) \sum_{j=0}^{1} \sum_{i=0}^{1} a_{0,0} a_{0,1} a_{1,0} a_{1,1} / a_{i,j}}{a_1 a_0 (a_{0,0} + a_{0,1} + a_{1,0} + a_{1,1}) + (a_1 + a_0)(a_{1,1} + a_{0,1})(a_{1,0} + a_{0,0})}.$$

Macroscale model

- By Inverse Fourier Transform, macroscopic model to errors $\mathcal{O}(\partial_x^4)$

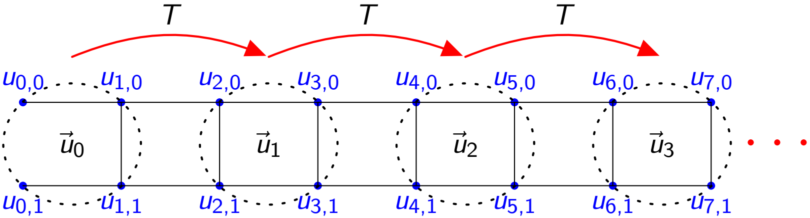
$$\frac{\partial U}{\partial t} = A\frac{\partial^2 U}{\partial x^2},$$

where A is

$$\frac{a_0 a_1\left(a_{0,1}+a_{0,0}\right)\left(a_{1,1}+a_{1,0}\right)+\left(a_0+a_1\right)\sum_{j=0}^{1}\sum_{i=0}^{1} a_{0,0}a_{0,1}a_{1,0}a_{1,1}/a_{i,j}}{a_1 a_0\left(a_{0,0}+a_{0,1}+a_{1,0}+a_{1,1}\right)+\left(a_1+a_0\right)\left(a_{1,1}+a_{0,1}\right)\left(a_{1,0}+a_{0,0}\right)}.$$

Spatial Evolution gives boundary conditions

- Fix time evolution



- The mapping T is

$$\begin{bmatrix} a_{1,0} & 0 & 0 & 0 \\ 0 & a_{1,1} & 0 & 0 \\ -a_{1,0}-a_{0,0}-a_0 & a_0 & a_{0,0} & 0 \\ a_0 & -a_{1,1}-a_{0,1}-a_0 & 0 & a_{0,1} \end{bmatrix}^{-1} \begin{bmatrix} a_{0,0} & 0 & -a_{0,0}-a_{1,0}-a_1 & a_1 \\ 0 & a_{0,1} & a_1 & -a_{0,1}-a_{1,1}-a_1 \\ 0 & 0 & a_{1,0} & 0 \\ 0 & 0 & 0 & a_{1,1} \end{bmatrix}$$

Boundary layers simplifies macroscale boundary conditions

- Eigenvectors $\vec{v}_1, \vec{v}_2, \vec{v}_3$ and $\vec{v}_4$ and corresponding eigenvalues $\mu_1 < 1$, $\mu_4 > 1$ and $\mu_2 = \mu_3 = 1$.

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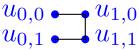
- As the eigenvectors are linearly independent

$\vec{u}_0 =$ 

$= c_1\vec{v}_1 + c_2\vec{v}_2 + c_3\vec{v}_3 + c_4\vec{v}_4.$

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- In general

$$\vec{u}_n = c_1\vec{v}_1\mu_1^n + c_2\vec{v}_2 + c_3\left(\vec{v}_3 + n\vec{v}_2\right) + c_4\vec{v}_4\mu_4^n.$$

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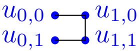

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- c_1 and c_4 associate with boundary layers.

- $c_4 = 0$

Derivation of Macroscale Boundary Conditions

- Given boundary conditions are the first two components of vector $\vec{u}_0$

$$u_{0,0} = c_1 v_{11} + c_2 v_{21} + c_3 v_{31}, \quad (1)$$

$$u_{0,1} = c_1 v_{12} + c_2 v_{22} + c_3 v_{32}. \quad (2)$$

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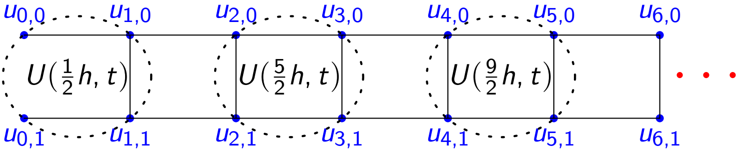
- At second cell

$$\vec{u}_1 = c_1 \vec{v}_1 \mu_1 + c_2 \vec{v}_2 + c_3 (\vec{v}_2 + \vec{v}_3).$$

Derivation of Macroscale Boundary Conditions



- The average of first cell

$$U(x = 0.5h) \quad = \quad \tfrac{1}{4}\vec{u}_0 \cdot \vec{1}.$$

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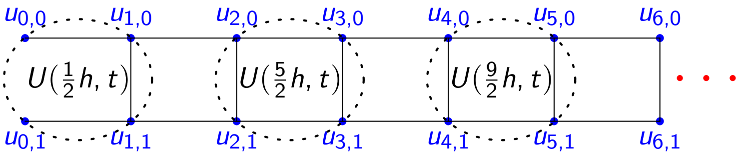

- The average of first cell

$$U(x = 0.5h) \quad = \quad \frac{1}{4}\vec{u}_0 \cdot \vec{1}.$$

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$$U(x = 2.5h) \quad = \quad \frac{1}{4}\vec{u}_1 \cdot \vec{1}.$$

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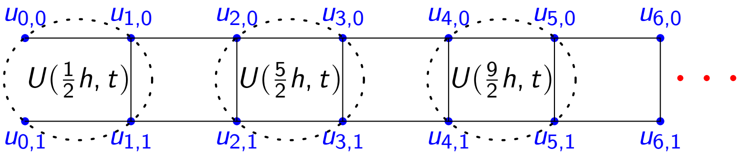

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- By extrapolation

$$\frac{\partial U}{\partial x} = \frac{U(x = 2.5h) - U(x = 0.5h)}{2h} = \frac{\frac{1}{4}\left[c_3\vec{v}_2 + c_1\vec{v}_1(\mu_1 - 1)\right] \cdot \vec{1}}{2h} \quad (3)$$

Subtracting boundary layers

- By extrapolation again

$$
\begin{aligned}
U(x=0) &= U(x=0.5) - 0.5h\frac{\partial U}{\partial x} \\
&= \tfrac{1}{4}\left[c_1\vec{v}_1(1.25-\mu_1/4) + c_2\vec{v}_2 + c_3(\vec{v}_3 - \tfrac{1}{4}\vec{v}_2)\right](4)
\end{aligned}
$$

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- Put equations (1), (2), (3) and (4) in a system

$$\begin{bmatrix} v_{11} & v_{21} & v_{31} \\ v_{12} & v_{22} & v_{32} \\ \frac{1}{4}\left(1.25-\mu_1/4\right)\vec{v}_1\cdot\vec{1} & \frac{1}{4}\vec{v}_2\cdot\vec{1} & \left(\frac{1}{4}\vec{v}_3\cdot\vec{1} - \frac{1}{16}\vec{v}_2\cdot\vec{1}\right) \\ \frac{1}{8h}(\mu_1-1)\vec{v}_1\cdot\vec{1} & 0 & \frac{1}{8h}\vec{v}_2\cdot\vec{1} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} u_{00} \\ u_{01} \\ U\big|_{x=0} \\ \frac{\partial U}{\partial x}\Big|_{x=0} \end{bmatrix}$$

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Macroscale boundary condition

- Subtracting the boundary layer effect

$$\begin{bmatrix} v_{11} & v_{21} & v_{31} \\ v_{12} & v_{22} & v_{32} \\ 0 & \frac{1}{4}\vec{v}_2 \cdot \vec{1} & \left(\frac{1}{4}\vec{v}_3 \cdot \vec{1} - \frac{1}{16}\vec{v}_2 \cdot \vec{1}\right) \\ 0 & 0 & \frac{1}{8h}\vec{v}_2 \cdot \vec{1} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} u_{00} \\ u_{01} \\ U\big|_{x=0} \\ \frac{\partial U}{\partial x}\Big|_{x=0} \end{bmatrix}$$

- Compute $\vec{z} = (-z_1, -z_2, 1, z_4)$ such that

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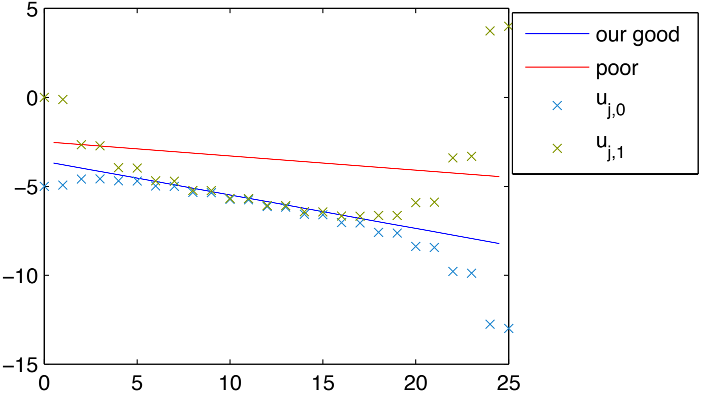
- Pre-multiply $\vec{z}$

$$U + z_4\frac{\partial U}{\partial x} = z_1 u_{00} + z_2 u_{01}.$$

Numerics verifies analytical results

$$U + 0.11\frac{\partial U}{\partial x} = 0.74u_{00} + 0.26u_{01}.$$



- Generalise to wave equation