The macroscale boundary conditions for diffusion
in a material with two layer and periodic diffusivities

Chen Chen supervised by Tony Roberts, Judith Bunder and Tony Miller

School of Mathematical Science, the University of Adelaide

`chen.chen@adelaide.edu.au`

Abstract

Homogenization and other multiscale modelling techniques allow us to build efficient mathematical model for simulating systems such as materials with complicated microstructure. But the modelling rarely addresses systematical method to derive boundary conditions for macroscale model. In this paper, we build a smooth macroscale model for a two-layer one-dimensional diffusion system with rapidly varying diffusivity and finite scale separation. I will discuss how to derive macroscopic boundary conditions for some one dimensional discrete diffusion problems. The result can be applied to a range of multiscale modelling problems including wave equations.

The microscale diffusion problem

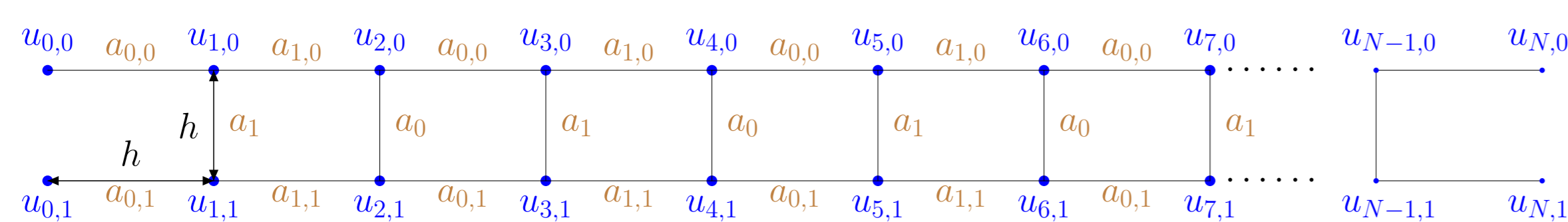We have the a discrete diffusion system to model as show in the following graph.

Figure 1: The discrete diffusion has a periodicity of two.

The associated microscale equations are

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

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

- u_{ij} are the temperature at position (i,j).
- h are the distance between two adjacent nodes.
- a_{ij} are the lateral diffusivities and a_k are the cross diffusivities. These diffusivities are all a two-periodic.

We need more accurate macroscale model and boundary conditions which allow infinitesimally small scale separation

Our objectives are the following:

1. *Create a macroscale model $\frac{\partial U}{\partial t} = A\frac{\partial^2 U}{\partial x^2}$ of the original microscale dynamics for 'mean' $U(x,t)$.*

2. *Propose a Macroscale boundary condition in the form of $U + B\frac{\partial U}{\partial x} = C(t)$ at the left and right boundaries.* We provide a systematic way to derive constant coefficient B and spatial constant $C(t)$ which can be carried to a more complicated problem such as wave equations. We proved coefficient B is in $\mathcal{O}(h)$ and $C(t)$ at one end is a weighted average of two boundary conditions at that end.

3. *The model and boundary conditions are valid for finite scale separation.* The microscale periodicity cannot be infinitesimally small because of computationally feasibility. If our methodology requires scale separation to be infinitesimally small, then the domain has to be infinitely long [1]. But we have a finite domain in the boundary value problem. So methods which require infinitesimally small is not helping our boundary value problem.

4. *Compare our result with the boundary conditions other researchers generally used.* We showed that our model is better for problems with finite inter nodes distance h.

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

$$U + B\frac{\partial U}{\partial x} = C(t)$$

Figure 2: We derive a macroscale model and its corresponding macroscale boundary conditions.

Systematic methods provide a framework for complex problems

Although the diffusion problem is relatively simple, we want our methodology to be general and systematic so that we have use a similar approach to more complicated problems. To have a macroscale model, we need macroscale equations corresponding to the microscale diffusion equations and macroscale boundary conditions. We define macroscale variable as the average of every four adjacent nodes in a cell as shown below.
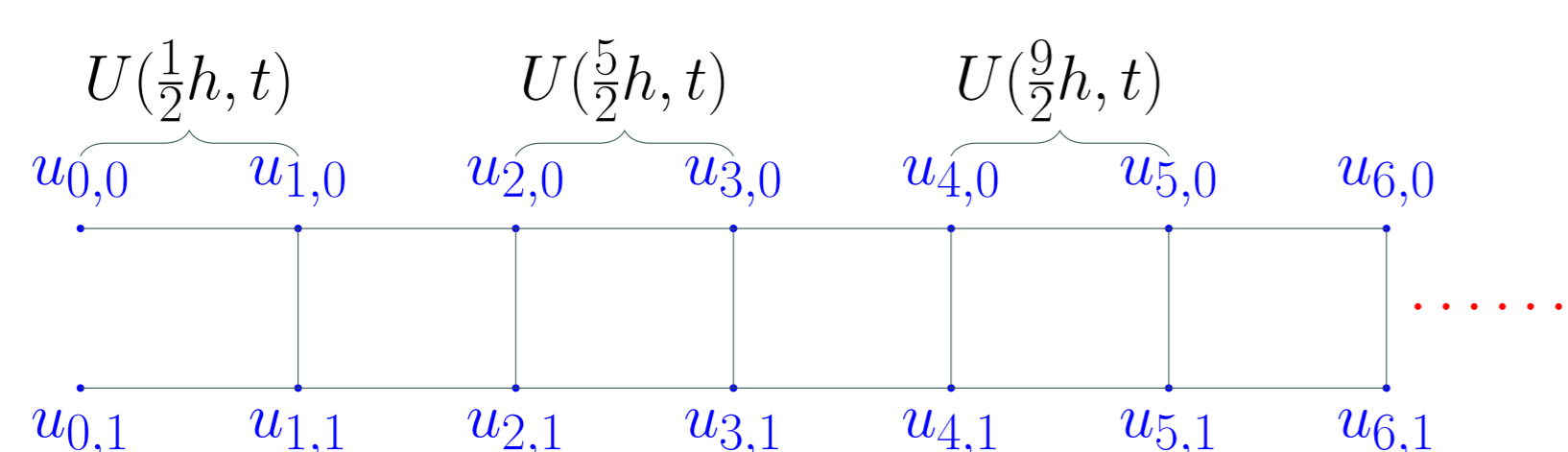

Figure 3: Macroscale variable U is chosen to be the average of a cell.

Centre manifold theory provides a iterative scheme to derive macroscale evolution

We applied Fourier Transform to discretise the eigenspectrum of the diffusion system, and then we are able to use centre manifold theory to create a macroscale model for the diffusion system. We showed the diffusion system has a eigenvalue of zero, which corresponding to the slow manifold. We proved that all the other eigenvalues are real and negative providing all the diffusivities constants are positive. These real and negative eigenvalues are corresponding to the centre stable manifold, and they are decaying to the slow manifold exponentially quickly. Centre manifold theory gives a time evolution of macroscale model as

$$\frac{\partial U}{\partial t} = \frac{a_0 a_1\left(a_{0,1} + a_{0,0}\right)\left(a_{1,1} + a_{1,0}\right) + (a_0 + a_1)\sum_{j=0}^{1}\sum_{i=0}^{1}a_{0,0}a_{0,1}a_{1,0}a_{1,1}/a_{i,j}}{a_1 a_0(a_{0,0} + a_{0,1} + a_{1,0} + a_{1,1}) + (a_1 + a_0)(a_{1,1} + a_{0,1})(a_{1,0} + a_{0,0})}\frac{\partial^2 U}{\partial x^2}.$$

Local analysis by spatial evolution deliver sound macroscale boundary conditions

I applied a method of spatial evolution adopted by Roberts [2] to propose the macroscale boundary conditions. I defined the spatial evolution mapping T as the mapping from the four nodes from nth cell $\vec{u}_n$ to the four nodes in $(n+1)$th cell $\vec{u}_{n+1}$ for arbitrary non-negative integer n as shown below.
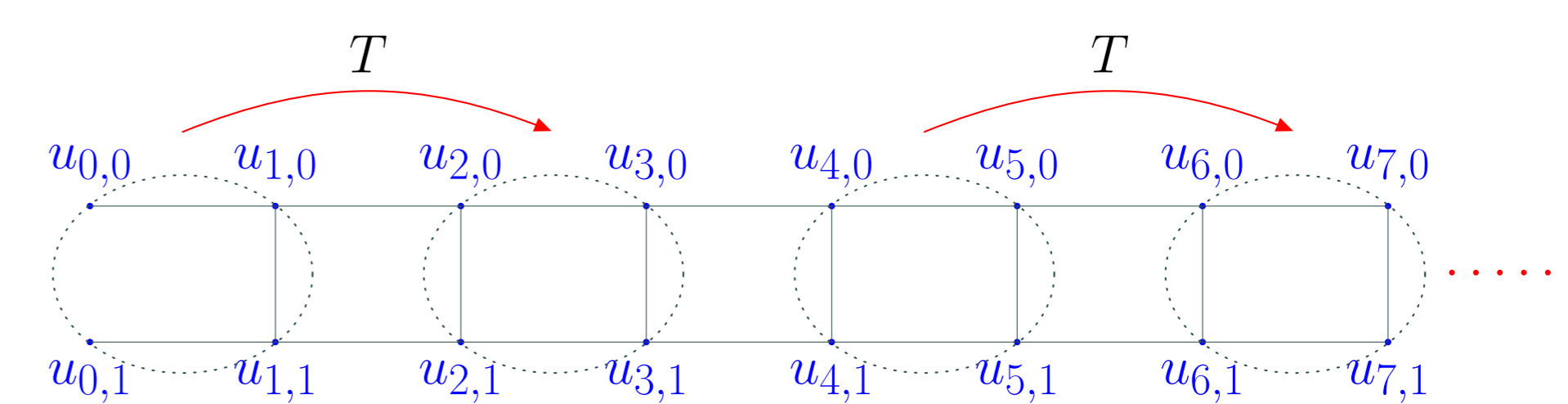

Figure 4: Mapping T maps nth cell $\vec{u}_n$ to $(n+1)$th cell $\vec{u}_{n+1}$.

Computation of this mapping T involves considering equilibrium equations at four interior nodes within two adjacent cells. Let v_1, v_2, v_3 and v_4 be the eigenvectors of mapping T with corresponding eigenvalues $\mu_1 < 1$ (decaying mode), $\mu_4 > 1$ (growing mode) and $\mu_2 = \mu_3 = 1$. It turns out v_3 is a generalised eigenvector. Then I write the nodes in first cell as a linear combination of the eigenvectors $\vec{u}_0 = c_1 v_1 + c_2 v_2 + c_3 v_3 + c_4 v_4$. But $c_4 = 0$ because otherwise the right boundary will be exponentially large. So the second cell is $\vec{u}_1 = c_1 v_1 + c_2 v_2 + c_3(v_2 + v_3)$.

We force that macroscale variables should only know the global behaviour and do not recognise the boundary layers. So the macroscale variable should not have any component in the direction of decay mode v_1. With this knowledge, we write macroscale variables at the very left boundary as a weighted sum of the mean of eigenvector $\bar{v}_2$ and mean of generalised eigenvector $\bar{v}_3$. Let v_{ij} be the jth component of vector v_i and adjoin the two macroscale boundary conditions with the macroscale equations

$$\begin{bmatrix} v_{11} & v_{21} & v_{31} \\ v_{12} & v_{22} & v_{32} \\ 0 & \bar{v}_2 & (\bar{v}_3 - \frac{1}{4}\bar{v}_2) \\ 0 & 0 & \frac{1}{2h}\bar{v}_2 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} u_{00} \\ u_{01} \\ U(x=0) \\ \frac{\partial U}{\partial x}\big|_{x=0} \end{bmatrix}. \quad (1)$$

Let G be the left hand side 4×3 matrix in systems of equations (1). Compute the basis vector $\vec{z} = (z_1, z_2, 1, z_4)$ for null space of G^T and pre-multiply $\vec{z}^T$ to system of equations (1), we have the macroscale boundary condition

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

Numerically we find z_4 is significant when the internode spacing h is not too small and we verify this by showing $z_4 \sim h$. We also showed $z_3 + z_4 = 1$, which means the right hand side of boundary condition () is a weighted average of the microscale boundary conditions.

We use a similar approach to derive the boundary conditions at the right end by setting up a different coordinate system looking from right to left.

Numerical results verify analysis

We ran numerous numerical example to verify our analytical result and they agree well. I will show one example with the domain from 0 to 2π and internodes distance $h = 2\pi/25$. The lateral diffusivities in this example are $a_{0,0} = 0.2061$, $a_{0,1} = 0.2969$, $a_{1,0} = 0.9456$ and $a_{1,1} = 1.1463$. The cross diffusivities are $a_0 = 0.1209$ and $a_1 = 0.1255$. The microscale boundary conditions are $u_{0,0} = 1.0224$, $u_{0,1} = 0$, $u_{N,0} = 3.1921$ and $u_{N,1} = 1.5643$.
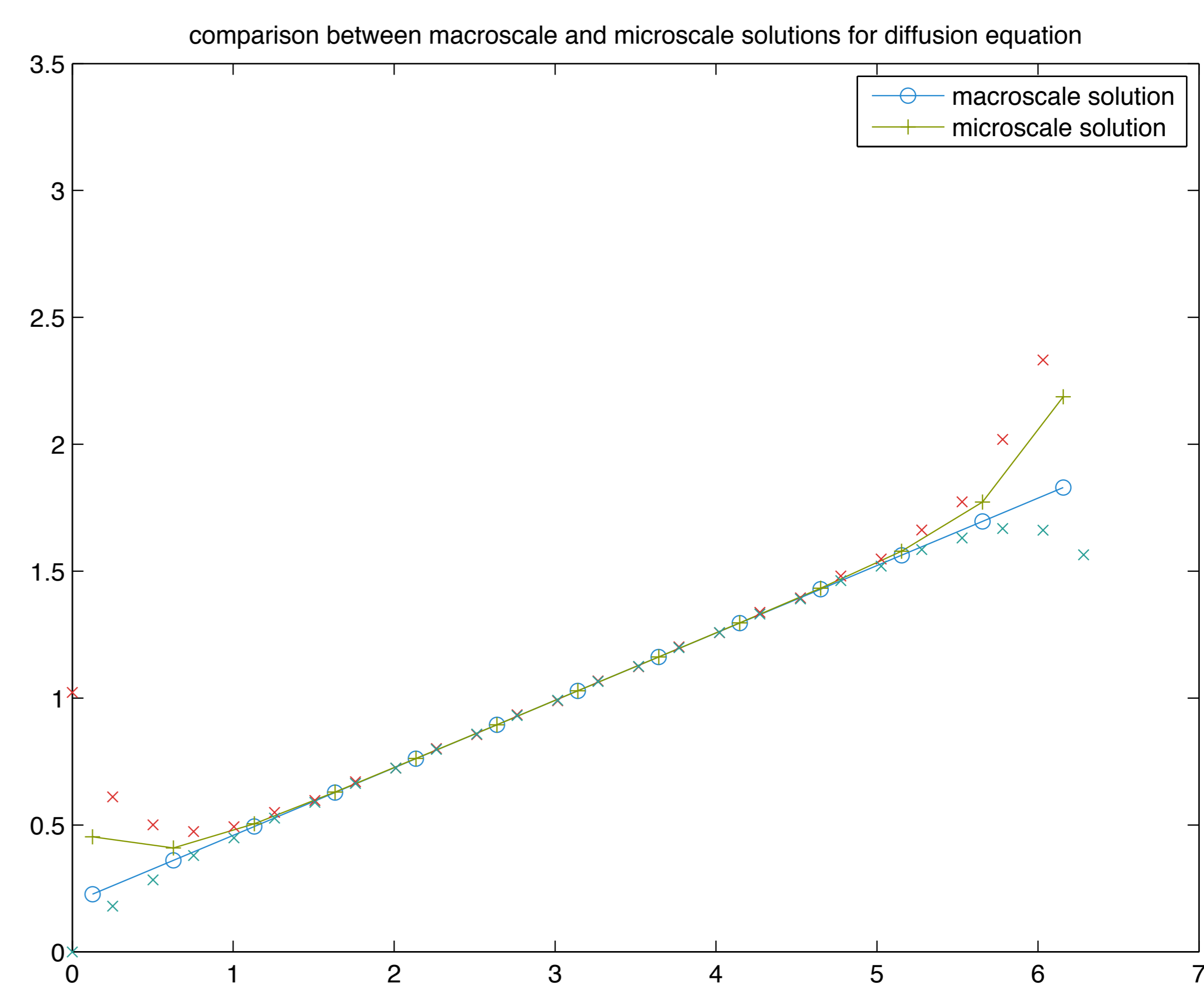

Figure 5: Comparison between macroscale and microscale solution

Figure 5 illustrates a pair of accurate macroscale boundary conditions. The red crosses are the temperatures u at the top layer and the blue crosses are those at the bottom layer. The green curve is the microscale solution to the diffusion problem and the blue curve are our macroscale model. The macroscale solution fits the global behaviour well while ignoring the boundary layers, which is the desired outcome.

The methodology is valid for more complicated problems such as waves

We would like to see the possibility of extend our methodology to higher dimensions and other problems. We are currently extend this methodology to wave equations. Another particular area we would like to consider afterwards is beams.

References

[1] Mei, C. C. and Vernescu, B. [2010], *Homogenization methods for multiscale mechanics*, World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ.

[2] Roberts, A. J. [1992], 'Boundary conditions for approximate differential equations', *Journal of Australian Mathematical Society* **34**, 54–80.
URL: *http://dx.doi.org/10.1017/S0334270000007384*

Acknowledgements