Dynamical system based macroscale models of multiphase materials

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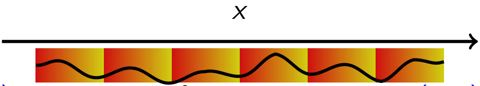
Overview



$u(0,t) = b_0$ $\quad$ $\rho(x)\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial u}{\partial x}\right)$ $\quad$ $u(L,t) = b_L$

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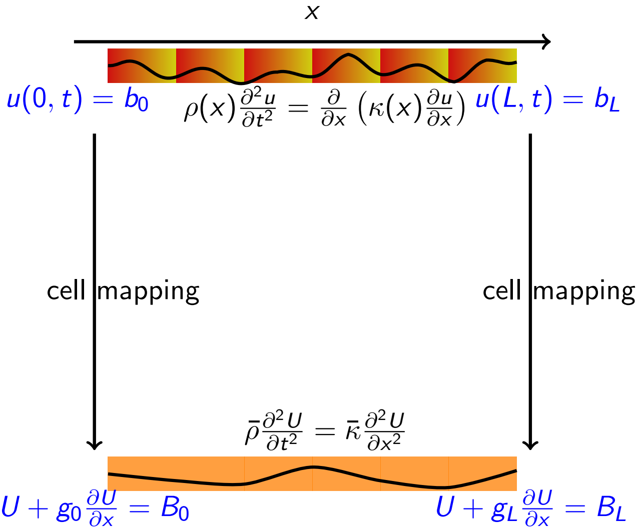
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cell mapping
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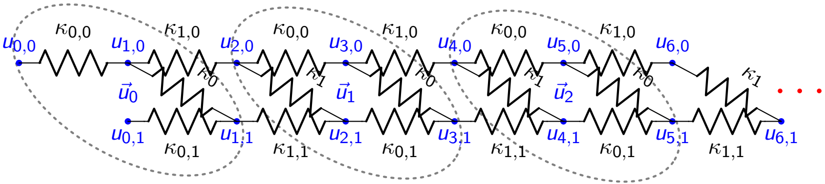
$U + g_0\frac{\partial U}{\partial x} = B_0$
$U + g_L\frac{\partial U}{\partial x} = B_L$

Wave equation in a two-strand material



$$\rho_{m,0}\frac{\partial^2 u_{m,0}}{\partial t^2} = \kappa_{m-1,0}(u_{m-1,0}-u_{m,0})+\kappa_{m,0}(u_{m+1,0}-u_{m,0})+\kappa_m(u_{m,1}-u_{m,0}),$$
$$\rho_{m,1}\frac{\partial^2 u_{m,1}}{\partial t^2} = \kappa_{m-1,1}(u_{m-1,1}-u_{m,1})+\kappa_{m,1}(u_{m+1,1}-u_{m,1})+\kappa_m(u_{m,0}-u_{m,1}).$$

- spatial domain $m = 1, 2, \ldots, N-1$,
- ρ_m and κ_m are two periodic horizontally,
- with Dirichlet boundary conditions, i.e. specified $u_{0,i}$ and $u_{N,i}$.

Simulation

The domain is $0 \leq x \leq \pi$, $0 \leq t \leq 35$. The boundary values are $u_{0,0} = 0$, $u_{0,1} = 1$, $u_{N,0} = 5$ and $u_{N,1} = 10$. Initial values are $u_{m,0} = 0.5 - 2e^{-x^2/3}$ and $u_{m,1} = 0.3 - 3e^{-x/3}$.

Homogenization theory derives macroscale model

$$\bar{\rho}\frac{\partial^2 U(x,t)}{\partial t^2} = \bar{\kappa}\frac{\partial^2 U(x,t)}{\partial x^2}.$$

- Spatial domain $[0, L]$, equivalent density is the arithmetic mean

$$\bar{\rho} = \frac{1}{4}\sum_{i=0}^{1}\sum_{j=0}^{1}\rho_{i,j}$$

and equivalent spring constant is a kind of harmonic mean

$$\bar{\kappa} = \left[\kappa_0\kappa_1\left(\kappa_{0,1}+\kappa_{0,0}\right)\left(\kappa_{1,1}+\kappa_{1,0}\right)+\left(\kappa_0+\kappa_1\right)\sum_{j=0}^{1}\sum_{i=0}^{1}\kappa_{0,0}\kappa_{0,1}\kappa_{1,0}\kappa_{1,1}/\kappa_{i,j}\right]/D$$

where

$$D = \kappa_1\kappa_0(\kappa_{0,0}+\kappa_{0,1}+\kappa_{1,0}+\kappa_{1,1})+(\kappa_1+\kappa_0)(\kappa_{1,1}+\kappa_{0,1})(\kappa_{1,0}+\kappa_{0,0})$$

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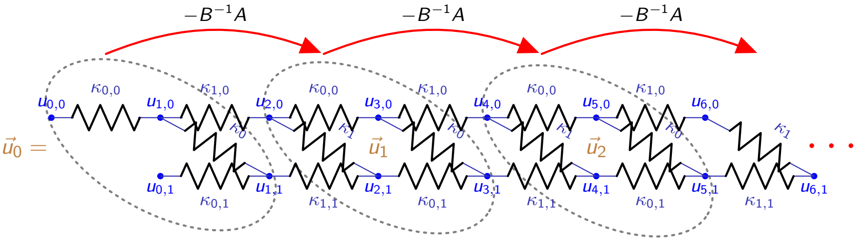
- with Robin boundary conditions $U(0,t)+g_0\left.\frac{\partial U}{\partial x}\right|_{x=0} = B_0$ and $U(L,t)+g_L\left.\frac{\partial U}{\partial x}\right|_{x=L} = B_L$.

Assuming quasi-steady state gives cell mapping



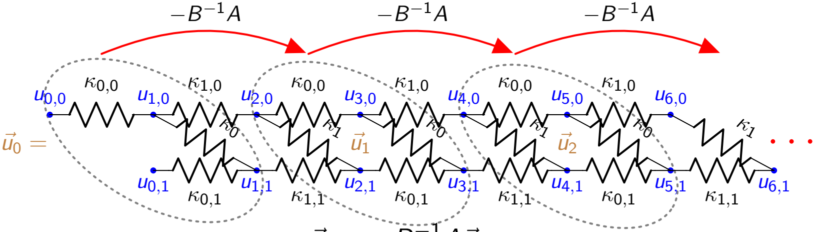
$$\begin{bmatrix} A & B \end{bmatrix} \begin{bmatrix} \vec{u}_0 \\ \vec{u}_1 \end{bmatrix} = \vec{0},$$

where

$$A = \begin{bmatrix} \kappa_{0,0} & 0 & -\kappa_{0,0} - \kappa_{1,0} - \kappa_1 & \kappa_1 \\ 0 & \kappa_{0,1} & \kappa_1 & -\kappa_{0,1} - \kappa_{1,1} - \kappa_1 \\ 0 & 0 & \kappa_{1,0} & 0 \\ 0 & 0 & 0 & \kappa_{1,1} \end{bmatrix},$$

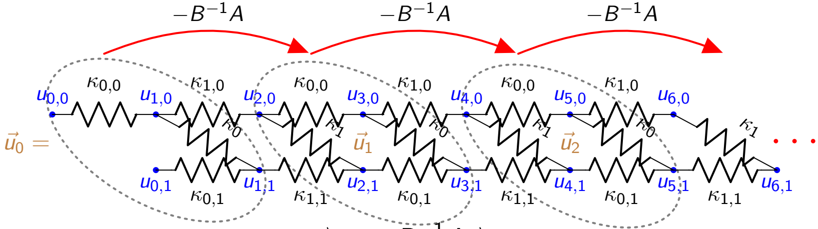
$$B = \begin{bmatrix} \kappa_{1,0} & 0 & 0 & 0 \\ 0 & \kappa_{1,1} & 0 & 0 \\ -\kappa_{1,0} - \kappa_{0,0} - \kappa_0 & \kappa_0 & \kappa_{0,0} & 0 \\ \kappa_0 & -\kappa_{1,1} - \kappa_{0,1} - \kappa_0 & 0 & \kappa_{0,1} \end{bmatrix}.$$

Assuming quansi-steady state gives cell mapping



$$\vec{u}_1 = -B^{-1}A\vec{u}_0,$$

Assuming quansi-steady state gives cell mapping



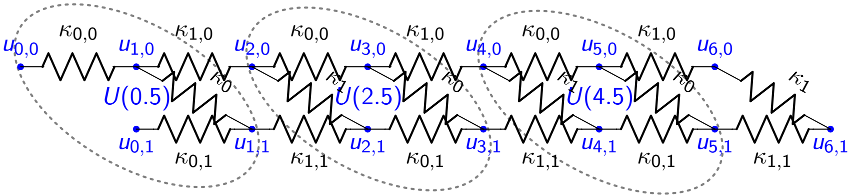
$$\vec{u}_1 = -B^{-1}A\vec{u}_0,$$

$$\vec{u}_{\nu+1} = -B^{-1}A\vec{u}_\nu,$$

$$\vec{u}_0 = \underbrace{c_1\vec{v}_1}_{\mu_1<1} + \underbrace{c_2\vec{v}_2}_{\mu_2=1} + \underbrace{c_3\vec{v}_3}_{\mu_3=1} + \underbrace{c_4\vec{v}_4}_{\mu_4>1},$$

where $\vec{v}_i$ is the eigenvectors of mapping matrix $-B^{-1}A$.

Cell mapping derives macroscale model and boundary conditions

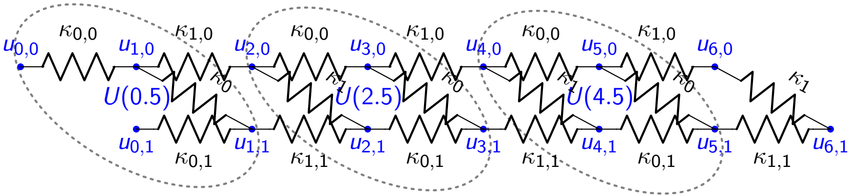


- $c_4 = 0$
-

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

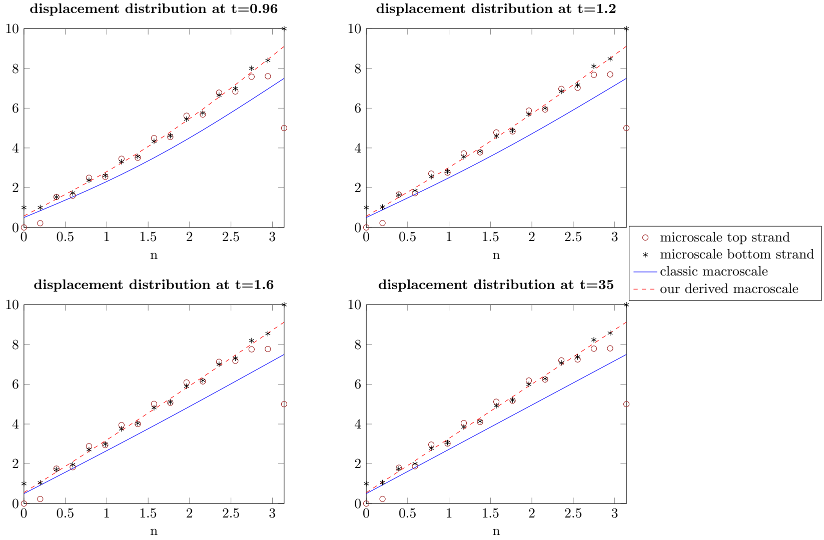
- Write U and $\frac{\partial U}{\partial x}$ as a function of $\vec{u}_\nu$.
- Boundary condition comes from considering the basis vector of the null space.

Use Levenberg–Marquardt algorithm check the improved boundary conditions

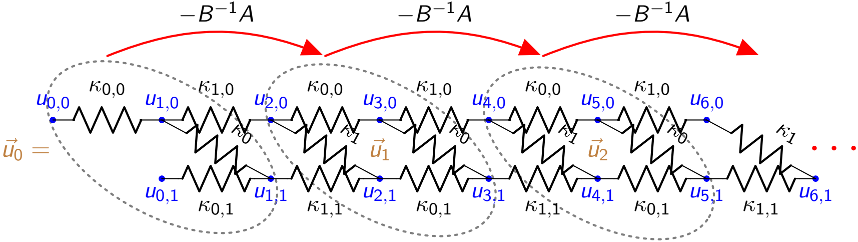


- This method captures out of equilibrium.
- Require solve the full microscale problem once and solve the macroscale problem many times.
- $$\min_{g_0, g_L} \left|\vec{v}_{\text{macro}} - \vec{v}_{\text{micro}}\right|^2$$
- The theory of Rayleigh quotient justifies eigenvectors are more sensitive.
- This algorithm verifies the derived boundary conditions.

Numerical results



Mapping methods generalise to more complicated problems



- Extend to any number of strands.
- Any periodicity.
- The method can be applied to non-linear problems.
- The algebraically complicated part of derivation can be done in Maple.

Other type of microscale boundary conditions

microscale boundary conditions	macroscale boundary conditions
Dirichlet, $u = 0$	Robin, $U + g\frac{\partial U}{\partial x} = 0$
Neumann, $\frac{\partial u}{\partial x} = 0$	the same Neumann, $\frac{\partial U}{\partial x} = 0$
Robin, $u + g_1\frac{\partial u}{\partial x} = 0$	a different Robin, $U + g_2\frac{\partial U}{\partial x} = 0$

Non-linear problems

- Assume Quasi-equilibrium and regard the problem as a spatial evolution.
- Deduce centre, stable and unstable manifold.
- Set the coefficients of unstable model to zero.
- Project the boundary conditions from centre stable manifold to centre manifold.

Future research

- Consider highly oscillatory initial conditions.
- Extend to three-dimensional multiphase materials.
- Model near-periodic multiphase materials.