Periodic Homogenization: Exercises

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Exercise 1

In this exercise we study the model problem in the theory analytically to get the first taste of the homogenization technique in action without numerical implementation. First, the model problem in the lecture reads

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}x}\left[C(x)\frac{\mathrm{d}u}{\mathrm{d}x}\right] + f(x) &= 0, \\ u(x=0) &= u_0, \\ C\frac{\mathrm{d}u}{\mathrm{d}x}\Big|_{x=L} &= t_0. \end{aligned} \tag{1}$$

This boundary value problem, as explained in the lecture, can be replaced with the homogenized problem consisting of the microscopic and macroscopic boundary value problems:

- Macroscopic boundary value problem

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\overline{x}}\left[\overline{C}(\overline{x})\frac{\mathrm{d}\overline{u}}{\mathrm{d}\overline{x}}\right] + f(\overline{x}) &= 0, \\ \overline{u}(\overline{x}=0) &= u_0, \\ \overline{C}\frac{\mathrm{d}\overline{u}}{\mathrm{d}\overline{x}}(\overline{x}=L) &= t_0. \end{aligned} \tag{2}$$

- Mircorsopic boundary value problem

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}x}\sigma(x) &= 0, \\ \sigma(x) &= C(x)[\epsilon(\widetilde{u}(x)) + \overline{\epsilon}], \end{aligned} \tag{3}$$

  with the boundary conditions: $\widetilde{u}$ is periodic, σn is antiperiodic. The strain denotation ϵ is considered as an operator acting on the displacement field in the sense that

$$\epsilon(u(x)) = \frac{\mathrm{d}u}{\mathrm{d}x}.$$

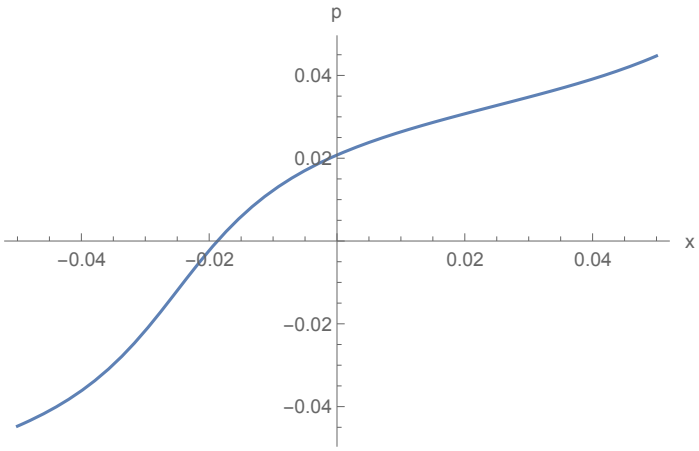


Figure 1: Graph of p(x)

Solution method First, we solve the microscopic BVP. The equilibrium equation gives

$$\sigma(x) = \text{const} = \kappa.$$

It is clear that this solution satisfy the antiperiodic condition for the traction $t = \sigma n$. According this, the equation for $\widetilde{u}(x)$ is given by

$$\frac{\mathrm{d}\widetilde{u}}{\mathrm{d}x} = \frac{\kappa}{C(x)} - \overline{\epsilon} = \frac{\kappa}{3/2 + \sin(2\pi k x)} - \overline{\epsilon}.$$

Integration of this equation gives

$$\widetilde{u}(x) = \frac{2\kappa \arctan \frac{2+3\tan(\pi k x)}{\sqrt{5}}}{\sqrt{5} k \pi} - \overline{\epsilon} x = p(x) - \overline{\epsilon} x.$$

The periodic boundary condition on $\widetilde{u}$ allows us to determine the constant κ. A typical graph of $p(x)$ with $\kappa = 1$, $k = 10$ is given Fig. Fig: graph of p(x). In this sample figure with $k = 10$ the wavelength of the $C(x)$ is then $2\pi/(2\pi k) = 1/10$. The periodic condition on $\widetilde{u}$ requires $\widetilde{u}(-\lambda/2) = \widetilde{u}(\lambda/2)$, that is

$$\widetilde{u}(x \to \lambda/2) = \widetilde{u}(x \to -\lambda/2) \quad \Leftrightarrow \quad p(x \to \lambda/2) - \overline{\epsilon}\frac{\lambda}{2} = p(x \to -\lambda/2) + \overline{\epsilon}\frac{\lambda}{2},$$

It can be deduced that

$$p(x)\Big|_{x \to -\lambda/2}^{x \to \lambda/2} = \frac{2\kappa}{k\sqrt{5}}.$$

Plugging this result into the equation for the periodic boundary condition of $\widetilde{u}$ we have just obtained the constant κ as follows

$$\frac{2\kappa}{k\sqrt{5}} = \overline{\epsilon} \underbrace{\lambda}_{1/k} \quad \Leftrightarrow \quad \kappa = \frac{\sqrt{5}}{2}\overline{\epsilon}.$$

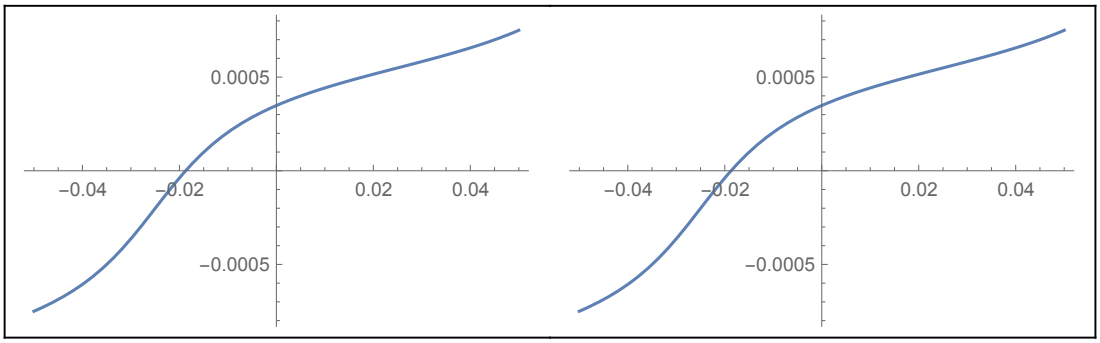


Figure 2: Numerical and analytical solutions for the displacement $u(x) = \widetilde{u}(x) + \overline{\epsilon}x$.

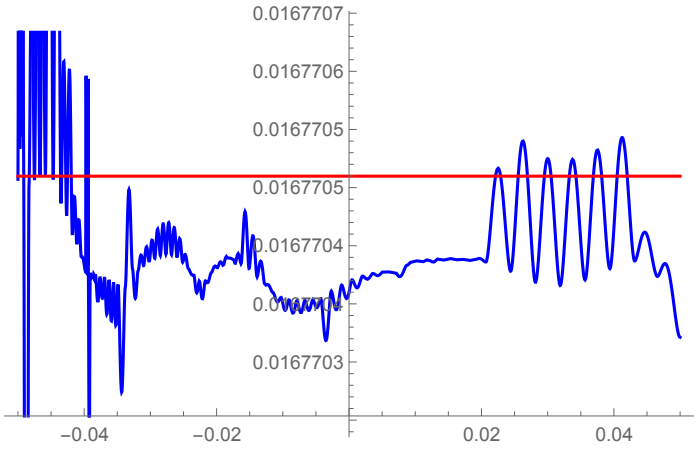


Figure 3: Numerical and analaytical solutions for the stress $\sigma(x)$.

In summary, we have just obtained the solution of the microscopic BVP as follows

$$\sigma(x) = \kappa = \frac{\sqrt{5}}{2}\overline{\epsilon},$$

$$u(x) = \widetilde{u}(x) + \overline{\epsilon}x = p(x) = \frac{2\kappa \arctan\frac{2+3\tan(\pi k x)}{\sqrt{5}}}{\sqrt{5}k\pi} = \frac{\arctan\frac{2+3\tan(\pi k x)}{\sqrt{5}}}{k\pi}\overline{\epsilon}.$$

The microscopic boundary value problem has been solved numerically using the Mathematica software (see "Periodic Homogenization.pdf"). The numerical and analytical solutions are presented in the Fig. 2 and Fig. 3. The comparison shows the excellent agreement, and thus justifies the solution method presented above.

As the stress is constant throughout the periodic mircostructure, namely the RVE, the mean stress or the average stress is identical to κ:

$$\overline{\sigma} = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} \sigma(x)\mathrm{d}x = \kappa = \frac{\sqrt{5}}{2}\overline{\epsilon}.$$

Accordingly, we can immediately see that the effective stiffness is constant

$$\overline{C} = \frac{\partial \overline{\sigma}}{\partial \overline{\epsilon}} = \frac{5}{2}.$$

Remark It must be noted that constitutive law $\overline{\sigma} = \sqrt{5}/2\overline{\epsilon}$ is linear because the original constitutive law $\sigma(x) = C(x)\epsilon(x)$ is also linear in terms of ϵ. This result is not surprising in the periodic homogenization framework. It will be explained further why it is not an accident in the variational framework in the subsequent exercise.

After solving the microscopic BVP (3), we come back to the macroscopic BVP (2) which is simply

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\overline{x}}\left[\frac{\sqrt{5}}{2}\frac{\mathrm{d}\overline{u}}{\mathrm{d}\overline{x}}\right] + f(\overline{x}) &= 0, \\ \overline{u}(\overline{x}=0) &= u_0, \\ \frac{\sqrt{5}}{2}\frac{\mathrm{d}\overline{u}}{\mathrm{d}\overline{x}}(\overline{x}=L) &= t_0. \end{aligned}$$

The analytical solution is given by

$$\overline{u}(\overline{x}) = u_0 - \frac{\overline{x}\,(-6t_0 + \overline{x}^2 - 3)}{3\sqrt{5}}.$$

With the boundary parameters $u_0 = 0$, $t_0 = 0$ the exact solution reads

$$\overline{u}(\overline{x}) = -\frac{\overline{x}(\overline{x}^2 - 3)}{3\sqrt{5}}.$$

The numerical solution for the full-field BVP (1) with $k = 50$ and the analytical of the homogenized BVP is illustrated in Fig. Fig: Full-field-vs-homogenization comparison. These two solutions demonstrates that the full-field solution and the homogenized solution are comparable, which justify, at least in the current example, the theory of the first-order homogenization.

Remark In the mathematical language we may not "forget" the macroscale and the microscale and consider the $\overline{u}$ as a function of x which is a "good" replacement of the full-field solution. In this sense the replacement of the full-field boundary value problem is actually

$$\begin{aligned} \frac{\mathrm{d}v}{\mathrm{d}x}\left[\frac{\sqrt{5}}{2}\frac{\mathrm{d}v}{\mathrm{d}x}\right] + f(x) &= 0, \\ v(x=0) &= u_0, \\ \frac{\sqrt{5}}{2}\frac{\mathrm{d}v}{\mathrm{d}x}(x=L) &= t_0. \end{aligned}$$

The bar over u says that $\overline{u}$ is essentially different from u. However, the bar over the coordinate x is actually not necessary. The rigorous theory behind the periodic homogenization does not need to distinguish x and $\overline{x}$. In the lecture we used $\overline{x}$ on purpose to make the "engineering sense" out of it.

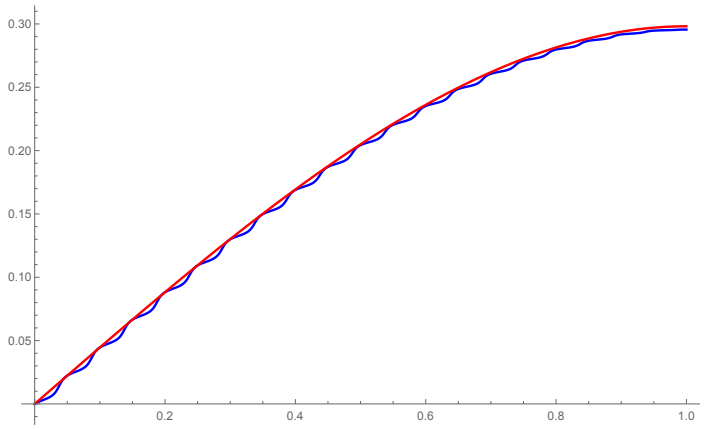


Figure 4: Comparison between the full-field solution (blue) and the homogenized solution (red)

Exercise 2

In this exercise we shall state the periodic homogenization problem in the variational formulation using the model problem (1). First, we see that the full-field BVP (1) is equivalent to the following variational principle

$$\inf_{u\in\mathcal{U}} \Pi(u) = \inf_{u\in\mathcal{U}} \left\{ \frac{1}{2}\int_0^L C(x)\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)^2 \mathrm{d}x - \int_0^L f(x)u(x)\mathrm{d}x - t_0\, u|_{x=L} \right\},$$

in which $\mathcal{U}$ is a function space consisting of function $u \in H^1(0, L)$ that satisfy the essential boundary condition $u(x = 0) = u_0$. The solution is obtained through the variational equation

$$\delta\left\{ \frac{1}{2}\int_0^L C(x)\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)^2 \mathrm{d}x - \int_0^L f(x)u(x)\mathrm{d}x - t_0 u|_{x=L} \right\} = 0.$$

We shall not go further in computing this variation. Instead, we shall argue formally why we motivate the periodic homogenization theory.

It is clear that the internal and external energies of the system are

$$\Pi_{\text{int}} = \frac{1}{2}\int_0^L C(x)\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)^2 \mathrm{d}x,$$
$$\Pi_{\text{ext}} = \int_0^L f(x)u(x)\mathrm{d}x - t_0 u\Big|_{x=L}.$$

In our example $f(x) = x$ and $C(x) = 3/2 + \sin(2\pi kx)$ with quite large k. It is obvious that $C(x)$ is periodic and very oscillatory within the domain $\Omega = (0, L)$. On the other hand $f(x) = x$ does not oscillate at all within Ω. The wavelength of the periodic function $C(x)$ is $2\pi/(2\pi k) = 1/k$ which is very small as compared to L when $k \to \infty$. This makes us "feel" that there exists two scales in our problem: $\lambda \sim 1/k$ and $\Lambda \sim L$. The ratio between these two scales is $\eta = \frac{1}{kL}$ which tends to zero as k

tends to infinity. The numerical observation suggests that the solution is "almost" periodic and indeed oscillating very fast. The overall trend of the solution u seems to be the average of these all oscillations in several small windows. This observation leads us to the idea of averaging out the fast oscillation in the full-field solution. To this end, we hope that such average solution is what we want to have as a replacement of the full-field solution.

In order to clarify the averaging idea, we shall now study a simple example

$$g(x) = \sin(2\pi kx) + q(x),$$

where $q(x)$ does not oscillate with the same scale of $\sin(2\pi kx)$, k is quite large. For example, $q(x)$ can be a polynomial of any order. We take in our example

$$q(x) = x^2 \quad \Rightarrow \quad g(x) = \sin(2\pi kx) + x^2, \quad \forall x \in (0, L).$$

This function has two parts, one of which oscillates with the wavelength $\lambda = 1/k$ while the other has no oscillation in its structure. The plot of this function suggests that there exists an average function behind $g(x)$. Assume that we are standing at point $\overline{x}$. As the wavelength in this example is constant, a small window around $\overline{x}$ that completes an oscillation would be $(\overline{x} - \lambda/2, \overline{x} + \lambda/2)$. We may average out the "fast" oscillation of g in this window and assign this value to a new function, called the average function $\bar{g} = \bar{g}(\overline{x})$. In this sense we see that $\overline{x}$ indeed plays the same role as x so that $\bar{g}$ is defined by

$$\bar{g}(x) = \frac{1}{\lambda} \int_{x-\lambda/2}^{x+\lambda/2} g(\xi)\, \mathrm{d}\xi.$$

For visualization we choose $k = 10$ and the graphs of $g(x)$ and $\bar{g}(x)$ is shown in Fig. Fig: function and its average 1

We add one more example

$$h(x) = \sin(k(x)x) + \sqrt{x}, \quad k(x) = 2\pi x^{1/3},$$

in which the wavenumber k now depends on the coordinate x. The wavelength is given by $\lambda(x) = 2\pi/k(x) = 1/x^{1/3}$. The average function is once again defined as follows

$$\overline{h}(x) = \frac{1}{\lambda(x)} \int_{x-\lambda(x)/2}^{x+\lambda(x)/2} h(\xi)\, \mathrm{d}\xi.$$

The results are presented in Fig. Fig: function and its average 2.

Averaging "out" the fast oscillation in the involved energies is essential in the first-order homogenization theory. It is seen that $C(x)$ oscillates with the wavelength $\lambda = 1/k$ and henceforth the internal

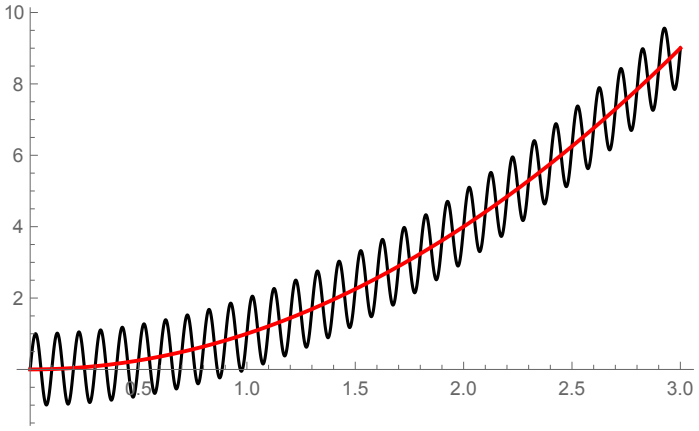


Figure 5: Function $g(x)$ (black) and its average $\bar{g}(x)$ over the fast oscillation within one wavelength (red).

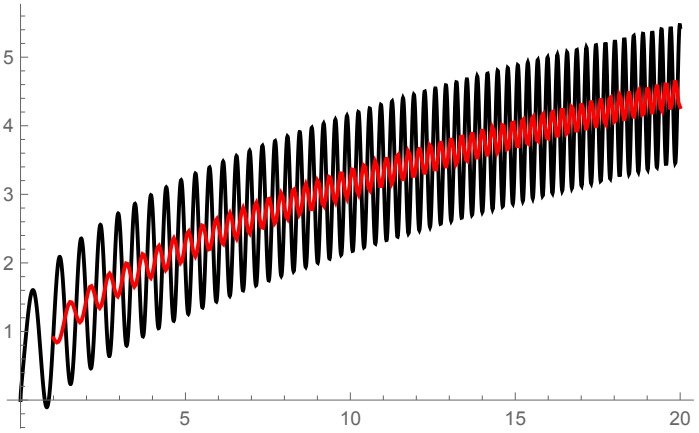


Figure 6: Function $h(x)$ (black) and its average $\bar{h}(x)$ over the fast oscilation within one wavelength (red).

energy Π_{int} is expected to do so. Using the strain definition $\epsilon = \mathrm{d}u/\mathrm{d}x$, we rewrite the internal energy as

$$\Pi_{\text{int}} = \frac{1}{2}\int_0^L C(x)\epsilon(u(x))^2 \mathrm{d}x.$$

The energy density

$$W(\epsilon) = \frac{1}{2}C(x)\epsilon^2 \tag{4}$$

characterizes the internal energy as the integral

$$\Pi_{\text{int}} = \int_0^L W(\epsilon(u(x))\mathrm{d}x.$$

The entire idea is briefly explained here. A "replacement" of the full-field internal energy is obtained by averaging the full-field internal energy density with respect to the wavelength of the solution which is in this case characterized by the wavelength of $C(x)$. This is the because the oscillation lies in the energy density $W(\epsilon)$. After averaging out this fast oscillation, we obtain the energy density that depends on the averaged strain $\overline{\epsilon}$ which should be understood as a field which is compatible with the "averaged" solution $\overline{u}$: $\overline{\epsilon} = \mathrm{d}\overline{u}/\mathrm{d}x$, or equivalently $\overline{\epsilon}(x) = \epsilon(\overline{u})$. The external energy does not contain any oscillations in its structure. Thus, no averaging is needed for this external energy. This explains why we apply the zero external force in the microscopic boundary value problem: $\mathrm{d}\sigma/\mathrm{d}x = 0$[1]. As a consequence of these arguments, the "replacement" boundary value problem is completely characterized by the average internal energy density and the "original" external energy. The average internal energy density is defined as

$$\overline{W}(\overline{\epsilon}) = \frac{1}{\lambda_u(x)}\int_{x-\lambda_u(x)}^{x+\lambda_u(x)} W(\epsilon)\,\mathrm{d}x, \quad \epsilon(x) = u'(x).$$

where $\lambda_u(x)$ is the wavelength of the full-field solution. Unfortunately, there is a little counter-intuition in this approach because we basically do not know u a priori and hence the computation of $\overline{W}_{\text{int}}(\overline{\epsilon})$ seems "ridiculous". Luckily, the first-order homogenization theory says that $\overline{W}(\overline{\epsilon})$ can be computed as a minimization principle

$$\overline{W}(\overline{\epsilon}) = \inf_{u\in\mathcal{W}}\left\{\frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} W(\epsilon)\,\mathrm{d}x\right\}, \tag{5}$$

in which $\mathcal{W}$ is some appropriate function space. The consistency condition in the homogenization theory helps to describe such function space appropriately. In this example, we agree for now that $\mathcal{W}$ consists of functions u that is "pseudo-periodic" in an RVE $\omega = (-\lambda/2, \lambda/2)$, that is

$$[\![u]\!] = \overline{\epsilon}[\![x]\!] = \overline{\epsilon}\big[(\lambda/2) - (-\lambda/2)\big] = \overline{\epsilon}\lambda. \tag{6}$$

[1]Euler equation does not involve the external force as seen later

In addition such a u must produce the traction $\sigma(x)n(x) = C(x)\epsilon(u(x))n(x)$ that is anti-periodic on the RVE $\omega = (-\lambda/2, \lambda/2)$, that is

$$\sigma(-\lambda/2)\underbrace{n(-\lambda/2)}_{-1} = \sigma(\lambda/2)\underbrace{n(\lambda/2)}_{1} \quad \Leftrightarrow \quad \sigma(-\lambda/2) = \sigma(\lambda/2).$$

We notice that the "pseudo-periodic" condition on u is the motivation for decomposing the original displacement field into the periodic displacement field and the linear term contribution $\bar{\epsilon}x$:

$$u(x) = \widetilde{u}(x) + \bar{\epsilon}x \quad \forall x \in \omega = (-\lambda/2, \lambda/2). \tag{7}$$

We see immediately that this decomposition will automatically fulfill the condition (6) if and only if $\widetilde{u}(x)$ is periodic because

$$[\![u]\!] = \underbrace{[\![\widetilde{u}]\!]}_{0} + [\![\bar{\epsilon}x]\!] = \bar{\epsilon}[\![x]\!].$$

Remark In the minimization principle (5) the average strain $\bar{\epsilon}$ is considered as given. The "pseudo-periodic" condition (6), or equivalently displacement decomposition and the periodic condition on $\widetilde{u}$, already implies

$$\bar{\epsilon} = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} \epsilon(x)\,\mathrm{d}x.$$

This is because the integration of the strain over the RVE $\omega = (-\lambda/2, \lambda/2)$

$$\epsilon(x) = \frac{\mathrm{d}u}{\mathrm{d}x} = \frac{\mathrm{d}\widetilde{u}}{\mathrm{d}x} + \bar{\epsilon}.$$

gives

$$\frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} \epsilon(x)\mathrm{d}x = \underbrace{\widetilde{u}\Big|_{x\to\lambda/2}^{x\to\lambda/2}}_{0} + \bar{\epsilon} = \bar{\epsilon}$$

due to the periodicity of $\widetilde{u}$.

In summary, the average internal energy density $\overline{W}(\bar{\epsilon})$ as a function of $\bar{\epsilon}$ is completely determined by solving the boundary value problem that is the Euler equation of the minimization principle

$$\inf_{u\in\mathcal{W}(\bar{\epsilon})}\int_{\omega} W(\epsilon(u(x))) = 0 \quad \Leftrightarrow \quad \inf_{u\in\mathcal{W}(\bar{\epsilon})}\frac{1}{2}\int_{-\lambda/2}^{\lambda/2} C(x)\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)^2\mathrm{d}x = 0. \tag{8}$$

Varying the above function with respect to u taking into account the pseudo-periodic condition on u, the anti-periodic condition on the traction $t = \sigma(x)n(x) = C(x)\,\mathrm{d}u/\mathrm{d}x\,n(x)$, we obtain exactly the microscopic BVP (3).

Having obtained the microscopic solution $u(x)$ from the variational principle (8), we can compute the average internal energy density by substituting the microscopic solution $u(x)$ into the original energy density:

$$\overline{W}(\overline{\epsilon}) = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} W(\epsilon(u(x)))\,\mathrm{d}x,$$

in which $\epsilon(x)$ is computed in accordance with the microscopic displacement solution of (8).

Next, upgrading from the microscale to macroscale, we assume that the homogenized solution $\overline{u}$ is the solution behind the strain $\overline{\epsilon}$, that is

$$\overline{\epsilon}(x) = \frac{\mathrm{d}\overline{u}}{\mathrm{d}x}.$$

and the homogenized stress is the average stress

$$\overline{\sigma} = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} \sigma(x)\,\mathrm{d}x. \tag{9}$$

It can be seen that $\overline{\sigma}$ is obtained from the macroscopic constitutive law[2]

$$\overline{\sigma} = \frac{\partial \overline{W}}{\partial \overline{\epsilon}}.$$

The main concern of the first-order homogenization theory is the variational principle for the homogenized displacement solution $\overline{u}$ that is the "replacement" of the original solution. The most important result from the first-order homogenization theory is that the homogenized solution is the solution (the stationary point) of the macroscopic minimization principle

$$\inf_{\overline{u}\in\mathcal{U}} \overline{\Pi}(\overline{u}) = \inf_{\overline{u}\in\mathcal{U}} \left\{ \int_0^L \overline{W}(\overline{\epsilon})\mathrm{d}x - \int_0^L f(x)\overline{u}(x)\mathrm{d}x - t_0\overline{u}\big|_{x=L} \right\}.$$

The solution is the stationary point of the variational equation

$$\delta\left\{ \int_0^L \overline{W}(\overline{\epsilon})\mathrm{d}x - \int_0^L f(x)\overline{u}(x)\mathrm{d}x - t_0\overline{u}\big|_{x=L} \right\} = 0.$$

Remark This statement is for now accepted as a result of the asymptotic expansion of the internal energy with respect to $\overline{\epsilon}$ and only first-order approximation is kept. We shall prove it neither formally nor rigorously because the proof will be very involved. On the other hand, the consistency condition mentioned above helps to build a micro-macroscale bridge in the homogenization theory. Such consistency condition is indeed derivable from such truncation of the asymptotic expansion upto the first order of $\overline{\epsilon}$.

[2]This statement will be considered as homework.

Exercise 3

In this exercise we study the nonlinear boundary value problem in which we allow the nonlinear constitutive law. To this end we examine the following boundary value problem as our model problem which is stated as a variational principle

$$\inf_{u\in\mathcal{U}} \Pi = \inf_{u\in\mathcal{U}} \left\{ \int_0^L W(\epsilon(u(x)))\mathrm{d}x - \int_0^L f(x)u(x)\mathrm{d}x - t_0 u\Big|_{x=L} \right\},$$

where $\mathcal{U}$ is defined as before. Thus, the essential boundary condition of this minimization principle is $u(x=0) = u_0$.

The variational equation is obtained by varying the function Π with respect to u as follows

$$\delta\left\{ \int_0^L W(\epsilon(u(x)))\mathrm{d}x - \int_0^L f(x)u(x)\mathrm{d}x - t_0 u\Big|_{x=L} \right\} = 0.$$

In this example we study the constitutive law

$$\sigma = C(\sqrt{1+\epsilon}-1) \quad \Leftrightarrow \quad \frac{\partial W}{\partial \epsilon} = C(\sqrt{1+\epsilon}-1) \quad \Leftrightarrow \quad W = \int C(\sqrt{1+\epsilon}-1)\,\mathrm{d}\epsilon = C\left[\frac{2}{3}(1+\epsilon)^{3/2} - \epsilon\right].$$

Remark The term "-1" appears here to make the stress vanish at the zero strain. The stored energy density vanishes at zero strain. That is, the zero level for the stored energy density which is considered as a potential field is chosen at the state of rigid body motion.

The inhomogeneity is reflected in the material parameter C as a function of x. Once again, we take $C(x) = 3/2 + \sin(2\pi k x)$ with quite large k. The wavelength is $\lambda = 1/k$ as before. According this variational principle, the full-field boundary value problem is given as follows

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}x}\left[C(x)\left(\sqrt{1+\frac{\mathrm{d}u}{\mathrm{d}x}}-1\right)\right] + f(x) &= 0, \\ u(x=0) &= u_0, \\ \left\{C(x)\left(\sqrt{1+\frac{\mathrm{d}u}{\mathrm{d}x}}-1\right)\right\}|_{x=L} &= t_0. \end{aligned} \tag{10}$$

For $k = 10$, $f(x) = x$, $u_0 = 0$, t_0, the numerical solution of this BVP can be obtained by finite element method with very fine mesh and the solution is visually shown in Fig. 7.

Following exactly the same spirit and procedure described in Exercise 2 (see also exercise 1), the microscopic boundary value problem is derived from the minimization principle

$$\inf_{u\in\mathcal{W}} \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} W(\epsilon(u(x)))\mathrm{d}x,$$

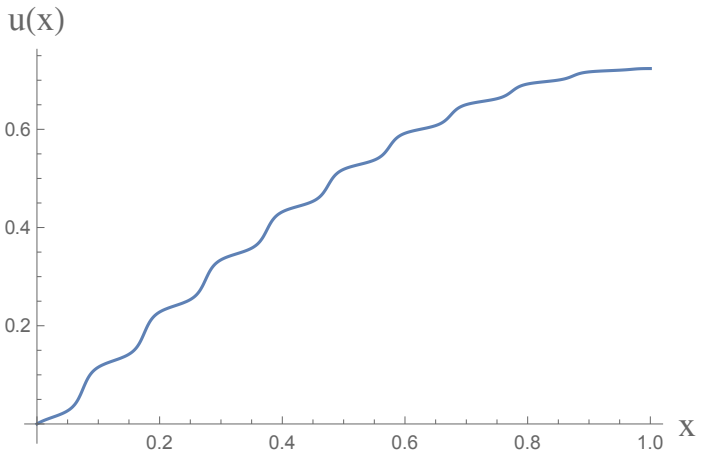


Figure 7: Full-field solution of the nonlinear boundary value problem (10).

where $\mathcal{W}$ is the function space defined as in Exercise 2. The Euler equations of this variational principle establish the microscopic boundary value

$$\frac{\mathrm{d}}{\mathrm{d}x}\sigma(x) = 0,$$

$$\sigma(x) = C(x)\big(\sqrt{1+\epsilon(u(x))}-1\big) = C(x)\left(\sqrt{1+\frac{\mathrm{d}\widetilde{u}}{\mathrm{d}x}+\overline{\epsilon}}-1\right) \quad \forall x \in (-\lambda/2, \lambda/2),$$

$\widetilde{u}$ is periodic,

σn is antiperiodic.

The first equation implies $\sigma(x) = \text{constant} = \kappa$ within the RVE $\omega = (-\lambda/2, \lambda/2)$. The second equation yields

$$\left[\frac{\kappa}{C(x)}+1\right]^2 - 1 - \overline{\epsilon} = \frac{\mathrm{d}\widetilde{u}}{\mathrm{d}x} \quad \Rightarrow \quad \frac{\mathrm{d}\widetilde{u}}{\mathrm{d}x} = \left[\frac{\kappa}{3/2+\sin(2\pi k x)}+1\right]^2 - 1 - \overline{\epsilon}.$$

Integration of this equation gives

$$\widetilde{u} = \int \left[\left(\frac{\kappa}{3/2+\sin(2\pi k x)}\right)^2 + 1\right]\mathrm{d}x - x - \overline{\epsilon}x = p(x) - \overline{\epsilon}x.$$

The periodic condition on $\widetilde{u}$ requires

$$p(x \to \lambda/2) - p(x \to -\lambda/2) = \overline{\epsilon}\lambda. \tag{11}$$

Evaluating the anti-derivative in definition of $p(x)$ using *Mathematica*, we obtain

$$\begin{aligned} p(x) &= \int \left\{\left[\left(\frac{\kappa}{3/2+\sin(2\pi k x)}\right)^2 + 1\right] - 1\right\}\mathrm{d}x \\ &= \frac{4\kappa\left(\sqrt{5}(5+3\kappa)\arctan\frac{2+3\tan(\pi k x)}{\sqrt{5}} + \frac{5+\cos(2\pi k x)}{3+\sin(2\pi k x)}\right)}{25\pi k} \end{aligned}$$

Again, with *Mathematica* the limits $p(x \to \pm\lambda/2)$ are evaluated as follows

$$\lim_{x\to\lambda/2} p(x) = \frac{2\kappa\big[-10\kappa + 3\sqrt{5}\pi(5+3\kappa)\big]}{75k\pi}, \quad \lim_{x\to-\lambda/2} = -\lim_{x\to\lambda/2} p(x).$$

Substituting these results into the condition (11), we obtain the equation for κ. The root of this equation is

$$\kappa_{\pm} = \frac{\pi\big[-3\sqrt{5} \pm \sqrt{3/\pi}\sqrt{15\pi - 10\overline{\epsilon} + 9\sqrt{5}\pi\overline{\epsilon}}\big]}{2(-2+9\pi/\sqrt{5})}.$$

The right solution corresponds to the "plus" branch, that is

$$\sigma(x) = \kappa = \frac{\pi\big[-3\sqrt{5} + \sqrt{3/\pi}\sqrt{15\pi - 10\overline{\epsilon} + 9\sqrt{5}\pi\overline{\epsilon}}\big]}{2(-2+9\pi/\sqrt{5})} \quad \forall x \in (-\lambda/2, \lambda/2).$$

The average stress is computed as follows

$$\overline{\sigma} = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2} \sigma(x)\mathrm{d}x = \kappa.$$

Thus, the macroscopic constitutive relation is given by

$$\overline{\sigma} = \frac{\pi\big[-3\sqrt{5} + \sqrt{3/\pi}\sqrt{15\pi - 10\overline{\epsilon} + 9\sqrt{5}\pi\overline{\epsilon}}\big]}{2(-2+9\pi/\sqrt{5})}.$$

The macroscopic energy density is given

$$\frac{\partial\overline{W}}{\partial\overline{\epsilon}} = \overline{\sigma}(\overline{\epsilon}) \quad \Rightarrow \quad \overline{W}(\overline{\epsilon}) = \int \overline{\sigma}(\overline{\epsilon})\mathrm{d}\overline{\epsilon}.$$

Using this marcosopic constitutive law, the macroscopic boundary value problem is set up as the minimization principle

$$\inf_{\overline{u}\in\mathcal{U}}\left\{\int_0^L \overline{W}(\overline{\epsilon})\mathrm{d}x - \int_0^L f(x)\overline{u}(x)\mathrm{d}x - t_0 u\big|_{x=L}\right\}.$$

The corresponding Euler equation is the macroscopic boundary value problem

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}x}\left[\overline{\sigma}\left(\frac{\mathrm{d}\overline{u}}{\mathrm{d}x}\right)\right] + f(x) &= 0, \\ \overline{u}(x=0) &= u_0, \\ \overline{\sigma}(x=L) &= t_0. \end{aligned} \tag{12}$$

We solve this macroscopic BVP using the finite element method in *Mathematica*. The numerical results of the original BVP (10) and the homogenized BVP (12) are shown in Fig. 8.

This result "numerically" justifies the first-order homogenization theory for the nonlinear problem.

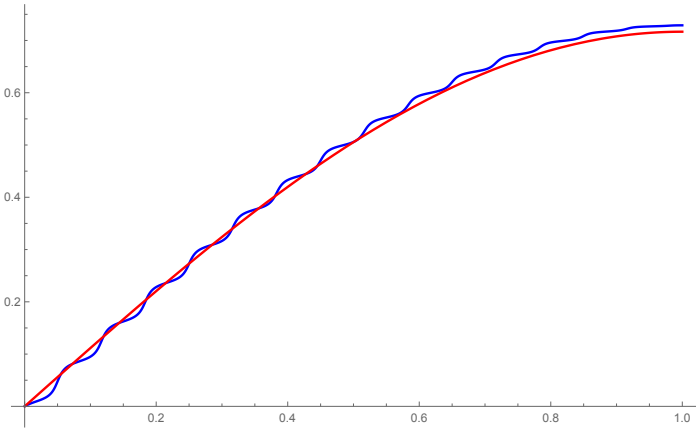


Figure 8: Comparison between the full-field solution of the original BVP (10) and the homogenized solution according to (12).

Exercise 4

There are many different possibilities of choosing $\mathbb{C}$, one of which is to mimic the isotropic linear material stiffness, that is

$$C^0_{ijkl} = \lambda^0 \delta_{ij}\delta_{kl} + \mu^0(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{13}$$

where λ^0 and μ^0 are two constants selected for the convergence of the fixed-point scheme which is presented later.

We can compute the acoustic tensor $\mathbf{K}^0(\boldsymbol{\xi})$ and and its inverse $\mathbf{N}^0(\boldsymbol{\xi})$ as follows

$$\begin{aligned}
K^0_{ij}(\boldsymbol{\xi}) &= (\lambda^0 + \mu^0)\xi_i\xi_j + \mu^0|\boldsymbol{\xi}|^2\delta_{ij},\\
N^0_{ij}(\boldsymbol{\xi}) &= \frac{1}{\mu^0\,|\boldsymbol{\xi}|^2}\left(\delta_{ij} - \frac{\lambda^0+\mu^0}{\lambda^0+2\mu^0}\frac{\xi_i\xi_j}{|\boldsymbol{\xi}|^2}\right),\\
\widehat{\Gamma^0}_{ijkl}(\boldsymbol{\xi}) &= -\frac{1}{4\mu^0\,|\boldsymbol{\xi}|^2}\big(\delta_{ik}\xi_j\xi_l + \delta_{jk}\xi_i\xi_l + \delta_{il}\xi_j\xi_k + \delta_{jl}\xi_i\xi_k\big) + \frac{\lambda^0+\mu^0}{\mu^0(\lambda^0+2\mu^0)}\frac{\xi_i\xi_j\xi_k\xi_l}{|\boldsymbol{\xi}|^4}.
\end{aligned} \tag{14}$$

Solution By definition the acoustic tensor $\mathbf{K}^0(\boldsymbol{\xi})$ is defined through

$$K^0_{ik}(\boldsymbol{\xi}) = C^0_{ijkl}\xi_j\xi_l.$$

Direct substitution of (13) into the above definition yields

$$\begin{aligned}
K^0_{ik} &= \lambda^0(\delta_{ij}\xi_j)(\delta_{kl}\xi_l) + \mu^0(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\xi_j\xi_l\\
&= \lambda^0\xi_i\xi_k + \mu^0\big[\delta_{ik}\underbrace{\xi_j\xi_j}_{|\boldsymbol{\xi}|^2} + \underbrace{(\delta_{il}\xi_l)}_{\xi_i}\underbrace{(\delta_{jk}\xi_j)}_{\xi_k}\big]\\
&= (\lambda^0+\mu^0)\xi_i\xi_k + \mu^0|\xi|^2\delta_{ik}.
\end{aligned}$$

This computation justifies the first result $(14)_1$.

In order to compute tensor $\mathbf{N}^0(\boldsymbol{\xi})$, we apply the formula

$$\mathbf{N}^0 = \big[\mathbf{K}^0\big]^{-1} = \frac{1}{\det\mathbf{K}^0}\mathrm{adj}[\mathbf{K}^0], \tag{15}$$

where $\mathrm{adj}\big[\mathbf{K}^0\big]$ denotes the adjugate of tensor $\mathbf{K}^0$ and the dependence on $\boldsymbol{\xi}$ is already dropped. First, we write down the tensor $\mathbf{K}^0$ explicitly as follows

$$\mathbf{K}^0 = \begin{bmatrix}
(\lambda^0+\mu^0)\xi_1^2 + \mu^0|\boldsymbol{\xi}|^2 & (\lambda^0+\mu^0)\xi_1\xi_2 & (\lambda^0+\mu^0)\xi_1\xi_3\\
K^0_{12} & (\lambda^0+\mu^0)\xi_2^2 + \mu^0|\boldsymbol{\xi}|^2 & (\lambda^0+\mu^0)\xi_2\xi_3\\
K^0_{13} & K^0_{23} & (\lambda^0+\mu^0)\xi_3^2 + \mu^0|\boldsymbol{\xi}|^2
\end{bmatrix}. \tag{16}$$

After some algebraic manipulation, we arrive at

$$\det \mathbf{K}^0 = (\lambda^0 + 2\mu^0)(\mu^0)^2 |\boldsymbol{\xi}|^6. \tag{17}$$

Again, some dummy computation gives

$$\begin{aligned}
\operatorname{adj}\big[\mathbf{K}^0\big]_{11} &= (-1)^{1+1}\big(K^0_{22}K^0_{33} - K^0_{23}K^0_{32}\big) \\
&= \mu^0|\boldsymbol{\xi}|^2\big[\lambda^0(\xi_2^2\xi_3^2 + \mu^0(\xi_1^2 + 2(\xi_2^2 + \xi_3^2))\big] \\
&= \mu^0|\boldsymbol{\xi}|^2\big[\lambda^0(|\boldsymbol{\xi}|^2 - \xi_1^2) + \mu^0(2|\boldsymbol{\xi}|^2 - \xi_1^2)\big] \\
&= \mu^0|\boldsymbol{\xi}|^2\big[(\lambda + 2\mu)|\boldsymbol{\xi}|^2 - (\lambda^0 + \mu^0)\xi_1^2\big], \\
\operatorname{adj}\big[\mathbf{K}^0\big]_{12} &= (-1)^{1+2}\big(K^0_{21}K_{33} - K^0_{31}K^0_{23}\big) \\
&= -\mu^0(\lambda^0 + \mu^0)\xi_1\xi_2|\boldsymbol{\xi}|^2.
\end{aligned}$$

It is not difficult to recognize the special algebraic structure of the above result. Observing the structure of $\mathbf{K}^0$, it is easily seen that further computation would give the values of $\operatorname{adj}\big[\mathbf{K}^0\big]_{ij}$ with only the permutation of the wavenumbers ξ_1, ξ_2 and ξ_3 in an appropriate manner. Without much computation effort we can easily derive

$$\begin{aligned}
\operatorname{adj}\big[\mathbf{K}^0\big]_{12} &= \operatorname{adj}\big[\mathbf{K}^0\big]_{21} = -\mu^0(\lambda^0 + \mu^0)\xi_1\xi_2|\boldsymbol{\xi}|^2, \\
\operatorname{adj}\big[\mathbf{K}^0\big]_{13} &= \operatorname{adj}\big[\mathbf{K}^0\big]_{31} = -\mu^0(\lambda^0 + \mu^0)\xi_1\xi_3|\boldsymbol{\xi}|^2, \\
\operatorname{adj}\big[\mathbf{K}^0\big]_{23} &= \operatorname{adj}\big[\mathbf{K}^0\big]_{32} = -\mu^0(\lambda^0 + \mu^0)\xi_2\xi_3|\boldsymbol{\xi}|^2, \\
\operatorname{adj}\big[\mathbf{K}^0\big]_{11} &= \mu^0|\boldsymbol{\xi}|^2\big[(\lambda + 2\mu^0)|\boldsymbol{\xi}|^2 - (\lambda^0 + \mu^0)\xi_1\xi_1\big], \\
\operatorname{adj}\big[\mathbf{K}^0\big]_{22} &= \mu^0|\boldsymbol{\xi}|^2\big[(\lambda + 2\mu^0)|\boldsymbol{\xi}|^2 - (\lambda^0 + \mu^0)\xi_2\xi_2\big], \\
\operatorname{adj}\big[\mathbf{K}^0\big]_{33} &= \mu^0|\boldsymbol{\xi}|^2\big[(\lambda + 2\mu^0)|\boldsymbol{\xi}|^2 - (\lambda^0 + \mu^0)\xi_3\xi_3\big].
\end{aligned}$$

Thus, we may summarize the above results into the following form

$$\operatorname{adj}\big[\mathbf{K}^0\big]_{ij} = \mu^0(\lambda^0 + 2\mu^0)|\boldsymbol{\xi}|^4\delta_{ij} - \mu^0(\lambda^0 + \mu^0)\xi_i\xi_j|\boldsymbol{\xi}|^2. \tag{18}$$

Combination of two results (17) and (18) in tandem with the inverse formula (15) leads to

$$\begin{aligned}
\mathbf{N}^0(\boldsymbol{\xi}) &= \frac{\mu^0(\lambda^0 + 2\mu^0)|\boldsymbol{\xi}|^4\delta_{ij} - \mu^0(\lambda^0 + \mu^0)\xi_i\xi_j|\boldsymbol{\xi}|^2}{(\lambda^0 + 2\mu^0)(\mu^0)^2|\boldsymbol{\xi}|^6} \\
&= \frac{\delta_{ij}}{\mu^0|\boldsymbol{\xi}|^2} - \frac{(\lambda^0 + \mu^0)\xi_i\xi_j}{\mu^0(\lambda^0 + 2\mu^0)|\boldsymbol{\xi}|^4} \\
&= \frac{1}{\mu^0|\boldsymbol{\xi}|^2}\left[\delta_{ij} - \frac{(\lambda^0 + \mu^0)\xi_i\xi_j}{(\lambda^0 + 2\mu^0)|\boldsymbol{\xi}|^2}\right],
\end{aligned}$$

which justifies equation $(14)_2$.

The last result is verified by substitution of $(14)_2$ into the definition

$$\widehat{\Gamma^0}_{ijkl} = -\frac{1}{4}\big[N^0_{ik}\xi_j\xi_l + N^0_{jk}\xi_i\xi_l + N^0_{il}\xi_j\xi_k + N_{jl}\xi_i\xi_k\big]. \tag{19}$$

Simple derivation is given in the following

$$\begin{aligned}
\widehat{\Gamma^0}_{ijkl} = &-\frac{1}{4}\Bigg\{\frac{1}{\mu^0|\boldsymbol{\xi}|^2}\delta_{ik}\xi_j\xi_l + \frac{1}{\mu^0|\boldsymbol{\xi}|^2}\delta_{jk}\xi_i\xi_l + \frac{1}{\mu^0|\boldsymbol{\xi}|^2}\delta_{il}\xi_j\xi_k + \frac{1}{\mu^0|\boldsymbol{\xi}|^2}\delta_{jl}\xi_i\xi_k \\
&- \frac{1}{\mu^0|\boldsymbol{\xi}|^2}\frac{\lambda^0+\mu^0}{\lambda^0+2\mu^0}\frac{\xi_i\xi_k}{|\boldsymbol{\xi}|^2}\xi_j\xi_l - \frac{1}{\mu^0|\boldsymbol{\xi}|^2}\frac{\lambda^0+\mu^0}{\lambda^0+2\mu^0}\frac{\xi_j\xi_k}{|\boldsymbol{\xi}|^2}\xi_i\xi_l \\
&- \frac{1}{\mu^0|\boldsymbol{\xi}|^2}\frac{\lambda^0+\mu^0}{\lambda^0+2\mu^0}\frac{\xi_i\xi_l}{|\boldsymbol{\xi}|^2}\xi_j\xi_k - \frac{1}{\mu^0|\boldsymbol{\xi}|^2}\frac{\lambda^0+\mu^0}{\lambda^0+2\mu^0}\frac{\xi_j\xi_l}{|\boldsymbol{\xi}|^2}\xi_i\xi_k\Bigg\} \\
= &-\frac{1}{4\mu^0\,|\boldsymbol{\xi}|^2}\big(\delta_{ik}\xi_j\xi_l + \delta_{jk}\xi_i\xi_l + \delta_{il}\xi_j\xi_k + \delta_{jl}\xi_i\xi_k\big) + \frac{\lambda^0+\mu^0}{\mu^0(\lambda^0+2\mu^0)}\frac{\xi_i\xi_j\xi_k\xi_l}{|\boldsymbol{\xi}|^4}.
\end{aligned} \tag{20}$$

Exercise 5

In this exercise we shall study a two-dimensional simple laminate microstructure with only two phases of linear isotropic materials characterized by two sets of Lame's constants (λ_1, μ_1) and (λ_2, μ_2). For this simple microstructure, analytical solutions can be made available by solving the microscopic boundary value problems

$$\begin{aligned} \sigma_{ij,j} &= 0 \quad \forall \mathbf{x} \in \omega, \\ \sigma_{ij}(\mathbf{x}) &= C_{ijkl}(\mathbf{x})\big[\epsilon_{kl}(\widetilde{\mathbf{u}}) + \overline{\epsilon}_{kl}\big] = C_{ijkl}(\mathbf{x})\big[\widetilde{\epsilon}_{kl} + \overline{\epsilon}_{kl}\big], \\ \widetilde{\mathbf{u}} &\text{ is periodic on } \omega, \\ \sigma_{ij} n_j &\text{ is antiperiodic on } \omega. \end{aligned} \tag{21}$$

The domain ω is depicted in Fig. 9. The parameters λ_i, μ_i are the Lame's constants corresponding to the i^{th} phase.

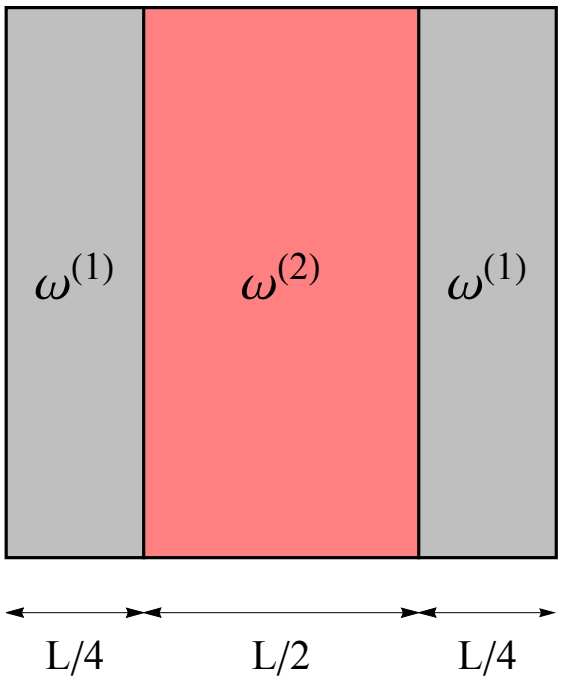


Figure 9: Microstructure of the laminate composite under investigation.

In this boundary value problem all the indices take value either 1 or 2. The equilibrium equation $(21)_1$ is explicitly written as

$$\begin{aligned} \sigma_{11,1} + \sigma_{12,2} &= 0, \\ \sigma_{21,1} + \sigma_{21,2} &= 0. \end{aligned} \tag{22}$$

The compatibility condition on the strain field is

$$(\nabla \times \boldsymbol{\epsilon}) \times \nabla = \mathbf{0},$$

whose two-dimensional reduction for plane strain problems is given by

$$\epsilon_{11,22} - 2\epsilon_{12,12} + \epsilon_{22,11} = 0. \tag{23}$$

Recalling that the compatibility condition is to say that the displacement field is a true potential field in the following sense. If the strain field is given, its path integral must be path-independent. Generally speaking, this can be guaranteed when the mixed derivatives are smooth throughout the whole definition domain. In the two-dimensional setting, we have

$$\epsilon_{11} = u_{1,1}, \quad \epsilon_{12} = \frac{1}{2}(u_{1,2} + u_{2,1}), \quad \epsilon_{22} = u_{2,2}.$$

The following relation must be fulfilled

$$u_{1,122} + u_{2,211} - 2 \times \frac{1}{2}(u_{1,212} + u_{2,112}) = 0,$$

which is nothing else but the reduced compatibility condition (23).

Let us denote $(\diamond)^{(1)}$ and $(\diamond)^{(1)}$ be the value of the field $(\diamond)$ at phase 1 and phase 2, respectively. For example, $\sigma_{ij}^{(1)}$ and $\sigma_{ij}^{(2)}$ are the stress distribution of phase 1 and phase 2, respectively. As the material structure is assembled only along the X1 direction and the RVE is periodic, it can be proved that all the variables occurring in equation $(21)_1$ are only dependent on x_1, that is

$$\sigma_{ij} = \sigma_{ij}(x_1), \qquad \epsilon_{ij} = \epsilon_{ij}(x_1). \tag{24}$$

The equilibrium equations (22) give

$$\sigma_{11,1} = 0, \quad \sigma_{21,1} = 0, \tag{25}$$

which deduce that σ_{11} and σ_{12} are strictly constants (independent of both x_1 and x_2

$$\sigma_{11} = \text{const}, \quad \sigma_{21} = \text{const}. \tag{26}$$

Two constants are not necessarily identical. Similar argument applied to equation (23) implies

$$\epsilon_{22} = \text{const}. \tag{27}$$

As we have only two phases in the microstructure, the following identities hold true

$$\sigma_{11}^{(1)} = \sigma_{11}^{(2)} = \text{const}, \quad \sigma_{21}^{(1)} = \sigma_{21}^{(2)} = \text{const} \tag{28}$$

and

$$\epsilon_{22}^{(1)} = \epsilon_{22}^{(2)} = \text{const}. \tag{29}$$

The constitutive relations

$$\sigma_{ij}^{(\alpha)} = \lambda_\alpha \delta_{ij} \epsilon_{kk}^{(\alpha)} + 2\mu \epsilon_{ij}^{(\alpha)} \quad \alpha = 1, 2$$

bring two equations (28) to equations for $\boldsymbol{\epsilon}^{(1)}$ and $\boldsymbol{\epsilon}^{(2)}$, that is

$$\begin{cases} \sigma_{11}^{(1)} = \sigma_{11}^{(2)} \\ \sigma_{21}^{(1)} = \sigma_{21}^{(2)} \end{cases} \quad \Leftrightarrow \quad \begin{cases} \lambda_1\big(\epsilon_{11}^{(1)} + \epsilon_{22}^{(1)}\big) + 2\mu_1 \epsilon_{11}^{(1)} & = \lambda_2\big(\epsilon_{11}^{(2)} + \epsilon_{22}^{(2)}\big) + 2\mu_2 \epsilon_{11}^{(2)}, \\ 2\mu_1 \epsilon_{12}^{(1)} & = 2\mu_2 \epsilon_{12}^{(2)} \end{cases} \tag{30}$$

In addition to the consideration of the equilibrium equations and the compatibility condition, we are left with only the average conditions

$$\begin{aligned} \frac{1}{|\omega|}\int_\omega \epsilon_{11}(\mathbf{x})\mathrm{d}\mathbf{x} &= \frac{1}{2}\epsilon_{11}^{(1)} + \frac{1}{2}\epsilon_{11}^{(2)} = \overline{\epsilon}_{11}, \\ \frac{1}{|\omega|}\int_\omega \epsilon_{12}(\mathbf{x})\mathrm{d}\mathbf{x} &= \frac{1}{2}\epsilon_{12}^{(1)} + \frac{1}{2}\epsilon_{12}^{(2)} = \overline{\epsilon}_{12}, \\ \frac{1}{|\omega|}\int_\omega \epsilon_{22}(\mathbf{x})\mathrm{d}\mathbf{x} &= \frac{1}{2}\epsilon_{22}^{(1)} + \frac{1}{2}\epsilon_{22}^{(2)} = \overline{\epsilon}_{22}, \end{aligned} \tag{31}$$

where use has be made of the fact that the fraction $1/2$ comes from the volume fraction $1/2 - 1/2$ of two phases and that the strain $\epsilon_{ij}^{(\alpha)}$, $\alpha = 1, 2$ are constant in each phase.

We summarize three set of equations (29), (30), (31) into a system of six equations for six variables $\epsilon_{11}^{(\alpha)}$, $\epsilon_{12}^{(\alpha)}$, $\epsilon_{22}^{(\alpha)}$, $\alpha = 1, 2$ as follows

$$\boxed{\begin{aligned} \lambda_1\big(\epsilon_{11}^{(1)} + \epsilon_{22}^{(1)}\big) + 2\mu_1 \epsilon_{11}^{(1)} &= \lambda_2\big(\epsilon_{11}^{(2)} + \epsilon_{22}^{(2)}\big) + 2\mu_2 \epsilon_{11}^{(2)}, \\ 2\mu_1 \epsilon_{12}^{(1)} &= 2\mu_2 \epsilon_{12}^{(2)}, \\ \epsilon_{22}^{(1)} &= \epsilon_{22}^{(2)}, \\ \frac{1}{2}\epsilon_{11}^{(1)} + \frac{1}{2}\epsilon_{11}^{(2)} &= \overline{\epsilon}_{11}, \\ \frac{1}{2}\epsilon_{12}^{(1)} + \frac{1}{2}\epsilon_{12}^{(2)} &= \overline{\epsilon}_{12}, \\ \frac{1}{2}\epsilon_{22}^{(1)} + \frac{1}{2}\epsilon_{22}^{(2)} &= \overline{\epsilon}_{22}. \end{aligned}} \tag{32}$$

Numerical example As for numerical investigation the following material parameters and the prescribed macroscopic strain are used:

- Material parameters

$$\lambda_1 = 1, \quad \lambda_2 = 2, \quad \mu_1 = 1, \quad \mu_2 = 2.$$

- Input macroscopic strain

$$\bar{\epsilon}_{11} = 1/100, \quad \bar{\epsilon}_{12} = 0, \quad \bar{\epsilon}_{22} = 2/100.$$

Solving system (32) with the aforementioned input variables yields

$$\begin{aligned} \epsilon_{11}^{(1)} &= \frac{7}{450} \approx 0.01555, & \epsilon_{11}^{(2)} &= \frac{1}{225} \approx 0.00444, \\ \epsilon_{12}^{(1)} &= 0, & \epsilon_{12}^{(2)} &= 0, \\ \epsilon_{22}^{(1)} &= \frac{1}{50} = 0.02, & \epsilon_{22}^{(2)} &= \frac{1}{50} = 0.02. \end{aligned}$$

These analytical solution is completely in agreement with the numerical result obtained by the fixed-point iteration scheme programmed in MATLAB using the Lippmann-Schwinger equation, see Fig. 10.

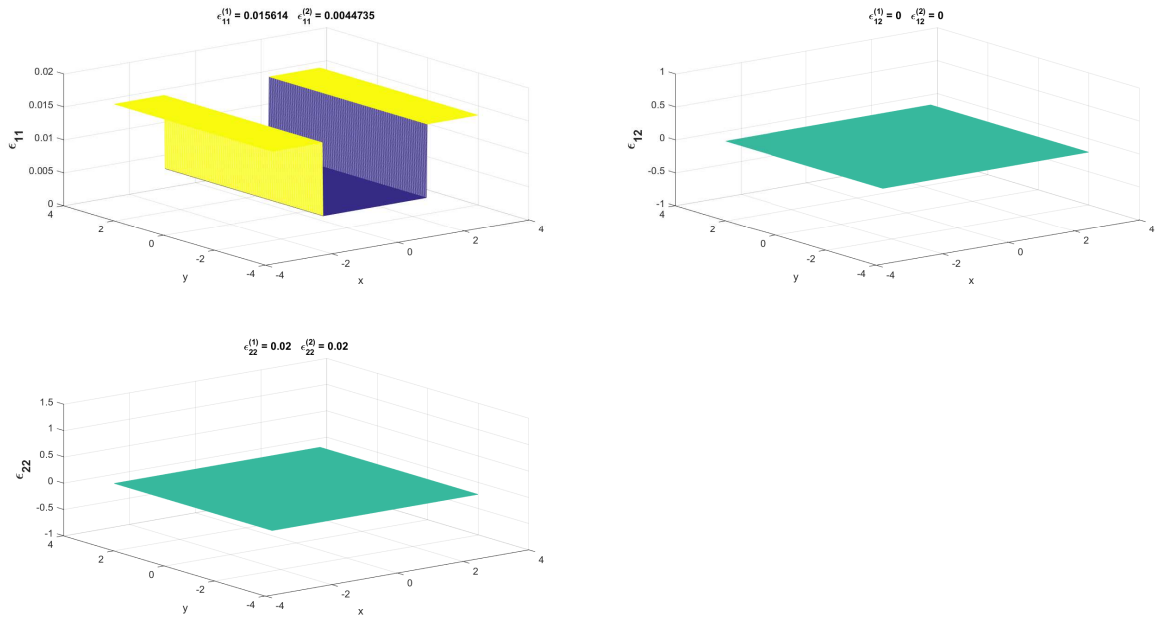


Figure 10: Distribution of the strain field throughout the microscopic domain ω

Exercise 6

The homogenization method is definitely not a method exclusively used in computational mechanics. The idea of homogenization method in fact comes from physicists and mathematicians at the first place. In this exercise we shall apply the technique to the Poisson equation with periodic variable coefficient. In the following we describe three boundary value problems:

- Full-field boundary value problem

$$\begin{aligned} \nabla \cdot \mathbf{q} &= 0 \quad \mathbf{x} \in \Omega, \\ \mathbf{q} &= \mathbf{C}(\mathbf{x}) \cdot \mathbf{p}, \quad \mathbf{p} = \nabla \phi, \\ \phi\big|_{\Gamma_D} &= u_0, \\ \mathbf{q} \cdot \mathbf{n}\big|_{\Gamma_N} &= t_0. \end{aligned} \tag{33}$$

- Macroscopic boundary value problem

$$\begin{aligned} \nabla \cdot \overline{\mathbf{q}} &= 0 \quad \mathbf{x} \in \Omega \\ \overline{\mathbf{q}} &= \overline{\mathbf{q}}(\overline{\mathbf{p}}), \quad \overline{\mathbf{p}} = \nabla \overline{\phi} \\ \overline{\phi}\big|_{\Gamma_D} &= u_0, \\ \overline{\mathbf{q}} \cdot \mathbf{n}\big|_{\Gamma_N} &= t_0. \end{aligned} \tag{34}$$

- Microscopic boundary value problem

$$\begin{aligned} \nabla \cdot \mathbf{q} &= \mathbf{0} \quad \forall \mathbf{x} \in \omega, \\ \mathbf{q} &= \mathbf{C}(\mathbf{x}) \cdot \mathbf{p}, \quad \mathbf{p} = \nabla \phi, \\ \phi &= \widetilde{\phi} + \overline{\mathbf{p}} \cdot \mathbf{x}, \\ &\widetilde{\phi} \text{ is periodic}, \\ &\mathbf{q} \cdot \mathbf{n} \text{ is antiperiodic}. \end{aligned} \tag{35}$$

In this exercise we shall mostly focus on solving the microscopic BVP (35) by resorting to the corresponding Lippmann-Schwinger equation. To this end, we rewrite the equilibrium equation in the indicial form

$$q_{i,i} = 0 \quad q_{i,i} - \left(C^0_{ij} p_j + C^0_{ij} p_j\right)_{,i} = 0 \quad \Leftrightarrow \quad C^0_{ij} p_{j,i} = -\tau_{i,i}, \tag{36}$$

where the polarization tensor is defined by

$$\tau_i = q_i - C^0_{ij} p_j.$$

The average condition on the gradient field is the consequence of the periodic condition on $\widetilde{\phi}$ and the decomposition $\phi = \widetilde{\phi} + \overline{\mathbf{p}} \cdot \mathbf{x}$ and given by

$$\frac{1}{|\omega|} \int_{\omega} \mathbf{p}(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \overline{\mathbf{p}} \tag{37}$$

Two equations (36) and (37) can be rephrased as the Lippmann-Schwinger equation as follows

$$\boxed{p_i(\mathbf{x}) = \widehat{\Gamma^0}_{ij} * \tau_j(\mathbf{x}) + \overline{p}_i \quad \Leftrightarrow \quad \mathbf{p}(\mathbf{x}) = \boldsymbol{\Gamma}^0 * \boldsymbol{\tau}(\mathbf{x}) + \overline{\mathbf{p}}.} \tag{38}$$

Derivation of Lippmann-Schwinger equation In the Fourier space the equilibrium equation (36) takes the form

$$\mathrm{i}\, \xi_i \widehat{q}_i = 0.$$

The definition equation for $\boldsymbol{\tau}$ in the Fourier space reads

$$\widehat{\tau}_i = \widehat{q}_i - C^0_{ij} \widehat{p}_j \quad \Leftrightarrow \quad \widehat{q}_i = \widehat{\tau}_i + C^0_{ij} \widehat{p}_j.$$

On the other hand, the link between $\mathbf{p}$ and ϕ, namely $\mathbf{p} = \nabla \phi$ or $p_i = \phi_{,i}$ in the Fourier reads

$$\widehat{p}_i = \mathrm{i}\, \xi_i \widehat{\phi},$$

which upon substitution into the equation for $\widehat{\mathbf{q}}$ gives

$$\widehat{q}_i = \widehat{\tau}_i + \mathrm{i}\, C^0_{ij} \xi_j \widehat{\phi}.$$

Elimination of $\widehat{\mathbf{q}}$ from the last equation using the relation $\mathrm{i}\, \xi_i \widehat{q}_i = 0$ leads to

$$\mathrm{i} \xi_i \widehat{q}_i = \mathrm{i} \xi_i \widehat{\tau}_i - C^0_{ij} \xi_i \xi_j \widehat{\phi} = 0 \quad \Rightarrow \quad \widehat{\phi} = \mathrm{i}\, \frac{\xi_i \widehat{\tau}_i}{C^0_{ij} \xi_i \xi_j} = \mathrm{i} \frac{\xi_j \widehat{\tau}_j}{C^0_{ij} \xi_i \xi_j}.$$

We have just arrived at

$$\widehat{p}_i = \mathrm{i}\, \xi_i \widehat{\phi} = -\frac{\xi_i \widehat{\tau}_j \xi_j}{C^0_{ij} \xi_i \xi_j} = -\frac{\xi_i \xi_j}{C^0_{ij} \xi_i \xi_j} \widehat{\tau}_j = \widehat{\Gamma^0}_{ij} \tau_j, \tag{39}$$

with the Green operator in the Fourier space given by

$$\widehat{\Gamma^0}_{ij} = -\frac{\xi_i \xi_j}{C^0_{ij} \xi_i \xi_j} \quad \forall \boldsymbol{\xi} \neq \mathbf{0}$$

Defining the Green operator as follows

$$\boxed{\widehat{\boldsymbol{\Gamma}^0} = \begin{cases} -\dfrac{\boldsymbol{\xi} \otimes \boldsymbol{\xi}}{\boldsymbol{\xi} \cdot \mathbf{C}^0 \cdot \boldsymbol{\xi}} & \boldsymbol{\xi} \neq \mathbf{0} \\ \mathbf{0} & \boldsymbol{\xi} = \mathbf{0}, \end{cases}}$$

equations (39) together with (37) prove the Lippmann-Schwinger equation (38).

Fixed-pointer iteration scheme We rewrite the Lippmann-Schwinger equation in the Fourier space as follows

$$\begin{aligned}\widehat{p}_i &= \widehat{\Gamma^0}_{ij}\,\widehat{\tau}_j(p_i),\\ \tau_i &= \big[C_{ij}(\mathbf{x}) - C^0_{ij}\big]p_j,\\ \widehat{p}_i(\mathbf{0}) &= \overline{p}_i.\end{aligned}$$

In accordance with this set of equations the following fixed-point scheme is naturally proposed

$$\boxed{\begin{aligned}\widehat{p}_i^{[n+1]} &= \widehat{\Gamma^0}_{ij}\,\widehat{\tau}_j^{[n]},\\ \widehat{\tau}_i^{[n]} &= \mathcal{F}\Big\{\big[C_{ij}(\mathbf{x}) - C^0_{ij}\big]\Big\}\mathcal{F}^{-1}\big[\widehat{p}_j^{[n]}\Big\},\\ \widehat{p}_i^{[n+1]}(\mathbf{0}) &= \overline{p}_i.\end{aligned}}$$

Modified fixed-pointer iteration scheme The modified fixed-point iteration scheme is developed according to the observation

$$p_i = -\Gamma^0_{ij} * (C^0_{jk}p_k) + \overline{p}_i \quad \Leftrightarrow \quad \begin{cases} \widehat{p}_i = -\widehat{\Gamma^0}_{ij} * (C^0_{jk}\widehat{p}_k),\\ \widehat{p}_i(\mathbf{0}) = \overline{p}_i.\end{cases}$$

This relation can be easily proved by using the same argument for the elasticity problems. That is, we start with a true statement

$$q^*_{i,i} = 0 \quad \text{with } \mathbf{q}^* = \mathbf{0}.$$

Following strictly the derivation of Lippmann-Schwinger equation (38) with the polarization tensor defined by

$$\tau_i = q^*_i - C^0_{ij}p_j = -C^0_{ij}p_j,$$

it can be deduced that

$$p_i = \Gamma^0_{ij} * (-C^0_{jk}p_k) + \overline{p}_i = -\Gamma^0_{ij} * C^0_{jk}p_k + \overline{p}_i.$$

We compute right-hand side of equation (39)

$$\widehat{\Gamma^0}_{ij}\widehat{\tau}_j = \widehat{\Gamma^0}_{ij}\big[\widehat{q}_j - C^0_{ik}\widehat{p}_k\big] = \widehat{\Gamma^0}_{ij}\widehat{q}_j - \underbrace{\widehat{\Gamma^0}_{ij}C^0_{ik}\widehat{p}_k}_{-\widehat{p}_i} = \widehat{\Gamma^0}_{ij}\widehat{q}_j + \widehat{p}_i.$$

Using this identity, we may replace the above fixed-point scheme with the improved one

$$\boxed{\begin{aligned}\widehat{p}_i^{[n+1]} &= \widehat{\Gamma^0}_{ij}\,\widehat{q}_j^{[n]} + \widehat{p}_i^{[n]},\\ \widehat{q}_i^{[n]} &= \mathcal{F}\big\{C_{ij}(\mathbf{x})p_j^{[n]}\big\},\\ \widehat{p}_i^{[n+1]}(\mathbf{0}) &= \overline{p}_i.\end{aligned}}$$

Exercise 7

We have learned the Lippmann-Schwinger equation for elasticity problems

$$\epsilon_{ij} = \Gamma^0_{ijkl} * \tau_{kl} + \overline{\epsilon}_{ij}$$

and the reduction to the one-dimensional counterpart is

$$\epsilon = \Gamma^0 * \tau + \overline{\epsilon}. \tag{40}$$

The fixed-point scheme for solving the Lippmann-Schwinger equation for the elasticity problems

$$\begin{aligned}
\widehat{\epsilon}^{[n+1]}_{ij} &= \widehat{\Gamma^0}_{ijkl}\, \widehat{\tau}^{[n]}_{kl}, \\
\widehat{\tau}^{[n]}_{kl} &= \mathcal{F}\Big\{ \big[C_{klij}(\mathbf{x}) - C^0_{klij}\big] : \mathcal{F}^{-1}\big[\widehat{\epsilon}^{[n]}_{ij}\big] \Big\}, \\
\widehat{\epsilon}^{[n+1]}_{ij}(\mathbf{0}) &= \overline{\epsilon}_{ij}
\end{aligned}$$

while the reduction of this system to that in one-dimensional setting reads

$$\begin{aligned}
\widehat{\epsilon}^{[n+1]} &= \widehat{\Gamma^0}\ \widehat{\tau}^{[n]}, \\
\widehat{\tau}^{[n]} &= \mathcal{F}\Big\{ \big[C(x) - C^0\big] \mathcal{F}^{-1}\big[\widehat{\epsilon}^{[n]}\big] \Big\}, \\
\widehat{\epsilon}^{[n+1]}(0) &= \overline{\epsilon}.
\end{aligned}$$

Goal In this exercise we shall investigate the question of how to choose the reference material constants by using the one-dimensional Lippman-Schwinger equation as a sample problem. Thus, we are mainly concerned with choosing C^0 for a stable fixed-point scheme.

Stability for the fixed-point iteration method Having the fixed-point iteration in the form

$$\mathbf{v}^{[n+1]} = \mathbf{A} \cdot \mathbf{v}^{[n]} + \mathbf{B}, \tag{41}$$

where $\mathbf{A}$ is the discretized system matrix and $\mathbf{B}$ a discrete constant vector, $\mathbf{v}$ the solution vector, the spectral radius is defined as the maximum eigenvalues $\lambda_{\max}$ of $\mathbf{A}$

$$\rho = \lambda_{\max} = \max_i |\lambda_i(\mathbf{A})|.$$

Here $\lambda_i(\mathbf{A})$ denotes the set of eigenvalues of matrix $\mathbf{A}$. The fixed-point iteration scheme converges for spectral radius lower than one, that is

$$\rho = \max_i |\lambda_i(\mathbf{A})| < 1.$$

Additionally, the spectral radius influences the convergence rate. Due to the linearity of Lippmann-Schwinger equation (linear integral equation) and by comparing (40) with (41), we can identify the system matrix $\mathbf{A}$ in the real space as

$$\mathbf{A} = \mathsf{F}^{-1}\big[\widehat{\underline{\Gamma}}\,\mathsf{F}\,C^{\Delta}\big],$$

where F and F^{-1} denote the discrete Fourier and inverse Fourier transform matrices, respectively, $\underline{C}^{\Delta} = \big\{C^{\Delta}(x_\alpha)\big\}_{\alpha=1}^{N}$ vector of values of C^{Δ} at the spectral collocation points, $\widehat{\underline{\Gamma}} = \big\{\Gamma(\xi_k)\big\}_{k=-N/2}^{N/2-1}$ the vector values of the Green operator at the spectral collocation points. We recall that $C^{\Delta}(x) = C(x) - C^0$. In this computation approach we have used F as the matrix performing the discrete Fourier transform. We recall that the discrete Fourier transform is a linear operator acting on the input vector $\mathbf{v}$ and returning its discrete Fourier transform $\mathsf{FFT}(\mathbf{v}) = \mathsf{F}\cdot\mathbf{v}$. The fast Fourier transform FFT is only a fast algorithm implementing the discrete Fourier transform and hence equivalent to the performance of F. Such matrix F can be constructed as follows (comparable to the differentiation matrix in our lecture)

$$\mathsf{F} = \left(\frac{\omega^{jk}}{\sqrt{N}}\right)_{j,k=0,\ldots,N-1} = \left(\frac{\big[\exp(-2\pi\mathrm{i}\,N)\big]^{jk}}{\sqrt{N}}\right)_{j,k=0,\ldots,N-1},$$

or equivalently

$$\mathsf{F} = \frac{1}{\sqrt{N}}\begin{bmatrix} 1 & 1 & 1 & 1 & \ldots & 1 \\ 1 & \omega & \omega^2 & \omega^3 & \ldots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \omega^6 & \ldots & \omega^{2(N-1)} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \omega^{3(N-1)} & \ldots & \omega^{(N-1)(N-1)} \end{bmatrix},$$

By using the modified-fixed point scheme

$$\widehat{\epsilon}^{[n+1]} = \widehat{\Gamma^0}\,\widehat{\sigma}^{[n]} + \widehat{\epsilon}^{[n]},$$
$$\widehat{\sigma}^{[n]} = \mathcal{F}\big\{C(x)\epsilon^{[n]}\big\}.$$

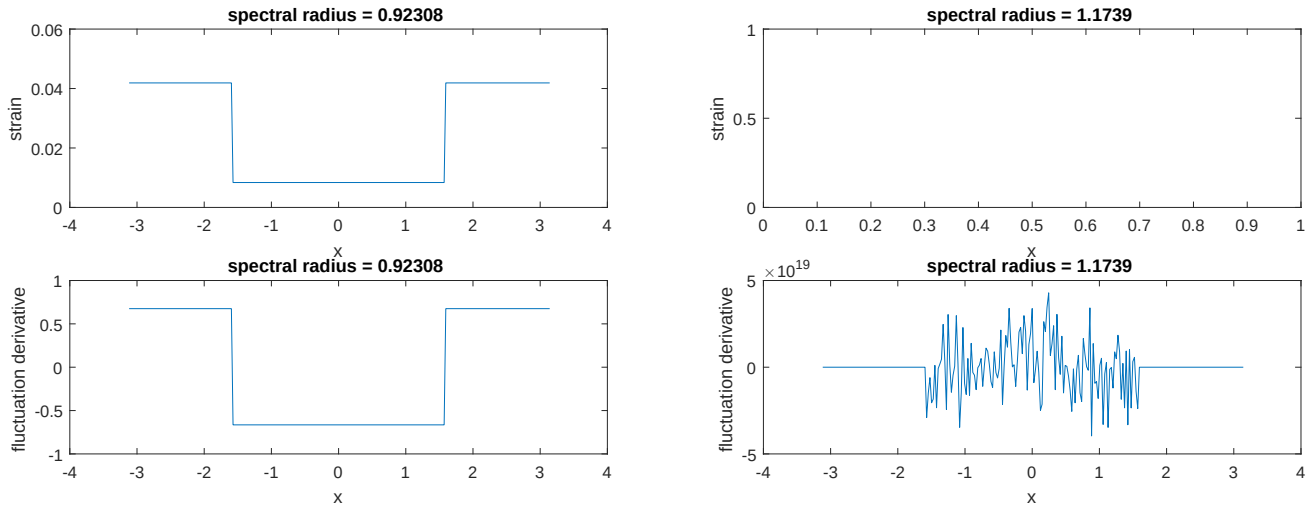
The corresponding matrix for studying the stability of the fixed-point method is given by

$$\mathbf{A} = \mathbf{I} + \underbrace{\widehat{\Gamma^0}}_{-1/C^0}\,\mathsf{F}\,\mathrm{diag}(\underline{C})\,\mathsf{F}^{-1}.$$

In the MATLAB code this equation is paraphrased into

```
% DFT matrix.
W = exp(-2*pi/N*1i*(k' * (0:N-1)));
% Convergence study of the strain solution.
equilibriumMatrix = eye(N,N) + fGamma * W * diag(C) * (1/N * conj(W));
```

Sample program A simple MATLAB code for illustrating how the choice of C^0 could influence the convergence of the fixed-point iteration scheme is given in the end of this exercise. Varying the parameter C^0, we may see that the numerical perform is completely in line with the theory: the solution is stable with spectral radius less than or equal to 1 and unstable otherwise. A numerical result is given in Fig. 11 in which a stable solution is observed when the spectral radius is less than 1 ($C^0 = 2.6$) and unstable solution with spectral radius larger than 1 ($C^0 = 2.4$).



(a) Stable solution with $\rho < 1$.

(b) Unstable solution with $\rho > 1$.

Figure 11: The stable scheme is obtained when the spectral radius is less than 1.

```
%% INITIALIZATION FOR PROBLEM DOMAIN.
% Problem domain is [-L, L].
radius = pi;
% Number of grid points.
N = 2^8;
% Distance between grid points.
h = radius/(N/2);

% Coordinates of collocation points.
scale = radius/pi;
x = scale * (2*pi/N) * (-N/2+1 : N/2);

```

```
%% PROBLEM SETTING.
% Phase one is recorded with value 1 and phase two with value 2. For
% example, phase(i,1) = 1 means x(i) belongs to phase 1, phase(i,2) = 2
% means x(i) belongs to phase 2.
phase = 2*ones(size(x));
phase(x < -radius/2 | x > radius/2) = 1;

% Material parameters: Here we only need scalar for constitutive relations
% in 1-dimensional problem. We use two phases of linear elasticity.
% E(1) -- material of phase 1, E(2) -- material of phase 2.
E = [1   5];

% Wave number used in Discrete Fourier Transform.
k = [0:N/2-1, N/2, -N/2+1 : -1]/scale;

% Prescribed deformation gradient (scalar in our case).
perturb = 0.0;
strain0 = 0.025*(1 + perturb);

% Compute C matrix at collocation points.
C = zeros(size(x));
C(phase == 1) = E(1);
C(phase == 2) = E(2);

% Reference Medium.
C0 = 2.5;

% Green operator in Fourier space.
fGamma = -1/C0;
%% SOLUTION OF LIPPMANN-SCHWINGER EQUATION.
% Maximum number of iteration.
```

```
maxIter1 = 10000;
maxIter2 = 500;
% Tolerance for stopping the iterative scheme.
TOL = 1e-16;

% Initialize the search variable.
strain = strain0*ones(size(x));
stress = C .* strain;
% Iterative scheme resorting  modified fixed-point method.
for iter = 1:maxIter1
    fourierStress = fft(stress);
    % Convergence test.
    if 1/N*norm(sum(k .* fourierStress)) / norm(fourierStress(1)) < TOL &&
        iter > 1
        disp(['Solver stops at step i = ', num2str(iter)]);
        break;
    end
    % If the solution does not converge, improve the solution.
    %-----------------------------------------
    % Updated strain in Fourier space.
    fourierStrain = fft(strain) + fGamma * fourierStress;
    fourierStrain(1) = N * strain0;
    % Updated strain in physical space.
    strain = ifft(fourierStrain);
    % Compute the stress for next step.
    stress = C .* strain;
end

%% SOLUTION FOR FLUCTUATIVE PART.
% Initialize the search variable.
alpha = 0*ones(size(x));
```

```
% Iterative scheme resorting to fixed point method.
delta_C = C - C0;
for iter = 1:maxIter2
    % Updated solution in Fourier space.
    falpha = fGamma * fft(delta_C) + fGamma * fft((delta_C).*alpha);

    falpha(1) = 0;
    % Updated solution in physical space.
    alpha = ifft(falpha);
end

%% Iterative scheme resorting to the MATLAB built-in CG-Solver
% b = -ifft( fGamma * fft(C - C0) )';
%% fv = @(v)  ifft( fGamma * fft((C-C0)' .* v))  - v;
% fv = @(v) fa(v, fGamma, C, C0);
% alpha = cgs(fv,b, 1e-8, maxIter);

%% COMPUTATION OF EFFECTIVE STIFFNESS.
vol = 2*radius;
meanStress = 1/vol * ( trapz(x,stress) + h*mean(stress([end, 1])) );
% Effective stiffness.
beta = C .* (1 + alpha);
Ceffective = 1/vol * ( trapz(x,beta) + h*mean(beta([end, 1])) );


%% Study the convergence of the solution based on the fixed-point schemes.
% DFT matrix.
W = exp(-2*pi/N*1i*(k' * (0:N-1)));
% Convergence study of the strain solution.
equilibriumMatrix = eye(N,N) + fGamma * W * diag(C) * (1/N * conj(W));
spectralRaidus1 = max(abs(eig(equilibriumMatrix)));
```

```
105 subplot(2,1,1), plot(x,strain),
106 title(['spectral radius = ', num2str(spectralRaidus1)]);
107 xlabel('x'), ylabel('strain')
108
109 % Convergence study of the fluctuation derivatives.
110 fluctuationMatrix = fGamma * (W .* repmat(delta_C,N,1)) * (1/N * conj(W));
111 spectralRadius2 = max(abs(eig(fluctuationMatrix)));
112 subplot(2,1,2), plot(x,alpha),
113 title(['spectral radius = ', num2str(spectralRadius2)]);
114 xlabel('x'), ylabel('fluctuation derivative');
```