PERIOD HOMOGENIZATION USING SPECTRAL METHODS

* First-taste example.

Consider the simple boundary value problem.

$$\begin{cases} \dfrac{d}{dx}\left[C(x)\dfrac{du}{dx}\right] + f(x) = 0 & x \in (0,L) \\ u(x=0) = u_0 & \text{Left-end boundary} \\ C\dfrac{du}{dx}\Big|_{x=L} = t_0 & \text{Right-end boundary} \end{cases} \quad (\star)$$

* Assume that $C(x)$ oscillates extremely fast.

For example

$$C(x) = \frac{3}{2} + \sin(2\pi kx) \qquad k \in \mathbb{Z}^+$$
$$= C_k(x).$$

* Question : According to numerical results, we may ask if it is possible to replace the BVP with an equivalent BVP in the limit $k \to \infty$. Important oberservation: There are two scales in the BVP.

separated

* Multiscale analysis : We "average out" the small oscillation to observe the bigger scale picture.

Only 2 scales in our problem

* Flowchart of problem solving

(i) Set up the microscale problem, solve the macroscale BVP while acquiring information from the microscale problem. (ii)

(ii) Set up the microscale problem, solve the microscale BVP, synthesize the solution to provide macroscale information to problem (i)

We shall use (☆) to illustrate the technique. We don't address the theory behind the whole first-order homogenization schem.

* Macroscale variable $\overline{(\cdot)}$
* Microscale variable $(\cdot)$

(A) The original BVP.

$$\begin{cases} \dfrac{d}{dx}\left[\left(\dfrac{3}{2}+\sin(2\pi kx)\right)\dfrac{du}{dx}\right] + f(x) = 0. & x \in (0, L) \\ u(x=0) = u_0 \\ C\dfrac{du}{dx}\Big|_{x=L} = t_0 \end{cases}$$

(B) The homogenized BVP as an equivalent replacement of the original BVP (Δ) $\Longrightarrow$ the solution converges to the solution of (Δ) in the limit $k \to \infty$.

The wavenumber $2k\pi$ defines the wavelength $\lambda = \dfrac{2\pi}{2\pi k} = \dfrac{1}{k}$.
The ratio between two scales (small scale $\sim \lambda$, large scale $\Lambda \sim 1$)

$$\underbrace{\eta = \frac{\lambda}{\Lambda} \sim \frac{1}{kL} \longrightarrow 0}_{\text{Two scales are well-separated}} \quad \text{as } k \to \infty$$

(i) MACROSCALE BOUNDARY VALUE PROBLEM

$$\begin{cases} \dfrac{d}{d\bar{x}}\left[\bar{C}(\bar{x})\dfrac{d\bar{u}}{d\bar{x}}\right] + f(\bar{x}) = 0 & \bar{x} \in (0, L) \\ \bar{u}(\bar{x}=0) = u_0 \\ \bar{C}\dfrac{d\bar{u}}{d\bar{x}}\Big|_{\bar{x}\to L} = t_0 \end{cases}$$

(ii) MICROSCALE BVP USING STRAIN-DRIVEN FORMULATION

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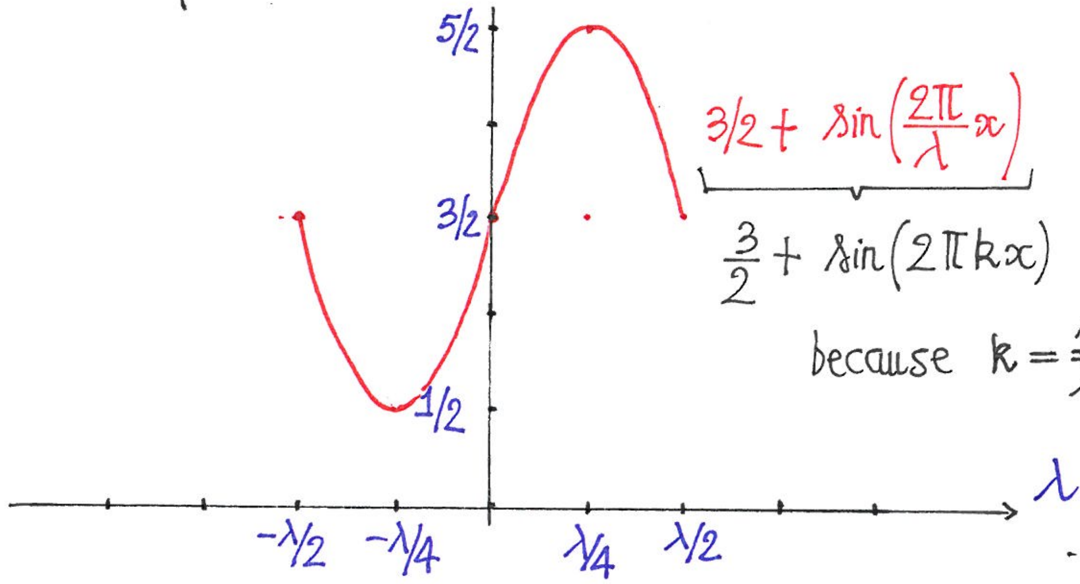
(ii) MICROSCALE BVP USING STRAIN-DRIVEN FORMULATION

$$\varepsilon(u(x)) = \varepsilon(u^*(x)) + \overline{\varepsilon} \Leftrightarrow u(x) = u^*(x) + \overline{\varepsilon}x.$$

$$\begin{cases} \dfrac{d}{dx}\sigma(x) = 0 \\ \sigma(x) = c(x)\big[\underbrace{\varepsilon(u^*(x)) + \overline{\varepsilon}}\big] \quad \forall x \in \text{RVE } \Omega \quad (\square) \\ u^* \text{ is periodic} \\ \sigma n \text{ is antiperiodic}, \quad \varepsilon(u^*(x)) = \dfrac{du^*}{dx} \end{cases}$$

act as an operator

* RVE — Representative volume element



$$\underbrace{\frac{3}{2} + \sin\left(\frac{2\pi}{\lambda}x\right)}_{\frac{3}{2} + \sin(2\pi k x)}$$

because $k = \frac{1}{\lambda}$ or $\lambda = \frac{1}{k}$

* $\varepsilon(u^*(x)) = \dfrac{du^*}{dx} \Longrightarrow \varepsilon$ acts as operator in our denotation.

* u^* represents the fluctuating term due to the decomposition

$$\varepsilon = \varepsilon^* + \overline{\varepsilon}$$

microscale strain; fluctuating; macroscale strain (Constant)

such that $\dfrac{1}{\lambda}\displaystyle\int_\Omega \varepsilon\, dx = \overline{\varepsilon}$ or equivalently $\dfrac{1}{\lambda}\displaystyle\int_\Omega \varepsilon^* dx = 0.$

* $c(x)$ represents the microstructure information.

In our example $c(x) = \dfrac{3}{2} + \sin\left(\dfrac{2\pi}{\lambda}x\right)$

(A) Solve microscopic BVP. & Extract Macroscale information

* The periodic Lippmann-Schwinger equation.

Recall The main assumption in the microscale problem

$$u(x) = u^*(x) + \overline{E}x.$$

$$\Updownarrow$$

$$\varepsilon(u(x)) = \varepsilon(u^*(x)) + \overline{\varepsilon}$$

The averaging gives the macaoscale quantity

$$\frac{1}{\lambda}\int_{\Omega} \varepsilon(u(x))dx = \overline{\varepsilon} \quad (1) \quad \text{or} \quad \frac{1}{\lambda}\int_{\Omega} \varepsilon(u^*(x))dx = 0. \quad \Omega = \left(-\frac{\lambda}{2}, \frac{\lambda}{2}\right)$$

Rewrite (□)

$$\frac{d}{dx}\sigma(x) = \frac{d}{dx}\left[\sigma(x) - c^\circ\varepsilon(u(x)) + c^\circ\varepsilon(u(x))\right] = 0.$$

$$\Rightarrow \frac{d}{dx} c^\circ \varepsilon(u(x)) = -\frac{d}{dx}\tau(x), \quad (2) \quad \text{where } \tau(x) = \sigma(x) - c^\circ\varepsilon(u(x))$$

$$= c(x)\,\varepsilon(u(x)) - c^\circ\varepsilon(u(x))$$

$$= (c - c^\circ)\,\varepsilon(u(x))$$

Combining (1) (2) we know that u (or equivalently u^*) is the solution of the Lippmann-Schwinger equation.

$$\varepsilon(u(x)) = \Gamma^\circ * \tau(x) + \overline{\varepsilon} \quad (3)$$

$$\Updownarrow \text{ equivalent}$$

$$\varepsilon(u^*(x)) = \Gamma^\circ * \tau(x) \quad (4), \quad \text{where } \tau(x) = (c - c^\circ)(\varepsilon(u^*) + \overline{\varepsilon})$$

$\Gamma^\circ \to$ Green operator

Question (i) How to obtain Green operator

(ii) Really ! How can we see (3) and (2) are equivalent/connected ?

Answer Work in Fourier space !

$$\frac{d}{dx} c^\circ \underbrace{\varepsilon(u(x))}_{\varepsilon(x)} = -\frac{d}{dx}\tau(x)$$

Step 1. Apply the Fourier transform:

$$c^\circ \hat{\varepsilon}(\xi)\, i\xi = -\, i\xi\, \hat{\tau}(\xi)$$

ξ is the wavenumber/ Fourier variable in the Fourier space.

$$\Rightarrow \begin{cases} c^\circ \hat{\varepsilon}(\xi) = -\hat{\tau}(\xi) & \forall \xi \neq 0. \\ \hat{\varepsilon}(0) = \frac{1}{\lambda}\int_\Omega \varepsilon\, dV = \bar{\varepsilon} \text{ (by definition)} \end{cases}$$

We use ξ to avoid confusion with k

τ is a function of ε by itself

$$\overset{\forall \xi \neq 0}{\Rightarrow} \hat{\varepsilon}(\xi) = -\frac{1}{c^\circ}\hat{\tau}(\xi) = \hat{\Gamma}^\circ \hat{\tau}(\xi), \text{ where } \Gamma^\circ = -\frac{1}{c^\circ}$$

Step 2 Apply the inverse Fourier transform:

$$\varepsilon(u(x)) = \Gamma^\circ * \tau(x) + \bar{\varepsilon}$$

because $\widehat{\Gamma^\circ * \tau}(\xi) = \hat{\Gamma}^\circ(\xi)\hat{\tau}(\xi)$ || Important property for periodic Fourier transform

Summary

$$\boxed{\begin{gathered} \varepsilon(u(x)) = \Gamma^\circ * \tau(x) + \bar{\varepsilon} \\ \Updownarrow \\ \begin{cases} \hat{\varepsilon}(\xi) = \hat{\Gamma}^\circ(\xi)\,\hat{\tau}(\xi) & , \forall \xi \neq 0 \\ \hat{\varepsilon}(0) = \frac{1}{\lambda}\int_\Omega \varepsilon\, dx = \bar{\varepsilon} & , \xi = 0. \end{cases} \\ \Updownarrow \\ \frac{d}{dx} c^\circ \varepsilon(x) = -\frac{d}{dx}\tau(x) \end{gathered}}$$

In the Fourier space, we have explicit closed-form of $\Gamma^\circ(\xi)$, Green operator, and the equation is an algebraic equation for $\hat{\varepsilon}(\xi)$.

* Fixed-point method for Lippmann-Schwinger equation

Initialization :

$$\varepsilon^{0}(x) = \bar{\varepsilon} \qquad \forall x \in \Omega$$

$$\sigma^{0}(x) = c(x)\ \varepsilon^{0}(x) \qquad \forall x \in \Omega$$

Iterative $i+1$ $\quad \varepsilon^{i}$ and σ^{i} being known

(a) $\tau^{i}(x) = \sigma^{i}(x) - c^{0}\ \varepsilon^{i}(x) \rightarrow$ according to def. of τ

(b) $\hat{\tau}^{i} := FFT(\tau^{i})$

(c) Convergence test $\rightarrow$ test equilibrium equation $\frac{d\sigma}{dx} = 0$

(d) $\begin{cases} \hat{\varepsilon}^{i+1}(\xi) = \hat{\Gamma}^{0}(\xi)\,\hat{\tau}^{i}(\xi) \\ \hat{\varepsilon}^{i+1}(0) = \bar{\varepsilon} \end{cases}$ update solution in Fourier space

(e) $\varepsilon^{i+1} = IFFT(\hat{\varepsilon}^{i+1}) \rightarrow$ pull solution back to physical space

(f) $\sigma^{i+1} = c(x)\,\varepsilon^{i+1}(x)$ $\rightarrow$ update stress solution.

* Compute macroscale strain, stress & effective stiffness.

+ Macroscale strain : $\bar{\varepsilon} = \frac{1}{\lambda}\int_{\Omega} \varepsilon\, dx$ (given from macroscale problem, constant in the microscale problem)

+ Macroscale stress : $\bar{\sigma} = \frac{1}{\lambda}\int_{\Omega} \sigma\, dx$

+ Macroscale/Effective stiffness : $\bar{C} = \frac{\partial \bar{\sigma}}{\partial \bar{\varepsilon}} \simeq \frac{\Delta \bar{\sigma}}{\Delta \bar{\varepsilon}}$

(B) Solve macroscale BVP by using the information supplied from microscale BVP

$$\begin{cases} \displaystyle\int_0^L \frac{d\delta\bar{u}}{d\bar{x}}\,\bar{C}(\bar{x})\,\frac{d\bar{u}}{d\bar{x}}\,d\bar{x} = \int_0^L f(\bar{x})\,\delta\bar{u}\,dx + t_0\,\delta\bar{u}\Big|_{\bar{x}=L} \\ \bar{u}(\bar{x}=0) = u_0 \end{cases}$$

SOLVE THIS BVP BY FEM.

* Derivation of consistent macroscopic tangent

(i) Macroscopic boundary value problem

$$\begin{cases} \dfrac{d}{d\bar{x}}\left(\bar{\sigma}(\bar{x})\right) + f(\bar{x}) = 0. \\ \bar{u}(\bar{x}=0) = \bar{u}_0 \\ \bar{C}\,\dfrac{d\bar{u}}{d\bar{x}}\Big|_{\bar{x}=L} = t_0 \end{cases}$$

(ii) Microscopic boundary value problem

$$\begin{cases} \dfrac{d}{dx}\sigma(x) = 0 \\ \sigma(x) = c(x)\left[\varepsilon(\tilde{u}(x)) + \bar{\varepsilon}\right] = c(x)\,\underbrace{\varepsilon(u(x))}_{\frac{d}{dx}\left(\tilde{u}(x) + \bar{\varepsilon}x\right)} \\ \tilde{u} \text{ is periodic.} \\ \sigma n \text{ is antiperiodic.} \end{cases}$$

We formally write down the stress incremement in terms of the strain increment

$$\Delta\bar{\sigma} = \frac{\partial\bar{\sigma}}{\partial\bar{\varepsilon}}\,\Delta\bar{\varepsilon}$$

in which

$$\begin{cases} \varepsilon = \bar{\varepsilon} + \tilde{\varepsilon} \quad \Rightarrow \varepsilon \text{ is decomposed into the average part \& the fluctuation part} \\ \bar{\sigma} = \dfrac{1}{\lambda}\displaystyle\int_\Omega \sigma(\varepsilon(x))\,dx. \\ \bar{\varepsilon} = \dfrac{1}{\lambda}\displaystyle\int_\Omega \varepsilon(u(x))\,dx. \end{cases}$$

$\Rightarrow$ Consistent macroscopic tangent: $\bar{C} = \dfrac{\partial\bar{\sigma}}{\partial\bar{\varepsilon}} \Rightarrow$ Computation ?

General denotation:

- Volume of a representative volume element: $V = |\Omega| = \lambda$
- Microscopic constitutive tangent: $C = \dfrac{\partial\sigma}{\partial\varepsilon}$

General denotation:

- Volume of an RVE : $V = |\Omega| = \lambda$
- Microscopic constitutive tangent : $C = \dfrac{\partial \sigma}{\partial \varepsilon}$
- Macroscopic stress

$$\overline{\sigma} = \frac{1}{V}\int_{\Omega} \sigma \, dx$$

- Macroscopic strain

$$\overline{\varepsilon} = \frac{1}{V}\int_{\Omega} \varepsilon \, dx.$$

- Strain decomposition

$$\underbrace{\varepsilon}_{\text{microscopic strain}} = \underbrace{\widetilde{\varepsilon}}_{\text{fluctuation part : periodic}} + \underbrace{\overline{\varepsilon}}_{\text{macroscopic strain}}$$

This decomposition is in principle equivalent to

$$u(x) = \widetilde{u}(x) + \overline{\varepsilon}\, x$$

* We compute the derivative

$$\overline{C} = \frac{\partial \overline{\sigma}}{\partial \overline{\varepsilon}} = \frac{\partial}{\partial \overline{\varepsilon}}\left\{\frac{1}{V}\int_{\Omega} \sigma \, dx\right\} = \frac{1}{V}\int_{\Omega} \frac{\partial \sigma}{\partial \varepsilon}\frac{\partial \varepsilon}{\partial \overline{\varepsilon}}\, dx.$$

$$= \frac{1}{V}\int_{\Omega} C\left[\frac{\partial}{\partial \overline{\varepsilon}}\left(\widetilde{\varepsilon} + \overline{\varepsilon}\right)\right] dx = \frac{1}{V}\int_{\Omega} C\left(\frac{\partial \widetilde{\varepsilon}}{\partial \overline{\varepsilon}} + 1\right) dx.$$

Thus, in order to compute the effective stiffness, we need to evaluate the integral

$$\overline{C} = \frac{1}{V}\int_{\Omega}\left[C + C\frac{\partial \widetilde{\varepsilon}}{\partial \overline{\varepsilon}}\right] dx.$$

and hence a way of computing the derivative $\underbrace{\dfrac{\partial \widetilde{\varepsilon}}{\partial \overline{\varepsilon}}}_{\text{Derivative of the fluctuation part}}$.

∗ Computation of derivative the fluctuation part

We recall the Lippmann–Schwinger equation

$$\varepsilon = \Gamma^\circ * \tau + \bar{\varepsilon} \iff \tilde{\varepsilon} = \Gamma^\circ * \tau. \quad (\Delta)$$

with

$$\tau = \sigma - c^\circ \varepsilon.$$

Taking derivative of (Δ) w.r.t. $\bar{\varepsilon}$, we obtain

$$\frac{\partial \tilde{\varepsilon}}{\partial \bar{\varepsilon}} = \Gamma^\circ * \frac{\partial \tau}{\partial \bar{\varepsilon}} = \Gamma^\circ * \left[\frac{\partial \sigma}{\partial \bar{\varepsilon}} - c^\circ\left(1 + \frac{\partial \tilde{\varepsilon}}{\partial \bar{\varepsilon}}\right)\right]$$

$$= \Gamma^\circ * \Big[\frac{\partial \sigma}{\partial \varepsilon} . \underbrace{\frac{\partial \varepsilon}{\partial \bar{\varepsilon}}}_{1+\frac{\partial \tilde{\varepsilon}}{\partial \bar{\varepsilon}}} - c^\circ\left(1 + \frac{\partial \tilde{\varepsilon}}{\partial \bar{\varepsilon}}\right)\Big] = \Gamma^\circ * \Big[\underbrace{(c - c^\circ)}_{C^\Delta}\left(1 + \frac{\partial \tilde{\varepsilon}}{\partial \bar{\varepsilon}}\right)\Big]$$

$$\Rightarrow \boxed{\frac{\partial \tilde{\varepsilon}}{\partial \bar{\varepsilon}} = \Gamma^\circ * \left[C^\Delta + C^\Delta : \frac{\partial \tilde{\varepsilon}}{\partial \bar{\varepsilon}}\right]} \quad (\star)$$

This is the linear integral equation for the derivative of the fluctuation part $\partial \tilde{\varepsilon}/\partial \bar{\varepsilon}$.

Normal mistake : We see that equation ($\star$) is a Lippmann–Schwinger type equation for $\partial \tilde{\varepsilon}/\partial \bar{\varepsilon}$. The average condition $\frac{1}{V}\int_\Omega \varepsilon \, dV = \bar{\varepsilon}$ or $\frac{1}{V}\int_\Omega \tilde{\varepsilon} \, dV = 0$ "must be" transfered to some average condition on $\partial \tilde{\varepsilon}/\partial \bar{\varepsilon}$.

It is clear that

$$\frac{1}{V}\int_\Omega \frac{\partial \tilde{\varepsilon}}{\partial \bar{\varepsilon}} dV = \frac{\partial}{\partial \bar{\varepsilon}}\left[\frac{1}{V}\int_\Omega \tilde{\varepsilon} \, dV\right] = 0.$$

Thus, the average condition for $\partial \tilde{\varepsilon}/\partial \bar{\varepsilon}$ is

$$\frac{1}{V}\int_\Omega \frac{\partial \tilde{\varepsilon}}{\partial \bar{\varepsilon}} dV = 0.$$

As equation (✯) is basically a Lippmann-Schwinger type equation for $\partial\tilde{\varepsilon}/\partial\bar{\varepsilon}$, it is convenient to solve it using the discrete Fourier transform. To this end, we work it out in the Fourier space (10)

$$\widehat{\frac{\partial\tilde{\varepsilon}}{\partial\bar{\varepsilon}}} = \hat{\Gamma}^0 \mathcal{F}\left\{C^\Delta + C^\Delta \frac{\partial\tilde{\varepsilon}}{\partial\bar{\varepsilon}}\right\}$$

$$\Rightarrow \hat{\alpha} = \hat{\Gamma}^0 \mathcal{F}\left\{C^\Delta + C^\Delta \alpha\right\} \qquad \text{with } \alpha = \frac{\partial\tilde{\varepsilon}}{\partial\bar{\varepsilon}}$$

$$\Rightarrow \hat{\alpha} = \hat{\Gamma}^0 \mathcal{F}\left\{C^\Delta + C^\Delta \mathcal{F}^{-1}[\hat{\alpha}]\right\}$$

Henceforth, we can now apply the fixed-point method to obtain the iteration scheme

$$\hat{\alpha}^{[n+1]} = \hat{\Gamma}^0 \mathcal{F}\left\{C^\Delta + C^\Delta \mathcal{F}^{-1}\left[\hat{\alpha}^{[n]}\right]\right\}.$$