PERIODIC HOMOGENIZATION USING SPECTRAL METHODS

* First-taste example

- Consider the simple boundary value problem

$$\frac{d}{dx}\left[C(x)\,\frac{du}{dx}\right] + f(x) = 0 \qquad x \in (0, L)$$

$$u(x=0) = u_0 \qquad \text{Left-end boundary}$$

$$C\,\frac{du}{dx}\Big|_{x=L} = t_0. \qquad \text{Right-end boundary}$$

- Assume that $C(x)$ oscillates extremely fast; for example

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

* 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 observation: There are two separated scales in the BVP.

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

  Multiscale: $\longrightarrow$ only two scales in our current problem

* **Flowchart of problem solving**

  (i) Set up the macroscopic problem, solve the macroscopic BVP while acquiring information from the microscopic problem (ii)

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

We shall use the BVP ($\bigstar$) to illustrate the technique. We do not address the theory behind the whole first-order periodic homogenization scheme.

* **Two-scale variables throughout the subject**
  - Macroscopic variable $\quad \overline{(\cdot)}$
  - Microscopic variable $\quad (\cdot)$

Repeat (A) The original BVP

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

(B) The homogenized BVP as an equivalent replacement of the original BVP (A)

$\Rightarrow$ The solution converges to the solution of in the limit $k \to \infty$.

The wavenumber $2\pi k$ defines the wavelength $\lambda = \dfrac{2\pi}{2\pi k} = \dfrac{1}{k}$.

The ratio between two scales (small scales $\sim \lambda$, large scale $\Lambda \sim L$)

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

The homogenization theory is only valid on the assumption of well-separated scales.

Replacement of the original BVP with the homogenized BVP

(i) MACROSCOPIC BOUNDARY VALUE PROBLEM

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

(ii) MICROSCOPIC BVP USING STRAIN-DRIVEN FORMULATION

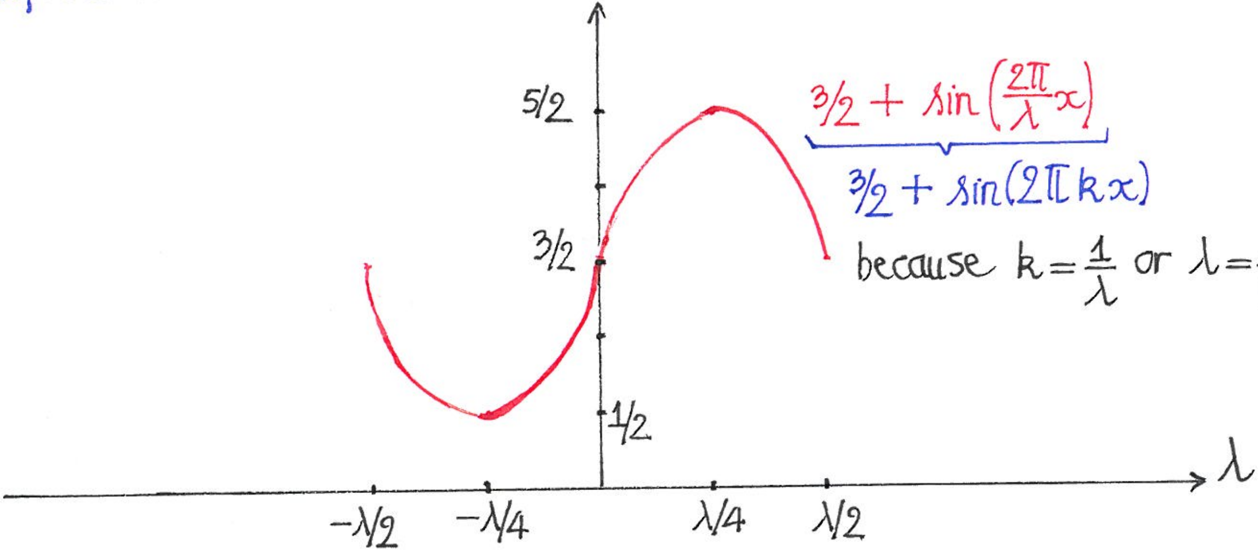
$$\begin{cases} \dfrac{d}{dx}\sigma(x) = 0 & \\ \sigma(x) = c(x)\underbrace{\left[\varepsilon(u^*(x)) + \bar{\varepsilon}\right]} & \forall x \in \text{RVE } \Omega \\ u^* \text{ is periodic} & \\ \sigma n \text{ is antiperiodic} & \end{cases}$$

$$\varepsilon(u(x)) = \varepsilon(u^*(x)) + \bar{\varepsilon} \iff u(x) = u^*(x) + \bar{\varepsilon}\,x$$

$\varepsilon(u^*(x)) = \dfrac{d}{dx}u^*$: $\varepsilon(\cdot)$ acts as an opertor

operator

* Reprensentative 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 $\lambda = \frac{1}{k}$.

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

* u^* represents the fluctuating term (from/as compared to the averaged term) due to the decomposition

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

microscopic strain — ε; ε^* — fluctuating; $\overline{\varepsilon}$ — macroscopic strain (constant)

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

* $c(x)$ represents the microstructure information

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

Numerical Procedure

(A) Solve the microscopic BVP & Extract the macroscopic information

$$\begin{cases} \frac{d}{dx}\sigma(x) = 0 \\ \sigma(x) = c(x)\left[\frac{du^*}{dx} + \overline{\varepsilon}\right] \\ u^* \text{ is periodic} \\ \sigma n \text{ is antiperiodic} \end{cases} \quad \forall x \in \text{RVE } \Omega \Rightarrow \text{Compute } \overline{\sigma} = \frac{1}{\lambda}\int_\Omega \sigma\, dx.$$

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

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

Solve this BVP by Finite Element Method.

* Circular convolution / Periodic convolution

Let f be a function with a well-defined periodic summation f_T where

$$f_T(x) \stackrel{\text{def}}{=} \sum_{k=-\infty}^{\infty} f(x-kT) = \sum_{k=-\infty}^{\infty} f(x+kT) \Rightarrow f_T \text{ is periodic with period } T$$

If h is any other function for which the convolution $f_T * h$ exists, then the convolution $f_T * h$ is periodic and identical to

$$(f_T * h)(x) \stackrel{\text{def}}{=} \int_{-\infty}^{\infty} h(\tau)\, f_T(x-\tau)\, d\tau$$

$$= \int_{t_0}^{t_0+T} h_T(\tau)\, f_T(x-\tau)\, d\tau$$

where t_0 is an arbitrary parameter and h_T is a periodic summation of h.

Question In order to apply the numerical methods, we need to discretize the continuous setting of formulas. What is the corresponding discrete form?

* Circular convolution / Periodic convolution

Assume that we have two periodic grid functions f and g. which are determined by the grid data $\{(x_j, f_j)\}_{j=1}^{N}$, and $\{x_j, g_j\}_{j=1}^{N}$ respectively.
We can extend f and g in a periodic sense as follows

$$F_j = (f_N)_j := f_{j(\mathrm{mod}\ N)} \qquad j \in \mathbb{Z}$$

$$G_j = (g_N)_j := g_{j(\mathrm{mod}\ N)} \qquad j \in \mathbb{Z}$$

Periodic convolution:

$$(f*g)_j := \sum_{\ell=1}^{N} f_\ell G_{j-\ell} = \sum_{\ell=1}^{N} g_\ell F_{j-\ell} = (g*f)_j$$

Periodic convolution theorem:

$$\mathcal{F}\{f*g\}(k) = \mathcal{F}\{f\}(k)\,\mathcal{F}\{g\}(k) \Longleftrightarrow \mathcal{F}^{-1}\{\mathcal{F}[f]\,\mathcal{F}[g]\}_j = (f*g)_j$$

(A) Solve the microscopic BVP

$\ast$ Recall: The main assumption in the microscopic problem

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

$$\Updownarrow$$

$$\varepsilon(u(x)) = \varepsilon(u^*(x)) + \overline{\varepsilon} \iff \frac{du}{dx} = \frac{du^*}{dx} + \overline{\varepsilon}$$

The averaging gives the macroscopic quantity

$$\frac{1}{\lambda}\int_\Omega \varepsilon(u(x))\,dx = \overline{\varepsilon} \quad \text{or equivalently} \quad \frac{1}{\lambda}\int_\Omega \varepsilon(u^*(x))\,dx = 0 \text{ with}$$

$$\Omega = (-\lambda/2, \lambda/2)$$

We rewrite the microscopic stress equilibrium equation: $\frac{d\sigma}{dx} = 0$.

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

$$\Rightarrow \frac{d}{dx} c^\circ \varepsilon(u(x)) = -\frac{d}{dx}\underbrace{\left[\sigma(x) - c^\circ \varepsilon(u(x))\right]}_{\tau(x)} = -\frac{d}{dx}\Big[\underbrace{c(x)\varepsilon(u(x)) - c^\circ \varepsilon(u(x))}_{(c-c^\circ)\varepsilon(u(x))}\Big]$$

$$\tau(x) = \sigma(x) - c^\circ \varepsilon(u(x)) = [c(x) - c^\circ]\,\varepsilon(u(x))$$

Repeat The averaging condition: $\frac{1}{\lambda}\int_{\Omega} \varepsilon(u(x))\,dx = \overline{\varepsilon}$ (☆)$_1$

The stress equilibrium: $\frac{d}{dx} c^{\circ} \varepsilon(u(x)) = -\frac{d}{dx}\tau(x),$ (☆)$_2$

where $\tau(x) = [c(x) - c^{\circ}]\, \varepsilon(u(x))$

(A)

Combining (☆)$_1$ & (☆)$_2$ we know that u (or equivalently u^*) is the solution of the Lippmann–Schwinger equation

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

$\Updownarrow$ equivalent

$$\varepsilon(u^*(x)) = \underbrace{\Gamma^{\circ}}_{\text{Green operator}} * \tau(x), \quad \text{where } \tau(x) = [c(x) - c^{\circ}]\left(\varepsilon(u^*) + \overline{\varepsilon}\right)$$

Question (i) How to obtain Green operator

(ii) Really ! How can we see (A) and (B) are equivalent/connected?

Answer Work in the Fourier space !

* Derivation of Lippmann-Schwinger equation

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

Step 1 Apply the Fourier transform

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

$$\Rightarrow \begin{cases} c^{\circ}\hat{\varepsilon}(\xi) = -\hat{\tau}(\xi) \quad \forall \xi \neq 0. \\ \hat{\varepsilon}(0) = \frac{1}{\lambda}\int_{\Omega} \varepsilon \underbrace{\exp(-i\xi(k)x)}_{\text{Substitute: } k=0} dx. \end{cases}$$

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

ξ is the (scaled) wavenumbers/ Fourier variable in the Fourier space

We use ξ to avoid confusion with interger wavenumber k and also the parameter k in our original boundary value problem

Step 2 Apply the inverse Fourier transform:

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

because $\widehat{\Gamma^{\circ} * \tau}(\xi) = \hat{\Gamma}^{\circ}(\xi)\,\hat{\tau}(\xi)$

Important property for periodic convolution

Summary

$$\varepsilon(u(x)) = \Gamma^0 * \tau(x) + \overline{\varepsilon}.$$

$$\Updownarrow$$

$$\begin{cases} \hat{\varepsilon}(\xi) = \widehat{\Gamma^0}(\xi)\,\hat{\tau}(\xi) & \forall \xi \neq 0 \\ \hat{\varepsilon}(0) = \dfrac{1}{\lambda}\displaystyle\int_{\Omega} \varepsilon \, dx = \overline{\varepsilon} & \xi = 0 \end{cases}$$

$$\Updownarrow$$

$$\frac{d}{dx} c^0 \varepsilon(x) = -\frac{d}{dx}\tau(x)$$: Stress equilibrium

In the Fourier space, we have explicit closed form of $\Gamma^0(\xi)$, Green operator, and the equation is an algebraic equation for $\hat{\varepsilon}(\xi)$.

* Fixed-point method for Lippmann-Schwinger equation

(A.) Initialization

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

$$\sigma^0(x) = c(x)\,\varepsilon^0(x)$$

(B) Iteration for solution at step i+1: ε^i and σ^i being known

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

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

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

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

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

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

(C) Outputs: Microscopic strain field $\varepsilon = \varepsilon(x)$, Microscopic stress field $\sigma = \sigma(x)$

* Macroscopic strain, stress and effective stiffness

Homogenized boundary value problem/ macroscopic BVP

$$\frac{d}{d\bar{x}}\underbrace{\left[\bar{C}(\bar{x})\frac{d\bar{u}}{d\bar{x}}\right]}_{} + f(\bar{x}) = 0 \qquad \bar{x} \in (0, L)$$

$$\bar{\sigma}(\bar{x}) = \bar{C}(\bar{x})\frac{d\bar{u}}{d\bar{x}} = \bar{C}(\bar{x})\bar{\varepsilon}(\bar{x})$$

$$\bar{\sigma} = \frac{1}{\lambda}\int \sigma\, dx$$

$$\bar{C} = \frac{\partial\bar{\sigma}}{\partial\bar{\varepsilon}} \quad (\bar{\sigma} \text{ is linearly dependent on } \bar{\varepsilon})$$

- Macroscopic strain $\quad \bar{\varepsilon} = \frac{1}{\lambda}\int_{\Omega} \varepsilon\, dx, \quad \varepsilon$: microscopic strain
- Macroscopic stress $\quad \bar{\sigma} = \frac{1}{\lambda}\int_{\Omega} \sigma\, dx \quad \sigma$: microscopic stress
- Effective stiffness $\quad \bar{C} = \frac{\partial\bar{\sigma}}{\partial\bar{\varepsilon}} \simeq \frac{\Delta\bar{\sigma}}{\partial\bar{\varepsilon}}$ (using finite difference for example)

$\Rightarrow$ At the macroscopic level, we inquire the macroscopic strain, macroscopic stress, macroscopic/effective stiffness.

* Computation of effective stiffness using finite difference

$$\overline{C} = \frac{\partial \overline{\sigma}}{\partial \overline{\varepsilon}} \simeq \frac{\Delta \overline{\sigma}}{\Delta \overline{\varepsilon}} = \frac{\overline{\sigma}^{(+)} - \overline{\sigma}^{(-)}}{\overline{\varepsilon}^{(+)} - \overline{\varepsilon}^{(-)}} = \frac{\overline{\sigma}^{(+)}(\overline{\varepsilon}^{(+)}) - \overline{\sigma}^{(-)}(\overline{\varepsilon}^{(-)})}{\overline{\varepsilon}^{(+)} - \overline{\varepsilon}^{(-)}}$$

- $\overline{\varepsilon}^{(+)}, \overline{\varepsilon}^{(-)} \Longrightarrow$ perturbate $\overline{\varepsilon}$ with a small perturbation p:

$$\begin{cases} \overline{\varepsilon}^{(+)} = \overline{\varepsilon} + p \\ \overline{\varepsilon}^{(-)} = \overline{\varepsilon} - p \end{cases}$$

- $\overline{\sigma}^{(+)}, \overline{\sigma}^{(-)} \Rightarrow$ Solve two microscopic Boundary Value Problems, each associated with $\overline{\varepsilon}^{(+)}$ and $\overline{\varepsilon}^{(-)} \Rightarrow$ Obtain the corresponding microspic stress field $\sigma^{(+)}$ and $\sigma^{(-)}$

  Compute the averages/macroscopic stress

$$\overline{\sigma}^{(+)} = \frac{1}{\lambda}\int_{\Omega} \sigma^{(+)} dx \qquad \overline{\sigma}^{(-)} = \frac{1}{\lambda}\int_{\Omega} \sigma^{(-)} dx$$

- $\overline{C} = \dfrac{\overline{\sigma}^{(+)}(\overline{\varepsilon}^{(+)}) - \overline{\sigma}^{(-)}(\overline{\varepsilon}^{(-)})}{2p} \Longrightarrow$ Central finite difference formula

* Derivation of consistent macroscopic tangent

(i) Macroscopic boundary value problem

$$\begin{cases} \dfrac{d}{dx}\overline{\sigma}(x) + f(\overline{x}) = 0 \\ \overline{u}(\overline{x}=0) = u_0 \\ \overline{C}\,\dfrac{d\overline{u}}{d\overline{x}}\Big|_{\overline{x}=L} = t_0 \end{cases}$$

(ii) Microscopic boundary value problem

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

We formally write the stress increment in terms of the macroscopic strain increment

$$\Delta\overline{\sigma} = \frac{\partial\overline{\sigma}}{\partial\overline{\varepsilon}}\Delta\overline{\varepsilon} \Longrightarrow \text{Consistent macroscopic tangent } \overline{C} = \frac{\partial\overline{\sigma}}{\partial\overline{\varepsilon}}$$

* Consistent macroscopic tangent

$$\Delta\bar{\sigma} = \frac{\partial\bar{\sigma}}{\partial\bar{\varepsilon}}\Delta\bar{\varepsilon} \Rightarrow \bar{C} = \frac{\partial\bar{\sigma}}{\partial\bar{\varepsilon}} : \text{consistent macroscopic tangent}$$

in which

$$\bar{\varepsilon} = \frac{1}{\lambda}\int_\Omega \varepsilon(u(x))\,dx$$

$$\bar{\sigma} = \frac{1}{\lambda}\int_\Omega \sigma(\varepsilon(x))\,dx$$

* Some general denotations:

- Volume of a representative volume element (RVE) : $V = |\Omega| = \lambda$
- Microscopic constitutive tangent : $C = \partial\sigma/\partial\varepsilon$
- Macroscopic strain : $\bar{\varepsilon} = \frac{1}{V}\int_\Omega \varepsilon\,dV = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2}\varepsilon\,dx.$
- Macroscopic stress: $\bar{\sigma} = \frac{1}{V}\int_\Omega \sigma\,dV = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2}\sigma\,dx$
- Differential element (volume) : $dV = dx.$

* Consistent macroscopic tangent.

- Recall the strain decomposition

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

This decomposition is in principle equivalent to : $u(x) = \tilde{u}(x) + \bar{\varepsilon}\, x$

- Compute the derivative $\partial\bar{\sigma}/\partial\bar{\varepsilon}$

$$\frac{\partial\bar{\sigma}}{\partial\bar{\varepsilon}} = \frac{\partial}{\partial\bar{\varepsilon}}\left\{\frac{1}{V}\int_\Omega \sigma\, dV\right\} = \frac{1}{V}\int_\Omega \frac{\partial}{\partial\bar{\varepsilon}}\sigma(\varepsilon)\, dV = \frac{1}{V}\int_\Omega \frac{\partial\sigma}{\partial\varepsilon}\frac{\partial\varepsilon}{\partial\bar{\varepsilon}}\, dV$$

$$= \frac{1}{V}\int_\Omega C\left[\frac{\partial}{\partial\bar{\varepsilon}}(\tilde{\varepsilon} + \bar{\varepsilon})\right] dV = \frac{1}{V}\int_\Omega C\left(1 + \frac{\partial\tilde{\varepsilon}}{\partial\bar{\varepsilon}}\right) dV$$

Thus, in order to compute the consistent macroscopic tangent/effective stiffness, we need to compute the integral

$$\boxed{\bar{C} = \frac{1}{V}\int_\Omega \left(C + C\frac{\partial\tilde{\varepsilon}}{\partial\bar{\varepsilon}}\right) dV}$$

Question We need to compute $\partial\tilde{\varepsilon}/\partial\bar{\varepsilon}$

$*$ Computation of the derivative of the fluctuation part $\partial\tilde{\varepsilon}/\partial\bar{\varepsilon}$

- Recall the Lippmann–Schwinger equation:

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

with $\tau = \sigma - C^{\circ}\varepsilon$

Take derivative of (Δ) w.r.t. $\bar{\varepsilon}$:

$$\frac{\partial\tilde{\varepsilon}}{\partial\bar{\varepsilon}} = \Gamma^{\circ} * \frac{\partial\tau}{\partial\bar{\varepsilon}} = \Gamma^{\circ} * \left[\frac{\partial\sigma}{\partial\bar{\varepsilon}} - C^{\circ}\frac{\partial\varepsilon}{\partial\bar{\varepsilon}}\right] = \Gamma^{\circ} * \left[\frac{\partial\sigma}{\partial\varepsilon}\frac{\partial\varepsilon}{\partial\bar{\varepsilon}} - C^{\circ}\frac{\partial\varepsilon}{\partial\bar{\varepsilon}}\right]$$

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

Linear integral equation for the derivative of the fluctuation part $\partial\tilde{\varepsilon}/\partial\bar{\varepsilon}$

$$\boxed{\frac{\partial\tilde{\varepsilon}}{\partial\bar{\varepsilon}} = \Gamma^{\circ} * \left[C^{\Delta} + C^{\Delta}\frac{\partial\tilde{\varepsilon}}{\partial\bar{\varepsilon}}\right]}$$

REMARK The average condition $\frac{1}{V}\int_{\Omega}\varepsilon\, dV = \bar{\varepsilon} \iff \frac{1}{V}\int_{\Omega}\tilde{\varepsilon}\, dV = 0$ must be "transferred" to some average condition on $\partial\tilde{\varepsilon}/\partial\bar{\varepsilon}$:

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

* Fixed-point iteration scheme for the Lippmann–Schwinger type equation

$$\frac{\partial \tilde{\varepsilon}}{\partial \bar{\varepsilon}} = \Gamma^{0} * \left[C^{\Delta} + C^{\Delta} \frac{\partial \tilde{\varepsilon}}{\partial \bar{\varepsilon}} \right] \qquad (\star)$$

It is convenient to solve $(\star)$ using the discrete Fourier transform.

To this end, we work it out in the Fourier space