

Lec 12: FFT-based methods

- Fourier analysis
- Green's function
- FFT homogenization

Fourier analysis

Fourier transform

The Fourier transform of function $f: \mathbb{R} \rightarrow \mathbb{C}$ is $\hat{f}: \mathbb{R} \rightarrow \mathbb{C}$, defined as:

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(t) e^{-i2\pi\xi t} dt, \quad \xi \in \mathbb{R}.$$

The inverse transform of $\hat{f}(\xi)$ can recover $f(t)$:

$$f(t) = \int_{-\infty}^{\infty} \hat{f}(\xi) e^{i2\pi\xi t} d\xi, \quad t \in \mathbb{R}.$$

Fourier series

For periodic function (e.g., homogenization), Fourier series is convenient.

Assume $f(t)$ is a periodic function with period T . The Fourier transform of $f(t)$ is:

$$C[k] = \frac{1}{T} \int_0^T f(t) e^{-i2\pi \frac{k}{T} t} dt, \quad k \in \mathbb{Z}.$$

The inverse transform (Fourier series) is given by:

$$f(t) = \sum_{k=-\infty}^{\infty} C[k] e^{i2\pi \frac{k}{T} t}, \quad t \in \mathbb{R}.$$

- Note :**
- * Coefficients $C[k]$ capture discrete frequencies $\frac{k}{T}$.
 - * The dual of the (time-domain) Fourier series is discrete-time Fourier transform (DTFT), where frequency is continuous while time is discrete.

Discrete Fourier transform (DFT)

Both time and frequency are discrete in this case. Let us discretize $f(t)$ at N points: $t_n = n \Delta t$, where $\Delta t = \frac{T}{N}$. Define discrete signal $x_n = f(t_n)$ for $n=0, 1, \dots, N-1$. Then $\{x_n\}$ is one period of an infinite periodic sequence.

Approximate $C[k]$ with Riemann sums:

$$C[k] \approx \hat{f}_k = \frac{1}{N} \sum_{n=0}^{N-1} x_n e^{-i2\pi kn/N}, \quad k=0, 1, \dots, N-1$$

Let $X_k := N \cdot \hat{f}_k$, we can define discrete Fourier transform:

$$X_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi kn/N}, \quad k=0, 1, \dots, N-1$$

The inverse discrete Fourier transform is:

$$x_n = \frac{1}{N} \sum_{k=0}^{N-1} X_k e^{i2\pi kn/N}, \quad k=0, 1, \dots, N-1$$

Fast Fourier transform (FFT)

From $\{x_n\}$ to $\{X_k\}$, we may use the DFT matrix:

$$\begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{N-1} \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & w & \cdots & w^{N-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & w^{N-1} & \cdots & w^{(N-1)(N-1)} \end{bmatrix}}_W \begin{bmatrix} X_0 \\ X_1 \\ \vdots \\ X_{N-1} \end{bmatrix}$$

where $W_{kn} = w^{kn} = \left(e^{-i2\pi/N}\right)^{kn}$. FFT algorithms utilize the symmetries of the matrix to reduce computational time from $\mathcal{O}(N^2)$ to $\mathcal{O}(N \log N)$.

"FFT is the most important numerical algorithm of our lifetime."

- Gilbert Strang

Green's function

Green's function is a concept to solve PDEs, and Fourier analysis turns Green's function from abstract mathematical tools into practical computational engines.

A motivating problem: 1D Poisson's equation

Consider the equation $-\frac{d^2u}{dx^2} = f(x), \quad x \in [0, L]$

satisfying the conditions:

$$\begin{cases} u(0) = u(L) & \text{periodicity} \\ u'(0) = u'(L) \\ \frac{1}{L} \int_0^L u(x) dx = 0 & \text{solvability} \end{cases}$$

Assume that $G(x, x_0)$ is the solution if $f(x) = \delta(x - x_0)$:

$$-\frac{d^2 G}{dx^2} = \delta(x - x_0) \quad (G(x, x_0) \text{ is Green's function})$$

Physically speaking, $G(x, x_0)$ is the solution response at x due to an impulse at x_0 . Assume somehow we can find G , and let's how it is useful. Consider

$$\boxed{\int_0^L G(x, s) f(s) ds} = \int_0^L -G(x, s) \frac{d^2 u}{ds^2} ds = \int_0^L \frac{dG}{ds} \frac{du}{ds} ds - G \frac{du}{ds} \Big|_0^L$$

$$= - \int_0^L \frac{d^2 G}{ds^2} u ds + \cancel{\frac{dG}{ds} u \Big|_0^L} - G \frac{du}{ds} \Big|_0^L = - \int_0^L \frac{d^2 G}{ds^2} u ds = \int_0^L \delta(x-s) u(s) ds$$

$$= u(x)$$

*operator L is
translation invariant*

convolution

This means that $u(x) = \int_0^L G(x-s) f(s) ds = (G * f)(x)$.

Finally, let us trivially check $u(x) = \int_0^L G(x-s) \delta(s-x_0) ds = G(x-x_0)$

is indeed the solution due to impulse $\delta(x-x_0)$.

Next, we will let $f(x) = \sin(\frac{2\pi}{L}x)$ and use three approaches to solve for $u(x)$.

Method I: Direct approach

To apply $u(x) = (G_l * f)(x)$, we must first find $G_l(x, s)$.

$$-\frac{d^2 G_l(x, x_0)}{dx^2} = \delta(x - x_0) \Rightarrow \left. \frac{d G_l}{dx} \right|_{x=x_0^+} - \left. \frac{d G_l}{dx} \right|_{x=x_0^-} = -1 \quad (*)$$

$G_l(x, x_0) = \frac{1}{2L} (x - x_0)^2 - \frac{1}{2} |x - x_0| - \frac{L}{12}$ will satisfy (*) and

$$\begin{cases} G_l(0, x_0) = G_l(L, x_0) \\ G_l'(0, x_0) = G_l'(L, x_0) \\ \frac{1}{L} \int_0^L G_l(x, x_0) dx = 0 \end{cases}$$

$$\Rightarrow u(x) = (G_l * f)(x) = \int_0^L G_l(x, s) \sin\left(\frac{2\pi}{L}s\right) ds = \frac{L^2}{4\pi^2} \sin\left(\frac{2\pi x}{L}\right)$$

Method II : Fourier series

$$-\frac{d^2 u}{dx^2} = f$$

$$\text{By Fourier series : } u(x) = \sum_{k=-\infty}^{\infty} C_u[k] e^{i 2\pi \frac{k}{L} x}, \quad f(x) = \sum_{k=-\infty}^{\infty} C_f[k] e^{i 2\pi \frac{k}{L} x}$$

$$\Rightarrow \left(\frac{2\pi k}{L}\right)^2 C_u[k] = C_f[k] \quad (\text{matching terms})$$

Note that $C_f[k] = \frac{1}{L} \int_0^L \sin\left(\frac{2\pi x}{L}\right) e^{-i 2\pi \frac{k}{L} x} dx$. It can be shown that

$$C_f[1] = \frac{1}{2i}, \quad C_f[-1] = -\frac{1}{2i}, \quad C_f[k] = 0 \text{ for } k \neq \pm 1.$$

$$\Rightarrow C_u[1] = \frac{1}{2i} \cdot \left(\frac{L}{2\pi}\right)^2, \quad C_u[-1] = -\frac{1}{2i} \left(\frac{L}{2\pi}\right)^2, \quad C_u[k] = 0 \text{ for } k \neq \pm 1$$

$$\Rightarrow u(x) = \frac{L^2}{8i\pi^2} e^{izx\frac{x}{L}} - \frac{L^2}{8i\pi^2} e^{-izx\frac{x}{L}} = \frac{L^2}{4\pi^2} \sin\left(\frac{2\pi}{L}x\right).$$

But wait, how is this related to Green's function?

Consider

$$-\frac{d^2 G}{dx^2} = \delta(x) \quad (x_0=0 \Rightarrow G(x,0)=G(x))$$

$$\text{By Fourier series, } G(x) = \sum_{k=-\infty}^{\infty} C_G[k] e^{izx\frac{k}{L}}, \quad f(x) = \sum_{k=-\infty}^{\infty} C_f[k] e^{izx\frac{k}{L}}$$

$$\Rightarrow \left(\frac{2\pi k}{L}\right)^2 C_G[k] = C_f[k] \text{ (matching terms)}$$

$$\text{Note that } C_f[k] = \frac{1}{L} \int_0^L \delta(x) e^{-izx\frac{k}{L}} dx = \frac{1}{L}$$

$$\Rightarrow C_G[k] = \begin{cases} \frac{L}{4\pi^2} \frac{1}{k^2} & (\text{Green's function in the frequency domain}) \\ 0 & (\text{implying } \frac{1}{L} \int G(x) dx = 0) \end{cases}$$

$$\Rightarrow G(x) = \sum_{k \neq 0} \frac{L}{4\pi^2} \frac{1}{k^2} e^{izx\frac{k}{L}}.$$

$$\underline{\text{Convolution theorem: }} u(x) = (G * f)(x) \Rightarrow C_u[k] = L C_G[k] \cdot C_f[k]$$

For $f = \sin\left(\frac{2\pi}{L}x\right)$, we have $C_u[k] = L \cdot \frac{L}{4\pi^2} \cdot \frac{1}{k^2} \cdot \frac{1}{2i} \cdot k \quad (k=\pm 1)$. compute once and save it for future use

For $f = \delta(x)$, we have $C_u[k] = L \cdot \frac{L}{4\pi^2} \cdot \frac{1}{k^2} \cdot \frac{1}{L} = C_G[k]$.

Method III: FFT

$$\text{Assume } u(x) = \sum_{k=0}^{N-1} \hat{u}_k e^{i 2 \pi \frac{k}{L} x}, \quad f(x) = \sum_{k=0}^{N-1} \hat{f}_k e^{i 2 \pi \frac{k}{L} x}$$

$$\Rightarrow \left(\frac{2\pi k}{L}\right)^2 \hat{u}_k = \hat{f}_k \quad (\text{matching terms, } X_k^u = N \cdot \hat{u}_k, X_k^f = N \cdot \hat{f}_k)$$

$$\Rightarrow X_k^u = \frac{L^2}{(2\pi k)^2} X_k^f \Rightarrow u(n \cdot \frac{L}{N}) = u(n \Delta x) = x_n^u$$

Algorithm

Step 1: $\{X_k^f\} = \text{FFT}(\{x_n^f\})$ where $x_n^f = f(n \Delta x)$

Step 2: $X_k^u = \frac{L^2}{(2\pi k)^2} X_k^f \quad \left(\frac{L^2}{(2\pi k)^2} = L \cdot \frac{L}{(2\pi k)^2} = L \cdot \hat{G}_k, \text{ set } X_0^u = 0 \right)$

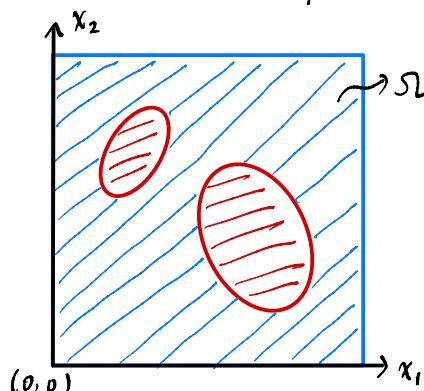
Step 3: $\{x_n^u\} = \text{inverse FFT}(\{X_k^u\})$

Question: What is the computational cost of this FFT-based algorithm compared with FEM?

FFT homogenization

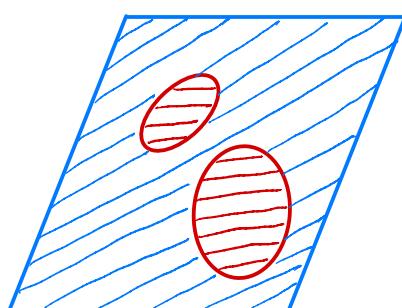
Problem setup

Consider a representative volume element (RVE):



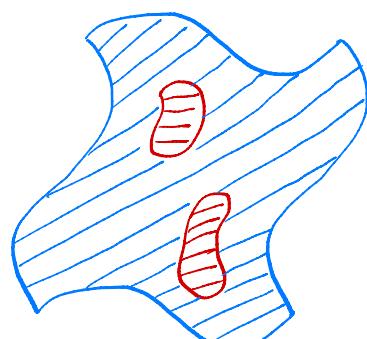
$$\underline{u}(x) = 0$$

$$\underline{\epsilon}(x) = 0$$



$$\underline{u}(x) = H \cdot x$$

$$\underline{\epsilon}(x) = H$$



$$\underline{u}(x) = H \cdot x + \underline{u}^*(x)$$

$$\underline{\epsilon}(x) = H + \nabla^s \underline{u}^*(x)$$

undeformed
configuration

(just for
illustration)

deformed
configuration

where $\underline{\underline{\epsilon}}$ is the prescribed macroscopic strain.

Proposition If we specify periodic B.C. for \underline{u}^* and anti-periodic B.C.

for $\underline{n} \cdot \underline{\underline{\epsilon}}$, the Hill-Mandel condition $\langle \underline{\underline{\epsilon}} : \underline{\underline{\epsilon}} \rangle = \langle \underline{\underline{\epsilon}} \rangle : \langle \underline{\underline{\epsilon}} \rangle$ can be satisfied.

Proof Define $\underline{\underline{\epsilon}}^*$ and $\underline{\underline{\epsilon}}^*$ to be: $\underline{\underline{\epsilon}} = \langle \underline{\underline{\epsilon}} \rangle + \underline{\underline{\epsilon}}^*$ and $\underline{\underline{\epsilon}} = \langle \underline{\underline{\epsilon}} \rangle + \underline{\underline{\epsilon}}^*$.

$$\text{Notice } \int_{\Omega} \nabla^s \underline{u}^*(x) = \int_{\Omega} \frac{1}{2} (\underline{u}_{i,j}^* + \underline{u}_{j,i}^*) = \int_{\Omega} \frac{1}{2} (\eta_j \underline{u}_i^* + n_i \underline{u}_j^*) = 0$$

$$\Rightarrow \langle \underline{\underline{\epsilon}} \rangle = \frac{1}{V} \int \underline{\underline{\epsilon}} = \underline{\underline{\epsilon}} + \frac{1}{V} \int \nabla^s \underline{u}^*(x) = \underline{\underline{\epsilon}} \Rightarrow \underline{\underline{\epsilon}}^* = \nabla^s \underline{u}^*$$

$$\langle \underline{\underline{\epsilon}} : \underline{\underline{\epsilon}} \rangle = \frac{1}{V} \int_{\Omega} (\langle \underline{\underline{\epsilon}} \rangle + \underline{\underline{\epsilon}}^*) : (\langle \underline{\underline{\epsilon}} \rangle + \underline{\underline{\epsilon}}^*)$$

$$= \langle \underline{\underline{\epsilon}} \rangle : \langle \underline{\underline{\epsilon}} \rangle + \underbrace{\langle \underline{\underline{\epsilon}} \rangle : \left(\frac{1}{V} \int_{\Omega} \underline{\underline{\epsilon}}^* \right)}_{(*)} + \underbrace{\left(\frac{1}{V} \int_{\Omega} \underline{\underline{\epsilon}}^* \right) : \langle \underline{\underline{\epsilon}} \rangle}_{(**)} + \underbrace{\frac{1}{V} \int_{\Omega} \underline{\underline{\epsilon}}^* : \underline{\underline{\epsilon}}^*}_{(***)}$$

$$\text{Since } \underline{\underline{\epsilon}} = \langle \underline{\underline{\epsilon}} \rangle + \underline{\underline{\epsilon}}^*, \frac{1}{V} \int \underline{\underline{\epsilon}} = \frac{1}{V} \int \langle \underline{\underline{\epsilon}} \rangle + \frac{1}{V} \int \underline{\underline{\epsilon}}^* \Rightarrow \langle \underline{\underline{\epsilon}}^* \rangle = 0 \Rightarrow (*) = 0.$$

$$\text{Since } \underline{\underline{\epsilon}} = \langle \underline{\underline{\epsilon}} \rangle + \underline{\underline{\epsilon}}^*, \frac{1}{V} \int \underline{\underline{\epsilon}} = \frac{1}{V} \int \langle \underline{\underline{\epsilon}} \rangle + \frac{1}{V} \int \underline{\underline{\epsilon}}^* \Rightarrow \langle \underline{\underline{\epsilon}}^* \rangle = 0 \Rightarrow (**) = 0.$$

$$\text{From equilibrium, } -\nabla \cdot \underline{\underline{\epsilon}} = 0 \Rightarrow -\nabla \cdot \underline{\underline{\epsilon}}^* = 0 \Rightarrow - \int_{\Omega} (\nabla \cdot \underline{\underline{\epsilon}}^*) \cdot \underline{u}^* = 0$$

$$\Rightarrow \int_{\Omega} \underline{\underline{\epsilon}}^* : \nabla \underline{u}^* - \int_{\partial\Omega} (\underline{n} \cdot \underline{\underline{\epsilon}}^*) \cdot \underline{u}^* = \int_{\Omega} \underline{\underline{\epsilon}}^* : \underline{\underline{\epsilon}}^* - \underbrace{\int_{\partial\Omega} (\underline{n} \cdot \underline{\underline{\epsilon}}) \cdot \underline{u}^*}_{0} + \underbrace{\int_{\partial\Omega} (\underline{n} \cdot \langle \underline{\underline{\epsilon}} \rangle) \cdot \underline{u}^*}_{0} = 0$$

$$\Rightarrow (**) = 0. \text{ Therefore, } \langle \underline{\underline{\epsilon}} : \underline{\underline{\epsilon}} \rangle = \langle \underline{\underline{\epsilon}} \rangle : \langle \underline{\underline{\epsilon}} \rangle.$$

FEM approach for the RVE problem

Strong form Find $\underline{u}^*(\underline{x})$ such that

$$-\nabla \cdot \underline{\underline{b}} = 0, \text{ where } \underline{\underline{b}}(\underline{x}) = \int_{\Omega} \underline{\underline{C}}(\underline{x}) : \underline{\underline{\epsilon}}(\underline{x})$$

$$\underline{\underline{\epsilon}}(\underline{x}) = \underline{\underline{H}} + \nabla^s \underline{u}^*(\underline{x})$$

Φ specified

$$\text{B.C. : } \begin{cases} \underline{u}^* & \text{periodic} \\ \underline{n} \cdot \underline{b} & \text{anti-periodic} \end{cases}$$

Weak form Find $\underline{u}^*(\underline{x}) \in V = \left\{ \underline{u} \mid \underline{u} \in [H^1(\Omega)]^{nd}, \underline{u} \text{ periodic on } \partial\Omega \right\}$

such that

$$\int_{\Omega} \underline{\underline{b}} : \nabla^s \underline{v} + \int_{\partial\Omega} (\underline{n} \cdot \underline{\underline{q}}) \cdot \underline{v} = 0, \forall \underline{v} \in V$$

Note: The periodic property of \underline{u}^* can be treated as constraints handled by substitution method or Lagrange multiplier method.

Recap: A summary of the methods:

	Dirichlet B.C.	periodic B.C.	nonlinear constraint
elimination method	✓	✗	✗
substitution method	✗	✓	✗
Lagrange multiplier method	✓	✓	✓

FFT methods for the RVE problem

From equilibrium: $\nabla \cdot \underline{\underline{\sigma}} = 0$ ($\sigma_{ij}, i=0$) inhomogeneous, can't do Fourier analysis

From constitutive relation: $\underline{\underline{\sigma}}(\underline{x}) = \underline{\underline{C}}(\underline{x}) : \underline{\underline{\epsilon}}(\underline{x})$

Introduce polarization stress $\underline{\underline{\tau}}(\underline{x})$ s.t. $\underline{\underline{\sigma}}(\underline{x}) = \underline{\underline{C}}^0 : \underline{\underline{\epsilon}}(\underline{x}) + \underbrace{(\underline{\underline{C}}(\underline{x}) - \underline{\underline{C}}^0) : \underline{\underline{\epsilon}}}_{\text{constant}}$

$$\Rightarrow \lambda u_{kk} \delta_{ij} + 2\mu u_{(ij)} + \tau_{ij} = 0 \quad (\text{isotropic material}) \quad \underline{\underline{\tau}}(\underline{x})$$

$$\Rightarrow \lambda u_{k,kj} \delta_{ij} + \mu(u_{ii,jj} + u_{jj,ii}) + \tau_{ij,i} = 0 \quad (\text{equilibrium})$$

$$\Rightarrow (\lambda + \mu) u_{k,kj} + \mu u_{jj,ii} + \tau_{ij,i} = 0$$

$$\text{Assume } u_j(\underline{x}) = \sum_{k_1=0}^{N_1-1} \sum_{k_2=0}^{N_2-1} \sum_{k_3=0}^{N_3-1} \hat{u}_j[\underline{k}] e^{i \frac{2\pi}{L} \underline{k} \cdot \underline{x}}$$

$$\epsilon_{ij}(\underline{x}) = \sum_{k_1=0}^{N_1-1} \sum_{k_2=0}^{N_2-1} \sum_{k_3=0}^{N_3-1} \hat{\epsilon}_{ij}[\underline{k}] e^{i \frac{2\pi}{L} \underline{k} \cdot \underline{x}} \quad (\text{truncated Fourier series})$$

$$\tau_{ij}(\underline{x}) = \sum_{k_1=0}^{N_1-1} \sum_{k_2=0}^{N_2-1} \sum_{k_3=0}^{N_3-1} \hat{\tau}_{ij}[\underline{k}] e^{i \frac{2\pi}{L} \underline{k} \cdot \underline{x}}$$

$$\Rightarrow i^2 \left((\lambda + \mu) g_k g_j \hat{u}_k + \mu g_i g_i \hat{u}_j \right) + i \cdot g_i \hat{\tau}_{ij} = 0 \quad (g_i = \frac{2\pi k_i}{L}) \quad \text{angular frequency}$$

$$\Rightarrow i \begin{bmatrix} (\lambda + \mu) g_1^2 + \mu |g|^2 & (\lambda + \mu) g_1 g_2 & (\lambda + \mu) g_1 g_3 \\ (\lambda + \mu) g_1 g_2 & (\lambda + \mu) g_2^2 + \mu |g|^2 & (\lambda + \mu) g_2 g_3 \\ (\lambda + \mu) g_1 g_3 & (\lambda + \mu) g_2 g_3 & (\lambda + \mu) g_3^2 + \mu |g|^2 \end{bmatrix} \begin{bmatrix} \hat{u}_1 \\ \hat{u}_2 \\ \hat{u}_3 \end{bmatrix} = - \begin{bmatrix} g_i \hat{\tau}_{i1} \\ g_i \hat{\tau}_{i2} \\ g_i \hat{\tau}_{i3} \end{bmatrix}$$

Inverting this matrix is OK!

$$= N_{jk}$$

symmetry of $\hat{\tau}$

$$\Rightarrow i \cdot \hat{u}_j = - \underbrace{\frac{1}{\mu |\underline{g}|^2} \left(\delta_{jk} - \frac{g_j g_k}{|\underline{g}|^2} \cdot \frac{n+\mu}{n+2\mu} \right)}_{= N_{jk}} g_h \hat{\tau}_{hk} \stackrel{\downarrow}{=} - \frac{1}{2} (N_{jk} g_h + N_{jh} g_k) \hat{\tau}_{hk}$$

Notice $\underline{\varepsilon}_{ij} = u_{(i,j)} \Rightarrow \hat{\varepsilon}_{ij} = \frac{i}{2} (g_j \hat{u}_i + g_i \hat{u}_j)$

$$\Rightarrow \hat{\varepsilon}_{ij} = - \underbrace{\frac{1}{4} (g_i N_{jk} g_h + g_j N_{ih} g_k + g_i N_{jh} g_h + g_i N_{jk} g_k)}_{\hat{G}_{ijkh} \text{ (Green's function)}} \hat{\tau}_{kh}$$

$$\Rightarrow \hat{G}_{ijkh} = \frac{1}{4\mu |\underline{g}|^2} (\delta_{ik} g_j g_h + \delta_{ih} g_j g_k + \delta_{jk} g_i g_h + \delta_{jh} g_i g_k) - \frac{n+\mu}{\mu(n+2\mu)} \frac{g_i g_j g_k g_h}{|\underline{g}|^4}$$

$$\Rightarrow \hat{\varepsilon}_{ij} = - \hat{G}_{ijkh} \hat{\tau}_{kh} \Leftrightarrow \underbrace{N_1 N_2 N_3 \hat{\varepsilon}_{ij}}_{\text{numpy.fft convention}} = - \hat{G}_{ijkh} \underbrace{N_1 N_2 N_3 \hat{\tau}_{kh}}$$

Algorithm

Initialization: $\underline{\varepsilon}^0(\underline{x}_d) = \underline{\underline{H}}$, $\underline{b}^0(\underline{x}_d) = \underline{\underline{C}}(\underline{x}_d) = \underline{\varepsilon}^0(\underline{x}_d)$, $\underline{x}_d = \left(\frac{n_1 L_1}{N_1}, \frac{n_2 L_2}{N_2}, \frac{n_3 L_3}{N_3} \right)$

At iteration $i+1$ with $\underline{\varepsilon}^i$ and \underline{b}^i known:

$$n_1 = 0, 1, \dots, N_1 - 1$$

$$n_2 = 0, 1, \dots, N_2 - 1$$

$$n_3 = 0, 1, \dots, N_3 - 1$$

$$(a) \underline{\tau}^i(\underline{x}_d) = \underline{b}^i(\underline{x}_d) - \underline{\underline{C}}^0: \underline{\varepsilon}^0(\underline{x}_d)$$

$$(b) N_1 N_2 N_3 \hat{\underline{\tau}}^i = \text{FFT}(\underline{\tau}^i)$$

$$(c) N_1 N_2 N_3 \hat{\underline{\varepsilon}}^{i+1} = - \hat{\underline{\underline{G}}}^i: N_1 N_2 N_3 \hat{\underline{\tau}}^i \quad (\hat{\underline{\varepsilon}}^{i+1}[0] = \underline{\underline{H}} \text{ to ensure } \frac{1}{V} \int_V \underline{\varepsilon} = \underline{\underline{H}})$$

$$(d) \underline{\varepsilon}^{i+1} = \text{inverse FFT}(N_1 N_2 N_3 \hat{\underline{\varepsilon}}^{i+1})$$

$$(e) \underline{b}^{i+1}(\underline{x}_d) = \underline{\underline{C}}(\underline{x}_d): \underline{\varepsilon}^{i+1}(\underline{x}_d)$$

Remarks:

- * The algorithm can be slightly modified by using $\hat{\underline{\varepsilon}}^i = - \hat{\underline{\underline{G}}}^i: \hat{\underline{\tau}}^i + \hat{\underline{\underline{G}}}^i: \hat{\underline{b}}^i$ so that step (c) can be changed to $\hat{\underline{\varepsilon}}^{i+1} = \hat{\underline{\varepsilon}}^i - \hat{\underline{\underline{G}}}^i: \hat{\underline{b}}^i$.

- * We have use angular frequency $\omega_i = \frac{2\pi k_i}{L}$, but you may also use frequency $\underline{\omega}_i = \frac{k_i}{L}$ or just k_i , and the results will remain the same.
- * The size of the RVE L does not play a (big) role.
- * By specifying different \underline{h} , i.e., $\langle \underline{\epsilon} \rangle$ and compute $\langle \underline{b} \rangle$, we can obtain the "homogenized" modulus.
- * Refer to the code we provide and the Moulinec 1998 paper for more details.