Introduction to FFT-based numerical methods for the homogenization of random materials (14–18 march 2022)

Introduction: the Green operator and the Lippmann–Schwinger equation

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Outline of the session on spatial discretization

- Lecture 1 — Introduction: the Green operator and the Lippmann–Schwinger (LS) equation
- Lecture 2 — Consistent discretization of the LS equation
- Lecture 3 — Asymptotically consistent discretization**s** of the LS equation

Outline of Lecture 1

- Homogenization in a nutshell
- The "corrector" problem
- Formal definition of the Green operator
- The Lippmann–Schwinger (LS) equation
- The "basic" scheme
- Fourier series in a nutshell
- Derivation of the periodic Green operator (homogeneous material)

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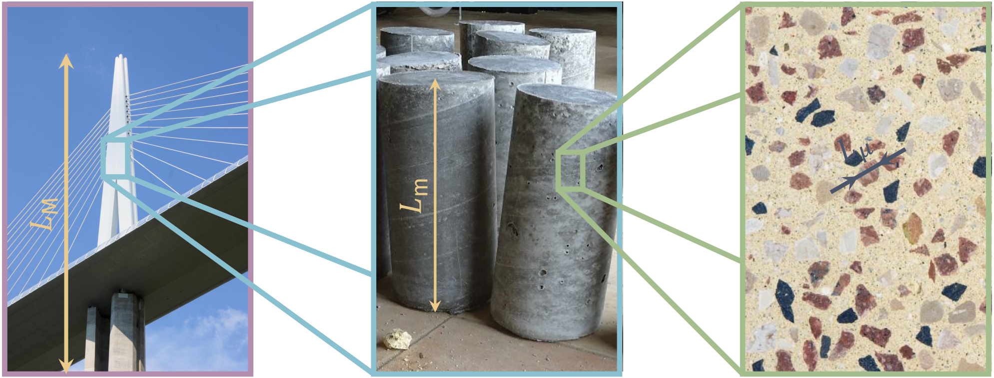
Random homogenization



Macroscopic scale

Mesoscopic scale

Microscopic scale

Separation of scales

$$L_\mu \ll L_\mathrm{m} \ll L_\mathrm{M}$$

Source: Structurae, BGEA Labo and Aménagements Déco Lafarge

What is homogenization?

Homogenization is the process of replacing the complex **microstructure** (cementitious matrix + aggregates) with an "equivalent", **homogeneous material**.

The goal is to establish the (quantitative) rule that relates the **geometry** and **mechanical properties** of the constituants to the **macroscopic mechanical properties**.

At the scale of the structure (the pylons of the cable-stayed bridge), material heterogeneities (aggregates, ...) are **ignored**.
The response of the structure is computed as if it was **homogeneous**.

Effective (macroscopic) linear elastic properties

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{C}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}) \qquad \Rightarrow \qquad \langle \boldsymbol{\sigma} \rangle = \mathbf{C}^{\text{eff}} : \langle \boldsymbol{\varepsilon} \rangle$$

Effective properties are found at the mesoscopic scale, experimentally or from an upscaling prediction

From random to periodic homogenization

A conceptual gap that will be discussed by F. Willot (Lecture 7)

Some structures are indeed periodic

Waffle slab (source: Holedeck)

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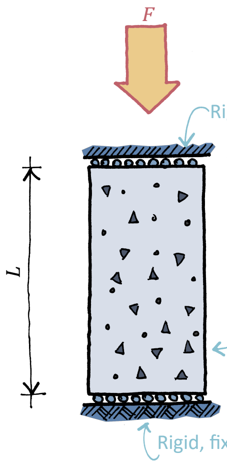
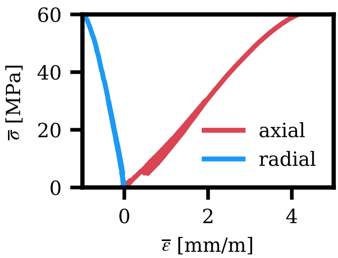
Experimental characterization (top-down approach)



Macroscopic variables

- Macro. stress: F/A
- Macro. strain: δ/L



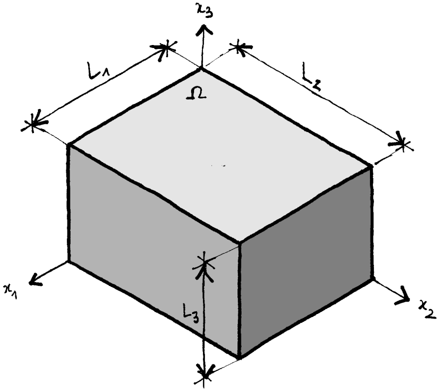
Compression test on a concrete sample
(Courtesy S. Bahafid, S. Ghabezloo)

Upscaling prediction (bottom-up approach)

"Corrector" problem reproduces physical experiment in-silico!

The unit-cell

$$\Omega = (0, L_1) \times \cdots \times (0, L_d)$$



Field equations

$$\begin{cases} \operatorname{div} \boldsymbol{\sigma} = 0 \\ \boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon} \\ \boldsymbol{\varepsilon} = \operatorname{sym} \operatorname{grad} \mathbf{u} \end{cases}$$

Periodic boundary conditions

$$\begin{cases} \mathbf{u}(\mathbf{x}) - \overline{\boldsymbol{\varepsilon}} \cdot \mathbf{x} \text{ is } \Omega\text{-periodic} \\ \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) \text{ is } \Omega\text{-skew-periodic} \end{cases} \Leftrightarrow \begin{cases} \mathbf{u}(\mathbf{x} + L_i\, \mathbf{e}_i) = \mathbf{u}(\mathbf{x}) + L_i\, \overline{\boldsymbol{\varepsilon}} \cdot \mathbf{e}_i \\ \boldsymbol{\sigma}(\mathbf{x} + L_i\, \mathbf{e}_i) \cdot \mathbf{e}_i = \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{e}_i \end{cases}$$

(no summation on i)

Post-processing the effective stiffness

Macroscopic strain is prescribed!

$$\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}$$

The corrector problem is linear!

There exists $\mathbf{L}$ such that $\langle \boldsymbol{\sigma} \rangle = \mathbf{L} : \bar{\boldsymbol{\varepsilon}} = \mathbf{L} : \langle \boldsymbol{\varepsilon} \rangle \quad \Rightarrow \quad \mathbf{L} = \mathbf{C}^{\mathrm{eff}}$

The homogenization workflow

- Solve corrector problem for **6 independent load cases**

$$\bar{\boldsymbol{\varepsilon}} = \mathbf{sym}\left(\mathbf{e}_i \otimes \mathbf{e}_j\right)$$

- Find the components of the effective stiffness

$$C_{ijkl} = \langle \sigma_{ij} \rangle$$

Introducing eigenstresses

$$\begin{cases} \operatorname{div} \boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma}(\mathbf{x} + L_i\,\mathbf{e}_i) \cdot \mathbf{e}_i = \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{e}_i \\ \boldsymbol{\varepsilon} = \operatorname{sym} \operatorname{grad} \mathbf{u} \\ \mathbf{u}(\mathbf{x} + L_i\,\mathbf{e}_i) = \mathbf{u}(\mathbf{x}) + L_i\,\overline{\boldsymbol{\varepsilon}} \cdot \mathbf{e}_i \\ \boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \end{cases}$$

Loading parameters

- $\overline{\boldsymbol{\varepsilon}} \in \mathcal{T}$: symmetric, second-order tensor
- $\boldsymbol{\varpi} \in \mathcal{T}(\Omega)$: symmetric, second-order tensor **field**
  (with square-integrable coefficients)

Eigenstresses?

- A very cheap extension
- Useful for: thermoelasticity, poroelasticity, elastoplasticity, ...

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Displacements are of no importance

For homogenization purposes, only $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ matter!

The subspace of self-equilibrated stresses

$$\boldsymbol{\sigma} \in \mathcal{S}(\Omega) \iff \begin{cases} \operatorname{\mathbf{div}} \boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma}(\mathbf{x} + L_i\,\mathbf{e}_i) \cdot \mathbf{e}_i = \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{e}_i \end{cases}$$

The subspace of compatible strains

$$\boldsymbol{\varepsilon} \in \mathcal{E}(\Omega) \iff \text{there exists } \mathbf{u} \text{ such that } \begin{cases} \boldsymbol{\varepsilon} = \operatorname{\mathbf{sym\,grad}} \mathbf{u} \\ \mathbf{u}(\mathbf{x} + L_i\,\mathbf{e}_i) = \mathbf{u}(\mathbf{x}) \end{cases}$$

Equivalent formulation of the corrector problem

Find $\boldsymbol{\sigma} \in \mathcal{S}(\Omega)$ and $\boldsymbol{\varepsilon} \in \overline{\boldsymbol{\varepsilon}} + \mathcal{E}(\Omega)$ such that $\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi}$ (v1)

Find $\boldsymbol{\varepsilon} \in \overline{\boldsymbol{\varepsilon}} + \mathcal{E}(\Omega)$ such that $\mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \in \mathcal{S}(\Omega)$ (v2)

Abstracting the corrector problem

The abstract prestressed corrector problem

$$\mathcal{P}(\mathbf{C}, \boldsymbol{\varpi}, \overline{\boldsymbol{\varepsilon}}) \quad \begin{cases} \text{Given } \overline{\boldsymbol{\varepsilon}} \in \mathcal{T} \text{ and } \boldsymbol{\varpi} \in \mathcal{T}(\Omega) \\ \text{Find } \boldsymbol{\varepsilon} \in \overline{\boldsymbol{\varepsilon}} + \mathcal{E}(\Omega) \text{ such that } \mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \in \mathcal{S}(\Omega) \end{cases}$$

Axioms

1. **Linearity:** $\mathcal{S}(\Omega)$ and $\mathcal{E}(\Omega)$ are vector subspaces of $\mathcal{T}(\Omega)$
2. $\mathcal{S}(\Omega)$ contains the **constant stress fields**
3. **Strain control:** for all $\boldsymbol{\varepsilon} \in \mathcal{E}(\Omega)$, $\langle \boldsymbol{\varepsilon} \rangle = 0$
4. **Hill–Mandel lemma:** $\langle \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \rangle = \mathbf{0}$ for all $\boldsymbol{\sigma} \in \mathcal{S}(\Omega)$ and $\boldsymbol{\varepsilon} \in \mathcal{E}(\Omega)$
5. **Well-posedness:** $\mathcal{P}(\mathbf{C}, \boldsymbol{\varpi}, \overline{\boldsymbol{\varepsilon}})$ always has a unique solution

   (ellipticity condition on $\mathbf{C}$)

The Green operator for strains

$$\mathcal{P}(\mathbf{C}, \boldsymbol{\varpi}, \bar{\boldsymbol{\varepsilon}}) \quad \begin{cases} \text{Given } \bar{\boldsymbol{\varepsilon}} \in \mathcal{T} \text{ and } \boldsymbol{\varpi} \in \mathcal{T}(\Omega) \\ \text{Find } \boldsymbol{\varepsilon} \in \bar{\boldsymbol{\varepsilon}} + \mathcal{E}(\Omega) \text{ such that } \mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \in \mathcal{S}(\Omega) \end{cases}$$

Definition [1–3]

The Green operator $\boldsymbol{\Gamma}$ associated with the (possibly heterogeneous) material $\mathbf{C}$ is the mapping $\boldsymbol{\Gamma} : \mathcal{T}(\Omega) \longrightarrow \mathcal{E}(\Omega)$ such that

$$\boldsymbol{\varepsilon} = -\boldsymbol{\Gamma}(\boldsymbol{\varpi}) \text{ is the solution to } \mathcal{P}(\mathbf{C}, \boldsymbol{\varpi}, \bar{\boldsymbol{\varepsilon}} = \mathbf{0})$$

Straightforward properties

- $\boldsymbol{\Gamma}$ is a linear operator
- $\langle \boldsymbol{\Gamma}(\boldsymbol{\varpi}) \rangle = \mathbf{0}$ for all $\boldsymbol{\varpi} \in \mathcal{T}(\Omega)$
- The solution to $\mathcal{P}(\mathbf{C}, \boldsymbol{\varpi}, \bar{\boldsymbol{\varepsilon}} \neq \mathbf{0})$ is $\boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} - \boldsymbol{\Gamma}(\boldsymbol{\varpi})$ when $\mathbf{C}$ is homogeneous!

[1] J. Korringa, *Journal of Mathematical Physics* **1973**, *14*, 509–513.
[2] R. Zeller, P. H. Dederichs, *Physica Status Solidi (B)* **1973**, *55*, 831–842.
[3] E. Kröner in Topics in Applied Continuum Mechanics, (Eds.: J. L. Zeman, F. Ziegler), Springer Verlag Wien, Vienna, **1974**, pp. 22–38.

Properties of the Γ operator

- $\mathbf{\Gamma}(\boldsymbol{\sigma}) = \mathbf{0}$ for all $\boldsymbol{\sigma} \in \mathcal{S}(\Omega)$
- $\langle \boldsymbol{\varpi}_1 : \mathbf{\Gamma}(\boldsymbol{\varpi}_2) \rangle = \langle \mathbf{\Gamma}(\boldsymbol{\varpi}_1) : \boldsymbol{\varpi}_2 \rangle$ for all $\boldsymbol{\varpi}_1, \boldsymbol{\varpi}_2 \in \mathcal{T}(\Omega)$
- $\mathbf{\Gamma}\big[\mathbf{C} : \mathbf{\Gamma}(\boldsymbol{\varpi})\big] = \mathbf{\Gamma}(\boldsymbol{\varpi})$ for all $\boldsymbol{\varpi} \in \mathcal{T}(\Omega)$

TODO: write proof

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The Lippmann–Schwinger equation (1/2)

Introduce a homogeneous reference material $\mathbf{C}_0$ with Green operator $\mathbf{\Gamma}_0$

Stress-polarization

$$\boldsymbol{\tau} = \boldsymbol{\sigma} - \mathbf{C}_0 : \boldsymbol{\varepsilon} = \left(\mathbf{C} - \mathbf{C}_0\right) : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \quad \Rightarrow \quad \mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} = \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau}$$

Equivalent formulations of the corrector problem

Find $\boldsymbol{\varepsilon} \in \overline{\boldsymbol{\varepsilon}} + \mathcal{E}(\Omega)$ such that $\mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \in \mathcal{S}(\Omega)$

Find $\begin{cases} \boldsymbol{\varepsilon} \in \overline{\boldsymbol{\varepsilon}} + \mathcal{E}(\Omega) \\ \boldsymbol{\tau} \in \mathcal{T}(\Omega) \end{cases}$ such that $\begin{cases} \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau} \in \mathcal{S}(\Omega) \\ \boldsymbol{\tau} = \left(\mathbf{C} - \mathbf{C}_0\right) : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \end{cases}$

Find $\boldsymbol{\varepsilon}, \boldsymbol{\tau} \in \mathcal{T}(\Omega)$ such that $\begin{cases} \boldsymbol{\varepsilon} = \overline{\boldsymbol{\varepsilon}} - \mathbf{\Gamma}_0(\boldsymbol{\tau}) \\ \boldsymbol{\tau} = \left(\mathbf{C} - \mathbf{C}_0\right) : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \end{cases}$

The Lippmann–Schwinger equation (2/2)

Equivalent formulation of the corrector problem

Find $\boldsymbol{\varepsilon}, \boldsymbol{\tau} \in \mathcal{T}(\Omega)$ such that $$\begin{cases} \boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} - \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \\ \boldsymbol{\tau} = \boldsymbol{\sigma} - \mathbf{C}_0 : \boldsymbol{\varepsilon} = \left(\mathbf{C} - \mathbf{C}_0\right) : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \end{cases}$$

Strain-based form of LS equation [1–3]

Find $\boldsymbol{\varepsilon} \in \mathcal{T}(\Omega)$ such that $$\begin{cases} \boldsymbol{\varepsilon} + \boldsymbol{\Gamma}_0(\boldsymbol{\sigma} - \mathbf{C}_0 : \boldsymbol{\varepsilon}) = \bar{\boldsymbol{\varepsilon}} \\ \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \end{cases}$$

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Non-linearities

To be further discussed during the week!

Non-linear elasticity [1]

Find $\boldsymbol{\varepsilon} \in \mathcal{T}(\Omega)$ such that $\begin{cases} \boldsymbol{\varepsilon} + \boldsymbol{\Gamma}_0(\boldsymbol{\sigma} - \mathbf{C}_0 : \boldsymbol{\varepsilon}) = \overline{\boldsymbol{\varepsilon}} \\ \boldsymbol{\sigma} = \mathcal{F}(\boldsymbol{\varepsilon}) \end{cases}$

Generalized standard materials

Use successive linearizations *à la* Newton–Raphson [2]
or **condensed pseudo-potentials** [3, 4]

Geometric non-linearities

Similar formulation with the **F**, **P** (Piola I) pair [5]

[1] H. Moulinec, P. Suquet, *Comptes rendus de l'Académie des sciences. Série II Mécanique physique chimie astronomie* **1994**, *318*, 1417–1423.
[2] L. Gélébart, R. Mondon-Cancel, *Computational Materials Science* **2013**, *77*, 430–439.
[3] N. Lahellec, P. Suquet, *Journal of the Mechanics and Physics of Solids* **2007**, *55*, 1932–1963.
[4] M. Schneider, D. Wicht, T. Böhlke, *Computational Mechanics* **2019**, *64*, 1073–1095.
[5] M. Kabel, T. Böhlke, M. Schneider, *Computational Mechanics* **2014**, *54*, 1497–1514.

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LS as a fixed-point problem

Find $\boldsymbol{\varepsilon} \in \mathcal{T}(\Omega)$ such that $\quad \boldsymbol{\varepsilon} + \boldsymbol{\Gamma}_0\left[\left(\mathbf{C} - \mathbf{C}_0\right) : \boldsymbol{\varepsilon}\right] = \overline{\boldsymbol{\varepsilon}}$

Standard linear problem

$$\left(I + H\right) \cdot x = b \iff x = \left(I - H + H^2 - H^3 + \cdots\right) \cdot b$$
$$= b - H \cdot \left[b - H \cdot \left(b - H \cdots\right)\right]$$

Fixed-point iterations

$$x_0 = b \quad \text{and} \quad x_{n+1} = b - H \cdot x_n$$

Conditional convergence

Converges if $\|H\| < 1$!

The “basic” scheme [1, 2]

Fixed-point iterations for the LS equation

$$\boldsymbol{\varepsilon}_0 = \bar{\boldsymbol{\varepsilon}} \quad \text{and} \quad \begin{cases} \boldsymbol{\sigma}_n = \mathcal{F}(\boldsymbol{\varepsilon}_n) \\ \boldsymbol{\varepsilon}_{n+1} = \bar{\boldsymbol{\varepsilon}} - \boldsymbol{\Gamma}_0\big(\boldsymbol{\sigma}_n - \mathbf{C}_0 : \boldsymbol{\varepsilon}_n\big) \end{cases}$$

Only conditionally convergent! [3, 4]

A classical simplification [1, 2]

$$\boldsymbol{\varepsilon}_0 = \bar{\boldsymbol{\varepsilon}} \quad \text{and} \quad \begin{cases} \boldsymbol{\sigma}_n = \mathcal{F}(\boldsymbol{\varepsilon}_n) \\ \boldsymbol{\varepsilon}_{n+1} = \boldsymbol{\varepsilon}_n - \boldsymbol{\Gamma}_0(\boldsymbol{\sigma}_n) \end{cases}$$

TODO: write proof!

[1] H. Moulinec, P. Suquet, *Comptes rendus de l’Académie des sciences. Série II Mécanique physique chimie astronomie* **1994**, *318*, 1417–1423.

[2] H. Moulinec, P. Suquet, *Computer Methods in Applied Mechanics and Engineering* **1998**, *157*, 69–94.

[3] J. C. Michel, H. Moulinec, P. Suquet, *International Journal for Numerical Methods in Engineering* **2001**, *52*, 139–160.

[4] H. Moulinec, P. Suquet, G. W. Milton, *International Journal for Numerical Methods in Engineering* **2018**, *114*, 1103–1130.

Time to take a step back...

Reference material?

- For the LS equation to be of use, **Γ_0 must be known**
- **Reference material must be homogeneous!** (see next slides)

Solve first, then discretize?

- **In principle**, fixed-point iterations is a viable solution procedure
- **But** unknowns are **fields** that require **spatial discretization**

Discretize first, then solve?

- Spatial discretization (e.g. Galerkin) leads to a linear system [1, 2]
- Use **any** (matrix-free) linear solver [3, 4]
- Allows convergence analysis wrt discretization parameter [1, 2, 5]

[1] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, *217–220*, 197–212.

[2] J. Vondřejc, J. Zeman, I. Marek, *Computers & Mathematics with Applications* **2014**, *68*, 156–173.

[3] J. Zeman et al., *Journal of Computational Physics* **2010**, *229*, 8065–8071.

[4] S. Brisard, L. Dormieux, *Computational Materials Science* **2010**, *49*, 663–671.

[5] M. Schneider, *Mathematical Methods in the Applied Sciences* **2015**, *38*, 2761–2778.

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Fourier series in a nutshell (1/2)

Input data is a periodic function;
output data is an infinite, discrete set of numbers

Multi-indices (tuples)

- $m = (m_1, \dots, m_d), n = (n_1, \dots, n_d)$: frequency indices
- $p = (p_1, \dots, p_d), q = (q_1, \dots, q_d)$: cell indices (pixels, voxels)

Discrete wave vectors over unit-cell $\Omega = (0, L_1) \times \cdots \times (0, L_d)$

$$\mathbf{k}_n = \frac{2\pi n_1}{L_1}\mathbf{e}_1 + \cdots + \frac{2\pi n_d}{L_d}\mathbf{e}_d$$

Fourier coefficients of a periodic function

$$\tilde{f}_n \overset{\text{def}}{=} \frac{1}{|\Omega|}\int_{\mathbf{x}\in\Omega} f(\mathbf{x})\, e^{-i\mathbf{k}_n\cdot\mathbf{x}}\, \mathrm{d}x_1 \dots \mathrm{d}x_d$$

Extends to tensor fields!

Fourier series in a nutshell (2/2)

Basic properties

$$\langle \mathsf{T} \rangle = \tilde{\mathsf{T}}_0 \qquad \widetilde{\mathbf{grad}\,\mathsf{T}}_n = \tilde{\mathsf{T}}_n \otimes i\mathbf{k}_n \qquad \widetilde{\mathbf{div}\,\mathsf{T}}_n = \tilde{\mathsf{T}}_n \cdot i\mathbf{k}_n$$

Inversion (under mild regularity conditions)

$$f(\mathbf{x}) = \sum_{n \in \mathbb{Z}^d} \tilde{f}_n \, e^{i\mathbf{k}_n \cdot \mathbf{x}}$$

Plancherel theorem and Parseval's identity

$$\langle f^* \, g \rangle = \sum_{n \in \mathbb{Z}^d} \tilde{f}_n^* \, \tilde{g}_n \qquad \langle |f|^2 \rangle = \sum_{n \in \mathbb{Z}^d} |\tilde{f}_n|^2$$

Circular convolution theorem

$$\widetilde{f \star g}_n = \tilde{f}_n \, \tilde{g}_n \quad \text{with} \quad f \star g(\mathbf{x}) \overset{\text{def}}{=} \frac{1}{|\Omega|} \int_{\mathbf{y} \in \Omega} f(\mathbf{x} - \mathbf{y}) \, g(\mathbf{y}) \, \mathrm{d}y_1 \ldots \mathrm{d}y_d$$

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What should we expect?

Γ_0 is a translation-invariant, linear operator

Integral representation of the Γ_0 linear operator

$$\boldsymbol{\varepsilon} = -\boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \qquad \boldsymbol{\varepsilon}(\mathbf{x}) = -\frac{1}{|\Omega|}\int_\Omega \mathbf{Q}_0(\mathbf{x}, \mathbf{y}) : \boldsymbol{\tau}(\mathbf{y})\,\mathrm{d}y_1 \ldots \mathrm{d}y_d$$

Translation invariance

$$\boldsymbol{\varepsilon}(\mathbf{x}) = -\frac{1}{|\Omega|}\int_\Omega \mathbf{Q}_0(\mathbf{x} - \mathbf{y}) : \boldsymbol{\tau}(\mathbf{y})\,\mathrm{d}y_1 \ldots \mathrm{d}y_d$$

Circular convolution theorem

$$\tilde{\boldsymbol{\varepsilon}}_n = -\tilde{\mathbf{Q}}_{0,n} : \tilde{\boldsymbol{\tau}}_n$$

Note

$$\tilde{\boldsymbol{\varepsilon}}_0 = \mathbf{0} \quad \text{since} \quad \langle \boldsymbol{\varepsilon} \rangle = \mathbf{0}$$

Fourier expansion of Green operator (1/3)

Use Fourier expansions of all mechanical fields

$$\begin{Bmatrix} \mathbf{u}(\mathbf{x}) \\ \boldsymbol{\varepsilon}(\mathbf{x}) \\ \boldsymbol{\sigma}(\mathbf{x}) \\ \boldsymbol{\tau}(\mathbf{x}) \end{Bmatrix} = \sum_{n \in \mathbb{Z}^d} \begin{Bmatrix} \tilde{\mathbf{u}}_n \\ \tilde{\boldsymbol{\varepsilon}}_n \\ \tilde{\boldsymbol{\sigma}}_n \\ \tilde{\boldsymbol{\tau}}_n \end{Bmatrix} e^{i\mathbf{k}_n \cdot \mathbf{x}}$$

Fourier coefficients of the Green operator

$$\tilde{\boldsymbol{\varepsilon}}_n = -\hat{\boldsymbol{\Gamma}}_0^\infty(\mathbf{k}_n) : \tilde{\boldsymbol{\tau}}_n \quad \text{with} \quad \hat{\boldsymbol{\Gamma}}_0^\infty(\mathbf{k}) = \mathbf{I} : \left[\mathbf{k} \otimes \left(\mathbf{k} \cdot \mathbf{C}_0 \cdot \mathbf{k}\right)^{-1} \otimes \mathbf{k}\right] : \mathbf{I}$$

$$I_{ijkl} = \tfrac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)$$

$\hat{\boldsymbol{\Gamma}}_0^\infty(\mathbf{k})$ does not depend on $\|\mathbf{k}\|$!

Fourier expansion of Green operator (2/3)

Rewrite BVP in Fourier space

$$\operatorname{div}\boldsymbol{\sigma} = \mathbf{0} \longrightarrow \tilde{\boldsymbol{\sigma}}_n \cdot i\mathbf{k}_n = \mathbf{0} \tag{1}$$

$$\boldsymbol{\sigma} = \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau} \longrightarrow \tilde{\boldsymbol{\sigma}}_n = \mathbf{C}_0 : \tilde{\boldsymbol{\varepsilon}}_n + \tilde{\boldsymbol{\tau}}_n \tag{2}$$

$$\boldsymbol{\varepsilon} = \operatorname{sym}\operatorname{grad}\mathbf{u} \longrightarrow \tilde{\boldsymbol{\varepsilon}}_n = \operatorname{sym}(\tilde{\mathbf{u}}_n \otimes i\mathbf{k}_n) \tag{3}$$

($\mathbf{C}_0 =$ const. is crucial!)

Combine (2) and (3)

$$\left.\begin{aligned}\tilde{\boldsymbol{\sigma}}_n &= \mathbf{C}_0 : \tilde{\boldsymbol{\varepsilon}}_n + \tilde{\boldsymbol{\tau}}_n \\ \tilde{\boldsymbol{\varepsilon}}_n &= \operatorname{sym}(\tilde{\mathbf{u}}_n \otimes i\mathbf{k}_n)\end{aligned}\right\} \Rightarrow \tilde{\boldsymbol{\sigma}}_n = \left(\mathbf{C}_0 \cdot i\mathbf{k}_n\right) \cdot \tilde{\mathbf{u}}_n + \tilde{\boldsymbol{\tau}}_n$$

Plug into (1)

$$\tilde{\boldsymbol{\sigma}}_n \cdot i\mathbf{k}_n = \mathbf{0} \Rightarrow \left(\mathbf{k}_n \cdot \mathbf{C}_0 \cdot \mathbf{k}_n\right) \cdot \tilde{\mathbf{u}}_n = i\tilde{\boldsymbol{\tau}}_n \cdot \mathbf{k}_n$$

Fourier expansion of Green operator (3/3)

General expression of displacement

$$\begin{aligned}\tilde{\mathbf{u}}_n &= i\left(\mathbf{k}_n\cdot\mathsf{C}_0\cdot\mathbf{k}_n\right)^{-1}\cdot\tilde{\boldsymbol{\tau}}_n\cdot\mathbf{k}_n\\ &= i\left[\left(\mathbf{k}_n\cdot\mathsf{C}_0\cdot\mathbf{k}_n\right)^{-1}\otimes\mathbf{k}_n\right]:\tilde{\boldsymbol{\tau}}_n\\ &= i\left[\left(\mathbf{k}_n\cdot\mathsf{C}_0\cdot\mathbf{k}_n\right)^{-1}\otimes\mathbf{k}_n\right]:\left(\mathsf{I}:\tilde{\boldsymbol{\tau}}_n\right)\\ &= i\left\{\left[\left(\mathbf{k}_n\cdot\mathsf{C}_0\cdot\mathbf{k}_n\right)^{-1}\otimes\mathbf{k}_n\right]:\mathsf{I}\right\}:\tilde{\boldsymbol{\tau}}_n\end{aligned}$$

General expression of strain

$$\tilde{\boldsymbol{\varepsilon}}_n = \mathbf{sym}\left(i\mathbf{k}_n\otimes\tilde{\mathbf{u}}_n\right) = \mathsf{I}:\left(i\mathbf{k}_n\otimes\tilde{\mathbf{u}}_n\right) = -\hat{\mathsf{\Gamma}}_0^\infty(\mathbf{k}_n):\tilde{\boldsymbol{\tau}}_n$$

with

$$\hat{\mathsf{\Gamma}}_0^\infty(\mathbf{k}) = \mathsf{I}:\left[\mathbf{k}\otimes\left(\mathbf{k}\cdot\mathsf{C}_0\cdot\mathbf{k}\right)^{-1}\otimes\mathbf{k}\right]:\mathsf{I}$$

Isotropic reference material

$$\mathbf{C}_0 = 2\mu_0\left(\frac{1+\nu_0}{1-2\nu_0}\mathbf{J}+\mathbf{K}\right) \qquad \mathbf{J} = \tfrac{1}{3}\boldsymbol{\delta}\otimes\boldsymbol{\delta} \qquad \mathbf{K} = \mathbf{I}-\mathbf{J}$$

$$\|\mathbf{t}\| = 1: \quad \mathbf{t}\cdot\mathbf{C}_0\cdot\mathbf{t} = \mu_0\left(\boldsymbol{\delta}+\frac{1}{1-2\nu_0}\mathbf{t}\otimes\mathbf{t}\right)$$

$$\left(\mathbf{t}\cdot\mathbf{C}_0\cdot\mathbf{t}\right)^{-1} = \frac{1}{\mu_0}\left[\boldsymbol{\delta}-\frac{1}{2\left(1-\nu_0\right)}\mathbf{t}\otimes\mathbf{t}\right]$$

Remember that $\mathbf{p} = \mathbf{t}\otimes\mathbf{t}$ and $\mathbf{q} = \boldsymbol{\delta}-\mathbf{t}\otimes\mathbf{t}$ are orthogonal projectors

$$\mathbf{p}:\mathbf{p} = \mathbf{p} \qquad \mathbf{q}:\mathbf{q} = \mathbf{q} \qquad \mathbf{p}:\mathbf{q} = \mathbf{q}:\mathbf{p} = \mathbf{0}$$

$$\begin{cases} \hat{\Gamma}^{\infty}_{0,ijhl}(\mathbf{k}) = \dfrac{\delta_{ih}t_jt_l+\delta_{il}t_jt_h+\delta_{jh}t_it_l+\delta_{jl}t_it_h}{4\mu_0}-\dfrac{t_it_jt_ht_l}{2\mu_0\left(1-\nu_0\right)} \\ \mathbf{t} = \mathbf{k}/\|\mathbf{k}\| \end{cases}$$

Applies to 3D and plane strain elasticity!

The Green operator in the real space

Integral expression of the Green operator

$$\boldsymbol{\varepsilon} = -\boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \qquad \boldsymbol{\varepsilon}(\mathbf{x}) = -\frac{1}{|\Omega|}\int_\Omega \mathbf{Q}_0(\mathbf{x}-\mathbf{y}) : \boldsymbol{\tau}(\mathbf{y})\,\mathrm{d}y_1 \ldots \mathrm{d}y_d$$

Formal expression using Fourier series

$$\mathbf{Q}_0(\mathbf{r}) = \sum_{n\in\mathbb{Z}^d} \underbrace{\left\{\mathbf{I} : \left[\mathbf{k}_n \otimes \left(\mathbf{k}_n \cdot \mathbf{C}_0 \cdot \mathbf{k}_n\right)^{-1} \otimes \mathbf{k}_n\right] : \mathbf{I}\right\}}_{\hat{\boldsymbol{\Gamma}}_0^\infty(\mathbf{k}_n)} e^{i\mathbf{k}_n\cdot\mathbf{r}}$$

Formal expression using Poisson summation formula [1]

$$\mathbf{Q}_0(\mathbf{r}) = \sum_{n\in\mathbb{Z}^d} \boldsymbol{\Gamma}_0^\infty(\mathbf{r} + n_1 L_1 \mathbf{e}_1 + \cdots + n_d L_d \mathbf{e}_d)$$

Non convergent series – Use at your own risk!

[1] M. Zecevic, R. A. Lebensohn, *International Journal for Numerical Methods in Engineering* **2021**, *122*, 7536–7552.

Conclusion

Summary of Lecture 1

- The "corrector" problem
- Formal definition of the Green operator
- The Lippmann–Schwinger (LS) equation
- The "basic scheme" and the need for spatial discretization
- Derivation of the Green operator

In Lecture 2

Consistent Galerkin discretization of the LS equation

Thank you for your attention!

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https://cv.archives-ouvertes.fr/sbrisard
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