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

LABORATOIRE NAVIER

Asymptotically consistent discretizations of the LS equation

Sébastien Brisard

Laboratoire Navier, École des Ponts, Univ. Gustave Eiffel, CNRS, Marne-la-Vallée, France

Université franco-allemande Deutsch-Französische Hochschule

École des Ponts ParisTech

Université Gustave Eiffel

cnrs

In the previous episode…

The discretized LS equation

$$\left(\mathbf{C}^N - \mathbf{C}_0\right)^{-1} : \boldsymbol{\tau}^N + \boldsymbol{\Gamma}_0^N(\boldsymbol{\tau}^N) = \bar{\boldsymbol{\varepsilon}}^N$$

Exact discretization of the operators

$$\bar{\boldsymbol{\varepsilon}}_p^N = \bar{\boldsymbol{\varepsilon}} + \langle\left(\mathbf{C} - \mathbf{C}_0\right)^{-1} : \boldsymbol{\varpi}\rangle_p \qquad \boldsymbol{\Gamma}_0^N(\boldsymbol{\tau}^N) = \mathrm{DFT}^{-1}\left[\hat{\boldsymbol{\Gamma}}_0^N : \mathrm{DFT}(\boldsymbol{\tau}^N)\right]$$

$$\mathbf{C}_p^N = \mathbf{C}_0 + \left[\langle\left(\mathbf{C} - \mathbf{C}_0\right)^{-1}\rangle_p\right]^{-1} \qquad \hat{\boldsymbol{\Gamma}}_{0,n}^N = \sum_{m\in\mathbb{Z}^d} \left(W_{n+mN}^N\right)^2 \hat{\boldsymbol{\Gamma}}_0^\infty(\mathbf{k}_{n+mN})$$

$$\mathbf{k}_n = \frac{2\pi n_1}{L_1}\mathbf{e}_1 + \cdots + \frac{2\pi n_d}{L_d}\mathbf{e}_d \qquad W_n^N = \mathrm{sinc}\,\frac{\pi n_1}{N_1} \cdots \mathrm{sinc}\,\frac{\pi n_d}{N_d}$$

Outline of Lecture 3

- Consistent discretization… so what?
- On asymptotically consistent discretizations
- Asymptotically consistent discretizations of the microstructure
- Asymptotically consistent discretizations of the Green operator
- Comparison of some discretizations

Outline of Lecture 3

- Consistent discretization… so what?
- On asymptotically consistent discretizations
- Asymptotically consistent discretizations of the microstructure
- Asymptotically consistent discretizations of the Green operator
- Comparison of some discretizations

Consistent discretization… so what? (1/2)

Consistent equivalent stiffness of heterogeneous cells

$$\mathbf{C}_p^N = \mathbf{C}_0 + \left[\langle \left(\mathbf{C} - \mathbf{C}_0\right)^{-1} \rangle_p\right]^{-1}$$

"The Brisard–Dormieux mixing rule is necessary to ensure that the computed effective properties constitute a bound on the effective stiffness [1], and thus tend to increase the error."

Kabel, Merkert, and Schneider [2]

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

[2] M. Kabel, D. Merkert, M. Schneider, *Computer Methods in Applied Mechanics and Engineering* **2015**, *294*, 168–188.

Consistent discretization… so what? (2/2)

Consistent discrete Green operator

$$\hat{\boldsymbol{\Gamma}}^N_{0,n} = \sum_{m \in \mathbb{Z}^d} \left(W^N_{n+mN}\right)^2 \hat{\boldsymbol{\Gamma}}^\infty_0(\mathbf{k}_{n+mN})$$

$$\mathbf{k}_n = \frac{2\pi n_1}{L_1}\mathbf{e}_1 + \cdots + \frac{2\pi n_d}{L_d}\mathbf{e}_d \qquad W^N_n = \operatorname{sinc}\frac{\pi n_1}{N_1} \cdots \operatorname{sinc}\frac{\pi n_d}{N_d}$$

"The second disadvantage of the discretization concerns the practical computation of the operator $\boldsymbol{\Gamma}^N_0$. Although explicit expressions for the Fourier coefficients of the operator $\boldsymbol{\Gamma}^N_0$ are available, **the involved series converges rather slowly** in three spatial dimensions [1]."

Schneider [2]

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

[2] M. Schneider, *Acta Mechanica* **2021**, *232*, 2051–2100.

These are fair comments!

Looking back at the history

- "FFT-based methods" [1, 2] predate the Galerkin setting [3]!
- It all started with the derivation of rigorous **bounds** [4, 5]
- "What if the reference material is not stiffer or softer than all phases?"
- The Galerkin setting allowed to prove convergence (w.r.t. grid-size) for **any** reference material!
- General setting can be extended to **any** flavour of "FFT-based method": asymptotically consistent discretizations [6]

[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] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, *217–220*, 197–212.
[4] Z. Hashin, S. Shtrikman, *Journal of the Mechanics and Physics of Solids* **1962**, *10*, 335–342.
[5] S. Brisard, L. Dormieux, *Computational Materials Science* **2010**, *49*, 663–671.
[6] A. Ern, J.-L. Guermond, *Theory and Practice of Finite Elements*, Springer-Verlag, New York, **2004**.

Outline of Lecture 3

- Consistent discretization… so what?
- On asymptotically consistent discretizations
- Asymptotically consistent discretizations of the microstructure
- Asymptotically consistent discretizations of the Green operator
- Comparison of some discretizations

What is a variational crime?

The initial problem

Find $u \in V$ such that, for all $v \in V$: $\quad a(u,v) = \ell(v)$

Exhaustive exploration of V is not possible!

Consistent discretization

Find $u^h \in V^h$ such that, for all $v^h \in V^h$: $\quad a(u^h,v^h) = \ell(v^h)$

$V^h \subset V$ and $\dim V^h < \infty$: exhaustive exploration is possible!
Exact evaluation of the bilinear and linear forms!

Asymptotically consistent discretization

Find $u^h \in V^h$ such that, for all $v^h \in V^h$: $\quad a^h(u^h,v^h) = \ell^h(v^h)$

Approximations of linear and bilinear forms must be asymptotically consistent [1]

[1] A. Ern, J.-L. Guermond, *Theory and Practice of Finite Elements*, Springer-Verlag, New York, **2004**.

We are all criminals

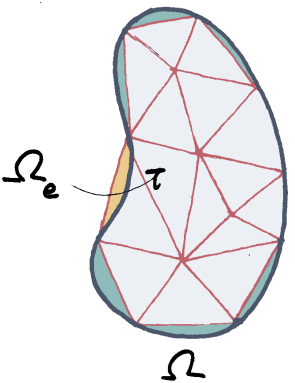
Examples of variational crimes (FEM)

- The bilinear form

$$a(\mathbf{u}, \mathbf{v}) = \int_{\Omega} \boldsymbol{\epsilon}(\mathbf{u}) : \mathbf{C} : \boldsymbol{\epsilon}(\mathbf{v})$$

- Geometry

$$\bigcup_e \Omega_e \neq \Omega$$



- Quadrature

$$\int_{\Omega_e} \boldsymbol{\epsilon}(\mathbf{u}) : \mathbf{C} : \boldsymbol{\epsilon}(\mathbf{v}) \simeq \sum_g w_g \, \boldsymbol{\epsilon}(\mathbf{u})(\mathbf{x}_g) : \mathbf{C}(\mathbf{x}_g) : \boldsymbol{\epsilon}(\mathbf{v})(\mathbf{x}_g)$$

Non-consistent vs. asymptotically consistent discretizations

- Additional error induced by lack of consistency must be of the same order as the inherent discretization error!
- See ref. [1] for a mathematical definition!
- Owing to the framework set in ref. [2], asymptotic consistency is the most important property you need to ensure to prove convergence (wrt grid-size) of your new fancy discretization scheme!

[1] A. Ern, J.-L. Guermond, *Theory and Practice of Finite Elements*, Springer-Verlag, New York, **2004**.

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

Outline of Lecture 3

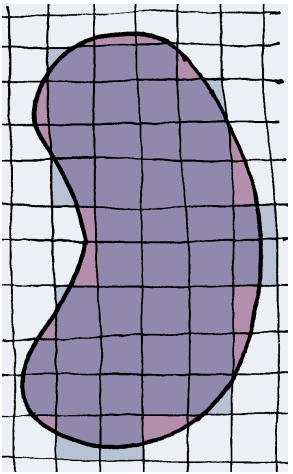
- Consistent discretization… so what?
- On asymptotically consistent discretizations
- Asymptotically consistent discretizations of the microstructure
- Asymptotically consistent discretizations of the Green operator
- Comparison of some discretizations

Handling heterogeneous cells (1/2)

Consistent mixing rule [1, 2]

$$\mathbf{C}_p^N = \mathbf{C}_0 + \left[\langle(\mathbf{C} - \mathbf{C}_0)^{-1}\rangle_p\right]^{-1}$$

This rule is sub-optimal! [3]



Alternative, non-consistent rules

- "Black-or-white"

$$\mathbf{C}_p^N = \mathbf{C}(\mathbf{x}_p) = \text{stiffness at cell center}$$

- Voigt, Reuss [4, 3]

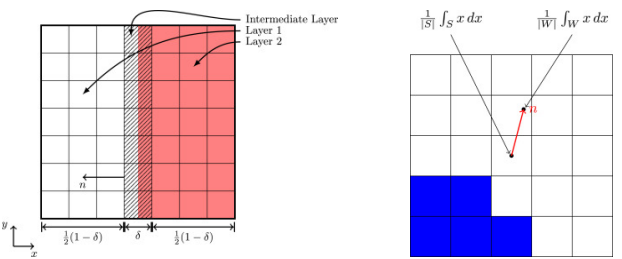
These rule omit information on local orientation of the interface!

[1] S. Brisard, L. Dormieux, *Computational Materials Science* **2010**, *49*, 663–671.
[2] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, *217–220*, 197–212.
[3] M. Kabel, D. Merkert, M. Schneider, *Computer Methods in Applied Mechanics and Engineering* **2015**, *294*, 168–188.
[4] J. Sanahuja, C. Toulemonde, *Cement and Concrete Research* **2011**, *41*, 1320–1329.

Handling heterogeneous cells (2/2)

Laminate approximation [1]

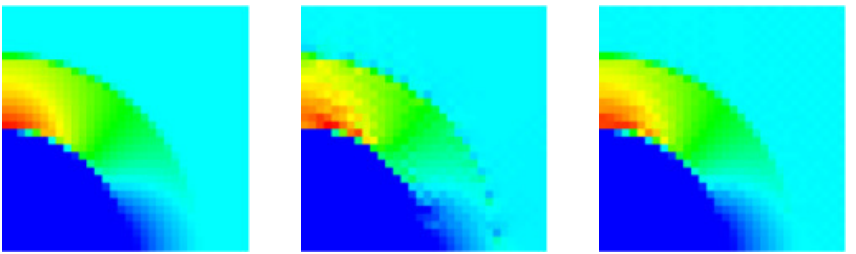
- Require sub-voxel microstructural information
- Approximate local normal
- Note: slightly different definition of consistency in this paper



Reproduced from [1]

[1] M. Kabel, D. Merkert, M. Schneider, *Computer Methods in Applied Mechanics and Engineering* **2015**, *294*, 168–188.

Mixing rules in action

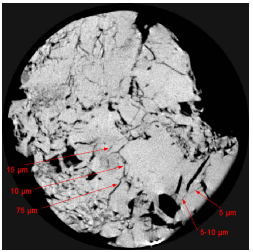


Analytical solution (left), black-or-white rule (middle), laminate rule (right) — Reproduced from [1]

[1] M. Kabel, D. Merkert, M. Schneider, *Computer Methods in Applied Mechanics and Engineering* **2015**, *294*, 168–188.

On the partial volume effect

100 µm slice through fractured limestone from the lower Ismay member of the Paradox Formation. Scan field of view is 21.5 mm, and individual pixels are 42 µm on a side. After scanning the entire volume, the sample was cut and fractures were measured in thin section. Fractures are visible despite being considerably thinner than the pixel width, because of partial volume effects. Sample and measurements courtesy of Dr. Brenda Kirkland, University of Texas at Austin.



(Reproduced from https://www.ctlab.geo.utexas.edu/about-ct/artifacts-and-partial-volume-effects/)

"Gray" voxels, even in two-phase (black and white) materials!
Mechanical properties?

Assigning stiffness to gray voxels

- Requires chemical composition (ill-posed problem) [1]
- Use mixing rule based on volume fraction only?
- Normal from neighbouring voxels?

[1] S. Scheiner et al., *Biomaterials* **2009**, *30*, 2411–2419.

Outline of Lecture 3

- Consistent discretization… so what?
- On asymptotically consistent discretizations
- Asymptotically consistent discretizations of the microstructure
- Asymptotically consistent discretizations of the Green operator
- Comparison of some discretizations

The need for non-consistent discrete Green operators

The consistent discrete Green operator

$$\hat{\boldsymbol{\Gamma}}^N_{0,n} = \sum_{m\in\mathbb{Z}^d} \left(W^N_{n+mN}\right)^2 \hat{\boldsymbol{\Gamma}}^\infty_0(\mathbf{k}_{n+mN}) \quad \text{with} \quad W^N_n = \operatorname{sinc}\frac{\pi n_1}{N_1}\cdots\operatorname{sinc}\frac{\pi n_d}{N_d}$$

Very slow convergence!

Non-consistent discrete Green operators

- "Approximate" in some sense the consistent operator
- Must be computed efficiently
- Keep the nice, block-diagonal structure!

$$\boldsymbol{\Gamma}^{N,\mathrm{nc}}_0(\boldsymbol{\tau}^N) = \mathrm{DFT}^{-1}\left[\hat{\boldsymbol{\Gamma}}^{N,\mathrm{nc}}_0 : \mathrm{DFT}(\boldsymbol{\tau}^N)\right]$$

A classical (though not too deep) trap…
…most of my students fall into!

When the spatial resolution is low and when the number N_j of discretization point is even, a special attention must be paid to the highest frequencies

$$\xi_j = \pm\left(\frac{N_j}{2} - 1\right)\frac{1}{T_j}, \quad j = 1 \text{ or } 2 .$$

In most FFT packages, the Fourier expansion at these frequencies consists of either $\cos(\xi_j x_j)$ or $\exp(-\mathrm{i}\xi_j x_j)$, instead of the correct expression consisting of the two terms $\exp(-\mathrm{i}\xi_j x_j)$ and $\exp(\mathrm{i}\xi_j x_j)$. Therefore, even when the stress $\boldsymbol{\sigma}$ is correctly approached by its Fourier expansion in step a) of the algorithm (10), the result of step d) may not approach accurately the Fourier expansion of the strain $\boldsymbol{\varepsilon}$ at these particular frequencies. This is because $\hat{\boldsymbol{F}}^0$ is neither even nor odd with respect to each individual component ξ_j. Oscillations were observed when (4) was used with relatively small values of N_j (lower than 128). This problem was fixed by using a different expression of $\hat{\boldsymbol{F}}^0$ in algorithm (10) at these frequencies.

$$\hat{\boldsymbol{F}}^0 = (\boldsymbol{c}^0)^{-1} .$$

In other terms, the stress $\boldsymbol{\sigma}$ is forced to $\mathbf{0}$ by the algorithm at these frequencies when convergence is reached.

Reproduced from Ref. [1]

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

The classical trap continued

DFT of a series of real numbers

$$\hat{x}_n = \hat{x}^*_{N-n}$$

Symmetry property of discrete Green operators

Discrete Green operators must map real fields onto real fields

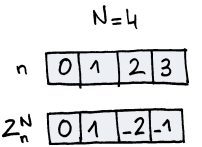
$$\hat{\Gamma}^{N,\mathrm{nc}}_{0,n} = \hat{\Gamma}^{N,\mathrm{nc},*}_{0,N-n}$$

The consistent discrete Green operator has this property by construction!

The "fftfreq" function

Definition

$$Z_n^N = \begin{cases} n & \text{if } 2n < N \\ n - N & \text{if } 2n \geq N \end{cases}$$



Important property

$$Z_{N-n}^N = \begin{cases} -Z_n^N & \text{if } 2n \neq N \\ Z_n^N & \text{if } 2n = N \end{cases}$$

$$Z_{N-n,N} = \begin{cases} N-n & \text{if } 2(N-n) < N \\ N-n-N & \text{if } 2(N-n) \geq N \end{cases} = \begin{cases} N-n & \text{if } 2n > N \\ -n & \text{if } 2n \leq N \end{cases} = \begin{cases} -n & \text{if } 2n > N \\ -n & \text{if } 2n = N \\ -(n-N) & \text{if } 2n > N \end{cases}$$

Extension to tuples

$$N = (N_1, \ldots, N_d) \text{ and } n = (n_1, \ldots, n_d): \quad Z_n^N = \left(Z_{n_1}^{N_1}, \ldots, Z_{n_d}^{N_d}\right)$$

Truncating high frequencies

The original discretization of Moulinec and Suquet [1, 2]

$$\hat{\boldsymbol{\Gamma}}^{N,\mathrm{MS}}_{0,n} \overset{\text{def}}{=} \hat{\boldsymbol{\Gamma}}^{\infty}_{0}(\mathbf{k}_{Z^N_n})$$

Symmetry property?

- If none of the n_i is equal to $2N_i$

$$\hat{\boldsymbol{\Gamma}}^{N,\mathrm{MS}}_{0,N-n} = \hat{\boldsymbol{\Gamma}}^{\infty}_{0}(\mathbf{k}_{Z^N_{N-n}}) = \hat{\boldsymbol{\Gamma}}^{\infty}_{0}(\mathbf{k}_{-Z^N_n}) = \hat{\boldsymbol{\Gamma}}^{\infty}_{0}(\mathbf{k}_{-Z^N_n}) = \hat{\boldsymbol{\Gamma}}^{N,\mathrm{MS}}_{0,n}$$

- If all the n_i are equal to $2N_i$, then

$$\hat{\boldsymbol{\Gamma}}^{N,\mathrm{MS}}_{0,N-n} = \hat{\boldsymbol{\Gamma}}^{N,\mathrm{MS}}_{0,n}$$

- If some (but not all) of the n_i are equal to $2N_i$, then we are in trouble

$$\hat{\boldsymbol{\Gamma}}^{N,\mathrm{MS}}_{0,n} = \mathbf{C}_0^{-1} \quad \text{or} \quad \hat{\boldsymbol{\Gamma}}^{N,\mathrm{MS}}_{0,n} = \mathbf{0}$$

[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.

Smoothly filtering out high frequencies

Using a "cosine window" [1]

$$\hat{\mathbf{\Gamma}}_{0,n}^{N,\mathrm{BD}} = \sum_{m\in\{-1,0\}^d} \left(C_{n+mN}^N\right)^2 \hat{\mathbf{\Gamma}}_0^\infty(\mathbf{k}_{n+mN}) \quad \text{with} \quad C_n^N = \cos\frac{\pi n_1}{2N_1}\cdots\cos\frac{\pi n_d}{2N_d}$$

Symmetry property?

Yes!

Connection with band-limited discretizations

- A radically different approach
- Discretization in the Fourier space rather than the real space
- See e.g. refs [2–4]

[1] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, *217–220*, 197–212.
[2] J. Zeman et al., *Journal of Computational Physics* **2010**, *229*, 8065–8071.
[3] J. Vondřejc, J. Zeman, I. Marek, *Computers & Mathematics with Applications* **2014**, *68*, 156–173.
[4] J. Vondřejc, J. Zeman, I. Marek, *Computer Methods in Applied Mechanics and Engineering* **2015**, *297*, 258–291.

Discretization in the real space

Remember definition of discrete Green operator

$$\boldsymbol{\tau}^N \in \mathcal{T}^N(\Omega) \mapsto \boldsymbol{\eta}^N = \boldsymbol{\Gamma}_0^N(\boldsymbol{\tau}^N) \in \mathcal{T}^N(\Omega) \quad \text{such that} \quad \boldsymbol{\eta}_p^N = \langle \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^N) \rangle_p$$

$\boldsymbol{\eta}^N$ is the cell-average of $\boldsymbol{\eta} = \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^N)$,
which itself solves an elasticity problem

The discrete Green operator as the solution to a BVP

$$\begin{cases} \mathbf{div}\,\boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma} = \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau}^N \\ \boldsymbol{\varepsilon} = \mathbf{sym}\,\mathbf{grad}\,\mathbf{u} \\ \mathbf{u} \text{ is } \Omega\text{-periodic!} \end{cases}$$

Discretize this problem and derive explicit solution
that defines a discrete Green operator.

Finite differences and DFT (1/2)

The 1d case, forward differences

$(x_p)_{0\le p<N}$ is given: $\Delta^+ x_p = x_{p+1} - x_p$

$$\widehat{\Delta^+ x}_n = \sum_p x_{p+1} \exp\left(-2i\pi np/N\right) - \hat{x}_n$$

$$= \sum_p x_p \exp\left[-2i\pi n\left(p-1\right)/N\right] - \hat{x}_n$$

$$= \exp\left(2i\pi n/N\right) \underbrace{\sum_p x_p \exp\left(-2i\pi np/N\right)}_{\hat{x}_n} - \hat{x}_n$$

$$= \left[\exp\left(2i\pi n/N\right) - 1\right]\hat{x}_n$$

$$= 2i \sin\left(\pi n/N\right) \exp\left(i\pi n/N\right)\hat{x}_n$$

Finite differences and DFT (2/2)

The 1d case, forward differences

$$\widehat{\Delta^{+}x}_n = 2i \sin(\pi n/N) \exp(i\pi n/N)\hat{x}_n$$

The 1d case, backward differences

$$\widehat{\Delta^{-}x}_n = 2i \sin(\pi n/N) \exp(-i\pi n/N)\hat{x}_n$$

The multi-dimensional case

$$\widehat{\Delta_i^{+}x}_n = 2i \sin(\pi n_i/N_i) \exp(i\pi n_i/N_i)\hat{x}_n$$
$$\widehat{\Delta_i^{-}x}_n = 2i \sin(\pi n_i/N_i) \exp(-i\pi n_i/N_i)\hat{x}_n$$

The seminal work of Willot & Pellegrini [1]

Forward differences for gradients, backwards differences for divergences

$$\begin{cases} \operatorname{div}\boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma} = \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau}^N \\ \boldsymbol{\varepsilon} = \mathbf{sym\,grad\,u} \end{cases} \longrightarrow \begin{cases} \hat{\boldsymbol{\sigma}}_n^N \cdot i\mathbf{b}_n^{N,*} = \mathbf{0} \\ \hat{\boldsymbol{\sigma}}_n^N = \mathbf{C}_0 : \hat{\boldsymbol{\varepsilon}}_n^N + \hat{\boldsymbol{\tau}}_n^N \\ \hat{\boldsymbol{\varepsilon}}_n^N = \frac{1}{2}\left[\hat{\mathbf{u}}_n^N \otimes \left(i\mathbf{b}_n^N\right) + \left(i\mathbf{b}_n^N\right) \otimes \hat{\mathbf{u}}_n^N\right] \end{cases}$$

$$\mathbf{b}_n^N = 2\sin\frac{\pi n_1}{N_1}\exp\frac{i\pi n_1}{N_1}\mathbf{e}_1 + \cdots + 2\sin\frac{\pi n_d}{N_d}\exp\frac{i\pi n_d}{N_d}\mathbf{e}_d$$

see Lecture 1

$$\hat{\boldsymbol{\varepsilon}}_n^N = -\hat{\boldsymbol{\Gamma}}_{0,n}^{N,\mathrm{WP08}} : \hat{\boldsymbol{\tau}} \qquad \hat{\boldsymbol{\Gamma}}_{0,n}^{N,\mathrm{WP08}} = \mathbf{I} : \left[\mathbf{b}_n^N \otimes \left(\mathbf{b}_n^{N,*} \cdot \mathbf{C}_0 \cdot \mathbf{b}_n^N\right)^{-1} \otimes \mathbf{b}_n^{N,*}\right] : \mathbf{I}$$

[1] F. Willot, Y.-P. Pellegrini, Fast Fourier Transform Computations and Build-up of Plastic Deformation in 2D, Elastic-Perfectly Plastic, Pixelwise Disordered Porous Media, arXiv e-print 0802.2488, **2008**.

More sophisticated FD schemes (1/2)

"Rotated grids" [1]

$$\hat{\boldsymbol{\Gamma}}^{N,\mathrm{Wil15}}_{0,n} = \hat{\boldsymbol{\Gamma}}^{\infty}_{0}(\mathbf{b}^N_n) \qquad \mathbf{b}^N_n = \frac{2N_1}{L_1}\tan\frac{\pi n_1}{N_1}\mathbf{e}_1 + \cdots + \frac{2N_d}{L_d}\tan\frac{\pi n_d}{N_d}\mathbf{e}_d$$

(proof of this operational formula can be found in ref. [2])

In the rest of this section, we derive a discrete scheme in 2D different from (22) and (23). In this scheme, the displacement field is evaluated at the 4 corners of the pixels and the strain and stress fields are evaluated at the centers of the pixels. We first express these fields in the 45°-rotated basis:

$$\mathbf{f}_1 = \frac{\mathbf{e}_1+\mathbf{e}_2}{\sqrt{2}}, \qquad \mathbf{f}_2 = \frac{\mathbf{e}_2-\mathbf{e}_1}{\sqrt{2}} \tag{30}$$

by:

$$u_i = R_{il}u_i, \qquad \varepsilon_{ij} = R_{il}\varepsilon_{IJ}R'_{jJ}, \qquad \sigma_{ij} = R_{il}\sigma_{IJ}R'_{jJ}, \qquad R_{iJ} = \frac{1-2\delta_{i1}\delta_{J2}}{\sqrt{2}} \tag{31}$$

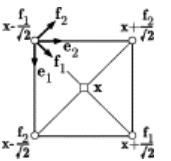
where uppercase indices refer to components in the rotated grid. We discretize (1) in the rotated basis by the centered differences (see Fig. 1):

$$\sigma_{IJ}(\boldsymbol{x}) = C_{IJ,KL}(\boldsymbol{x})\varepsilon_{KL}(\boldsymbol{x}) \tag{32a}$$

$$\sigma_{I1}(\boldsymbol{x}-\sqrt{2}\mathbf{f}_1) + \sigma_{I2}\left(\boldsymbol{x}+\frac{\mathbf{f}_2-\mathbf{f}_1}{\sqrt{2}}\right) - \sigma_{I2}\left(\boldsymbol{x}-\frac{\mathbf{f}_1+\mathbf{f}_2}{\sqrt{2}}\right) = 0 \tag{32b}$$

$$\varepsilon_{KL}(\boldsymbol{x}) = \frac{1}{2\sqrt{2}}\left[u_K\left(\boldsymbol{x}+\frac{\mathbf{f}_L}{\sqrt{2}}\right) - u_K\left(\boldsymbol{x}-\frac{\mathbf{f}_L}{\sqrt{2}}\right) + u_L\left(\boldsymbol{x}+\frac{\mathbf{f}_K}{\sqrt{2}}\right) - u_L\left(\boldsymbol{x}-\frac{\mathbf{f}_K}{\sqrt{2}}\right)\right] \tag{32c}$$

where $\boldsymbol{x}$ lie at the centers of the pixels and $\boldsymbol{x} \pm \mathbf{f}_i/\sqrt{2}$ lie at the corners.



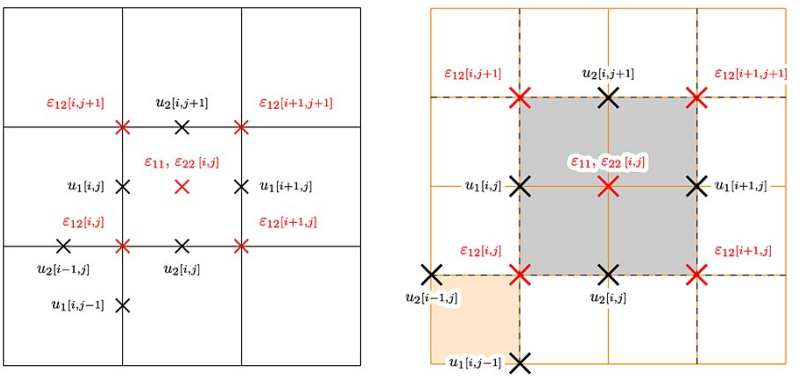
(reproduced from ref. [1])

[1] F. Willot, *Comptes Rendus Mécanique* **2015**, *343*, 232–245.

[2] S. Brisard, *International Journal for Numerical Methods in Engineering* **2017**, *109*, 459–486.

More sophisticated FD schemes (2/2)

Staggered grids [1]



(reproduced from ref. [1])

[1] M. Schneider, F. Ospald, M. Kabel, *International Journal for Numerical Methods in Engineering* **2015**, n/a–n/a.

Finite element discretizations

The discrete Green operator is a standard BVP

$$\begin{cases} \operatorname{div} \boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma} = \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau}^N \\ \boldsymbol{\varepsilon} = \mathbf{sym}\,\mathbf{grad}\,\mathbf{u} \end{cases}$$

Use finite elements?

On the resulting FE problem

- Homogeneous material, Cartesian grid ⇒ homogeneous element stiffness matrix
- "Nearly" closed-form solution in Fourier space!

$$\hat{\boldsymbol{\Gamma}}^{N,\mathrm{FE}}_{0,n} = h_1 \cdots h_d \, \mathbf{I} : \left(\hat{\mathbf{b}}^N_n \otimes \hat{\mathbf{K}}^N_n \otimes \hat{\mathbf{b}}^{N,*}_n \right) : \mathbf{I}$$

- See refs. [1, 2]

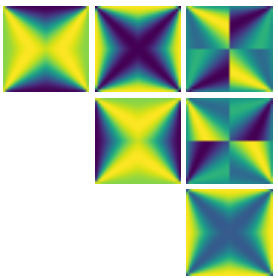
[1] M. Schneider, D. Merkert, M. Kabel, *International Journal for Numerical Methods in Engineering* **2017**, *109*, 1461–1489.

[2] S. Brisard, *International Journal for Numerical Methods in Engineering* **2017**, *109*, 459–486.

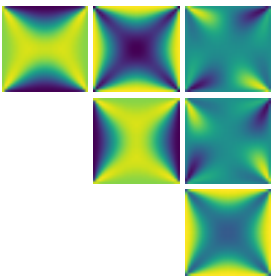
Outline of Lecture 3

- Consistent discretization… so what?
- On asymptotically consistent discretizations
- Asymptotically consistent discretizations of the microstructure
- Asymptotically consistent discretizations of the Green operator
- Comparison of some discretizations

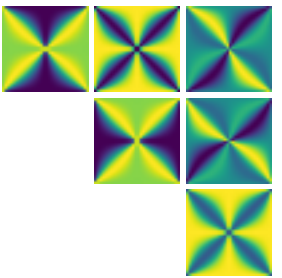
Comparison in Fourier space



Moulinec and Suquet [1]



Brisard and Dormieux [2]



Willot [3]

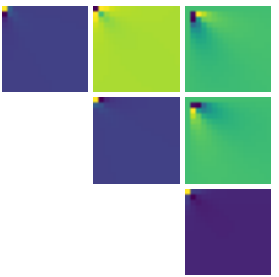
[1] H. Moulinec, P. Suquet, *Computer Methods in Applied Mechanics and Engineering* **1998**, *157*, 69–94.

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

[3] F. Willot, *Comptes Rendus Mécanique* **2015**, *343*, 232–245.

Comparison for impulse

Moulinec and Suquet [1]



Brisard and Dormieux [2]

Willot [3]

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

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

[3] F. Willot, *Comptes Rendus Mécanique* **2015**, *343*, 232–245.

Which operator should I use?

Moulinec and Suquet [1]

- Pros: cheap, no dependency on $\mathbf{C}_0$
- Cons: strong Gibbs

Willot [2] (recommended)

- Pros: quite cheap, no dependency on $\mathbf{C}_0$
- Cons: slight Gibbs

Brisard and Dormieux [3]

- Pros: virtually no Gibbs, "almost" delivers a bound
- Cons: costly, dependency on $\mathbf{C}_0$

Schneider, Merkert, and Kabel [4]

- Pros: no dependency on $\mathbf{C}_0$
- Cons: quite costly
- Gibbs?

[1] H. Moulinec, P. Suquet, *Computer Methods in Applied Mechanics and Engineering* **1998**, *157*, 69–94.
[2] F. Willot, *Comptes Rendus Mécanique* **2015**, *343*, 232–245.
[3] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, *217–220*, 197–212.
[4] M. Schneider, D. Merkert, M. Kabel, *International Journal for Numerical Methods in Engineering* **2017**, *109*, 1461–1489.

Conclusion (1/2)

Summary of Lecture 2

- Consistent discretization is useless (but for the sake of pedagogy)
- It paves the way to asymptotically consistent discretizations
- Many possible discretizations… pick your own!

Summary of this Block

- Homogenization requires the solution to the corrector problem
- This corrector problem can be transformed into a single integral equation: the Lippmann–Schwinger equation
- Upon Galerkin discretization, the discrete LS equation has a nice (block-diagonal plus block circulant) structure that calls for matrix-free implementation and the use of FFT
- Several strategies are possible to derive good asymptotically consistent discretizations

Conclusion (2/2)
Some personal thoughts

"FFT-based methods" = discretization scheme + a solver

A numerical code should be structured accordingly

continuous Green operators / discretization schemes / solvers

Ongoing projets

- Full rewrite of my code: `Scapin.jl`
  `https://github.com/sbrisard/Scapin.jl`
- Open-book: *An introduction to Lippmann–Schwinger solvers*
  `https://github.com/sbrisard/LS-intro`
  (although Matti did an excellent job already, see Ref. [1])

[1] M. Schneider, *Acta Mechanica* **2021**, *232*, 2051–2100.

Thank you for your attention!

sebastien.brisard@univ-eiffel.fr

https://navier-lab.fr/en/equipe/brisard-sebastien
https://cv.archives-ouvertes.fr/sbrisard
https://sbrisard.github.io