Colloque national mécamat 2021 – Semaine des GT

On the spatial discretization of the Lippmann–Schwinger equation

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26 january 2021

Motivation (1/2)

Outline of the Moulinec–Suquet method

- **Step 1 –** Start from the corrector problem (system of PDEs)
- **Step 2 –** Reformulate as an integral equation (Lippmann–Schwinger)
- **Step 3 –** Replace Fourier series with discrete Fourier transforms
- **Step 4 –** Introduce fixed-point iterations

We recognize a familiar pattern

- **Step 3** is the **discretization** step
- **Step 4** is the **solution** step (introduces an iterative linear solver)

Motivation (2/2)

Questions

- Convergence with respect to grid size? **(S. Brisard)**
  - Investigation of the **spatial discretization** (this talk)
  - Cast the method in a Galerkin setting
- Convergence of the **iterative solver**? **(M. Schneider)**
  - How to minimize number of iterations?
  - Can we do better than fixed-point iterations
- Strategies for complex material non-linearities? **(L. Gélébart)**
  - Use condensed potential (M. Schneider)
  - Alternative approach

Outline of this talk

This talk is devoted to the spatial discretization of the Lippmann–Schwinger equation

- Introducing the corrector problem
- Preliminaries
- The periodic, fourth-rank Green operator
- Strong and weak forms of the Lippmann–Schwinger (LS) equation
- Discretization of the LS equation
- Connexion with the discrete Fourier transform
- Consistent vs. asymptotically consistent discretizations

Introducing the corrector problem

- The corrector problem
- On periodic boundary conditions

The "corrector" problem

Field equations

$$\mathbf{div}\,\boldsymbol{\sigma} = \mathbf{0}$$

$$\boldsymbol{\sigma} = \mathsf{C} : \boldsymbol{\varepsilon}$$

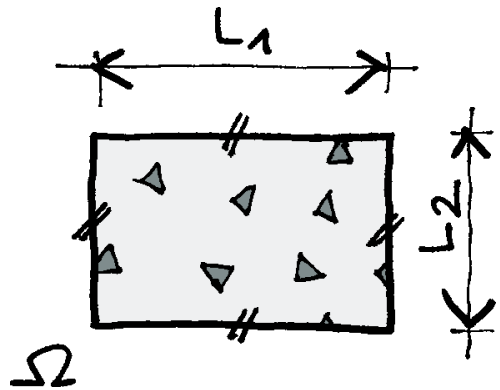
$$\boldsymbol{\varepsilon} = \mathbf{sym}\,\mathbf{grad}\,\mathbf{u}$$

C depends on observation point (material is heterogeneous!)

Periodic boundary conditions

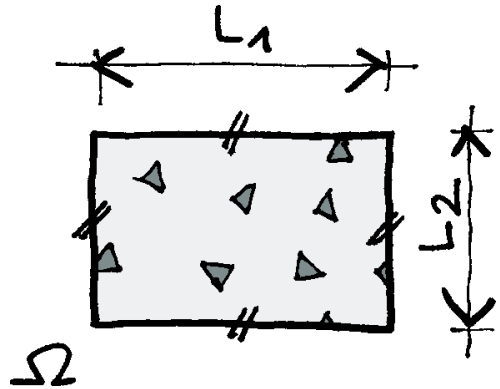
$$\Omega = (0, L_1) \times \cdots \times (0, L_d)$$

$$\mathrm{PBC}\{\bar{\boldsymbol{\varepsilon}}\} \overset{\text{def}}{=} \begin{cases} \mathbf{u}(\mathbf{x}) - \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{x} & \Omega\text{-periodic} \\ \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) & \Omega\text{-skew-periodic} \end{cases}$$



On periodic boundary conditions

$$\mathrm{PBC}\{\bar{\boldsymbol{\varepsilon}}\} \overset{\text{def}}{=} \begin{cases} \mathbf{u}(\mathbf{x}) - \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{x} & \Omega\text{-periodic} \\ \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) & \Omega\text{-skew-periodic} \end{cases}$$



- 2nd condition should be understood as

$$\boldsymbol{\sigma}(\mathbf{x} + L_i\,\mathbf{e}_i) \cdot \mathbf{e}_i = \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{e}_i \quad \text{for all} \quad i = 1, \dots, d$$

  (no summation)

- $\bar{\boldsymbol{\varepsilon}}$ (prescribed) is the macroscopic strain: $\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}$
- Hill–Mandel lemma holds!

Preliminaries

- On the Mandel–Voigt representation of tensors
- On Fourier series
- On the discrete Fourier transform
- Fourier series vs. discrete Fourier transforms

Mandel–Voigt representation of tensors

2nd order, symmetric, tensors

$$[\mathbf{s}] = \left[s_{11}, s_{22}, s_{33}, \Xi s_{23}, \Xi s_{31}, \Xi s_{12}\right]^{\mathsf{T}} \quad \text{with} \quad \Xi = \sqrt{2}$$

4th order tensors with minor symmetries

$$[\mathbf{T}] = \begin{bmatrix} T_{1111} & T_{1122} & T_{1133} & \Xi T_{1123} & \Xi T_{1131} & \Xi T_{1112} \\ T_{2211} & T_{2222} & T_{2233} & \Xi T_{2223} & \Xi T_{2231} & \Xi T_{2212} \\ T_{3311} & T_{3322} & T_{3333} & \Xi T_{3323} & \Xi T_{3331} & \Xi T_{3312} \\ \Xi T_{2311} & \Xi T_{2322} & \Xi T_{2333} & 2T_{2323} & 2T_{2331} & 2T_{2312} \\ \Xi T_{3111} & \Xi T_{3122} & \Xi T_{3133} & 2T_{3123} & 2T_{3131} & 2T_{3112} \\ \Xi T_{1211} & \Xi T_{1222} & \Xi T_{1233} & 2T_{1223} & 2T_{1231} & 2T_{1212} \end{bmatrix}$$

Some properties

$$\mathbf{s}_1 : \mathbf{s}_2 = [\mathbf{s}_1]^{\mathsf{T}} \cdot [\mathbf{s}_2] \qquad [\mathbf{T} : \mathbf{s}] = [\mathbf{T}] \cdot [\mathbf{s}] \qquad [\mathbf{T}^{-1}] = [\mathbf{T}]^{-1}$$

On Fourier series

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

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

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

Inversion (under mild regularity conditions)

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

On the discrete Fourier transform (1/2)

Input and output data are finite sets of numbers

$$(x_p)_p \quad \text{and} \quad (\hat{x}_n)_n \quad \text{with} \quad 0 \leq p_i, n_i < N_i \quad \text{and} \quad i = 1, \dots, d$$

Definition

$$\hat{x}_n \overset{\text{def}}{=} \sum_{p_1=0}^{N_1-1} \cdots \sum_{p_d=0}^{N_d-1} x_p \exp\left[-2\mathrm{i}\pi\left(\frac{p_1 n_1}{N_1} + \cdots + \frac{p_d n_d}{N_d}\right)\right]$$

Output can be seen as a discrete, periodic series

$$\hat{x}_{n+mN} = \hat{x}_n \quad \text{with} \quad n + mN \overset{\text{def}}{=} (n_1 + m_1 N_1, \dots, n_d + m_d N_d)$$

Implementation: fast Fourier transform (FFT)
$\mathcal{O}(N \log N)$ **rather than** $\mathcal{O}(N^2)$

On the discrete Fourier transform (2/2)

Inversion

$$x_p = \frac{1}{N_1 \cdots N_d} \sum_{n_1=0}^{N_1-1} \cdots \sum_{n_d=0}^{N_d-1} \hat{x}_n \exp\left[2\mathrm{i}\pi\left(\frac{p_1 n_1}{N_1} + \cdots + \frac{p_d n_d}{N_d}\right)\right]$$

$\Rightarrow$ input can **also** be seen as a discrete, **periodic** series ($x_{p+qN} \overset{\text{def}}{=} x_p$).

Circular convolution theorem

$$\widehat{x \star y}_n = \hat{x}_n \hat{y}_n \quad \text{with} \quad (x \star y)_p \overset{\text{def}}{=} \sum_{q_1=0}^{N_1-1} \cdots \sum_{q_d=0}^{N_d-1} x_{p-q}\, y_q$$

Fourier series vs. DFT

Cell-wise constant functions (over a grid)

$$f|_{\Omega_p} = f_p \quad \text{and} \quad \langle f \rangle_p = f_p$$

Fourier coefficients of cell-wise constant functions

$$\tilde{f}_n = \frac{1}{N} F(h\mathbf{k}_n)\hat{f}_n \quad \text{with} \quad F(\mathbf{K}) = \operatorname{sinc}\frac{K_1}{2} \cdots \operatorname{sinc}\frac{K_d}{2}$$

- $\tilde{f}_n$: Fourier coefficients of the **periodic function** f
- $\hat{f}_n$: discrete Fourier transform of the **cell values** f_p

Note: how to sum over $\mathbb{Z}^d$?

$$\sum_{n\in\mathbb{Z}^d} \tilde{f}_n\, g_n = \sum_{0\le n_i<N_i} \hat{f}_n \left[\frac{1}{N} \sum_{m\in\mathbb{Z}^d} F(h\mathbf{k}_{n+mN})\, g_{n+mN}\right]$$

The periodic, fourth-order Green operator

- Definition
- Elementary properties
- Expression in Fourier space

Definition

We consider here a homogeneous material!

The elementary problem

$$\begin{cases} \mathbf{div}\,\boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma} = \mathbb{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau} \\ \boldsymbol{\varepsilon} = \mathbf{sym}\,\mathbf{grad}\,\mathbf{u} \\ \mathrm{PBC}\{\bar{\boldsymbol{\varepsilon}}\} \end{cases}$$

Prescribed average strain is null!

$$\mathbb{C}_0 = \text{const.}$$

$$\boldsymbol{\tau}(\mathbf{x}) \neq \text{const.}$$

This is a linear problem

- Output depends **linearly** on input
- Loading parameters are $\bar{\boldsymbol{\varepsilon}}$ (const. tensor) and $\boldsymbol{\tau}$ (tensor field)

$$\boldsymbol{\varepsilon} = \mathbb{A} : \bar{\boldsymbol{\varepsilon}} - \Gamma_0(\boldsymbol{\tau}) = \bar{\boldsymbol{\varepsilon}} - \Gamma_0(\boldsymbol{\tau})$$

See Korringa [Kor73], Zeller and Dederichs [ZD73], and Kröner [Krö74]

Elementary properties

- Constant eigenstress: $\boldsymbol{\Gamma}_0(\langle\boldsymbol{\tau}\rangle) = \mathbf{0}$
- Volume average: $\langle\boldsymbol{\Gamma}_0(\boldsymbol{\tau})\rangle = \mathbf{0}$
- Symmetry: $\langle\boldsymbol{\tau}_1 : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}_2)\rangle = \langle\boldsymbol{\Gamma}_0(\boldsymbol{\tau}_1) : \boldsymbol{\tau}_2\rangle$
- "Idempotence": $\boldsymbol{\Gamma}_0[\mathbf{C}_0 : \boldsymbol{\Gamma}_0(\boldsymbol{\tau})] = \boldsymbol{\Gamma}_0(\boldsymbol{\tau})$
- Positivity: $\langle\boldsymbol{\tau} : \boldsymbol{\Gamma}_0(\boldsymbol{\tau})\rangle \geq 0$

$\boldsymbol{\Gamma}_0$ is a projector onto the space of geometrically compatible strain fields

See Willis [Wil77] and Bellis and Suquet [BS18]

Expression in Fourier space

Use Fourier series expansions of all mechanical fields

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

Expression of the Green operator in Fourier space

$$\tilde{\boldsymbol{\varepsilon}}_n = -\hat{\boldsymbol{\Gamma}}_0(\mathbf{k}_n) : \tilde{\boldsymbol{\tau}}_n, \quad \text{with} \quad \hat{\boldsymbol{\Gamma}}_0(\mathbf{k}) = \mathbf{I}_4 : \Big[\mathbf{k} \otimes \big(\mathbf{k} \cdot \mathbf{C}_0 \cdot \mathbf{k}\big)^{-1} \otimes \mathbf{k}\Big] : \mathbf{I}_4$$

In other words

$$\boldsymbol{\Gamma}_0(\boldsymbol{\tau})(\mathbf{x}) = \sum_{n \in \mathbb{Z}^d} \hat{\boldsymbol{\Gamma}}_0(\mathbf{k}_n) : \tilde{\boldsymbol{\tau}}_n \, \mathrm{e}^{\mathrm{i}\mathbf{k}_n \cdot \mathbf{x}}$$

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

The dirty details (1/2)

- Rewrite BVP in Fourier space ($\mathbf{C}_0 = \text{const.}$ is **crucial**!)

$$\mathbf{div}\,\boldsymbol{\sigma} = \mathbf{0} \longrightarrow \tilde{\boldsymbol{\sigma}}_n \cdot \mathrm{i}\mathbf{k}_n = \mathbf{0} \quad (1)$$

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

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

- Combine (2) and (3) (drop indices)

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

- Plug into (1)

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

The dirty details (2/2)

- General expression of displacement ($k = \|\mathbf{k}\|$ and $\mathbf{n} = \mathbf{k}/k$)

$$\begin{aligned}
\tilde{\mathbf{u}} &= \mathrm{i}\left(\mathbf{k}\cdot\mathbf{C}_0\cdot\mathbf{k}\right)^{-1}\cdot\tilde{\boldsymbol{\tau}}\cdot\mathbf{k}\\
&= \mathrm{i}\left[\left(\mathbf{k}\cdot\mathbf{C}_0\cdot\mathbf{k}\right)^{-1}\otimes\mathbf{k}\right]:\tilde{\boldsymbol{\tau}}\\
&= \mathrm{i}\left[\left(\mathbf{k}\cdot\mathbf{C}_0\cdot\mathbf{k}\right)^{-1}\otimes\mathbf{k}\right]:\left(\mathbf{I}_4:\tilde{\boldsymbol{\tau}}\right)\\
&= \mathrm{i}\left\{\left[\left(\mathbf{k}\cdot\mathbf{C}_0\cdot\mathbf{k}\right)^{-1}\otimes\mathbf{k}\right]:\mathbf{I}_4\right\}:\tilde{\boldsymbol{\tau}}\\
&= \mathrm{i}k^{-1}\left\{\left[\left(\mathbf{n}\cdot\mathbf{C}_0\cdot\mathbf{n}\right)^{-1}\otimes\mathbf{n}\right]:\mathbf{I}_4\right\}:\tilde{\boldsymbol{\tau}}
\end{aligned}$$

- General expression of strain

$$\tilde{\boldsymbol{\varepsilon}} = \mathbf{sym}(\mathrm{i}\mathbf{k}\otimes\tilde{\mathbf{u}}) = \mathbf{I}_4:\left(\mathrm{i}\mathbf{k}\otimes\tilde{\mathbf{u}}\right) = -\hat{\boldsymbol{\Gamma}}_0:\tilde{\boldsymbol{\tau}}$$

with

$$\hat{\boldsymbol{\Gamma}}_0 = \mathbf{I}_4:\left[\mathbf{n}\otimes\left(\mathbf{n}\cdot\mathbf{C}_0\cdot\mathbf{n}\right)^{-1}\otimes\mathbf{n}\right]:\mathbf{I}_4 \qquad \text{(QED)}$$

Isotropic reference material

$$\mathbf{C}_0 = 2\mu_0\left(\frac{1+\nu_0}{1-2\nu_0}\mathbf{J}_4 + \mathbf{K}_4\right) \qquad \mathbf{J}_4 = \frac{1}{3}\mathbf{I}_2 \otimes \mathbf{I}_2 \qquad \mathbf{K}_4 = \mathbf{I}_4 - \mathbf{J}_4$$

$$\mu_0^{-1}\mathbf{n}\cdot\mathbf{C}_0\cdot\mathbf{n} = \mathbf{I}_2 + \frac{\mathbf{n}\otimes\mathbf{n}}{1-2\nu_0} = \left(\mathbf{I}_2 - \mathbf{n}\otimes\mathbf{n}\right) + \frac{2\left(1-\nu_0\right)}{1-2\nu_0}\mathbf{n}\otimes\mathbf{n}$$

$$\mu_0\left(\mathbf{n}\cdot\mathbf{C}_0\cdot\mathbf{n}\right)^{-1} = \left(\mathbf{I}_2 - \mathbf{n}\otimes\mathbf{n}\right) + \frac{1-2\nu_0}{2\left(1-\nu_0\right)}\mathbf{n}\otimes\mathbf{n} = \mathbf{I}_2 - \frac{\mathbf{n}\otimes\mathbf{n}}{2\left(1-\nu_0\right)}$$

$$\hat{\Gamma}_{0,ijkl}(\mathbf{k}) = \frac{\delta_{ik}n_jn_l + \delta_{il}n_jn_k + \delta_{jk}n_in_l + \delta_{jl}n_in_k}{4\mu_0} - \frac{n_in_jn_kn_l}{2\mu_0\left(1-\nu_0\right)}$$

(applies also to plane strain elasticity)

The Lippmann–Schwinger equation

- Strong form of the LS equation
- Weak form of the LS equation
- The space of stress-polarizations

Derivation of the LS equation

Recall the corrector problem

$$\mathscr{P} \overset{\text{def}}{=} \begin{cases} \mathbf{div}\,\boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon} \\ \boldsymbol{\varepsilon} = \mathbf{sym\,grad\,u} \\ \mathrm{PBC}\{\bar{\boldsymbol{\varepsilon}}\} \end{cases}$$

Heterogeneous material!

$\mathbf{C}(\mathbf{x}) \neq \text{const.}$

Introduce one new unknown… and one new equation

$$\mathscr{P} \iff \begin{cases} \mathbf{div}\,\boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma} = \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau} \\ \boldsymbol{\varepsilon} = \mathbf{sym\,grad\,u} \\ \mathrm{PBC}\{\bar{\boldsymbol{\varepsilon}}\} \\ \boldsymbol{\tau} = \left(\mathbf{C} - \mathbf{C}_0\right) : \boldsymbol{\varepsilon} \end{cases}$$

Arbitrary reference material

$\mathbf{C}_0 = \text{const.}$

$\boldsymbol{\tau}$: stress-polarization

Strong form of the LS equation

From Hervé's talk

$$\text{Corrector problem} \iff \begin{cases} \boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} - \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \\ \boldsymbol{\tau} = \left(\mathbf{C} - \mathbf{C}_0\right) : \boldsymbol{\varepsilon} \end{cases}$$

LS equation: strong form #1

$$\boldsymbol{\varepsilon} + \boldsymbol{\Gamma}_0\left[\left(\mathbf{C} - \mathbf{C}_0\right) : \boldsymbol{\varepsilon}\right] = \bar{\boldsymbol{\varepsilon}}$$

LS equation: strong form #2

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

Simplify notation

$$\mathbf{L}(\mathbf{x}) \overset{\text{def}}{=} \mathbf{C}(\mathbf{x}) - \mathbf{C}_0 \quad \text{and} \quad \mathbf{M}(\mathbf{x}) = \mathbf{L}(\mathbf{x})^{-1}$$

See Korringa [Kor73], Zeller and Dederichs [ZD73], and Kröner [Krö74]

Weak form of the LS equation [Wil77]

Step 1 – Start from strong form of LS equation

Find $\boldsymbol{\tau} \in \mathbb{V}$ such that, for all $\mathbf{x} \in \Omega$:

$$\mathbf{M}(\mathbf{x}) : \boldsymbol{\tau}(\mathbf{x}) + \boldsymbol{\Gamma}_0(\boldsymbol{\tau})(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}}$$

Step 2 – "Multiply" with arbitrary test stress-polarization

Find $\boldsymbol{\tau} \in \mathbb{V}$ such that, for all $\mathbf{x} \in \Omega$ and $\boldsymbol{\varpi} \in \mathbb{V}$:

$$\boldsymbol{\varpi}(\mathbf{x}) : \mathbf{M}(\mathbf{x}) : \boldsymbol{\tau}(\mathbf{x}) + \boldsymbol{\varpi}(\mathbf{x}) : \boldsymbol{\Gamma}_0(\boldsymbol{\tau})(\mathbf{x}) = \boldsymbol{\varpi}(\mathbf{x}) : \bar{\boldsymbol{\varepsilon}}$$

Step 3 – Integrate over unit-cell Ω (take volume average)

Find $\boldsymbol{\tau} \in \mathbb{V}$ such that, for all $\boldsymbol{\varpi} \in \mathbb{V}$:

$$a(\boldsymbol{\tau}, \boldsymbol{\varpi}) \overset{\text{def}}{=} \langle \boldsymbol{\varpi} : \mathbf{M} : \boldsymbol{\tau} \rangle + \langle \boldsymbol{\varpi} : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \rangle = \langle \boldsymbol{\varpi} : \bar{\boldsymbol{\varepsilon}} \rangle \overset{\text{def}}{=} \ell(\boldsymbol{\varpi})$$

On the space of stress-polarizations

Find $\boldsymbol{\tau} \in \mathbb{V}$ such that, for all $\boldsymbol{\varpi} \in \mathbb{V}$:

$$a(\boldsymbol{\tau}, \boldsymbol{\varpi}) \overset{\text{def}}{=} \langle \boldsymbol{\varpi} : \mathbf{M} : \boldsymbol{\tau} \rangle + \langle \boldsymbol{\varpi} : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \rangle = \langle \boldsymbol{\varpi} : \bar{\boldsymbol{\varepsilon}} \rangle \overset{\text{def}}{=} \ell(\boldsymbol{\varpi})$$

- $\boldsymbol{\tau}$: **trial** function (stress-polarization),
- $\boldsymbol{\varpi}$: **test** function (stress-polarization),
- $\mathbb{V}$: space of second-rank, symmetric tensors fields with square integrable components [BD12].

Discretization of the Lippmann–Schwinger equation

- Galerkin discretization
- The approximation subspace
- The discrete variational problem
- Structure of the underlying linear system

Galerkin discretization in a nutshell

The initial problem

Find $\boldsymbol{\tau} \in \mathbb{V}$ such that $\quad a(\boldsymbol{\tau}, \boldsymbol{\varpi}) = \ell(\boldsymbol{\varpi}) \quad$ for all $\boldsymbol{\varpi} \in \mathbb{V}$

Exhaustive exploration of $\mathbb{V}$ is not possible!

Explore a finite-dimension subspace $\mathbb{V}^h \subset \mathbb{V}$

Find $\boldsymbol{\tau}^h \in \mathbb{V}^h$ such that $\quad a(\boldsymbol{\tau}^h, \boldsymbol{\varpi}^h) = \ell(\boldsymbol{\varpi}^h) \quad$ for all $\boldsymbol{\varpi}^h \in \mathbb{V}^h$

This is a linear system!

Our roadmap

- **Define** the approximation subspace $\mathbb{V}^h$
- **Evaluate** the linear form ℓ over $\mathbb{V}^h$
- **Evaluate** the bilinear form a over $\mathbb{V}^h$

Defining the approximation subspace (1/2)

Discretization over a grid

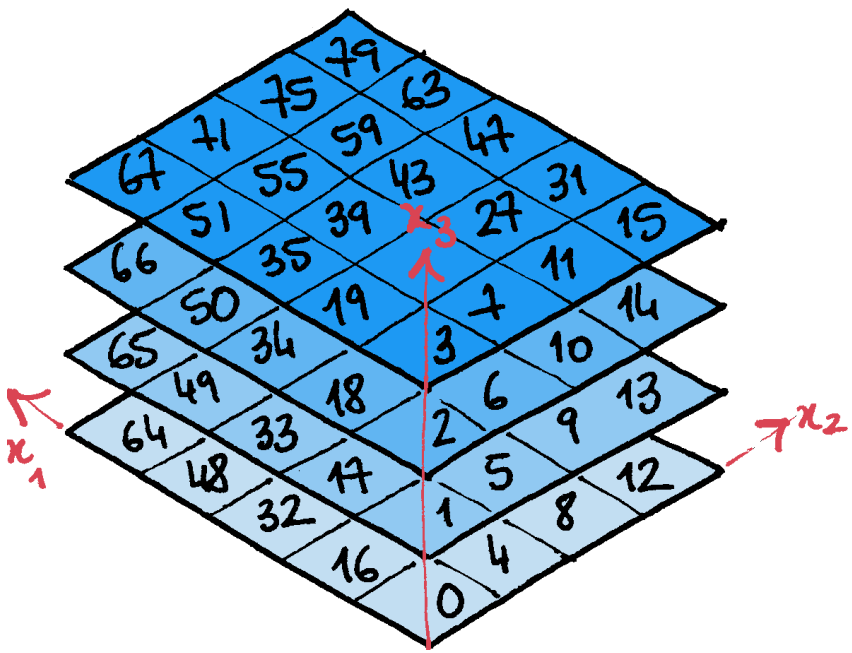
- Any mesh would do…but we anticipate on the use of FFTs!
- **Regular grid**: $N_1 \times \cdots \times N_d$
- Grid spacing: $h_i = L_i/N_i$; Total number of cells: $N = N_1 \cdots N_d$
- Convention: p, q cell indices (pixels); m, n frequency indices.

Cell average

$$\langle \mathbb{Q} \rangle_p \overset{\text{def}}{=} \frac{1}{|\Omega_p|} \int_{\Omega_p} \mathbb{Q}(\mathbf{x}) \, \mathrm{d}\mathbf{x}$$

Average over whole unit-cell

$$\langle \mathbb{Q} \rangle = \frac{1}{N} \sum_{p=0}^{N-1} \langle \mathbb{Q} \rangle_p$$



Defining the approximation subspace (2/2)

Two natural choices for square-integrable fields

- Trigonometric polynomials
  (outside the scope of this talk, see [VZM14; VZM15; Von16])
- **Cell-wise constant functions**

$$\mathcal{N}_{\text{dofs}} = \dim \mathbb{V}^h = sN \qquad\qquad s = d\big(d+1\big)/2$$

Some technical details

- Trial and test stress-polarization defined by their cell-values

$$\mathbf{x} \in \Omega_p \; : \quad \boldsymbol{\tau}^h(\mathbf{x}) = \boldsymbol{\tau}_p^h \quad \text{and} \quad \boldsymbol{\varpi}^h(\mathbf{x}) = \boldsymbol{\varpi}_p^h$$

- Cell-averages

$$\langle \boldsymbol{\tau}^h \rangle_p = \boldsymbol{\tau}_p^h \quad \text{and} \quad \langle \boldsymbol{\varpi}^h \rangle_p = \boldsymbol{\varpi}_p^h$$

Evaluating ℓ and a over $\mathbb{V}^h$

$$\left.\begin{aligned} \ell(\boldsymbol{\varpi}) &= \langle \boldsymbol{\varpi} \rangle : \bar{\boldsymbol{\varepsilon}} \\ \langle \boldsymbol{\varpi}^h \rangle_p &= \boldsymbol{\varpi}_p^h \end{aligned}\right\} \quad \Rightarrow \quad \ell(\boldsymbol{\varpi}^h) = \frac{1}{N} \sum_p \boldsymbol{\varpi}_p^h : \bar{\boldsymbol{\varepsilon}}$$

Evaluating a over $\mathbb{V}^h$

$$a(\boldsymbol{\tau}^h, \boldsymbol{\varpi}^h) = \langle \boldsymbol{\varpi}^h : \mathbf{M} : \boldsymbol{\tau}^h \rangle + \langle \boldsymbol{\varpi}^h : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^h) \rangle$$

$$\langle \boldsymbol{\varpi}^h : \mathbf{M} : \boldsymbol{\tau}^h \rangle = \frac{1}{N} \sum_p \langle \boldsymbol{\varpi}^h : \mathbf{M} : \boldsymbol{\tau}^h \rangle_p = \frac{1}{N} \sum_p \boldsymbol{\varpi}_p^h : \langle \mathbf{M} \rangle_p : \boldsymbol{\tau}_p^h$$

$$\langle \boldsymbol{\varpi}^h : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^h) \rangle = \frac{1}{N} \sum_p \langle \boldsymbol{\varpi}^h : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^h) \rangle_p = \frac{1}{N} \sum_p \boldsymbol{\varpi}_p^h : \langle \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^h) \rangle_p$$

The discrete Green operator

For $\boldsymbol{\tau}^h \in \mathbb{V}^h$, $(\boldsymbol{\tau}_1^h, \boldsymbol{\tau}_2^h, \ldots) \mapsto \langle \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^h) \rangle_p$ is linear with respect to the $\boldsymbol{\tau}_p^h$

$$\langle \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^h) \rangle_p = \sum_q \boldsymbol{\Gamma}_{0,pq}^h : \boldsymbol{\tau}_q^h$$

$-\boldsymbol{\Gamma}_{0,pq}^h : \boldsymbol{\tau}_q^h$ = average strain in cell p induced by constant eigenstress $\boldsymbol{\tau}_q^h$ in cell q!

The discrete variational problem

The discrete variational problem

Find $\boldsymbol{\tau}_0^h, \boldsymbol{\tau}_1^h, \dots, \boldsymbol{\tau}_{N-1}^h$ such that, for all $\boldsymbol{\varpi}_0^h, \boldsymbol{\varpi}_1^h, \dots, \boldsymbol{\varpi}_{N-1}^h$

$$\sum_p \boldsymbol{\varpi}_p^h : \langle \mathbf{M} \rangle_p : \boldsymbol{\tau}_p^h + \sum_{p,q} \boldsymbol{\varpi}_p^h : \boldsymbol{\Gamma}_{0,pq}^h : \boldsymbol{\tau}_q^h = \sum_p \boldsymbol{\varpi}_p^h : \bar{\boldsymbol{\varepsilon}}$$

The linear system

$$\langle \mathbf{M} \rangle_p : \boldsymbol{\tau}_p^h + \sum_q \boldsymbol{\Gamma}_{0,pq}^h : \boldsymbol{\tau}_q^h = \bar{\boldsymbol{\varepsilon}}$$

Convergence w.r.t grid-size

OK, classical Galerkin setting [BD12]

Assembling the linear system

The linear system

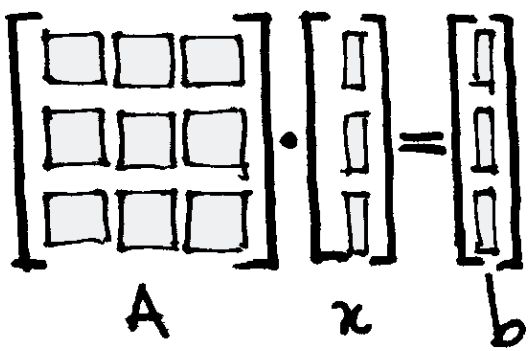
$$\langle \mathbf{M} \rangle_p : \boldsymbol{\tau}_p^h + \sum_q \boldsymbol{\Gamma}_{0,pq}^h : \boldsymbol{\tau}_q^h = \bar{\boldsymbol{\varepsilon}} \qquad \Longleftrightarrow \qquad A \cdot x = b$$

Use the Mandel–Voigt representation

- $\langle \mathbf{M} \rangle_p$, $\boldsymbol{\Gamma}_{0,pq}^h$: fourth-rank tensors $\rightarrow$ $s \times s$ blocks
- $\boldsymbol{\tau}_p^h$ and $\bar{\boldsymbol{\varepsilon}}$: second-rank tensors $\rightarrow$ $s \times 1$ blocks

$$x_p = [\boldsymbol{\tau}_p] \quad \text{and} \quad b_p = [\bar{\boldsymbol{\varepsilon}}]$$

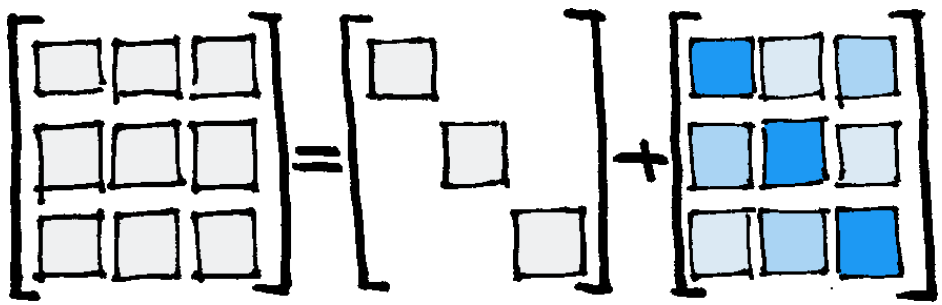
$$A_{pq} = \underbrace{\delta_{pq}[\langle \mathbf{M} \rangle_q]}_{\text{block-diagonal}} + \underbrace{[\boldsymbol{\Gamma}_{0,pq}^h]}_{\text{full matrix!}}$$



On the structure of the matrix

$$A_{pq} = \delta_{pq}[\langle \mathbf{M} \rangle_q] + [\boldsymbol{\Gamma}^h_{0,pq}] \qquad \Longleftrightarrow \qquad A = D + C.$$

- D: **block-diagonal**
- $\boldsymbol{\Gamma}^h_{0,pq}$: influence of cell q over cell p
- Translation invariant in periodic setting $\Rightarrow$ C: **block-circulant**!
- Convolution product in real space $\rightarrow$ local product in Fourier space (here comes the **discrete Fourier transform**!!!)



Connexion with the discrete Fourier transform

- Expression of the discrete Green operator
- Matrix-free implementation
- Wait a minute…

Expression of the discrete Green operator

Exact for cell-wise constant stress-polarizations!

$$\langle \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^h) \rangle_p = \mathrm{DFT}_p^{-1}[\hat{\boldsymbol{\eta}}_\bullet^h], \quad \text{with} \quad \hat{\boldsymbol{\eta}}_n^h = \hat{\boldsymbol{\Gamma}}_{0,n}^h : \hat{\boldsymbol{\tau}}_n^h \quad \text{and} \quad \hat{\boldsymbol{\tau}}_n^h = \mathrm{DFT}_n[\boldsymbol{\tau}_\bullet^h]$$

$$\hat{\boldsymbol{\Gamma}}_{0,n}^h = \sum_{m \in \mathbb{Z}^d} \left[F(h\mathbf{k}_{n+mN}) \right]^2 \hat{\boldsymbol{\Gamma}}_0(\mathbf{k}_{n+mN})$$

$$F(\mathbf{K}) = \operatorname{sinc} \frac{K_1}{2} \cdots \operatorname{sinc} \frac{K_d}{2}$$

$$\mathbf{k}_{n+mN} = 2\pi \left(\frac{n_1 + m_1 N_1}{L_1} \mathbf{e}_1 + \cdots + \frac{n_d + m_d N_d}{L_d} \mathbf{e}_d \right)$$

Proof is not difficult, but technical [BD10; BD12]

Wait a minute…

The consistent discrete Green operator

$$\hat{\Gamma}^h_{0,n} = \sum_{m \in \mathbb{Z}^d} \left[F(h\mathbf{k}_{n+mN}) \right]^2 \hat{\Gamma}_0(\mathbf{k}_{n+mN})$$

Above expression is exact, but its evaluation is difficult, if possible at all [BD10]!

Introduce an approximation of this operator (asymptotically consistent discretization)

Consistent vs. asymptotically consistent discretizations

- What is a variational crime?
- Asymptotically consistent approx. of local operator
- Asymptotically consistent approx. of non-local operator

On variational crimes

The initial problem

Find $\boldsymbol{\tau} \in \mathbb{V}$ such that $\quad a(\boldsymbol{\tau}, \boldsymbol{\varpi}) = \ell(\boldsymbol{\varpi}) \quad$ for all $\boldsymbol{\varpi} \in \mathbb{V}$

Exhaustive exploration of $\mathbb{V}$ is not possible!

Consistent discretization

Find $\boldsymbol{\tau}^h \in \mathbb{V}^h$ such that $\quad a(\boldsymbol{\tau}^h, \boldsymbol{\varpi}^h) = \ell(\boldsymbol{\varpi}^h) \quad$ for all $\boldsymbol{\varpi}^h \in \mathbb{V}^h$

Exact evaluation of the bilinear and linear forms!

Asymptotically consistent discretization

Find $\boldsymbol{\tau}^h \in \mathbb{V}^h$ such that $\quad a^h(\boldsymbol{\tau}^h, \boldsymbol{\varpi}^h) = \ell^h(\boldsymbol{\varpi}^h) \quad$ for all $\boldsymbol{\varpi}^h \in \mathbb{V}^h$

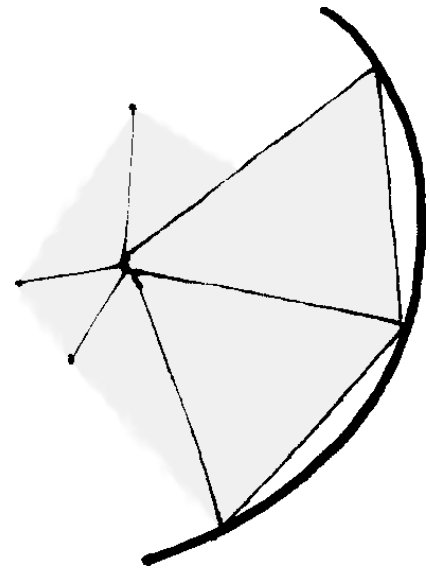
Approximations ℓ^h and a^h must be asymptotically consistent [EG04]

We are all criminals

Examples of variational crimes (FEM)

The bilinear form

$$a(\mathbf{u},\mathbf{v}) = \int_\Omega \mathbf{grad}[\mathbf{u}] : \mathsf{C} : \mathbf{grad}[\mathbf{v}]$$



Geometry

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

Quadrature

$$\int_{\Omega_e} \mathbf{grad}[\mathbf{u}] : \mathsf{C} : \mathbf{grad}[\mathbf{v}] \simeq \sum_g w_g \, \mathbf{grad}[\mathbf{u}](\mathbf{x}_g) : \mathsf{C} : \mathbf{grad}[\mathbf{v}](\mathbf{x}_g)$$

Handling heterogeneous cells

Consistent equivalent stiffness of cell [BD12]

$$\langle \boldsymbol{\varpi}^h : \mathbf{M} : \boldsymbol{\tau}^h \rangle = \frac{1}{N} \sum_p \boldsymbol{\varpi}_p^h : \langle \mathbf{M} \rangle_p : \boldsymbol{\tau}_p^h$$

$$= \frac{1}{N} \sum_p \boldsymbol{\tau}_p^h : \left(\mathbf{C}_p^h - \mathbf{C}^{\mathrm{ref}} \right)^{-1} : \boldsymbol{\varpi}_p^h$$

$$\mathbf{C}_p^h \overset{\mathrm{def}}{=} \mathbf{C}^{\mathrm{ref}} + \langle \mathbf{M} \rangle_p^{-1}$$

Although consistent, this rule sometimes leads to surprising convergence results in practice.

Alternative, non-consistent rules

- "Black-or-white": $\mathbf{C}_p^h$ = stiffness at cell center
- Laminate approximation [KMS15]: probably your best bet

Discrete Green operators

The consistent discrete Green operator

$$\langle \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^h) \rangle_p = \mathrm{DFT}_p^{-1}[\hat{\boldsymbol{\eta}}^h_\bullet], \quad \text{with} \quad \hat{\boldsymbol{\eta}}^h_n = \hat{\boldsymbol{\Gamma}}^{h,\mathrm{c}}_{0,n} : \hat{\boldsymbol{\tau}}^h_n$$

$$\hat{\boldsymbol{\Gamma}}^{h,\mathrm{c}}_{0,n} = \sum_{m \in \mathbb{Z}^d} \left[F(h\mathbf{k}_{n+mN}) \right]^2 \hat{\boldsymbol{\Gamma}}_0(\mathbf{k}_{n+mN})$$

Asymptotically consistent discrete Green operators

Retain the nice block-circulant structure!

$$\langle \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \rangle_p \simeq \mathrm{DFT}_p^{-1}[\hat{\boldsymbol{\eta}}^h_\bullet], \quad \text{with} \quad \hat{\boldsymbol{\eta}}^h_n = \hat{\boldsymbol{\Gamma}}^{h,\star}_{0,n} : \hat{\boldsymbol{\tau}}^h_n$$

Signal processing approaches

Filter out high frequencies!

Rectangular window [MS94; MS98]

Select $m_i \in \{-1, 0\}$ that minimizes $n_i + m_i N_i$

$$\hat{\Gamma}_{0,n}^{h,\mathrm{MS}} = \hat{\Gamma}_0(\mathbf{k}_{n+mN}) \quad \text{with} \quad m_i = \begin{cases} -1 & \text{if } 2n_i > N_i \\ 0 & \text{otherwise} \end{cases}$$

If any of the n_i is such that $2n_i = N_i$, then set $\hat{\Gamma}_{0,n}^{h,\mathrm{MS}} = \mathbb{C}_0$.

Cosine window [BD12]

$$\hat{\Gamma}_{0,n}^{h,\mathrm{BD}} = \sum_{m \in \{-1,0\}^d} \left[G(h\mathbf{k}_{n+mN})\right]^2 \hat{\Gamma}_0(\mathbf{k}_{n+mN}) \qquad G(\mathbf{K}) = \cos\frac{K_1}{4} \cdots \cos\frac{K_d}{4}$$

Strong connexion w. **band-limited** approximation of Zeman et al. [Zem+10] and Vondřejc [Von16]

Discretization in the real space

Discretize the homogeneous, eigenstressed problem!

Finite differences on rotated grids [Wil15; SOK15]

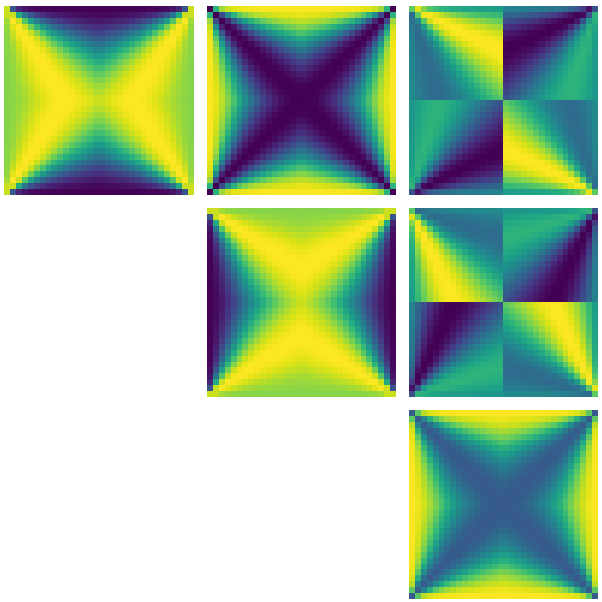
$$\hat{\Gamma}^{h,\star}_{0,n} = \hat{\Gamma}_0(\mathbf{k}^\star_n) \qquad \begin{cases} \mathbf{k}^{\mathrm{W}}_n = \dfrac{1}{h_1}\tan\dfrac{\pi n_1}{N_1}\mathbf{e}_1 + \cdots + \dfrac{1}{h_3}\tan\dfrac{\pi n_3}{N_3}\mathbf{e}_3 \\ \mathbf{k}^{\mathrm{SOK}}_n = \dfrac{\mathrm{e}^{\mathrm{i}2\pi n_1/N_1}-1}{h_1}\mathbf{e}_1 + \cdots + \dfrac{\mathrm{e}^{\mathrm{i}2\pi n_3/N_1}-1}{h_3}\mathbf{e}_3 \end{cases}$$

See also Willot and Pellegrini [WP08] and Willot et al. [WAP14]
The above, more operational formula for $\mathbf{k}^{\mathrm{W}}_n$ is proved in [Bri17]

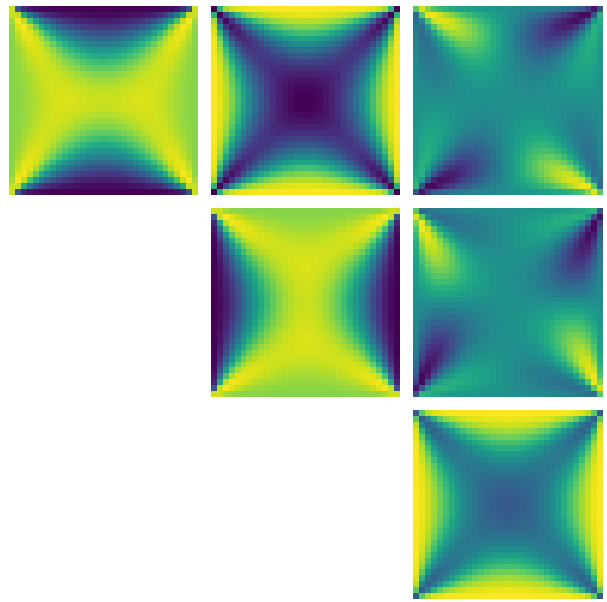
Finite elements [SMK17; Bri17]

No closed-form expression, but fairly easy implementation.

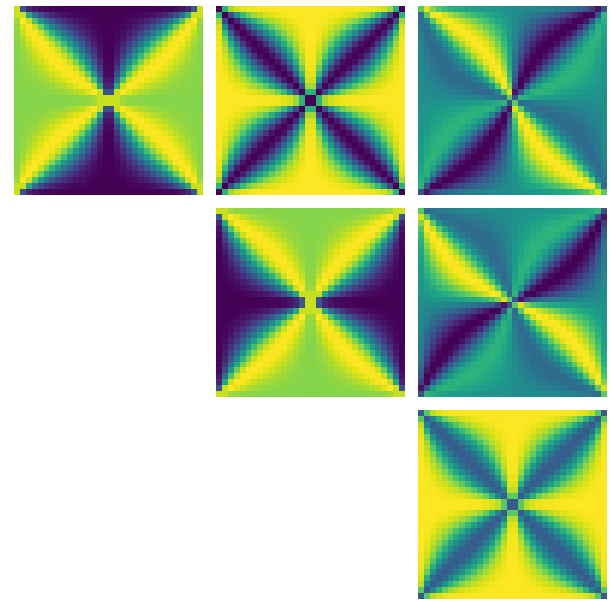
Comparison in Fourier space



Moulinec and Suquet [MS98]



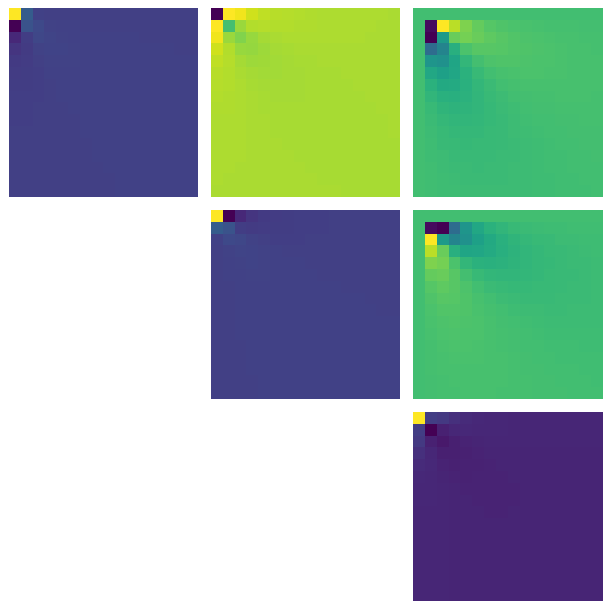
Brisard and Dormieux [BD12]



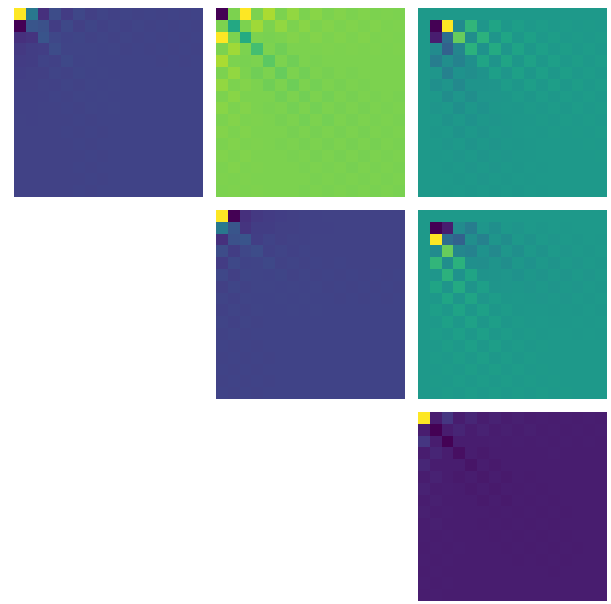
Willot [Wil15]

Comparison for impulse

Moulinec and Suquet [MS98]



Brisard and Dormieux [BD12]



Willot [Wil15]

Which operator should I use?

Moulinec and Suquet [MS98]

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

Brisard and Dormieux [BD12]

Pros: virtually no Gibbs **Cons:** costly, dependency on $\mathbf{C}_0$

Willot [Wil15] (recommended)

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

Schneider et al. [SMK17]

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

Conclusion

- Weak form of the Lippmann–Schwinger equation
- Galerkin discretization (cell-wise constant test functions)
- Consistent discretization impractical
- Introduce several asymptotically consistent discretizations

The problem is now ready to be handed to a solver!

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Thank you for your attention

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