FFT-based Galerkin method for homogenization of periodic media

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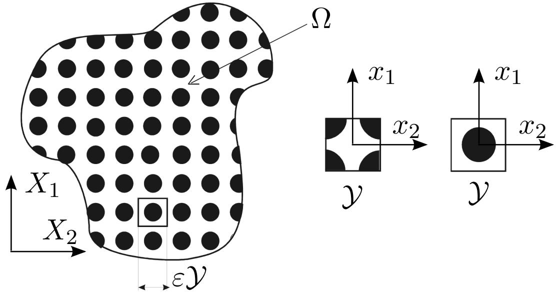
Model problem



- Coefficients $\boldsymbol{A}$ are periodic with period of $\varepsilon\mathcal{Y}$

$$-\nabla_{\boldsymbol{X}} \cdot \left(\boldsymbol{A}\left(\frac{\boldsymbol{X}}{\varepsilon}\right) \nabla_{\boldsymbol{X}} u^{\varepsilon}(\boldsymbol{X}) \right) = f \text{ in } \Omega$$

$$u^{\varepsilon} = 0 \text{ on } \partial\Omega$$

$$\downarrow$$

$$-\nabla_{\boldsymbol{X}} \cdot (\boldsymbol{A}_{\text{eff}} \nabla_{\boldsymbol{X}} U(\boldsymbol{X})) = f \text{ in } \Omega$$

$$U = 0 \text{ on } \partial\Omega$$

- Variational characterization of $\boldsymbol{A}_{\text{eff}} \in \mathbb{R}^{d\times d}$

$$\left(\boldsymbol{A}_{\text{eff}}\boldsymbol{E},\boldsymbol{E}\right) = \inf_{v\in H^1_{\text{per},0}(\mathcal{Y})} \frac{1}{|\mathcal{Y}|}\int_{\mathcal{Y}} \left(\boldsymbol{A}(\boldsymbol{x})\left[\boldsymbol{E}+\nabla_x v(\boldsymbol{x})\right], \boldsymbol{E}+\nabla_x v(\boldsymbol{x})\right)\mathrm{d}\boldsymbol{x}$$

for arbitrary $\boldsymbol{E} \in \mathbb{R}^d$

- Optimality conditions (cell problem)

$$\nabla_x \cdot \left[\boldsymbol{A}(\boldsymbol{x})\left(\boldsymbol{E}+\nabla_x u^*(\boldsymbol{x})\right)\right] = 0$$

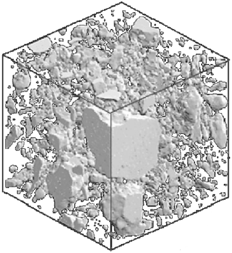
- Due to periodicity

$$\int_{\mathcal{Y}} \nabla_x u^*(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \boldsymbol{0}$$

- Traditionally solved by the Finite Element Method

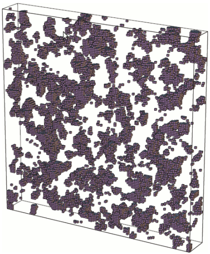
Examples of pixel- and voxel-based cells $\mathcal{Y}$

MicroComputed tomography



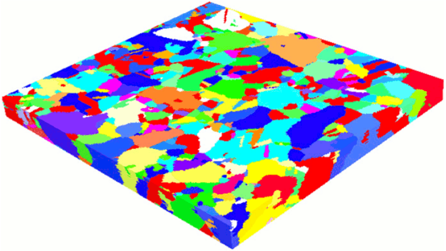
GALLUCCI ET AL, CCR (2006)

Microstructure reconstruction



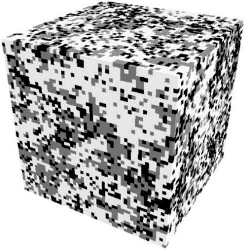
QUINTANILLA & JONES, PRE (2007)

Serial sectioning



ROLLETT ET AL, MSMSE (2010)

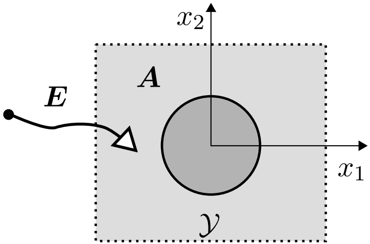
Microstructure models



ŠMILAUER & BAŽANT, CCR (2010)

Motivation

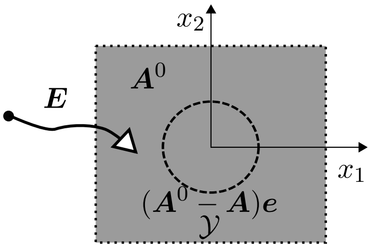
Cell problem – scalar setting (MILTON, 2002)



$$\nabla \times \boldsymbol{e}^*(\boldsymbol{x}) = \boldsymbol{0}, \quad \nabla \cdot \boldsymbol{\jmath}(\boldsymbol{x}) = \boldsymbol{0}, \quad \boldsymbol{\jmath}(\boldsymbol{x}) = \boldsymbol{A}(\boldsymbol{x})\left[\boldsymbol{E} + \boldsymbol{e}^*(\boldsymbol{x})\right] \qquad \boldsymbol{x} \in \mathcal{Y}$$

$$\int_{\mathcal{Y}} \boldsymbol{e}^*(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \boldsymbol{0}$$

- $\mathcal{Y} = \prod_{\alpha=1}^{d}(-Y_\alpha, Y_\alpha) \subset \mathbb{R}^d$: periodic cell
- $\boldsymbol{A}(\boldsymbol{x})$: periodic tensor of material coefficients
- $\boldsymbol{e}^*(\boldsymbol{x}) = \nabla_x u^*(\boldsymbol{x})$: periodic fluctuating gradient field
- $\boldsymbol{\jmath}(\boldsymbol{x})$: periodic flux field



- Lippmann-Schwinger equation: Seek for $\boldsymbol{e} = \boldsymbol{E} + \boldsymbol{e}^*$

$$\boldsymbol{e}(\boldsymbol{x}) + \int_{\mathcal{Y}} \boldsymbol{\Gamma}^0(\boldsymbol{x}-\boldsymbol{y})\Big(\boldsymbol{A}(\boldsymbol{y}) - \boldsymbol{A}^0\Big)\boldsymbol{e}(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \boldsymbol{E} \text{ for } \boldsymbol{x} \in \mathcal{Y}$$

with $\boldsymbol{A}^0 \succ \boldsymbol{0}$ and

$$\hat{\boldsymbol{\Gamma}}^0(\boldsymbol{k}) = \begin{cases} \boldsymbol{0} & \boldsymbol{k} = \boldsymbol{0} \\ \dfrac{\boldsymbol{\xi}(\boldsymbol{k}) \otimes \boldsymbol{\xi}(\boldsymbol{k})}{\boldsymbol{A}^0\boldsymbol{\xi}(\boldsymbol{k}) \cdot \boldsymbol{\xi}(\boldsymbol{k})} & \boldsymbol{k} \in \mathbb{Z}^d \backslash \{\boldsymbol{0}\}, \xi_\alpha = \frac{k_\alpha}{Y_\alpha}, \alpha = 1, \dots, d \end{cases}$$

- Cell problem

$$\nabla \cdot \left[\boldsymbol{A}(\boldsymbol{x}) \left(\boldsymbol{E} + \nabla u^*(\boldsymbol{x}) \right) \right] = 0$$

- Reformulation

$$\nabla \cdot \left[\left(\boldsymbol{A}(\boldsymbol{x}) + \boldsymbol{A}^0 - \boldsymbol{A}^0 \right) \left(\boldsymbol{E} + \nabla u^*(\boldsymbol{x}) \right) \right] = 0$$
$$\nabla \cdot \boldsymbol{A}^0 \nabla u^*(\boldsymbol{x}) = -\nabla \cdot \boldsymbol{b}(\boldsymbol{x})$$

with

$$\boldsymbol{b}(\boldsymbol{x}) = \left[\left(\boldsymbol{A}(\boldsymbol{x}) - \boldsymbol{A}^0 \right) \left(\boldsymbol{E} + \nabla u^*(\boldsymbol{x}) \right) \right]$$

- Can be solved in a closed form with the Fourier Transform techniques

- Fourier transform

$$\widehat{\boldsymbol{f}}(\boldsymbol{k}) = \overline{\widehat{\boldsymbol{f}}(-\boldsymbol{k})} = \frac{1}{|\mathcal{Y}|}\int_{\mathcal{Y}} \boldsymbol{f}(\boldsymbol{x})\varphi_{-\boldsymbol{k}}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \text{ for } \boldsymbol{k} \in \mathbb{Z}^d$$

$$\varphi_{\boldsymbol{k}}(\boldsymbol{x}) = \exp\Big(\mathrm{i}\pi\boldsymbol{\xi}(\boldsymbol{k})\cdot\boldsymbol{x}\Big) \text{ for } \boldsymbol{x} \in \mathcal{Y} \text{ and } \boldsymbol{k} \in \mathbb{Z}^d$$

$$\boldsymbol{\xi}(\boldsymbol{k}) = (k_\alpha/2Y_\alpha)_{\alpha=1}^d$$

- Plancherel theorem

$$\big(\boldsymbol{f},\boldsymbol{g}\big)_{L^2(\mathcal{Y},\mathbb{R}^d)} = |\mathcal{Y}|\sum_{\boldsymbol{k}\in\mathbb{Z}^d}\big(\widehat{\boldsymbol{f}}(\boldsymbol{k}),\widehat{\boldsymbol{g}}(\boldsymbol{k})\big)_{\mathbb{C}^d}.$$

- Gradient and divergence operators

$$\widehat{(\nabla f)}(\boldsymbol{k}) = \mathrm{i}\pi\boldsymbol{\xi}(\boldsymbol{k})\widehat{f}(\boldsymbol{k}) \qquad \widehat{(\nabla\cdot\boldsymbol{f})}(\boldsymbol{k}) = \mathrm{i}\pi\boldsymbol{\xi}(\boldsymbol{k})\cdot\widehat{\boldsymbol{f}}(\boldsymbol{k})$$

- Convolution is local in the Fourier space

$$\nabla \cdot \boldsymbol{A}^0 \nabla u^*(\boldsymbol{x}) = -\nabla \cdot \boldsymbol{b}(\boldsymbol{x})$$

- Apply Fourier transform $(\boldsymbol{k} \neq \boldsymbol{0})$

$$-\pi^2 \left(\boldsymbol{A}^0 \boldsymbol{\xi}(\boldsymbol{k}) \cdot \boldsymbol{\xi}(\boldsymbol{k}) \right) \widehat{u^*}(\boldsymbol{k}) = -\mathrm{i}\pi \boldsymbol{\xi}(\boldsymbol{k}) \cdot \widehat{\boldsymbol{b}}(\boldsymbol{k})$$

$$\widehat{u^*}(\boldsymbol{k}) = \frac{\mathrm{i}}{\pi} \frac{\boldsymbol{\xi}(\boldsymbol{k})}{\boldsymbol{A}^0 \boldsymbol{\xi}(\boldsymbol{k}) \cdot \boldsymbol{\xi}(\boldsymbol{k})} \cdot \widehat{\boldsymbol{b}}(\boldsymbol{k})$$

$$\widehat{\boldsymbol{e}^*}(\boldsymbol{k}) = -\frac{\boldsymbol{\xi}(\boldsymbol{k}) \otimes \boldsymbol{\xi}(\boldsymbol{k})}{\boldsymbol{A}^0 \boldsymbol{\xi}(\boldsymbol{k}) \cdot \boldsymbol{\xi}(\boldsymbol{k})} \widehat{\boldsymbol{b}}(\boldsymbol{k})$$

- Convolution property

$$\boldsymbol{e}^*(\boldsymbol{x}) = -\int_{\mathcal{Y}} \boldsymbol{\Gamma}^0(\boldsymbol{x} - \boldsymbol{y}) \boldsymbol{b}(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}$$

- Apply gradient decomposition $(\boldsymbol{E} = \boldsymbol{e} - \boldsymbol{e}^*)$ and expand $\boldsymbol{b}$

$$\boldsymbol{e}(\boldsymbol{x}) + \int_{\mathcal{Y}} \overbrace{\boldsymbol{\Gamma}^0(\boldsymbol{x}-\boldsymbol{y})}^{\text{step II}} \overbrace{\Big(\boldsymbol{A}(\boldsymbol{y}) - \boldsymbol{A}^0\Big)\boldsymbol{e}(\boldsymbol{y})}^{\text{step I}} \,\mathrm{d}\boldsymbol{y} = \boldsymbol{E} \text{ for } \boldsymbol{x} \in \mathcal{Y}$$

- Step I is local in the real space
- Step II is local in the Fourier space, and can be efficiently evaluated by the FFT
- Simple fixed-point algorithm

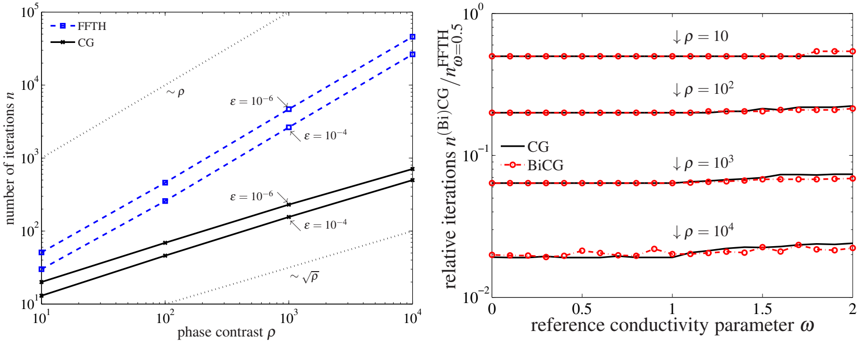
$$\boldsymbol{e}_{(k+1)}(\boldsymbol{x}) = \boldsymbol{E} - \int_{\mathcal{Y}} \boldsymbol{\Gamma}^0(\boldsymbol{x}-\boldsymbol{y})\Big(\boldsymbol{A}(\boldsymbol{y}) - \boldsymbol{A}^0\Big)\boldsymbol{e}_{(k)}(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}$$

- (Non-)convergence strongly influenced by the choice of $\boldsymbol{A}^0$ and the phase contrast
- More efficient than standard Finite Element Methods
- Many improvements of the original scheme available

Motivation

Some (computational) observations (ZEMAN ET AL, 2010)

- Lippmann-Schwinger equation → a non-symmetric linear system
- Trigonometric collocation method (SARANEN & VAINIKKO, 2002)
- System is solvable by the Conjugate Gradient algorithm
- Performance independent of A^0



- Why?

Outline

Weak formulation of unit cell problem

- Fluctuating gradient field: $\boldsymbol{e} = \boldsymbol{E} + \boldsymbol{e}^*$

$$\nabla \times \boldsymbol{e}^*(\boldsymbol{x}) = \boldsymbol{0}, \quad \nabla \cdot \boldsymbol{\jmath}(\boldsymbol{x}) = \boldsymbol{0}, \quad \boldsymbol{\jmath}(\boldsymbol{x}) = \boldsymbol{A}(\boldsymbol{x})\left[\boldsymbol{E} + \boldsymbol{e}^*(\boldsymbol{x})\right] \quad \boldsymbol{x} \in \mathcal{Y}$$

$$\int_{\mathcal{Y}} \boldsymbol{e}^*(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x} = \boldsymbol{0}$$

Weak solution

Find $\boldsymbol{e}^* \in \mathscr{E}$ such that

$$\left(\boldsymbol{A}\boldsymbol{e}^*, \boldsymbol{v}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} = -\left(\boldsymbol{A}\boldsymbol{E}, \boldsymbol{v}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} \quad \text{for all } \boldsymbol{v} \in \mathscr{E}$$

with

$$\mathscr{E} = \left\{ \boldsymbol{f} \in L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d) : \nabla \times \boldsymbol{f} = \boldsymbol{0}, \int_{\mathcal{Y}} \boldsymbol{f}(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x} = \boldsymbol{0} \right\}$$

Weak formulation of unit cell problem

Projection operator

Fundamental lemma

Operator $\mathcal{G}^0 : L^2_{\mathrm{per}}(\mathcal{Y}; \mathbb{R}^d) \to L^2_{\mathrm{per}}(\mathcal{Y}; \mathbb{R}^d)$, defined as

$$\mathcal{G}^0[\boldsymbol{f}](\boldsymbol{x}) = \int_{\mathcal{Y}} \boldsymbol{\Gamma}^0(\boldsymbol{x} - \boldsymbol{y}) \boldsymbol{A}^0 \boldsymbol{f}(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y},$$

is a *projection* on $\mathscr{E}$, self-adjoint and independent of $\boldsymbol{A}^0$ for $\boldsymbol{A}^0 = a^0 \boldsymbol{I}$ with $a^0 \neq 0$, i.e.

$$\big(\mathcal{G}[\boldsymbol{u}], \boldsymbol{v}\big)_{L^2(\mathcal{Y};\mathbb{R}^d)} = \big(\boldsymbol{u}, \mathcal{G}[\boldsymbol{v}]\big)_{L^2(\mathcal{Y};\mathbb{R}^d)} \quad \forall \boldsymbol{u}, \boldsymbol{v} \in L^2_{\mathrm{per}}(\mathcal{Y}; \mathbb{R}^d)$$

and

$$\widehat{\mathcal{G}}(\boldsymbol{k}) = \begin{cases} \boldsymbol{0} & \boldsymbol{k} = \boldsymbol{0} \\ \dfrac{\boldsymbol{\xi}(\boldsymbol{k}) \otimes \boldsymbol{\xi}(\boldsymbol{k})}{\boldsymbol{\xi}(\boldsymbol{k}) \cdot \boldsymbol{\xi}(\boldsymbol{k})} & \boldsymbol{k} \in \mathbb{Z}^d \backslash \{\boldsymbol{0}\}, \xi_\alpha = \frac{k_\alpha}{Y_\alpha}, \alpha = 1, \ldots, d \end{cases}$$

Weak formulation of unit cell problem

Properties of projection operator $\mathcal{G}$)

- Curl-free – from construction
- Zero-mean – $\widehat{\mathcal{G}}(\mathbf{0}) = \mathbf{0}$
- Indendence of a^0 –

$$\frac{\boldsymbol{\xi}(\boldsymbol{k}) \otimes \boldsymbol{\xi}(\boldsymbol{k}) a^0}{a^0 \boldsymbol{\xi}(\boldsymbol{k}) \cdot \boldsymbol{\xi}(\boldsymbol{k})}$$

- Projection – $(\boldsymbol{k} \neq \mathbf{0})$

$$\frac{\boldsymbol{\xi}(\boldsymbol{k}) \otimes \boldsymbol{\xi}(\boldsymbol{k})}{\boldsymbol{\xi}(\boldsymbol{k}) \cdot \boldsymbol{\xi}(\boldsymbol{k})} \frac{\boldsymbol{\xi}(\boldsymbol{k}) \otimes \boldsymbol{\xi}(\boldsymbol{k})}{\boldsymbol{\xi}(\boldsymbol{k}) \cdot \boldsymbol{\xi}(\boldsymbol{k})} = \frac{\boldsymbol{\xi}(\boldsymbol{k}) \otimes \boldsymbol{\xi}(\boldsymbol{k})}{\boldsymbol{\xi}(\boldsymbol{k}) \cdot \boldsymbol{\xi}(\boldsymbol{k})}$$

- Self-adjointness – apply the Plancherel theorem

$$\Big(\frac{\boldsymbol{\xi}(\boldsymbol{k}) \otimes \boldsymbol{\xi}(\boldsymbol{k})}{\boldsymbol{\xi}(\boldsymbol{k}) \cdot \boldsymbol{\xi}(\boldsymbol{k})} \widehat{\boldsymbol{u}}(\boldsymbol{k})\Big) \cdot \widehat{\boldsymbol{v}}(-\boldsymbol{k}) = \widehat{\boldsymbol{u}}(\boldsymbol{k}) \cdot \Big(\frac{\boldsymbol{\xi}(-\boldsymbol{k}) \otimes \boldsymbol{\xi}(-\boldsymbol{k})}{\boldsymbol{\xi}(-\boldsymbol{k}) \cdot \boldsymbol{\xi}(-\boldsymbol{k})} \widehat{\boldsymbol{v}}(-\boldsymbol{k})\Big)$$

- e.g., integral $\Rightarrow$ weak

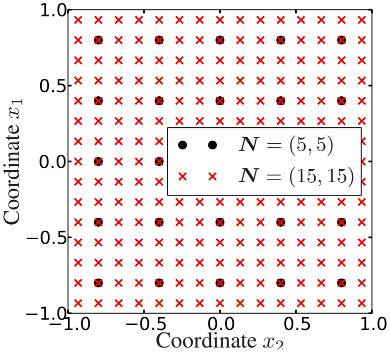
$$\begin{aligned}
\boldsymbol{e} + \mathcal{G}[(\boldsymbol{A}^0)^{-1}(\boldsymbol{A} - \boldsymbol{A}^0)\boldsymbol{e}] &= \boldsymbol{E} \quad \text{(Lippmann-Schwinger)} \\
\mathcal{G}[\boldsymbol{e}] &= \boldsymbol{e}^* \quad (\mathcal{G} \text{ maps to zero-mean}) \\
\mathcal{G}[(\boldsymbol{A}^0)^{-1}\boldsymbol{A}\boldsymbol{e}] &= \boldsymbol{0} \\
\big(\mathcal{G}[(\boldsymbol{A}^0)^{-1}\boldsymbol{A}\boldsymbol{e}^*], \boldsymbol{v}\big)_{L^2(\mathcal{Y};\mathbb{R}^d)} &= -\big((\boldsymbol{A}^0)^{-1}\mathcal{G}[\boldsymbol{A}\boldsymbol{E}], \boldsymbol{v}\big)_{L^2(\mathcal{Y};\mathbb{R}^d)} \\
\big((\boldsymbol{A}^0)^{-1}\boldsymbol{A}\boldsymbol{e}^*, \mathcal{G}[\boldsymbol{v}]\big)_{L^2(\mathcal{Y};\mathbb{R}^d)} &= -\big((\boldsymbol{A}^0)^{-1}\boldsymbol{A}\boldsymbol{E}, \mathcal{G}[\boldsymbol{v}]\big)_{L^2(\mathcal{Y};\mathbb{R}^d)} \\
\big(\boldsymbol{A}\boldsymbol{e}^*, \boldsymbol{v}\big)_{L^2(\mathcal{Y};\mathbb{R}^d)} &= -\big(\boldsymbol{A}\boldsymbol{E}, \boldsymbol{v}\big)_{L^2(\mathcal{Y};\mathbb{R}^d)} \quad \text{for all } \boldsymbol{v} \in \mathscr{E}
\end{aligned}$$

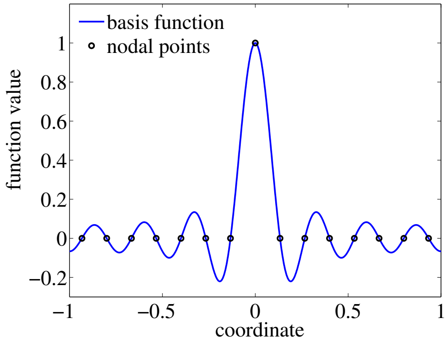
- existence of and uniqueness of the weak solution follows from Lax-Milgram lemma, under standard assumptions

$$c_A \boldsymbol{I} \preceq \boldsymbol{A}(\boldsymbol{x}) \preceq C_A \boldsymbol{I} \text{ a.e. in } \mathcal{Y}$$

Trigonometric polynomials

Saranen & Vainikko (2002)





$$\mathbb{Z}_{\boldsymbol{N}} = \left\{ \boldsymbol{k} \in \mathbb{Z}^d : -\frac{N_\alpha}{2} \leq k_\alpha \leq \frac{N_\alpha}{2}, \alpha = 1, \ldots, d \right\}$$

$$h_{\max} = \max_{\alpha} \frac{2Y_\alpha}{N_\alpha}, \quad \boldsymbol{x}^{\boldsymbol{k}} \text{ – nodal points}$$

- Technical assumption: N_α is odd

Trigonometric polynomials

Saranen & Vainikko (2002)

- Space of real-valued trigonometric polynomials

$$\mathscr{T}_{\boldsymbol{N}} = \left\{ \sum_{\boldsymbol{k}\in\mathbb{Z}_{\boldsymbol{N}}} \hat{\boldsymbol{c}}^{\boldsymbol{k}} \varphi_{\boldsymbol{k}}(\boldsymbol{x}) : \hat{\boldsymbol{c}}^{\boldsymbol{k}} \in \mathbb{C}^d, \hat{\boldsymbol{c}}^{\boldsymbol{k}} = \overline{\hat{\boldsymbol{c}}^{-\boldsymbol{k}}} \right\} \subset C^{\infty}_{\mathrm{per}}(\mathcal{Y}; \mathbb{R}^d)$$

- Two ways to represent a trigonometric polynomial $\boldsymbol{v}_{\boldsymbol{N}} \in \mathscr{T}_{\boldsymbol{N}}$
  - via Fourier coefficients

$$\boldsymbol{v}_{\boldsymbol{N}}(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathbb{Z}_{\boldsymbol{N}}} \hat{\boldsymbol{v}}_{\boldsymbol{N}}(\boldsymbol{k})\varphi_{\boldsymbol{k}}(\boldsymbol{x})$$

  - via interpolation of function values

$$\boldsymbol{v}_{\boldsymbol{N}}(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathbb{Z}_{\boldsymbol{N}}} \boldsymbol{v}_{\boldsymbol{N}}(\boldsymbol{x}^{\boldsymbol{k}})\varphi_{\boldsymbol{N},\boldsymbol{k}}(\boldsymbol{x})$$

  with

$$\varphi_{\boldsymbol{N},\boldsymbol{k}}(\boldsymbol{x}) = \frac{1}{|\boldsymbol{N}|} \sum_{\boldsymbol{m}\in\mathbb{Z}_{\boldsymbol{N}}} \exp\left\{ \mathrm{i}\pi \sum_{\alpha} m_\alpha \left(\frac{x_\alpha}{Y_\alpha} - \frac{2k_\alpha}{N_\alpha} \right) \right\} \quad \text{for } \boldsymbol{k} \in \mathbb{Z}_{\boldsymbol{N}}$$

Trigonometric polynomials

"Fourier" orthogonal projection

$\mathcal{P}_{\boldsymbol{N}} : L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d) \to \mathscr{T}_{\boldsymbol{N}}$

- Definition

$$\mathcal{P}_{\boldsymbol{N}}[\boldsymbol{f}](\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathbb{Z}_{\boldsymbol{N}}} \widehat{\boldsymbol{f}}(\boldsymbol{k})\varphi_{\boldsymbol{k}}(\boldsymbol{x})$$

- Approximation properties
  - For $\boldsymbol{f} \in L^2(\mathcal{Y};\mathbb{R}^d)$

$$\|\boldsymbol{f} - \mathcal{P}_{\boldsymbol{N}}[\boldsymbol{f}]\|_{L^2(\mathcal{Y};\mathbb{R}^d)} \to 0 \text{ as } |\boldsymbol{N}| \to \infty$$

  - For $\boldsymbol{f} \in H^s_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)$ with $s > 0$

$$\|\boldsymbol{f} - \mathcal{P}_{\boldsymbol{N}}[\boldsymbol{f}]\|_{L^2(\mathcal{Y};\mathbb{R}^d)} \le h^s_{\max}\|\boldsymbol{f}\|_{H^s(\mathcal{Y};\mathbb{R}^d)}$$

Trigonometric polynomials

Approximation properties of Fourier projection

- Convergence follows from density of $\{\varphi_{\boldsymbol{k}}\}_{\boldsymbol{k}\in\mathbb{Z}^d}$
- For more regular data

$$\begin{aligned}\left\|\boldsymbol{f}-\mathcal{P}_{\boldsymbol{N}}[\boldsymbol{f}]\right\|^2_{L^2(\mathcal{Y};\mathbb{R}^d)} &= |\mathcal{Y}|\sum_{\boldsymbol{k}\in\mathbb{Z}^d\setminus\mathbb{Z}_{\boldsymbol{N}}}\left\|\widehat{\boldsymbol{f}}(\boldsymbol{k})\right\|^2_{\mathbb{C}^d}\\ &= |\mathcal{Y}|\sum_{\boldsymbol{k}\in\mathbb{Z}^d\setminus\mathbb{Z}_{\boldsymbol{N}}}\left\|\boldsymbol{\xi}(\boldsymbol{k})\right\|^{-2s}_{\mathbb{R}^d}\left\|\boldsymbol{\xi}(\boldsymbol{k})\right\|^{2s}_{\mathbb{R}^d}\left\|\widehat{\boldsymbol{f}}(\boldsymbol{k})\right\|^2_{\mathbb{C}^d}\\ &\leq |\mathcal{Y}|h^{2s}_{\max}\sum_{\boldsymbol{k}\in\mathbb{Z}^d\setminus\mathbb{Z}_{\boldsymbol{N}}}\left\|\boldsymbol{\xi}(\boldsymbol{k})\right\|^{2s}_{\mathbb{R}^d}\left\|\widehat{\boldsymbol{f}}(\boldsymbol{k})\right\|^2_{\mathbb{C}^d}\\ &\leq h^{2s}_{\max}\left\|\boldsymbol{f}\right\|^2_{H^s(\mathcal{Y};\mathbb{R}^d)}\end{aligned}$$

Trigonometric polynomials
Interpolation projection

$\mathcal{Q}_{\boldsymbol{N}} : C_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d) \to \mathscr{T}_{\boldsymbol{N}}$

- Definition

$$\mathcal{Q}_{\boldsymbol{N}}[\boldsymbol{f}](\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathbb{Z}_{\boldsymbol{N}}} \boldsymbol{f}(\boldsymbol{x}^{\boldsymbol{k}})\varphi_{\boldsymbol{N},\boldsymbol{k}}(\boldsymbol{x})$$

- Approximation properties
  - For $\boldsymbol{f} \in H^s_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)$ with $s > d/2$

$$\|\boldsymbol{f} - \mathcal{P}_{\boldsymbol{N}}[\boldsymbol{f}]\|_{L^2(\mathcal{Y};\mathbb{R}^d)} \leq Ch^s_{\max}\|\boldsymbol{f}\|_{H^s(\mathcal{Y};\mathbb{R}^d)}$$

(constant C can be made explicit)

- Proof proceeds analogously as for $\mathcal{P}_{\boldsymbol{N}}$ (but is more tedious)

Galerkin method

Without variational crimes

- Approximation space: $\mathscr{E}_{\boldsymbol{N}} = \mathscr{T}_{\boldsymbol{N}} \cap \mathscr{E} = \mathcal{P}_{\boldsymbol{N}}[\mathscr{E}]$

Galerkin approximation

Find $\boldsymbol{e}^*_{\boldsymbol{N}} \in \mathscr{E}_{\boldsymbol{N}}$ such that

$$\left(\boldsymbol{A}\boldsymbol{e}^*_{\boldsymbol{N}}, \boldsymbol{v}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} = -\left(\boldsymbol{A}\boldsymbol{E}, \boldsymbol{v}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} \quad \forall \boldsymbol{v} \in \mathscr{E}_{\boldsymbol{N}} \qquad \text{(Ga)}$$

- Qualitative properties
  - Existence – from Lax-Milgram lemma
  - Convergence – from Cea lemma

$$\left\|\boldsymbol{e}^*_{\boldsymbol{N}} - \boldsymbol{e}^*\right\|_{L^2(\mathcal{Y};\mathbb{R}^d)} \leq \frac{C_A}{c_A} \inf_{\boldsymbol{v}_{\boldsymbol{N}} \in \mathscr{E}_{\boldsymbol{N}}} \left\|\boldsymbol{e}^* - \boldsymbol{v}_{\boldsymbol{N}}\right\|_{L^2(\mathcal{Y};\mathbb{R}^d)}$$
$$\leq \frac{C_A}{c_A} \left\|\boldsymbol{e}^* - \mathcal{P}_{\boldsymbol{N}}[\boldsymbol{e}^*]\right\|_{L^2(\mathcal{Y};\mathbb{R}^d)}$$

  - Rate of convergence for sufficiently regular solution, i.e. $\boldsymbol{e}^* \in H^s(\mathcal{Y}; \mathbb{R}^d)$

Galerkin method

With variational crimes

- Previous framework is elegant, but scalar products are difficult to evaluate exactly
- Integration rule for trigonometric polynomials $\boldsymbol{u_N}, \boldsymbol{v_N} \in \mathscr{T}_{\boldsymbol{N}}$

$$\left(\boldsymbol{u_N}, \boldsymbol{v_N}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} = \frac{|\mathcal{Y}|}{|\boldsymbol{N}|} \sum_{\boldsymbol{k}\in\mathbb{Z}_{\boldsymbol{N}}} \left(\boldsymbol{u_N}(\boldsymbol{x^k}), \boldsymbol{v_N}(\boldsymbol{x^k})\right)_{\mathbb{R}^d}$$

- Standard estimates still valid when the forms are evaluated approximately

$$\left(\boldsymbol{A}\boldsymbol{u_N}, \boldsymbol{v_N}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} \approx \left(\mathcal{Q}_{\boldsymbol{N}}[\boldsymbol{A}\boldsymbol{e}^*_{\boldsymbol{N}}], \boldsymbol{v_N}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)}$$

$$\left(\boldsymbol{A}\boldsymbol{E}, \boldsymbol{v_N}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} \approx \left(\mathcal{Q}_{\boldsymbol{N}}[\boldsymbol{A}\boldsymbol{E}], \boldsymbol{v_N}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)}$$

Galerkin methods

Galerkin approximation with numerical integration

Find $\boldsymbol{e}^*_{\boldsymbol{N}} \in \mathcal{V}_{\boldsymbol{N}}$ such that

$$\left(\mathcal{Q}_{\boldsymbol{N}}[\boldsymbol{A}\boldsymbol{e}^*_{\boldsymbol{N}}], \boldsymbol{v}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} = -\left(\mathcal{Q}_{\boldsymbol{N}}[\boldsymbol{A}\boldsymbol{E}], \boldsymbol{v}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} \quad \forall \boldsymbol{v} \in \mathscr{E}_{\boldsymbol{N}} \qquad \text{(GaNi)}$$

- Existence – from Lax-Milgram lemma
- Convergence – from (similar, but more tedious)
  - Second Strang lemma
  - Orthogonal projection
  - Interpolation projection
- Rate of convergence for sufficiently regular solutions
- Requires higher regularity of data, namely

$$\boldsymbol{A} \in W^{s,\infty}_{\mathrm{per}} \text{ with } s > d/2$$

- Admits fully discrete representation

- Fully discrete space

$$\mathbb{E}_{\boldsymbol{N}} = \{\mathbf{v} \in \mathbb{R}^{d\times \boldsymbol{N}} : \sum_{\boldsymbol{k}\in\mathbb{Z}_{\boldsymbol{N}}} \mathbf{v}^{\boldsymbol{k}} \varphi_{\boldsymbol{N},\boldsymbol{k}}(\boldsymbol{x}) \in \mathscr{E}_{\boldsymbol{N}}\}$$

- Evaluation of scalar products

$$\left(\mathcal{Q}_{\boldsymbol{N}}[\boldsymbol{A}\boldsymbol{e}^*_{\boldsymbol{N}}], \boldsymbol{v}_{\boldsymbol{N}}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} = \frac{|\mathcal{Y}|}{|\boldsymbol{N}|}\left(\mathbf{A}\mathbf{e}^*, \mathbf{v}\right)_{\mathbb{R}^{d\times\boldsymbol{N}}}$$

$$\left(\mathcal{Q}_{\boldsymbol{N}}[\boldsymbol{A}\boldsymbol{E}], \boldsymbol{v}_{\boldsymbol{N}}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} = \frac{|\mathcal{Y}|}{|\boldsymbol{N}|}\left(\mathbf{A}\mathbf{E}, \mathbf{v}\right)_{\mathbb{R}^{d\times\boldsymbol{N}}}$$

with sparse representations

$$\mathbf{A} = \begin{bmatrix} \mathsf{A}_{11} & \mathsf{A}_{12} & \mathsf{A}_{13} \\ \mathsf{A}_{12} & \mathsf{A}_{22} & \mathsf{A}_{23} \\ \mathsf{A}_{13} & \mathsf{A}_{23} & \mathsf{A}_{33} \end{bmatrix}, \quad \mathbf{e}^* = \begin{bmatrix} \mathsf{e}^*_1 \\ \mathsf{e}^*_2 \\ \mathsf{e}^*_3 \end{bmatrix}, \quad \mathbf{E} = \begin{bmatrix} \mathsf{E}_1 \\ \mathsf{E}_2 \\ \mathsf{E}_3 \end{bmatrix}, \quad \mathbf{v} = \begin{bmatrix} \mathsf{v}_1 \\ \mathsf{v}_2 \\ \mathsf{v}_3 \end{bmatrix}$$

- Recall that $\boldsymbol{A}^0 = a^0 \boldsymbol{I}$ with $a^0 \neq 0 \Rightarrow \mathcal{G}^0 \to \mathcal{G}$
- Discrete projection operator onto $\mathbb{E}_{\boldsymbol{N}}$: $\mathbf{G} = \mathbf{F}\widehat{\mathbf{G}}\mathbf{F}^{-1}$ with sparse representation

$$\mathbf{F} = \begin{bmatrix} \mathsf{F} & 0 & 0 \\ 0 & \mathsf{F} & 0 \\ 0 & 0 & \mathsf{F} \end{bmatrix}, \quad \widehat{\mathbf{G}} = \begin{bmatrix} \widehat{\mathsf{G}}_{11} & \widehat{\mathsf{G}}_{12} & \widehat{\mathsf{G}}_{13} \\ \widehat{\mathsf{G}}_{12} & \widehat{\mathsf{G}}_{22} & \widehat{\mathsf{G}}_{23} \\ \widehat{\mathsf{G}}_{13} & \widehat{\mathsf{G}}_{23} & \widehat{\mathsf{G}}_{33} \end{bmatrix}$$

  with the action of F implemented using FFT.
- $\mathbf{G}$ inherits all properties of $\mathcal{G}$
- Fully discrete formulation

$$\begin{aligned} \left(\mathbf{Ae}^*, \mathbf{v}\right)_{\mathbb{R}^{d\times \boldsymbol{N}}} &= -\left(\mathbf{AE}, \mathbf{v}\right)_{\mathbb{R}^{d\times \boldsymbol{N}}} && \forall \mathbf{v} \in \mathbb{E}_{\boldsymbol{N}} \\ \left(\mathbf{Ae}^*, \mathbf{Gv}\right)_{\mathbb{R}^{d\times \boldsymbol{N}}} &= -\left(\mathbf{AE}, \mathbf{Gv}\right)_{\mathbb{R}^{d\times \boldsymbol{N}}} && \forall \mathbf{v} \in \mathbb{R}^{d\times \boldsymbol{N}} \\ \left(\mathbf{GAe}^*, \mathbf{v}\right)_{\mathbb{R}^{d\times \boldsymbol{N}}} &= -\left(\mathbf{GAE}, \mathbf{v}\right)_{\mathbb{R}^{d\times \boldsymbol{N}}} && \forall \mathbf{v} \in \mathbb{R}^{d\times \boldsymbol{N}} \end{aligned}$$

Galerkin methods

Overview of discretization strategy

$$
\begin{array}{ccccc}
L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d) & \xmapsto{\mathcal{P}_{\boldsymbol{N}}} & \mathscr{T}^d_{\boldsymbol{N}} & \xmapsto{\mathcal{I}_{\boldsymbol{N}}} & \mathbb{R}^{d\times \boldsymbol{N}} \\
\downarrow \mathcal{G} & & \downarrow \mathcal{G} & & \downarrow \mathbf{G} \\
\mathcal{E} & \xmapsto{\mathcal{P}_{\boldsymbol{N}}} & \mathcal{E}_{\boldsymbol{N}} & \xmapsto{\mathcal{I}_{\boldsymbol{N}}} & \mathbb{E}_{\boldsymbol{N}}
\end{array}
$$

- Auxiliary operator

$$\mathcal{I}_{\boldsymbol{N}} : C_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d) \to \mathbb{R}^{d\times \boldsymbol{N}}$$

$$\mathcal{I}_{\boldsymbol{N}}[\boldsymbol{u}_{\boldsymbol{N}}] = \left(\boldsymbol{u}_{\boldsymbol{N}}(\boldsymbol{x}^{\boldsymbol{k}})\right)^{\boldsymbol{k}\in\mathbb{Z}_{\boldsymbol{N}}} \in \mathbb{R}^{d\times \boldsymbol{N}}$$

Galerkin methods

Linear system

Final result

Vector $\mathbf{e}^* \in \mathbb{E}_{\boldsymbol{N}}$ solves the system of linear equations

$$\underbrace{\mathbf{GA}}_{\mathbf{M}}\underbrace{\mathbf{e}^*}_{\mathbf{x}} = -\underbrace{\mathbf{GAE}}_{\mathbf{b}}$$

- Equivalent to discrete Lippmann-Schwinger equation from collocation
- Moulinec-Suquet FFT scheme $\equiv$ Galerkin Element method
- Very large non-symmetric system, but with sparse structure $\Rightarrow$ well-suited for iterative solvers (multiplication cost $\sim |\boldsymbol{N}| \log(|\boldsymbol{N}|)$)
- Matrix **M** is independent of $\boldsymbol{A}^0$
- Spectral radius of **M** corresponds to contrast in material properties $\rho_A \geq 1$

- GC method solves the problem

$$\mathbf{x} = \arg \min_{\mathbf{y} \in \mathbb{E}_{\boldsymbol{N}}} \frac{1}{2} \mathbf{y}^{\mathsf{T}} \mathbf{M} \mathbf{y} + \mathbf{y}^{\mathsf{T}} \mathbf{b}$$

iteratively on the Krylov subspace

$$\mathbb{K}_{(k)}(\mathbf{A}, \mathbf{r}_{(0)}) = \operatorname{span}\left\{\mathbf{r}_{(0)}, \mathbf{M}\mathbf{r}_{(0)}, \mathbf{M}^2\mathbf{r}_{(0)}, \dots, \mathbf{M}^k\mathbf{r}_{(0)}\right\}$$

with

$$\mathbf{r}_{(k)} = \mathbf{M}\mathbf{x}_{(k)} + \mathbf{b} = \mathbf{G}\mathbf{A}\left(\mathbf{x}_{(k)} + \mathbf{E}\right) \in \mathbb{E}_{\boldsymbol{N}}$$

- Therefore, $\mathbb{K}_{(0)} \subset \mathbb{K}_{(1)} \subset \mathbb{K}_{(2)} \subset \dots \mathbb{E}_{\boldsymbol{N}}$.
- Convergence rates $\sqrt{\rho_A}$ follows from standard theory orthogonal projection methods, e.g. (SAAD, 2003)

Conclusions and outlook

- Complex engineering methods may have simple structure
- Numerical results for the scalar case have been successfully explained
- Variational framework for FFT-based methods has been proposed
- Analysis exploits the underlying physics and existing engineering approaches, and results in
  - existence and approximation theory,
  - development of efficient iterative solvers,
  - treatment of even grids (not shown).
- Guaranteed error estimates $\to$ Part II
- Additional details are available at

  http://arxiv.org/abs/1311.0089

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INVESTICE DO ROZVOJE VZDĚLÁVÁNÍ