FFT-based Galerkin method for homogenization of periodic media - Part II

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Outline

1. Homogenized matrix
   - Primal and dual cell formulations
   - Helmholtz decomposition
   - Duality arguments
   - Basic properties
   - Fourier-Galerkin method
2. Guaranteed error bounds
   - Two-sided bounds
   - Error estimate
   - Computational issues
   - Integration rule
3. Examples
4. Conclusions and outlook

Cell problem revisited
(MILTON, 2002)

Primal and dual form

Find the matrix $\boldsymbol{A}_{\text{eff}} \in \mathbb{R}^{d\times d}$ satisfying

$$\left(\boldsymbol{A}_{\text{eff}}\boldsymbol{E}, \boldsymbol{E}\right)_{\mathbb{R}^d} = \min_{\boldsymbol{v}\in\mathscr{E}} \frac{1}{|\mathcal{Y}|}\left(\boldsymbol{A}(\boldsymbol{E}+\boldsymbol{v}), \boldsymbol{E}+\boldsymbol{v}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} \tag{P}$$

$$\left(\boldsymbol{A}_{\text{eff}}^{-1}\boldsymbol{J}, \boldsymbol{J}\right)_{\mathbb{R}^d} = \min_{\boldsymbol{w}\in\mathscr{J}} \frac{1}{|\mathcal{Y}|}\left(\boldsymbol{A}^{-1}(\boldsymbol{J}+\boldsymbol{w}), \boldsymbol{J}+\boldsymbol{w}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)} \tag{D}$$

for arbitrary $\boldsymbol{E}$ and $\boldsymbol{J} \in \mathbb{R}^d$, with

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

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

$L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)$ revisited
(MILTON, 2002)

- Helmholtz decomposition

$$L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d) = \mathbb{R}^d \oplus \mathscr{E} \oplus \mathscr{J}$$

- Projection operators (Fourier representation)

$$\widehat{\mathcal{G}}^{(0)}(\boldsymbol{k}) = \begin{cases} \boldsymbol{I} & \boldsymbol{k} = \boldsymbol{0} \\ \boldsymbol{0} \otimes \boldsymbol{0} & \boldsymbol{k} \in \mathbb{Z}^d \backslash \{\boldsymbol{0}\} \end{cases} \qquad \mathcal{G}^{(0)} : L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d) \to \mathbb{R}^d$$

$$\widehat{\mathcal{G}}^{(1)}(\boldsymbol{k}) = \begin{cases} \boldsymbol{0} \otimes \boldsymbol{0} & \boldsymbol{k} = \boldsymbol{0} \\ \frac{\boldsymbol{\xi}(\boldsymbol{k}) \otimes \boldsymbol{\xi}(\boldsymbol{k})}{\boldsymbol{\xi}(\boldsymbol{k}) \cdot \boldsymbol{\xi}(\boldsymbol{k})} & \boldsymbol{k} \in \mathbb{Z}^d \backslash \{\boldsymbol{0}\} \end{cases} \qquad \mathcal{G}^{(1)} : L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d) \to \mathscr{E}$$

$$\widehat{\mathcal{G}}^{(2)}(\boldsymbol{k}) = \begin{cases} \boldsymbol{0} \otimes \boldsymbol{0} & \boldsymbol{k} = \boldsymbol{0} \\ \boldsymbol{I} - \frac{\boldsymbol{\xi}(\boldsymbol{k}) \otimes \boldsymbol{\xi}(\boldsymbol{k})}{\boldsymbol{\xi}(\boldsymbol{k}) \cdot \boldsymbol{\xi}(\boldsymbol{k})} & \boldsymbol{k} \in \mathbb{Z}^d \backslash \{\boldsymbol{0}\} \end{cases} \qquad \mathcal{G}^{(2)} : L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d) \to \mathscr{J}$$

- Inner product

$$\left(\boldsymbol{u}, \boldsymbol{v}\right)_{L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)} := \frac{1}{|\mathcal{Y}|}\left(\boldsymbol{u}, \boldsymbol{v}\right)_{L^2(\mathcal{Y};\mathbb{R}^d)}$$

(P) = (D)

Perturbation-duality theorem (Ekeland and Temam, 1976)

Let $F : \mathscr{V} \to \mathbb{R}$ be a functional on a Hilbert space $\mathscr{V}$. Consider a Hilbert perturbation space $\mathscr{W}$ and a perturbation functional $\Phi : \mathscr{V} \times \mathscr{W} \to \mathbb{R}$, satisfying $F(\boldsymbol{v}) = \Phi(\boldsymbol{v}, \boldsymbol{0})$. Then

$$\min_{\boldsymbol{v}\in\mathscr{V}} F(\boldsymbol{v}) = \min_{\boldsymbol{v}\in\mathscr{V}} \Phi(\boldsymbol{v}, \boldsymbol{0}) = -\max_{\boldsymbol{w}^{\#}\in\mathscr{W}^{\#}} \Phi^{\#}(0; \boldsymbol{w}^{\#})$$

provided that F and Φ are convex, continuous and coercive on $\mathscr{V}$ and $\mathscr{V} \times \mathscr{W}$. Here, $\Phi^{\#} : \mathscr{V}^{\#} \times \mathscr{W}^{\#} \to \mathbb{R}$ is the Fenchel conjugate

$$\Phi^{\#}(\boldsymbol{v}^{\#}; \boldsymbol{w}^{\#}) = \max_{(\boldsymbol{v},\boldsymbol{w})\in\mathscr{V}\times\mathscr{W}} \left[\left\langle \boldsymbol{v}^{\#}, \boldsymbol{v} \right\rangle_{\mathscr{V}^{\#}\times\mathscr{V}} + \left\langle \boldsymbol{w}^{\#}, \boldsymbol{w} \right\rangle_{\mathscr{W}^{\#}\times\mathscr{W}} - \Phi(\boldsymbol{v}, \boldsymbol{w}) \right]$$

(P) = (D)

After Dvořák (1995)

- In our case

$$F(\boldsymbol{v}) = \frac{1}{2}\big(\boldsymbol{A}(\boldsymbol{E}+\boldsymbol{v}), \boldsymbol{E}+\boldsymbol{v}\big)_{L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)}$$

$$\Phi(\boldsymbol{v},\boldsymbol{w}) = \frac{1}{2}\big(\boldsymbol{A}(\boldsymbol{E}+\boldsymbol{v}+\boldsymbol{w}), \boldsymbol{E}+\boldsymbol{v}+\boldsymbol{w}\big)_{L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)}$$

$$\mathscr{V} = \mathscr{V}^{\#} = \mathscr{E}$$

$$\mathscr{W} = \mathscr{W}^{\#} = L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)$$

- Dual functional

$$\Phi^{\#}(\boldsymbol{0},\boldsymbol{w}^{\#}) = \max_{(\boldsymbol{v},\boldsymbol{w})\in\mathscr{V}\times\mathscr{W}} \Big[\big(\boldsymbol{w}^{\#},\boldsymbol{w}\big)_{L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)} - \Phi(\boldsymbol{v},\boldsymbol{w})\Big]$$

- Substitute $\boldsymbol{w}' = \boldsymbol{E} + \boldsymbol{v} + \boldsymbol{w}$

$$
\begin{aligned}
-\Phi^{\#}(\mathbf{0}, \boldsymbol{w}^{\#}) &= - \max_{(\boldsymbol{v},\boldsymbol{w}')\in\mathscr{V}\times\mathscr{W}} \left[\left(\boldsymbol{w}^{\#}, \boldsymbol{w}' - \boldsymbol{E} - \boldsymbol{v}\right)_{L^2_{\mathrm{per}}} - \frac{1}{2}\left(\boldsymbol{A}\boldsymbol{w}', \boldsymbol{w}'\right)_{L^2_{\mathrm{per}}} \right] \\
&= \left(\boldsymbol{w}^{\#}, \boldsymbol{E}\right)_{L^2_{\mathrm{per}}} + \min_{\boldsymbol{v}\in\mathscr{V}} \left(\boldsymbol{w}^{\#}, \boldsymbol{v}\right)_{L^2_{\mathrm{per}}} \\
&\quad - \max_{\boldsymbol{w}'\in\mathscr{W}} \left[\left(\boldsymbol{w}^{\#}, \boldsymbol{w}'\right)_{L^2_{\mathrm{per}}} - \frac{1}{2}\left(\boldsymbol{A}\boldsymbol{w}', \boldsymbol{w}'\right)_{L^2_{\mathrm{per}}} \right]
\end{aligned}
$$

- By Helmholtz

$$
\min_{\boldsymbol{v}\in\mathscr{V}} \left(\boldsymbol{w}^{\#}, \boldsymbol{v}\right)_{L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)} = \begin{cases} 0 & \text{if } \boldsymbol{w}^{\#} \in \mathbb{R}^d \times \mathscr{J} \\ -\infty & \text{otherwise} \end{cases}
$$

(P) = (D)
After DVOŘÁK (1995)

- By Lax-Milgram

$$\max_{\boldsymbol{w}'\in\mathscr{W}}\left[\left(\boldsymbol{w}^{\#},\boldsymbol{w}'\right)_{L^2_{\mathrm{per}}}-\frac{1}{2}\left(\boldsymbol{A}\boldsymbol{w}',\boldsymbol{w}'\right)_{L^2_{\mathrm{per}}}\right]=\frac{1}{2}\left(\boldsymbol{A}^{-1}\boldsymbol{w}^{\#},\boldsymbol{w}^{\#}\right)_{L^2_{\mathrm{per}}}$$

- Thus

$$\left(\boldsymbol{A}_{\mathrm{eff}}\boldsymbol{E},\boldsymbol{E}\right)_{\mathbb{R}^d}=\max_{\boldsymbol{w}^{\#}\in\mathbb{R}^d\times\mathscr{J}}\left[2\left(\boldsymbol{w}^{\#},\boldsymbol{E}\right)_{L^2_{\mathrm{per}}}-\left(\boldsymbol{A}^{-1}\boldsymbol{w}^{\#},\boldsymbol{w}^{\#}\right)_{L^2_{\mathrm{per}}}\right]$$

- Decompose $\boldsymbol{w}^{\#}=\boldsymbol{J}+\boldsymbol{w}$, with $\boldsymbol{J}\in\mathbb{R}^d$ and $\boldsymbol{w}\in\mathscr{J}$

$$\left(\boldsymbol{A}_{\mathrm{eff}}\boldsymbol{E},\boldsymbol{E}\right)_{\mathbb{R}^d}=\max_{\boldsymbol{J}\in\mathbb{R}^d}\left[2\left(\boldsymbol{J},\boldsymbol{E}\right)_{L^2_{\mathrm{per}}}-\min_{\boldsymbol{w}\in\mathscr{J}}\left(\boldsymbol{A}^{-1}(\boldsymbol{J}+\boldsymbol{w}),(\boldsymbol{J}+\boldsymbol{w})\right)_{L^2_{\mathrm{per}}}\right]$$

(P) = (D)

After DVOŘÁK (1995)

- Set

$$\big(\boldsymbol{B}_{\text{eff}}\boldsymbol{J},\boldsymbol{J}\big)_{\mathbb{R}^d} := \min_{\boldsymbol{w}\in\mathscr{J}}\big(\boldsymbol{A}^{-1}(\boldsymbol{J}+\boldsymbol{w}),(\boldsymbol{J}+\boldsymbol{w})\big)_{L^2_{\text{per}}}$$

  so that

$$\big(\boldsymbol{A}_{\text{eff}}\boldsymbol{E},\boldsymbol{E}\big)_{\mathbb{R}^d} = \max_{\boldsymbol{J}\in\mathbb{R}^d}\Big[2\big(\boldsymbol{J},\boldsymbol{E}\big)_{L^2_{\text{per}}} - \big(\boldsymbol{B}_{\text{eff}}\boldsymbol{J},\boldsymbol{J}\big)_{\mathbb{R}^d}\Big]$$

- Optimality conditions

$$\boldsymbol{E} = \boldsymbol{B}_{\text{eff}}\boldsymbol{J} \qquad (\star)$$

$$\big(\boldsymbol{A}_{\text{eff}}\boldsymbol{E},\boldsymbol{E}\big)_{\mathbb{R}^d} = \big((\boldsymbol{B}_{\text{eff}})^{-1}\boldsymbol{E},\boldsymbol{E}\big)_{\mathbb{R}^d}$$

- Therefore, $\boldsymbol{A}_{\text{eff}} = (\boldsymbol{B}_{\text{eff}})^{-1}$

- Voigt-Reuss-Hill bounds

$$\left(\frac{1}{|\mathcal{Y}|}\int_{\mathcal{Y}} \boldsymbol{A}^{-1}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}\right)^{-1} \preceq \boldsymbol{A}_{\text{eff}} \preceq \frac{1}{|\mathcal{Y}|}\int_{\mathcal{Y}} \boldsymbol{A}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$

- By linearity
  - $\boldsymbol{e}^{*} \in \mathscr{E}$ – Minimizer of (P) for a given $\boldsymbol{E}$
  - $\boldsymbol{e}^{*(\alpha)} \in \mathscr{E}$ – Minimizer of (P) for $\boldsymbol{E} = \boldsymbol{\epsilon}^{(\alpha)} = (\delta_{\alpha\beta})_{\beta=1}^{d}$, so that $\boldsymbol{e}^{*} = \sum_{\alpha} E_{\alpha}\boldsymbol{e}^{*(\alpha)}$
  - $\boldsymbol{\jmath}^{*} \in \mathscr{J}$ and $\boldsymbol{\jmath}^{*(\alpha)} \in \mathscr{J}$ defined by analogy
- Matrix entries

$$(\boldsymbol{A}_{\text{eff}})_{\alpha\beta} = \left(\boldsymbol{A}(\boldsymbol{\epsilon}^{(\alpha)} + \boldsymbol{e}^{*(\alpha)}), \boldsymbol{\epsilon}^{(\beta)} + \boldsymbol{e}^{*(\beta)}\right)_{L^2_{\text{per}}(\mathcal{Y};\mathbb{R}^d)}$$

$$(\boldsymbol{A}^{-1}_{\text{eff}})_{\alpha\beta} = \left(\boldsymbol{A}^{-1}(\boldsymbol{\epsilon}^{(\alpha)} + \boldsymbol{\jmath}^{*(\alpha)}), \boldsymbol{\epsilon}^{(\beta)} + \boldsymbol{\jmath}^{*(\beta)}\right)_{L^2_{\text{per}}(\mathcal{Y};\mathbb{R}^d)}$$

Homogenized matrix A_{eff}

There is a free lunch

- Constitutive equation and ($\star$)

$$\boldsymbol{J} + \boldsymbol{\jmath}^*(\boldsymbol{x}) = \boldsymbol{A}(\boldsymbol{x})\left[\boldsymbol{E} + \boldsymbol{e}^*(\boldsymbol{x})\right] \qquad \boldsymbol{E} = \boldsymbol{A}_{\text{eff}}^{-1}\boldsymbol{J}$$

- Dual solution is for free

$$\boldsymbol{\epsilon}^{(\beta)} + \boldsymbol{\jmath}^{*(\beta)} = \boldsymbol{A}(\boldsymbol{x})\left[\sum_{\alpha=1}^{d}\boldsymbol{\epsilon}^{(\alpha)} + E_\alpha \boldsymbol{e}^{*(\alpha)}\right] \text{ with } \boldsymbol{E} = \boldsymbol{A}_{\text{eff}}^{-1}\boldsymbol{\epsilon}^{(\beta)}$$

Only d solutions are needed to resolve (P) + (D) completely

Approximate homogenized matrix

Fourier-Galerkin method with numerical integration

- Finite-dimensional spaces (N_α is odd)

$$\mathscr{E}_{\boldsymbol{N}} = \mathcal{P}_{\boldsymbol{N}}[\mathscr{E}], \quad \mathscr{J}_{\boldsymbol{N}} = \mathcal{P}_{\boldsymbol{N}}[\mathscr{J}], \quad \mathscr{T}^d_{\boldsymbol{N}} = \mathbb{R}^d \oplus \mathscr{E}_{\boldsymbol{N}} \oplus \mathscr{J}_{\boldsymbol{N}}$$

Galerkin approximations

For all $\boldsymbol{E}$ and $\boldsymbol{J} \in \mathbb{R}^d$, solve

$$\left(\boldsymbol{A}_{\mathrm{eff},\boldsymbol{N}}\boldsymbol{E}, \boldsymbol{E}\right)_{\mathbb{R}^d} = \min_{\boldsymbol{v}_{\boldsymbol{N}} \in \mathscr{E}_{\boldsymbol{N}}} \left(\mathcal{Q}_{\boldsymbol{N}}[\boldsymbol{A}(\boldsymbol{E} + \boldsymbol{v}_{\boldsymbol{N}})], \boldsymbol{E} + \boldsymbol{v}_{\boldsymbol{N}}\right)_{L^2_{\mathrm{per}}} \qquad (\mathrm{P}_{\boldsymbol{N}})$$

$$\left(\boldsymbol{A}^{-1}_{\mathrm{eff},\boldsymbol{N}}\boldsymbol{J}, \boldsymbol{J}\right)_{\mathbb{R}^d} = \min_{\boldsymbol{w}_{\boldsymbol{N}} \in \mathscr{J}_{\boldsymbol{N}}} \left(\mathcal{Q}_{\boldsymbol{N}}[\boldsymbol{A}^{-1}(\boldsymbol{J} + \boldsymbol{w}_{\boldsymbol{N}})], \boldsymbol{J} + \boldsymbol{w}_{\boldsymbol{N}}\right)_{L^2_{\mathrm{per}}} \qquad (\mathrm{D}_{\boldsymbol{N}})$$

- By discrete Helmholtz and duality theory
  - the approximations are equivalent
  - solution to the dual problem is for free
  - only d calculations are needed to resolve ($\mathrm{P}_{\boldsymbol{N}}$) + ($\mathrm{D}_{\boldsymbol{N}}$) completely

Guaranteed error bounds

Computable values (DVOŘÁK, 1995; WIECKOWSKI, 1995)

- How far is $\boldsymbol{A}_{\text{eff}}$ from $\boldsymbol{A}_{\text{eff},\boldsymbol{N}}$?
- Upper bound from (P) and (P$_{\boldsymbol{N}}$)

$$\left(\boldsymbol{A}_{\text{eff}}\boldsymbol{E},\boldsymbol{E}\right)_{\mathbb{R}^d} = \min_{\boldsymbol{v}\in\mathscr{E}}\left(\boldsymbol{A}(\boldsymbol{E}+\boldsymbol{v}),\boldsymbol{E}+\boldsymbol{v}\right)_{L^2_{\text{per}}(\mathcal{Y};\mathbb{R}^d)}$$
$$\leq \left(\boldsymbol{A}(\boldsymbol{E}+\boldsymbol{e}^*_{\boldsymbol{N}}),\boldsymbol{E}+\boldsymbol{e}^*_{\boldsymbol{N}}\right)_{L^2_{\text{per}}(\mathcal{Y};\mathbb{R}^d)} =: \left(\overline{\boldsymbol{A}}_{\text{eff},\boldsymbol{N}}\boldsymbol{E},\boldsymbol{E}\right)_{\mathbb{R}^d}$$

- Lower bound from dual formulation

$$\left(\boldsymbol{A}^{-1}_{\text{eff}}\boldsymbol{J},\boldsymbol{J}\right)_{\mathbb{R}^d} = \min_{\boldsymbol{w}\in\mathscr{J}}\left(\boldsymbol{A}^{-1}(\boldsymbol{J}+\boldsymbol{w}),\boldsymbol{J}+\boldsymbol{w}\right)_{L^2_{\text{per}}(\mathcal{Y};\mathbb{R}^d)}$$
$$\leq \left(\boldsymbol{A}^{-1}(\boldsymbol{J}+\boldsymbol{\jmath}^*_{\boldsymbol{N}}),\boldsymbol{J}+\boldsymbol{\jmath}^*_{\boldsymbol{N}}\right)_{L^2_{\text{per}}(\mathcal{Y};\mathbb{R}^d)} = \left(\underline{\boldsymbol{A}}^{-1}_{\text{eff},\boldsymbol{N}}\boldsymbol{J},\boldsymbol{J}\right)_{\mathbb{R}^d}$$

- Guaranteed bounds (in d computations)

$$\underline{\boldsymbol{A}}_{\text{eff},\boldsymbol{N}} \preceq \boldsymbol{A}_{\text{eff}} \preceq \overline{\boldsymbol{A}}_{\text{eff},\boldsymbol{N}}$$

Guaranteed error bounds

Error estimate (Dvořák, 1995)

Convergence result

Let $c_A \boldsymbol{I} \preceq \boldsymbol{A} \preceq C_A \boldsymbol{I}$ with $0 < c_A \leq C_A$. Then

$$\operatorname{tr}\left(\overline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}} - \underline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}}\right) \leq C_A \sum_{\alpha} \left\| \boldsymbol{e}^{*(\alpha)} - \boldsymbol{e}_{\boldsymbol{N}}^{*(\alpha)} \right\|^2_{L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)} + \frac{(\operatorname{tr} \boldsymbol{A}_{\mathrm{eff}})^2}{c_A} \sum_{\alpha} \left\| \boldsymbol{\jmath}^{*(\alpha)} - \boldsymbol{\jmath}_{\boldsymbol{N}}^{*(\alpha)} \right\|^2_{L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)}$$

- From Part I:

$$\operatorname{tr}\left(\overline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}} - \underline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}}\right) \approx C h_{\max}^{2s} \text{ for } \boldsymbol{e}^{*(\alpha)} \in H^s_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)$$

Guaranteed error bounds

Error estimate (Dvořák, 1995)

- For $\mathbf{0} \preceq \boldsymbol{C} \preceq \boldsymbol{D}$

$$\mathrm{tr}(\boldsymbol{D} - \boldsymbol{C}) \leq (\mathrm{tr}\,\boldsymbol{D})^2\,\mathrm{tr}(\boldsymbol{C}^{-1} - \boldsymbol{D}^{-1})$$

- Thus

$$\begin{aligned}\mathrm{tr}\left(\overline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}} - \underline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}}\right) &= \mathrm{tr}\left(\overline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}} - \boldsymbol{A}_{\mathrm{eff}}\right) + \mathrm{tr}\left(\boldsymbol{A}_{\mathrm{eff}} - \underline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}}\right)\\ &\leq \mathrm{tr}(\overline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}} - \boldsymbol{A}_{\mathrm{eff}}) + (\mathrm{tr}\,\boldsymbol{A}_{\mathrm{eff}})^2\,\mathrm{tr}(\underline{\boldsymbol{A}}^{-1}_{\mathrm{eff},\boldsymbol{N}} - \boldsymbol{A}^{-1}_{\mathrm{eff}})\end{aligned}$$

- By self-adjointness of $\boldsymbol{A}$ and Galerkin orthogonality

$$\begin{aligned}\left(\boldsymbol{A}(\boldsymbol{e}^{*(\alpha)} - \boldsymbol{e}_{\boldsymbol{N}}^{*(\alpha)}), \boldsymbol{e}^{*(\alpha)} - \boldsymbol{e}_{\boldsymbol{N}}^{*(\alpha)}\right) &= (\boldsymbol{A}_{\mathrm{eff}})_{\alpha\alpha} + (\overline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}})_{\alpha\alpha}\\ &\quad - 2\left(\boldsymbol{A}(\boldsymbol{\epsilon}^{(\alpha)} + \boldsymbol{e}^{*(\alpha)}), \boldsymbol{\epsilon}^{(\alpha)} + \boldsymbol{e}_{\boldsymbol{N}}^{*(\alpha)}\right)\\ &= (\overline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}})_{\alpha\alpha} - (\boldsymbol{A}_{\mathrm{eff}})_{\alpha\alpha}\end{aligned}$$

- Scalar products in the two-sided bounds are difficult to evaluate (recall numerical integration in Part I)
- Computable approximation

$$\boldsymbol{A}(\boldsymbol{x}) \preceq \overline{\boldsymbol{A}}(\boldsymbol{x}) \text{ for } \boldsymbol{x} \in \mathcal{Y}$$

- By analogy to the 'exact' case

$$\underline{\underline{\boldsymbol{A}}}_{\mathrm{eff},\boldsymbol{N}} \preceq \underline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}} \preceq \boldsymbol{A}_{\mathrm{eff}} \preceq \overline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}} \preceq \overline{\overline{\boldsymbol{A}}}_{\mathrm{eff},\boldsymbol{N}}$$

- What are computable approximations?

$$\left(\overline{\boldsymbol{A}}\boldsymbol{u}_{\boldsymbol{N}}, \boldsymbol{v}_{\boldsymbol{N}}\right)_{L^2_{\mathrm{per}}(\mathcal{Y};\mathbb{R}^d)} \text{ for } \boldsymbol{u}_{\boldsymbol{N}}, \boldsymbol{v}_{\boldsymbol{N}} \in \mathscr{T}^d_{\boldsymbol{N}}$$

- Recall the two representations

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

- Relation between basis functions

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

- Use the double grid with $2N$ points

$$(\boldsymbol{u_N})_\alpha(\boldsymbol{v_N})_\beta(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathbb{Z}_{2\boldsymbol{N}}} (\boldsymbol{u_N}(\boldsymbol{x}_{2\boldsymbol{N}}^{\boldsymbol{k}}))_\alpha(\boldsymbol{v_N}(\boldsymbol{x}_{2\boldsymbol{N}}^{\boldsymbol{k}}))_\beta\varphi_{2\boldsymbol{N},\boldsymbol{k}}(\boldsymbol{x})$$

Guaranteed error bounds

Computing with trigonometric polynomials

- Exact integration rule

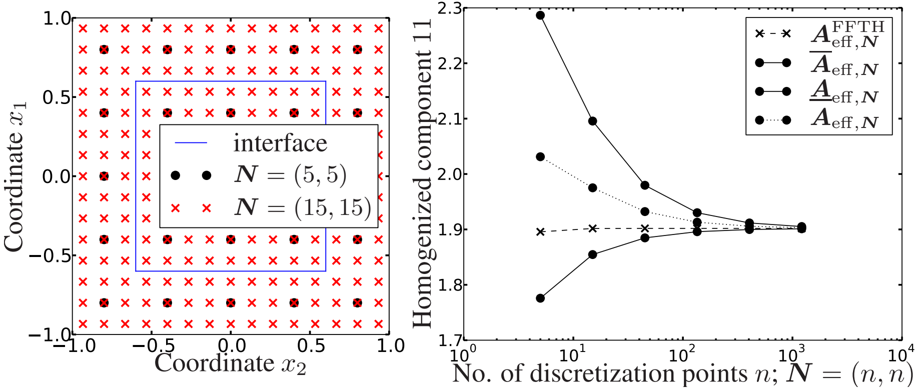
$$\left(\overline{\boldsymbol{A}}\boldsymbol{u}_{\boldsymbol{N}}, \boldsymbol{v}_{\boldsymbol{N}}\right)_{L^2_{\mathrm{per}}} = \sum_{\alpha,\beta} \sum_{\boldsymbol{k}\in\mathbb{Z}_{2\boldsymbol{N}}} \left(\overline{A}_{\alpha\beta}, \varphi_{2\boldsymbol{N},\boldsymbol{k}}\right)_{L^2_{\mathrm{per}}(\mathcal{Y})} (\boldsymbol{u}_{\boldsymbol{N}}(\boldsymbol{x}^{\boldsymbol{k}}_{2\boldsymbol{N}}))_\alpha (\boldsymbol{v}_{\boldsymbol{N}}(\boldsymbol{x}^{\boldsymbol{k}}_{2\boldsymbol{N}}))_\beta$$

$$\left(\overline{A}_{\alpha\beta}, \varphi_{2\boldsymbol{N},\boldsymbol{k}}\right)_{L^2_{\mathrm{per}}(\mathcal{Y})} = \frac{1}{|2\boldsymbol{N}|} \sum_{\boldsymbol{m}\in\mathbb{Z}_{2\boldsymbol{N}}} \omega_{\boldsymbol{N}}^{-\boldsymbol{m}\boldsymbol{k}} \left(\overline{A}_{\alpha\beta}, \varphi_{\boldsymbol{m}}\right)_{L^2_{\mathrm{per}}(\mathcal{Y})}$$

- For simple approximations (by constants, bi-linear ...), the integrals can be evaluated efficiently by FFT
- Example: Inclusion $\prod_\alpha(-L_\alpha, L_\alpha) \subset \mathcal{Y}$ with constant data

$$\left(\overline{A}_{\alpha\beta}, \varphi_{\boldsymbol{m}}\right)_{L^2_{\mathrm{per}}(\mathcal{Y})} = \overline{A}_{\alpha\beta} \prod_{\alpha}^{d} \frac{2Y_\alpha}{L_\alpha} \operatorname{sinc}\left(\frac{m_\alpha}{M_\alpha}\right)$$

Examples
Effective properties

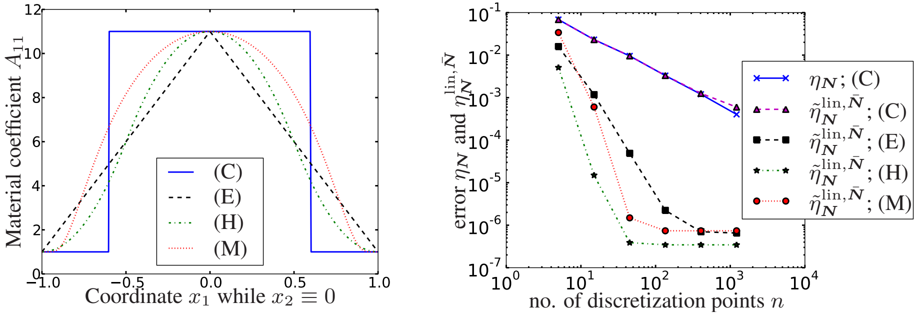


- Phase contrast set to 10^1
- Reasonable estimate

$$\frac{1}{2}\left(\overline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}} + \underline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}}\right)$$

Examples

Rates of convergence



- Increasing smoothness: $\mathrm{C} \to \mathrm{E} \to \mathrm{H} \to \mathrm{M}$
- Error norms

$$\eta_{\boldsymbol{N}} := \frac{\mathrm{tr}(\overline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}} - \underline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}})}{\mathrm{tr}(\overline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}} + \underline{\boldsymbol{A}}_{\mathrm{eff},\boldsymbol{N}})}, \qquad \tilde{\eta}_{\boldsymbol{N}} := \frac{\mathrm{tr}(\overline{\overline{\boldsymbol{A}}}_{\mathrm{eff},\boldsymbol{N}} - \underline{\underline{\boldsymbol{A}}}_{\mathrm{eff},\boldsymbol{N}})}{(\overline{\overline{\boldsymbol{A}}}_{\mathrm{eff},\boldsymbol{N}} + \underline{\underline{\boldsymbol{A}}}_{\mathrm{eff},\boldsymbol{N}})}$$

Conclusions and outlook

- Duality-based error estimates
  - Rely on the underlying physics (orthogonality)
  - Discretization is straightforward
  - Galerkin-Fourier method always produces conforming fields
- Interpolation operator can be avoided by a carefull integration on the double grid
- Possible extensions
  1. Stochastic problems
  2. Preconditioning by multi-grid
  3. More complex/real-world problems

Thank you for your patience!

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General grid

- Two index sets

$$\mathbb{Z}_{\boldsymbol{N}} = \left\{ \boldsymbol{k} \in \mathbb{Z}^d : |k_\alpha| < \frac{N_\alpha}{2} \right\}$$

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