FFT-accelerated solvers for computational micromechanics: A linear algebraic view



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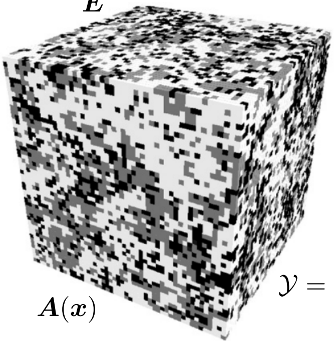
Corrector problem in (image-based) homogenization

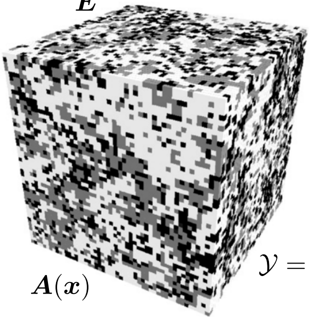


$$-\nabla \cdot \left[\boldsymbol{A}(\boldsymbol{x})\nabla u^*(\boldsymbol{x})\right] = \nabla \cdot \left[\boldsymbol{A}(\boldsymbol{x})\boldsymbol{E}\right] \text{ for } \boldsymbol{x} \in \mathcal{Y} \subset \mathbb{R}^d$$

$$u^* \text{ is periodic on } \partial\mathcal{Y}, \quad \int_{\mathcal{Y}} u^*(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = 0$$

$\hookleftarrow$ Claude Le Bris, Wednesday, 25 September (9:20, 9:36)

Reformulation using polarization

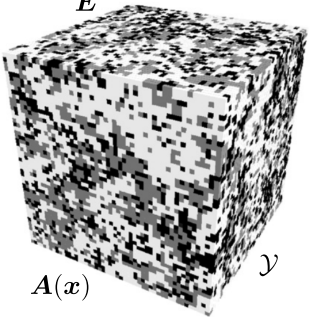


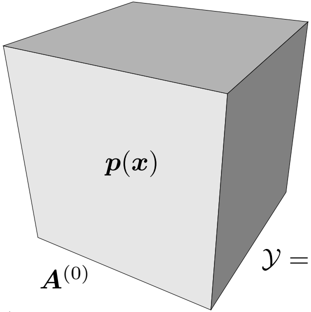
$$-\nabla \cdot \left[\left(\boldsymbol{A}(\boldsymbol{x}) - \boldsymbol{A}^{(0)} + \boldsymbol{A}^{(0)} \right) \nabla u^*(\boldsymbol{x}) \right] = \nabla \cdot \left[\left(\boldsymbol{A}(\boldsymbol{x}) - \boldsymbol{A}^{(0)} \right) \boldsymbol{E} \right] \text{ for } \boldsymbol{x} \in \mathcal{Y} \subset \mathbb{R}^d$$

$$u^* \text{ is periodic on } \partial\mathcal{Y}, \qquad \int_{\mathcal{Y}} \nabla u^*(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} = 0,$$

e.g., Z. Hashin, S. Shtrikman, *J Appl Phys* **33**, 3125 (1962)

Reformulation using polarization



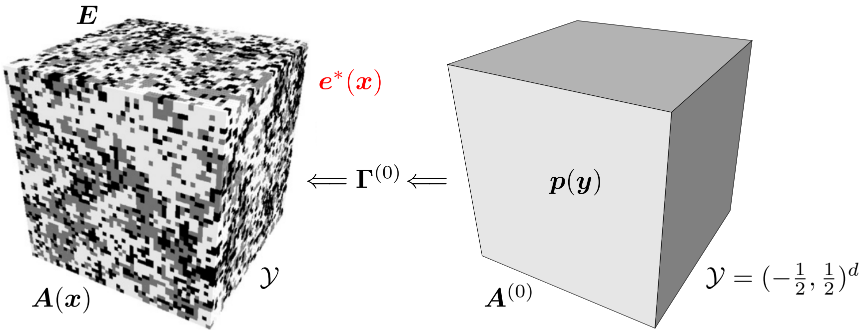


$$-\nabla \cdot \left[\boldsymbol{A}^{(0)} \boldsymbol{e}^*(\boldsymbol{x}) \right] = \nabla \cdot \overbrace{\left[\left(\boldsymbol{A}(\boldsymbol{x}) - \boldsymbol{A}^{(0)} \right) \left(\boldsymbol{E} + \boldsymbol{e}^*(\boldsymbol{x}) \right) \right]}^{\boldsymbol{p}(\boldsymbol{x})} \quad \text{for } \boldsymbol{x} \in \mathcal{Y} \subset \mathbb{R}^d$$

$$\boldsymbol{e}^* \text{ is periodic on } \partial\mathcal{Y}, \quad \int_{\mathcal{Y}} \boldsymbol{e}^*(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \boldsymbol{0}, \quad \boldsymbol{e}^* \text{ is compatible}$$

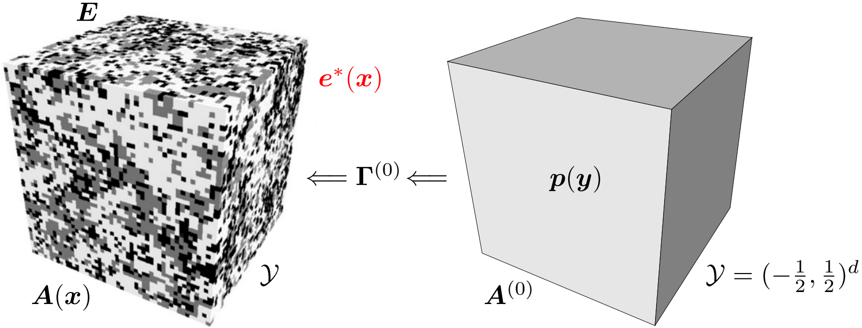
e.g., Z. Hashin, S. Shtrikman, *J Appl Phys* **33**, 3125 (1962)

Lippmann-Schwinger equation



$$\boldsymbol{e}^*(\boldsymbol{x}) = -\int_{\mathcal{Y}} \boldsymbol{\Gamma}^{(0)}(\boldsymbol{x}-\boldsymbol{y}) \overbrace{\left(\boldsymbol{A}(\boldsymbol{y}) - \boldsymbol{A}^{(0)}\right)(\boldsymbol{E} + \boldsymbol{e}^*(\boldsymbol{y}))}^{\boldsymbol{p}(\boldsymbol{y})} \,\mathrm{d}\boldsymbol{y}$$

Moulinec-Suquet basic scheme



$$\boldsymbol{e}^*_{(k+1)}(\boldsymbol{x}) = -\overbrace{\int_{\mathcal{Y}} \boldsymbol{\Gamma}^{(0)}(\boldsymbol{x}-\boldsymbol{y})}^{\text{convolution in Step II}} \overbrace{\Big(\boldsymbol{A}(\boldsymbol{y}) - \boldsymbol{A}^{(0)}\Big)\Big(\boldsymbol{E} + \boldsymbol{e}^*_{(k)}(\boldsymbol{y})\Big)}^{\boldsymbol{p}_{(k)}(\boldsymbol{y}) \text{ in Step I}} \, \mathrm{d}\boldsymbol{y}$$

H. Moulinec, P. Suquet, *C R Acad Sci Paris* **318**, 1417 (1994);
H. Moulinec, P. Suquet, *Comput Methods Appl Mech Eng* **157**, 69 (1998)

Moulinec-Suquet basic scheme

C. R. Acad. Sci. Paris, t. 318, Série II, p. 1417-1423, 1994 1417

Mécanique des solides/*Mechanics of Solids*

A fast numerical method for computing the linear and nonlinear mechanical properties of composites

Hervé Moulinec and Pierre Suquet

Abstract – This Note is devoted to a new iterative algorithm to compute the local and overall response of a composite from images of its (complex) microstructure. The elastic problem for a heterogeneous material is formulated with the help of a homogeneous reference medium and written under the form of a periodic Lippman-Schwinger equation. Using the fact that the Green's function of the pertinent operator is known explicitly in Fourier space, this equation is solved iteratively. The method is extended to the case where the individual constituents are elastic-plastic Von Mises materials with isotropic hardening.

Une méthode de calcul rapide des propriétés macroscopiques linéaires et non linéaires de composites

Résumé – *Cette Note est consacrée à un nouvel algorithme de détermination de la réponse locale et du comportement global d'un composite, à partir d'images complexes de sa microstructure. Le problème d'une hétérogénéité élastique est tout d'abord reformulé à l'aide d'un milieu homogène de référence ce qui conduit à une équation de Lippman-Schwinger périodique, Cette équation, dont la fonction de Green est explicitement connue dans l'espace de Fourier, est résolue itérativement. L'algorithme proposé est étendu à des phases présentant un comportement élasto-plastique avec écrouissage.*

Version française abrégée – Le but de cette étude est de développer une méthode de simulation numérique du comportement d'un matériau hétérogène à partir d'images réelles ou

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Comput. Methods Appl. Mech. Engrg. 157 (1998) 69–94

Computer methods in applied mechanics and engineering

A numerical method for computing the overall response of nonlinear composites with complex microstructure

H. Moulinec, P. Suquet*

L.M.A./C.N.R.S., 31 Chemin Joseph Aiguier, 13402 Marseille, Cedex 20, France

Received 28 May 1996; revised 1 May 1997

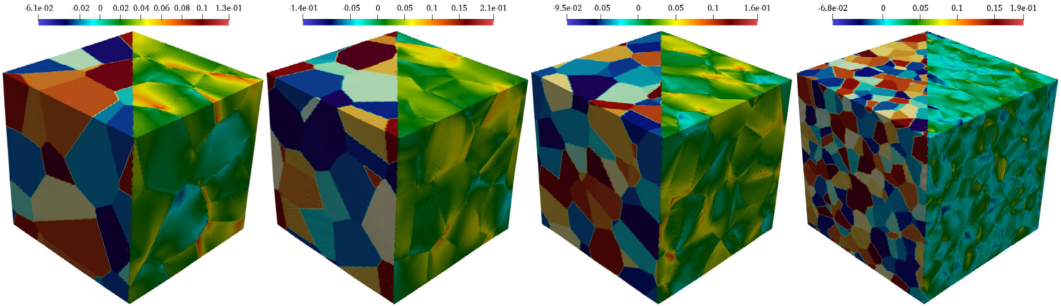
Abstract

The local and overall responses of nonlinear composites are classically investigated by the Finite Element Method. We propose an alternate method based on Fourier series which avoids meshing and which makes direct use of microstructure images. It is based on the exact expression of the Green function of a linear elastic and homogeneous comparison material. First, the case of elastic nonhomogeneous constituents is considered and an iterative procedure is proposed to solve the Lippman–Schwinger equation which naturally arises in the problem. Then, the method is extended to non-linear constituents by a step-by-step integration in time. The accuracy of the method is assessed by varying the spatial resolution of the microstructures. The flexibility of the method allows it to serve for a large variety of microstructures. © 1998 Elsevier Science S.A.

. . . alternative method to the Finite Element Method based on Fourier series . . .

H. Moulinec, P. Suquet, *C R Acad Sci Paris* **318**, 1417 (1994);
H. Moulinec, P. Suquet, *Comput Methods Appl Mech Eng* **157**, 69 (1998)

Fast and memory-efficient solver



- Easy to implement
- Matrix-free
- Convergence independent of mesh size + efficiency of FFT
- $\approx 10\times$ faster than finite elements

A. Vidyasagar, A. D. Tutcuoglu, D. M. Kochmann, *Comput Methods Appl Mech Eng* **335**, 584 (2018)

Why Moulinec-Suquet scheme works?

- Contributions in $\approx (1994 + 20)$ and (mostly) equivalent
- French stream: **Sébastien Brisard** and Luc Dormieux
  - Hashin-Shtrikman variational principles
- German stream: **Matti Schneider**
  - gradient descent
- Czech stream: **Jaroslav Vondřejc**, Jan Zeman, and Ivo Marek†
  - Fourier-Galerkin method

Outline

Preliminaries

Discrete Laplace/Green's function preconditioning

Application to corrector problem

Results

Conclusions

Preliminaries

- Model problem

$$
\begin{aligned}
-\boldsymbol{\nabla} \cdot \left[\boldsymbol{A}(\boldsymbol{x})\boldsymbol{\nabla} u(\boldsymbol{x})\right] &= f(\boldsymbol{x}) && \text{for } \boldsymbol{x} \in \Omega \\
u(\boldsymbol{x}) &= 0 && \text{for } \boldsymbol{x} \in \partial\Omega
\end{aligned}
$$

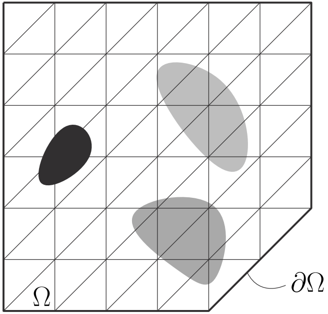
- Weak form: Find $u \in H_0^1(\Omega)$ such that

$$
\int_\Omega \boldsymbol{\nabla} v(\boldsymbol{x}) \cdot \boldsymbol{A}(\boldsymbol{x})\boldsymbol{\nabla} u(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_\Omega v(\boldsymbol{x}) f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \text{ for all } v \in H_0^1(\Omega)
$$

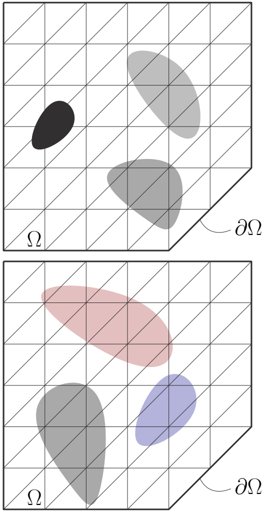
- Finite element approximation

$$
u(\boldsymbol{x}) \approx \sum_{i=1}^{N} u(\boldsymbol{x}_{\mathrm{N}}^{i})\varphi_i(\boldsymbol{x}) \text{ for } \boldsymbol{x} \in \Omega
$$

$$
v(\boldsymbol{x}) \approx \sum_{j=1}^{N} v(\boldsymbol{x}_{\mathrm{N}}^{j})\varphi_j(\boldsymbol{x}) \text{ for } \boldsymbol{x} \in \Omega
$$



Preliminaries



- Galerkin projection: Find $\mathbf{u} \in \mathbb{R}^N$ such that

$$\mathbf{v}^\mathsf{T}\mathbf{K}\mathbf{u} = \mathbf{v}^\mathsf{T}\mathbf{f} \text{ for all } \mathbf{v} \in \mathbb{R}^N$$

  where $(i, j = 1, \ldots, N)$

$$u_i = u(\boldsymbol{x}_\mathrm{N}^i), \quad v_j = v(\boldsymbol{x}_\mathrm{N}^j)$$

$$K_{ji} = \int_\Omega \boldsymbol{\nabla}\varphi_j(\boldsymbol{x}) \cdot \boldsymbol{A}(\boldsymbol{x})\boldsymbol{\nabla}\varphi_i(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x},$$

$$f_j = \int_\Omega \varphi_j(\boldsymbol{x}) f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$

- Reference problem

$$K_{ji}^{(0)} = \int_\Omega \boldsymbol{\nabla}\varphi_j(\boldsymbol{x}) \cdot \boldsymbol{A}^{(0)}(\boldsymbol{x})\boldsymbol{\nabla}\varphi_i(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$

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Preliminaries

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Discrete Laplace/Green's function preconditioning

Preconditioned system of equations

- Find $\mathbf{u} \in \mathbb{R}^N$ such that

$$\left(\mathbf{K}^{(0)}\right)^{-1}\mathbf{K}\mathbf{u} = \left(\mathbf{K}^{(0)}\right)^{-1}\mathbf{f}$$

- For the generalized eigenvalue problem

$$\mathbf{K}\phi_k = \lambda_k \mathbf{K}^{(0)}\phi_k \text{ for } k = 1, \ldots, N$$

characterize all eigenvalues λ_k.

- Previous works (mostly concerned with $N \to \infty$)

1. B. F. Nielsen, A. Tveito, W. Hackbusch, *IMA J Numer Anal* **29**, 24 (2009)
2. T. Gergelits, K.-A. Mardal, B. F. Nielsen, Z. Strakoš, *SIAM J Numer Anal* **57**, 1369 (2019)
3. T. Gergelits, B. F. Nielsen, Z. Strakoš, *SIAM J Numer Anal* **58**, 2193 (2020)
4. T. Gergelits, B. F. Nielsen, Z. Strakoš, *Numer Algorithms* **91**, 301 (2022)
5. B. F. Nielsen, Z. Strakoš, *SIAM Rev* **66**, 125 (2024)

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Our alternative to 2

Guaranteed upper-lower bounds on all eigenvalues

For each $j = 1, \ldots, N$, determine

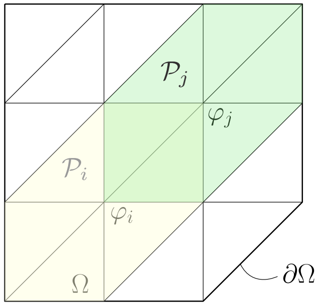
$$\underline{\lambda}_j = \text{ess inf}_{\boldsymbol{x} \in \mathcal{P}_j} \ \lambda_{\min}\Big(\big(\boldsymbol{A}^{(0)}(\boldsymbol{x})\big)^{-1}\boldsymbol{A}(\boldsymbol{x})\Big)$$
$$\overline{\lambda}_j = \text{ess sup}_{\boldsymbol{x} \in \mathcal{P}_j} \ \lambda_{\max}\Big(\big(\boldsymbol{A}^{(0)}(\boldsymbol{x})\big)^{-1}\boldsymbol{A}(\boldsymbol{x})\Big)$$

and sort them in the non-decreasing order

$$\{\underline{\lambda}_1, \underline{\lambda}_2, \cdots, \underline{\lambda}_N\} \to \underline{\lambda}_{r(1)} \leq \underline{\lambda}_{r(2)} \leq \cdots \leq \underline{\lambda}_{r(N)}$$
$$\{\overline{\lambda}_1, \overline{\lambda}_2, \cdots, \overline{\lambda}_N\} \to \overline{\lambda}_{s(1)} \leq \overline{\lambda}_{s(2)} \leq \cdots \leq \overline{\lambda}_{s(N)}$$

Then

$$\underline{\lambda}_{r(k)} \leq \lambda_k \leq \overline{\lambda}_{s(k)} \text{ for } k = 1, \ldots, N$$



M. Ladecký, I. Pultarová, J. Zeman, *Appl Math* **66**, 21 (2021)

Outline of the proof (for lower bounds)

Auxiliary lemma

For $\mathcal{D} \subseteq \Omega$, let

$$c^{\mathcal{D}} = \operatorname{ess\,inf}_{\boldsymbol{x}\in\mathcal{D}} \lambda_{\min}\Big(\big(\boldsymbol{A}^{(0)}(\boldsymbol{x})\big)^{-1}\boldsymbol{A}(\boldsymbol{x})\Big) \qquad (*)$$

Then for any $v \in H_0^1(\Omega), v \neq 0$

$$c^{\mathcal{D}} \leq \frac{\int_{\mathcal{D}} \nabla v(\boldsymbol{x}) \cdot \boldsymbol{A}(\boldsymbol{x}) \nabla v(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}}{\int_{\mathcal{D}} \nabla v(\boldsymbol{x}) \cdot \boldsymbol{A}^{(0)}(\boldsymbol{x}) \nabla v(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}}$$

From $(*)$, we have

$$c^{\mathcal{D}} \boldsymbol{w} \cdot \boldsymbol{A}^{(0)}(\boldsymbol{x}) \boldsymbol{w} \leq \boldsymbol{w} \cdot \boldsymbol{A}(\boldsymbol{x}) \boldsymbol{w} \text{ for all } \boldsymbol{w} \in \mathbb{R}^d \text{ and for almost all } \boldsymbol{x} \in \mathcal{D}$$

Take $\nabla v(\boldsymbol{x}) = \boldsymbol{w}$ for $\boldsymbol{x} \in \mathcal{D}$ and integrate over $\mathcal{D}$.

M. Ladecký, I. Pultarová, J. Zeman, *Appl Math* **66**, 21 (2021)

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Outline of the proof (for lower bounds)

Courant-Fischer (C-F) min-max theorem

For $\mathbf{K}$ and $\mathbf{K}^{(0)} \in \mathbb{R}^{N\times N}_{\text{spd}}$, the generalized eigenvalues satisfy

$$\lambda_k = \max_{\mathbb{S}\subseteq\mathbb{R}^N,\, \dim(\mathbb{S})=N-k+1} \; \min_{\mathbf{v}\in\mathbb{S},\, \mathbf{v}\neq\mathbf{0}} \frac{\mathbf{v}^\mathsf{T}\mathbf{K}\mathbf{v}}{\mathbf{v}^\mathsf{T}\mathbf{K}^{(0)}\mathbf{v}}$$

For $k=1$, set $\mathbb{I}=\{1,\dots,N\}$. By C-F theorem,

$$\lambda_1 = \min_{\mathbf{v}\in\mathbb{R}^N,\mathbf{v}_\mathbb{I}\neq\mathbf{0}} \frac{\mathbf{v}^\mathsf{T}\mathbf{K}\mathbf{v}}{\mathbf{v}^\mathsf{T}\mathbf{K}^{(0)}\mathbf{v}}$$

Auxiliary lemma with $\mathcal{D}=\cup_{k\in\mathbb{I}}\mathcal{P}_k$ and $v(\boldsymbol{x})=\sum_{i\in\mathbb{I}} v_i\varphi_i(\boldsymbol{x})$, $v\neq 0$ entails

$$\lambda_{r(1)} = c^{\mathcal{D}} \leq \min_{\mathbf{v}\in\mathbb{R}^N,\mathbf{v}_\mathbb{I}\neq\mathbf{0}} \frac{\int_\mathcal{D} \nabla v(\boldsymbol{x})\cdot \boldsymbol{A}(\boldsymbol{x})\nabla v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}}{\int_\mathcal{D} \nabla v(\boldsymbol{x})\cdot \boldsymbol{A}^{(0)}(\boldsymbol{x})\nabla v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}} = \min_{\mathbf{v}\in\mathbb{R}^N,\mathbf{v}_\mathbb{I}\neq\mathbf{0}} \frac{\mathbf{v}^\mathsf{T}\mathbf{K}\mathbf{v}}{\mathbf{v}^\mathsf{T}\mathbf{K}^{(0)}\mathbf{v}} = \lambda_1$$

e.g., G. H. Golub, C. F. Van Loan, *Matrix computations* (Johns Hopkins University Press, 2013), Theorem 8.1.2; M. Ladecký, I. Pultarová, J. Zeman, *Appl Math* **66**, 21 (2021)

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For $k = 2$, set $\mathbb{I} = \{1, \ldots, N\}\backslash\{r(1)\}$. By C-F theorem,

$$\lambda_2 \geq \min_{\mathbf{v}\in\mathbb{R}^N, \mathbf{v}_\mathbb{I}\neq\mathbf{0}} \frac{\mathbf{v}^\mathsf{T}\mathbf{K}\mathbf{v}}{\mathbf{v}^\mathsf{T}\mathbf{K}^{(0)}\mathbf{v}}$$

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$$\lambda_{r(2)} = c^{\mathcal{D}} \leq \min_{\mathbf{v}\in\mathbb{R}^N, \mathbf{v}_\mathbb{I}\neq\mathbf{0}} \frac{\int_\mathcal{D} \nabla v(\boldsymbol{x}) \cdot \boldsymbol{A}(\boldsymbol{x})\nabla v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}}{\int_\mathcal{D} \nabla v(\boldsymbol{x}) \cdot \boldsymbol{A}^{(0)}(\boldsymbol{x})\nabla v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}} = \min_{\mathbf{v}\in\mathbb{R}^N, \mathbf{v}_\mathbb{I}\neq\mathbf{0}} \frac{\mathbf{v}^\mathsf{T}\mathbf{K}\mathbf{v}}{\mathbf{v}^\mathsf{T}\mathbf{K}^{(0)}\mathbf{v}} \leq \lambda_2$$

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$$\lambda_2 \geq \min_{\mathbf{v}\in\mathbb{R}^N,\mathbf{v}_\mathbb{I}\neq\mathbf{0}} \frac{\mathbf{v}^\mathsf{T}\mathbf{K}\mathbf{v}}{\mathbf{v}^\mathsf{T}\mathbf{K}^{(0)}\mathbf{v}}$$

Auxiliary lemma with $\mathcal{D}=\cup_{k\in\mathbb{I}}\mathcal{P}_k$ and $v(\boldsymbol{x})=\sum_{i\in\mathbb{I}} v_i\varphi_i(\boldsymbol{x})$, $v\neq 0$ entails

$$\underline{\lambda}_{r(2)} = c^{\mathcal{D}} \leq \min_{\mathbf{v}\in\mathbb{R}^N,\mathbf{v}_\mathbb{I}\neq\mathbf{0}} \frac{\int_\mathcal{D}\nabla v(\boldsymbol{x})\cdot\boldsymbol{A}(\boldsymbol{x})\nabla v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}}{\int_\mathcal{D}\nabla v(\boldsymbol{x})\cdot\boldsymbol{A}^{(0)}(\boldsymbol{x})\nabla v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}} = \min_{\mathbf{v}\in\mathbb{R}^N,\mathbf{v}_\mathbb{I}\neq\mathbf{0}} \frac{\mathbf{v}^\mathsf{T}\mathbf{K}\mathbf{v}}{\mathbf{v}^\mathsf{T}\mathbf{K}^{(0)}\mathbf{v}} \leq \lambda_2$$

e.g., G. H. Golub, C. F. Van Loan, *Matrix computations* (Johns Hopkins University Press, 2013), Theorem 8.1.2; M. Ladecký, I. Pultarová, J. Zeman, *Appl Math* **66**, 21 (2021)

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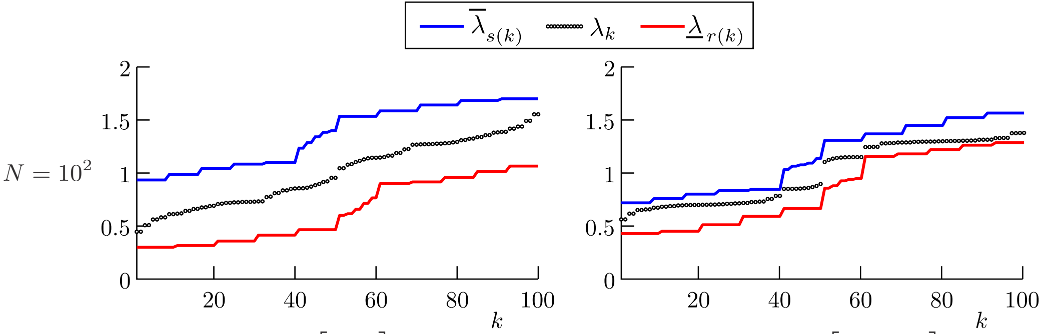
Example

$$\boldsymbol{A}(\boldsymbol{x}) = \begin{bmatrix} 1 & 0.3 \\ 0.3 & 1 \end{bmatrix} + \begin{bmatrix} 0.3\,\mathrm{sgn}(x_2) & 0.1\cos(x_1) \\ 0.1\cos(x_1) & 0.3\,\mathrm{sgn}(x_2) \end{bmatrix}$$ for $\boldsymbol{x} \in (-\pi, \pi)^2$, uniform Q_4 elements



$$\boldsymbol{A}^{(0)}(\boldsymbol{x}) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \boldsymbol{A}^{(0)}(\boldsymbol{x}) = \begin{bmatrix} 1 & 0.3 \\ 0.3 & 1 \end{bmatrix}$$

M. Ladecký, I. Pultarová, J. Zeman, *Appl Math* **66**, 21 (2021)

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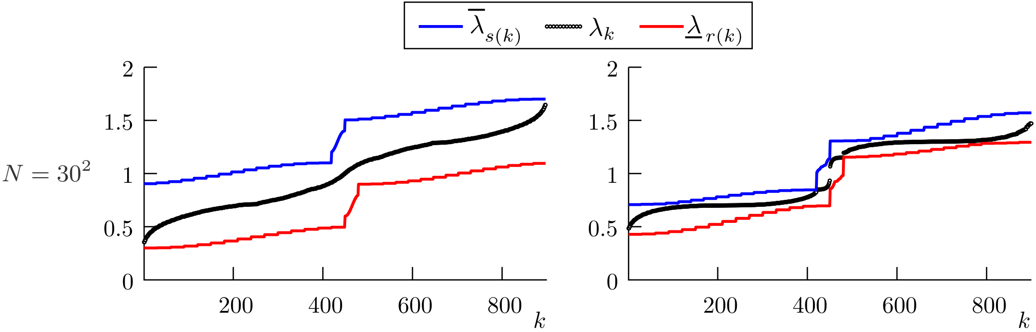

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Extensions

- M. Ladecký, I. Pultarová, J. Zeman, *Appl Math* **66**, 21 (2021)
  - Mixed boundary conditions
  - Periodic boundary conditions
  - Linear elasticity problems
- I. Pultarová, M. Ladecký, *Numer Linear Algebra Appl* **28**, e2382 (2021)
  - Algebraic multilevel preconditioning
  - Stochastic Galerkin finite element method
  - Finite difference method

$$\mathbf{K} = \sum_{e=1}^{M} \mathbf{K}_e, \qquad \mathbf{K}^{(0)} = \sum_{e=1}^{M} \mathbf{K}_e^{(0)}, \qquad \mathbf{K}_e \text{ and } \mathbf{K}_e^{(0)} \text{ are symmetric and have the same kernels}$$

- L. Gaynutdinova, et al., *Numer Linear Algebra Appl* **31**, e2549 (2024)
  - Elliptic problems discretized with Discontinuous Galerkin method (SIPG)
  - Convection-diffusion-reaction problems discretized with Galerkin method
  - Patches of indices (fully algebraic)

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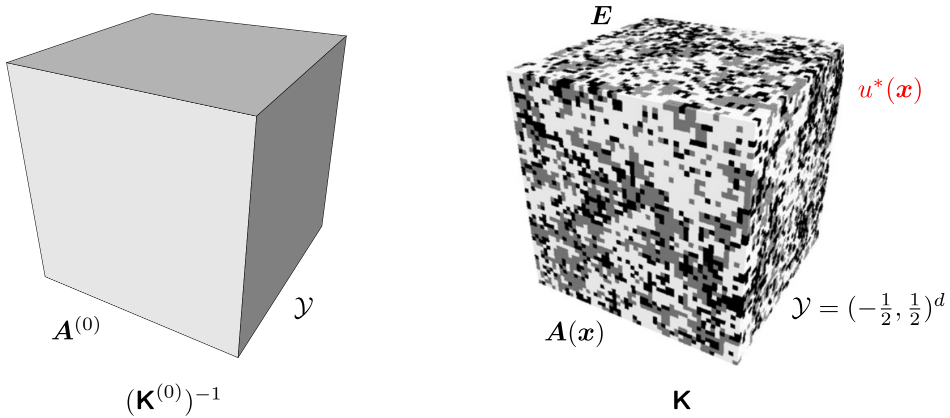
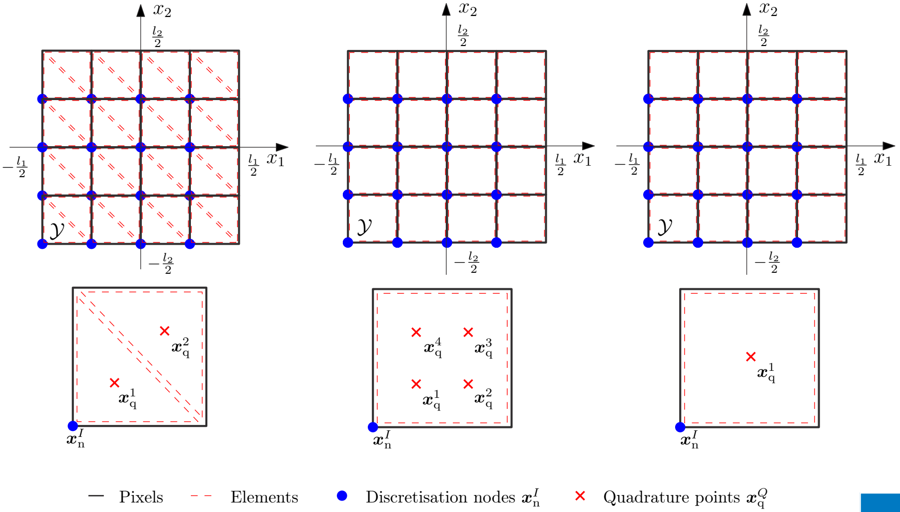
Laplace/Green's function preconditioning viewpoint



M. Schneider, D. Merkert, M. Kabel, *Int J Num Meth Engng* **109**, 1461 (2017), M. Leuschner, F. Fritzen, *Comput Mech* **62**, 359 (2018), S. Lucarini, J. Segurado, *Int J Eng Sci* **144**, 103131 (2019), ...

Regular finite element meshes



M. Ladecký, *et al.*, *Appl Math Comput* **446**, 127835 (2023)

Structure of the preconditioned problem

$$K^e_{ji} = \sum_{q=1}^{Q} w^q_{\mathrm{q}} \boldsymbol{\nabla}\varphi_j(\boldsymbol{x}^q_{\mathrm{q}}) \cdot \boldsymbol{A}(\boldsymbol{x}^q_{\mathrm{q}}) \boldsymbol{\nabla}\varphi_i(\boldsymbol{x}^q_{\mathrm{q}}), \qquad f^e_j = \sum_{q=1}^{Q} w^q_{\mathrm{q}} \boldsymbol{\nabla}\varphi_j(\boldsymbol{x}^q_{\mathrm{q}}) \cdot \boldsymbol{A}(\boldsymbol{x}^q_{\mathrm{q}}) \boldsymbol{E}, \quad e = 1, \dots, M$$

Preconditioned system of linear equations

$$\overbrace{\left(\mathbf{D}^{\mathsf{T}}\mathbf{W}\mathbf{A}^{(0)}\mathbf{D}\right)}^{\mathbf{K}^{(0)}}{}^{-1}\overbrace{\left(\mathbf{D}^{\mathsf{T}}\mathbf{W}\mathbf{A}\mathbf{D}\right)}^{\mathbf{K}}\mathbf{u} = -\overbrace{\left(\mathbf{D}^{\mathsf{T}}\mathbf{W}\mathbf{A}^{(0)}\mathbf{D}\right)}^{\mathbf{K}^{(0)}}{}^{-1}\overbrace{\left(\mathbf{D}^{\mathsf{T}}\mathbf{W}\mathbf{A}\mathbf{E}\right)}^{\mathbf{f}}$$

- (Block-) diagonal matrices $\mathbf{W}$, $\mathbf{A}$, and $\mathbf{A}^{(0)}$ at integration points
- Discrete gradient $\mathbf{D}$ and divergence $\mathbf{D}^{\mathsf{T}}$ matrices are structured and sparse (short stencil)
- Multiplication with $\mathbf{K}$ with linear complexity
- Spectrum of the preconditioned matrix (almost) discretization-independent
- How to apply preconditioner efficiently ($\equiv$ using FFT)?

M. Ladecký, *et al.*, *Appl Math Comput* **446**, 127835 (2023)

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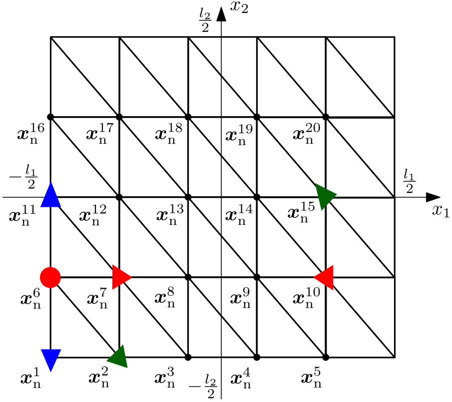

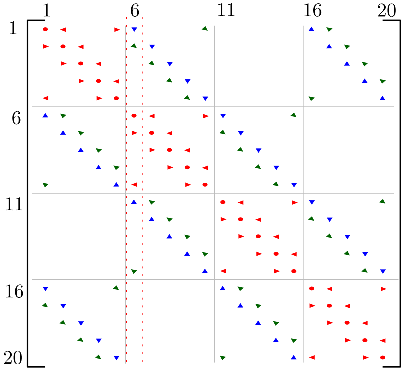

– Elements • Discretisation nodes - x_n^I

$\mathbf{K}^{(0)}$

$$\widehat{\mathbf{K}}^{(0)} = \mathbf{F}\mathbf{K}^{(0)}\mathbf{F}^{-1}$$ is diagonal and thus cheaply invertible

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Inversion of of $\mathbf{K}^{(0)}$

- Because $(\widehat{\mathbf{K}}^{(0)})^{-1}$ is diagonal

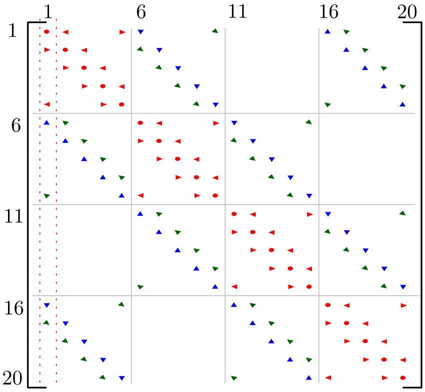
$$(\mathbf{K}^{(0)})^{-1} = \mathbf{F}^{-1}(\widehat{\mathbf{K}}^{(0)})^{-1}\mathbf{F}$$

- Row extraction ($\mathbf{K}^{(0)}$ is never assembled)

$$\mathbf{K}^{(0)}_{:,1} = \mathbf{K}^{(0)} \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

- Diagonal

$$\mathrm{diag}(\widehat{\mathbf{K}}^{(0)}) = \mathbf{F}\mathbf{K}^{(0)}_{:,1}$$



$\mathbf{K}^{(0)}$

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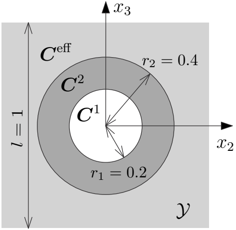
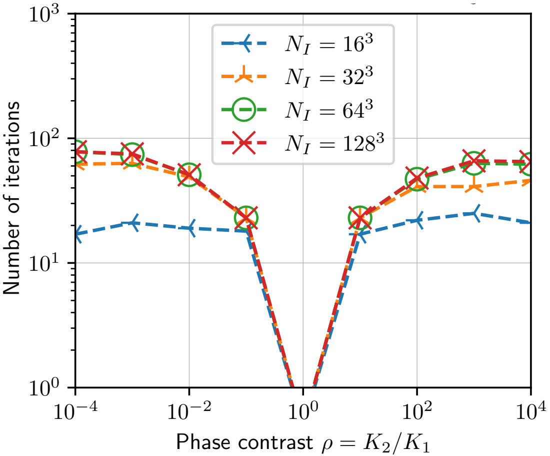
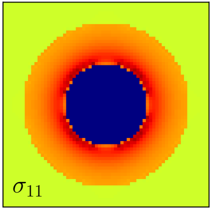
Results (3D small-strain elasticity)







- Independence of mesh size (Q_8 elements)

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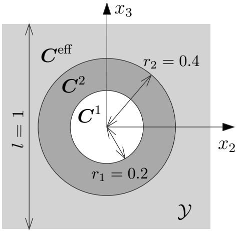
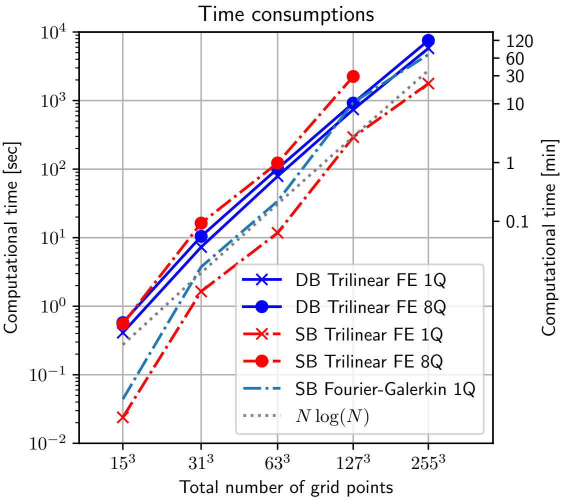
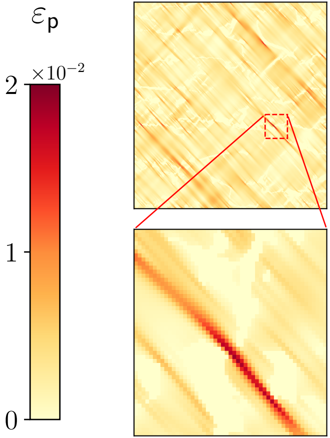
Results (3D small-strain elasticity)





- Quasi-linear scaling (3D linear elasticity)

Results (2D finite-strain elasto-plasticity)



$\boldsymbol{A}^{(0)}$		Fourier	linear FE	bilinear FE
Newton		11	9	10
	$\boldsymbol{I}$	1,012	861	761
(P)CG	$\boldsymbol{I}_{\mathrm{sym}}$	781	609	540
	$\boldsymbol{A}^{(0)}_{\mathrm{mean}}$	585	457	407

- Choice of reference problem's coefficients (T_3 and Q_4 elements)

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Conclusions

- Linear-algebraic perspective on FFT-based solvers $\equiv$ Laplace/Green's function preconditioning
- All eigenvalues of the preconditioned matrix can be bounded by coefficients
- Limited influence of grid spacing
- Extends to other scenarios, e.g., finite differences, stochastic Galerkin, discontinuous Galerkin
- Provides the basis for generic regular finite element discretization
- Preconditioner constructed by purely algebraic means
- WIP: Guaranteed (certified) bounds on discretization and algebraic errors

Thanks to the organizers for the opportunity and their courage and the audience for their time and patience!

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Interested in details?

1. Ladecký, M., Pultarová, I. & Z. J. Guaranteed two-sided bounds on all eigenvalues of preconditioned diffusion and elasticity problems solved by the finite element method. *Appl Math* **66**, 21–42 (2021).
2. Pultarová, I. & Ladecký, M. Two-sided guaranteed bounds to individual eigenvalues of preconditioned finite element and finite difference problems. *Numer Linear Algebra Appl* **28**, e2382 (2021).
3. **Leute, R.J.**, Ladecký, M., **Falsafi, A.**, **Jödicke, I.**, Pultarová, I., Z. J., **Junge, T.** & **Pastewka, L.** Elimination of ringing artifacts by finite-element projection in FFT-based homogenization. *J Comput Phys* **453**, 110931 (2022).
4. Ladecký, M., **Leute, R.J.**, **Falsafi, A.**, Pultarová, I., **Pastewka, L.**, **Junge, T.** & Z. J. An optimal preconditioned FFT-accelerated finite element solver for homogenization. *Appl Math Comput* **446**, 127835 (2023).
5. **Gaynutdinova, L.**, Ladecký, M., Pultarová, I., **Vlasák, M.** and Z. J., Preconditioned discontinuous Galerkin method and convection-diffusion-reaction problems with guaranteed bounds to resulting spectra. *Numer Linear Algebra Appl* **31**, e2382 (2024).