Discrete Green's operator preconditioning: Theory and applications

Martin Ladecký Ivana Pultarová Jan Zeman

Department of Mathematics
Faculty of Civil Engineering
Czech Technical University in Prague

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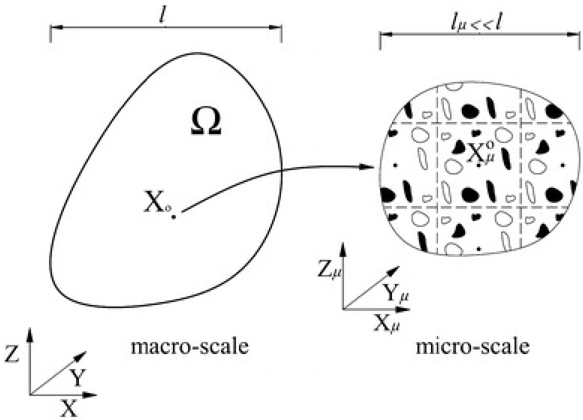
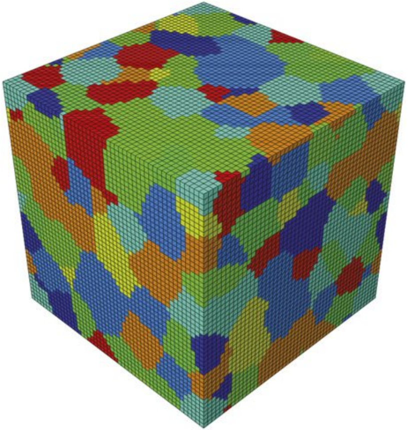
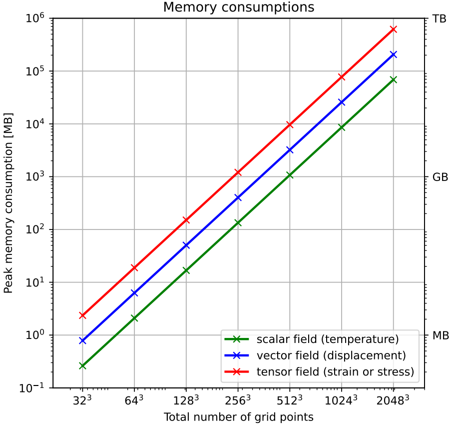
Two-scale material analysis



Adopted from: Multiscale Computational Homogenization. F. Otero et al., Archives of Computational Methods in Engineering (2018)

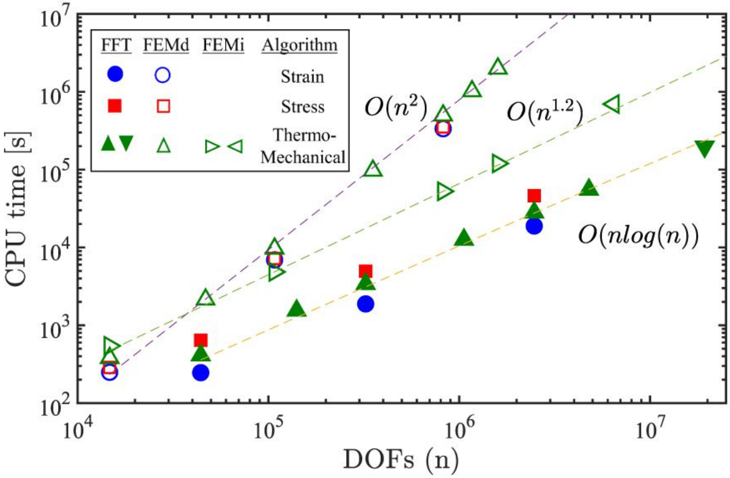
Computational demands





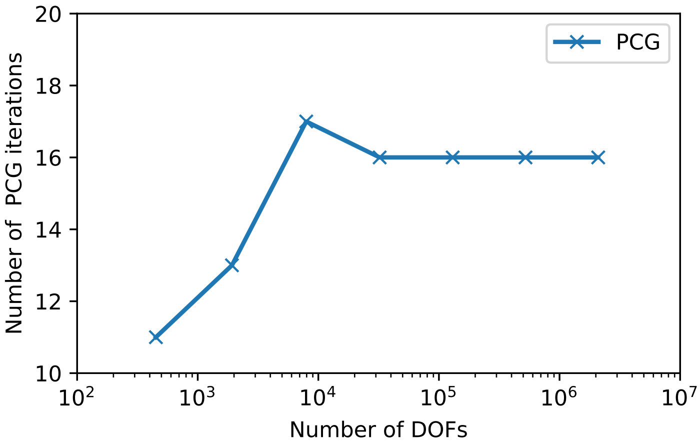
Adapted from: Computational Homogenization of Polycrystals, J. Segurado et al. Advances in Applied Mechanics (2018)

Time consumption



Adopted from: A variational fast Fourier transform method for phase-transforming materials," by A. Cruzado et al. Modelling and Simulation in Materials Science and Engineering (2021). Solved using Abaqus FEA software suite (formerly ABAQUS)

Grid size independence



The 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.

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Model problem

- elliptic problem

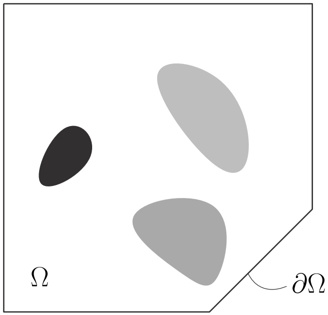
$$-\nabla \cdot \mathbf{A}(\boldsymbol{x})\nabla u(\boldsymbol{x}) = f(\boldsymbol{x}) \quad \boldsymbol{x} \in \Omega$$
$$u(\boldsymbol{x}) = 0 \qquad \boldsymbol{x} \in \partial\Omega$$

- weak form

$$\int_\Omega \nabla v(\boldsymbol{x})^\mathsf{T} \mathbf{A}(\boldsymbol{x})\nabla u(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_\Omega v(\boldsymbol{x})^\mathsf{T} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \quad v \in \mathcal{V}$$

- approximation

$$u(\boldsymbol{x}) \approx u^N(\boldsymbol{x}) = \sum_{i=1}^{N} u^N(\boldsymbol{x}_i^\mathrm{n})\varphi_i(\boldsymbol{x})$$



Model problem

- elliptic problem

$$
\begin{aligned}
-\nabla \cdot \mathbf{A}(\boldsymbol{x})\nabla u(\boldsymbol{x}) &= f(\boldsymbol{x}) \quad \boldsymbol{x} \in \Omega \\
u(\boldsymbol{x}) &= 0 \qquad\quad \boldsymbol{x} \in \partial\Omega
\end{aligned}
$$

- weak form

$$
\int_\Omega \nabla v(\boldsymbol{x})^\mathsf{T} \mathbf{A}(\boldsymbol{x}) \nabla u(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \int_\Omega v(\boldsymbol{x})^\mathsf{T} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \quad v \in \mathcal{V}
$$

- approximation

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u(\boldsymbol{x}) \approx u^N(\boldsymbol{x}) = \sum_{i=1}^{N} u^N(\boldsymbol{x}_i^\mathrm{n}) \varphi_i(\boldsymbol{x})
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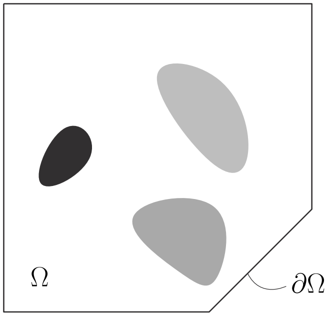

Model problem

- elliptic problem

$$\begin{aligned} -\nabla \cdot \mathbf{A}(\boldsymbol{x})\nabla u(\boldsymbol{x}) &= f(\boldsymbol{x}) \quad && \boldsymbol{x} \in \Omega \\ u(\boldsymbol{x}) &= 0 && \boldsymbol{x} \in \partial\Omega \end{aligned}$$

- weak form

$$\int_\Omega \nabla v(\boldsymbol{x})^\mathsf{T} \mathbf{A}(\boldsymbol{x}) \nabla u(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \int_\Omega v(\boldsymbol{x})^\mathsf{T} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} \quad v \in \mathcal{V}$$

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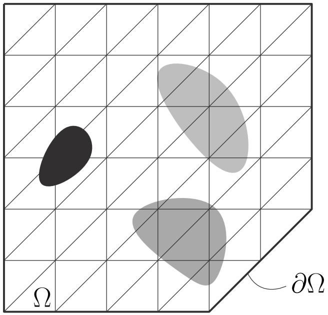


System of linear equations

$$\mathbf{K}\mathbf{u} = \mathbf{b}$$

- linear system matrix

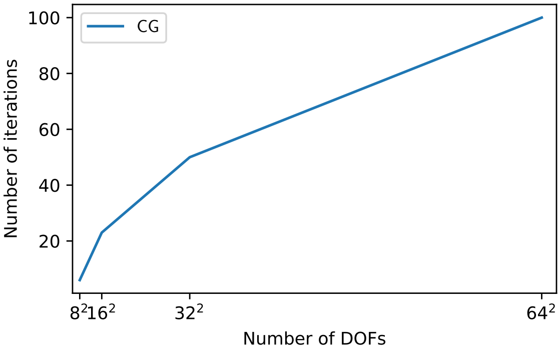
$$\mathbf{K}[j,i] = \int_\Omega \nabla\varphi_j(\boldsymbol{x})^\mathsf{T}\mathbf{A}(\boldsymbol{x})\nabla\varphi_i(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$

- unknown

$$\mathbf{u}[i] = u^N(\boldsymbol{x}_i^\mathrm{n})$$

- right-hand side

$$\mathbf{b}[j] = \int_\Omega \varphi_j(\boldsymbol{x}) f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$



- preconditioned system

$$\mathbf{M}^{-1}\mathbf{K}\mathbf{u} = \mathbf{M}^{-1}\mathbf{b}$$

- preconditioner

$$\mathbf{M}^{-1}\mathbf{K} \approx \mathbf{I}$$

- symmetric form

$$\mathbf{M}^{-1/2}\mathbf{K}\mathbf{M}^{-1/2}\mathbf{z} = \mathbf{M}^{-1/2}\mathbf{b}, \qquad \mathbf{z} = \mathbf{M}^{1/2}\mathbf{u}$$

procedure PCG($\boldsymbol{u}_0$, $\mathbf{K}$, $\mathbf{b}$, $\mathbf{M}$, tol, $it_{\max}$)
  $\mathbf{r}_0 := \mathbf{b} - \mathbf{K}\boldsymbol{u}_0$
  $\mathbf{z}_0 := \mathbf{M}^{-1}\mathbf{r}_0$
  $nr_0 := \|\mathbf{r}_0\|$ ▷ initial residual
  $\mathbf{p}_0 := \mathbf{z}_0$

  while $k \le it_{max}$ **do** ▷ $k = 0, 1, \ldots, it_{max}$
    $\mathbf{Kp}_k = \mathbf{K}\mathbf{p}_k$
    $\alpha_k = \dfrac{\mathbf{r}_k^\top \mathbf{z}_k}{\mathbf{p}_k^\top \mathbf{Kp}_k}$
    $\delta\tilde{\boldsymbol{u}}_{k+1} = \delta\tilde{\boldsymbol{u}}_k + \alpha_k \mathbf{p}_k$
    $\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k \mathbf{Kp}_k$
    $\mathbf{z}_{k+1} = \mathbf{M}^{-1}\mathbf{r}_{k+1}$
    $nr_{k+1} = \left\|\mathbf{r}_{k+1}\right\|$
    if $\dfrac{nr_{k+1}}{nr_0} < tol$ **then**
      return $\boldsymbol{u}_{k+1}$
    $\beta_k = \dfrac{\mathbf{r}_{k+1}^\top \mathbf{z}_{k+1}}{\mathbf{r}_k^\top \mathbf{z}_k}$
    $\mathbf{p}_{k+1} = \mathbf{z}_{k+1} + \beta_k \mathbf{p}_k$

    $k = k + 1$
  return $\boldsymbol{u}_k$

Preconditioning approaches

- diagonal scaling or Jacobi

$$\mathbf{M} = \mathrm{diag}(\mathbf{K})$$

$$\mathbf{M}^{-1} = \begin{bmatrix} \mathbf{K}_{1,1}^{-1} & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \mathbf{K}_{N,N}^{-1} \end{bmatrix}$$

- incomplete Cholesky or LU factorization

$$\mathbf{M} \approx \mathbf{L}\mathbf{L}^{\mathsf{T}}$$

$$\mathbf{L}^{\mathsf{T}} = \begin{pmatrix} \times & \times & 0 & 0 & \times \\ & \times & \times & \times & 0 \\ & & \times & \times & 0 \\ & \mathbf{0} & & \times & \times \\ & & & & \times \end{pmatrix}$$

$$\vdots$$

- operator (Laplace, discrete Green's) preconditioning

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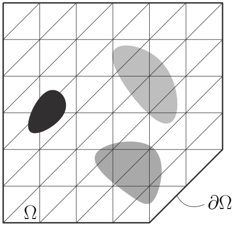
Discrete Green's operator preconditioning

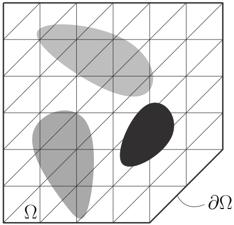
- original problem

$$\mathbf{K} = \int_\Omega \nabla v(\boldsymbol{x})^\mathsf{T} \mathbf{A}(\boldsymbol{x}) \nabla u(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x}$$



- reference problem

$$\mathbf{K}^{\mathsf{ref}} = \int_\Omega \nabla v(\boldsymbol{x})^\mathsf{T} \mathbf{A}^{\mathsf{ref}}(\boldsymbol{x}) \nabla u(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x}$$



- discrete Green's (Laplace) operator preconditioned linear system

$$\left(\mathbf{K}^{\mathsf{ref}}\right)^{-1} \mathbf{K}\mathbf{u} = \left(\mathbf{K}^{\mathsf{ref}}\right)^{-1} \mathbf{b}$$

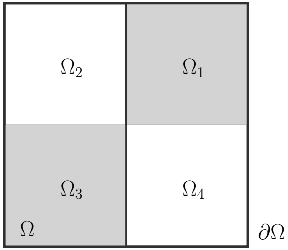
Example 1: Setting

- original problem

$$-\nabla \cdot \mathbf{A}(\boldsymbol{x})\nabla u(\boldsymbol{x}) = 0 \quad \boldsymbol{x} \in \Omega$$

$$\mathbf{A}(\boldsymbol{x}) = 161.45 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{x} \in \Omega_{1,3}$$

$$\mathbf{A}(\boldsymbol{x}) = 1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{x} \in \Omega_{2,4}$$

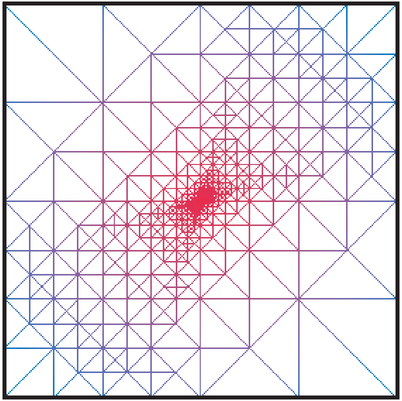


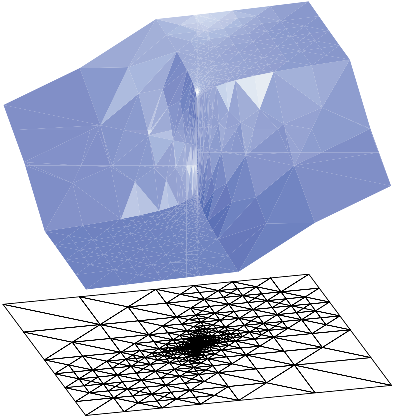
- reference problem

$$-\nabla \cdot I\nabla u(\boldsymbol{x}) = 0 \quad \boldsymbol{x} \in \Omega$$

Adopted from: Laplacian Preconditioning of Elliptic PDEs: Localization of the Eigenvalues of the Discretized Operator," by T. Gergelits et al.

Example 1: Mesh and solution





Adapted from: Convergence of Adaptive Finite Element Methods, by P. Morin, et al.

Example 1: Convergence

- condition number

$$\kappa(\mathbf{K}) = \lambda_N / \lambda_1$$

- bound

$$\frac{\|\mathbf{x} - \mathbf{x}_k\|_{\mathbf{K}}}{\|\mathbf{x} - \mathbf{x}_0\|_{\mathbf{K}}} \leq 2 \left(\frac{\sqrt{\kappa(\mathbf{K})} - 1}{\sqrt{\kappa(\mathbf{K})} + 1} \right)^k$$

- condition numbers

$$\kappa_{\mathsf{ICHOL}} \approx 16$$
$$\kappa_{\mathsf{Laplace}} \approx 161$$

J. W. Daniel, The conjugate gradient method for linear and nonlinear operator equations, SIAM J. Numer. Anal., 4 (1967), pp. 10–26.

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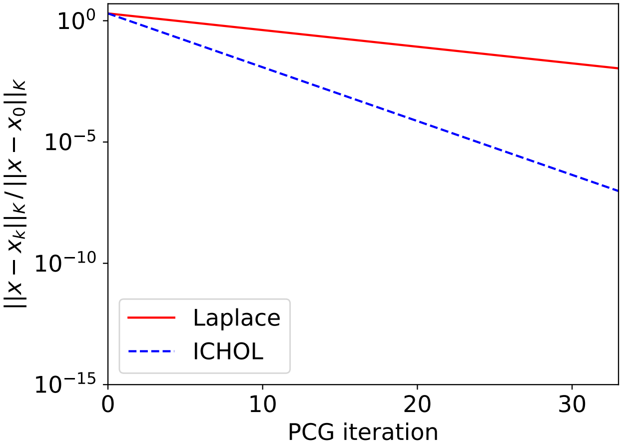

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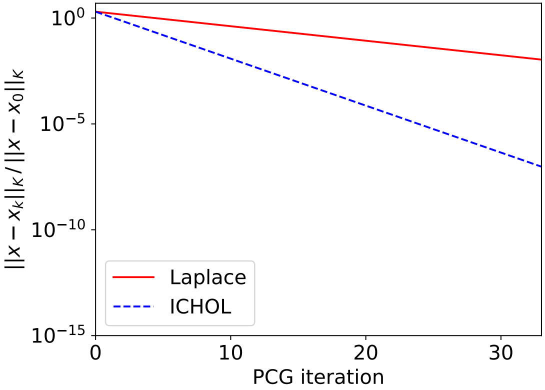

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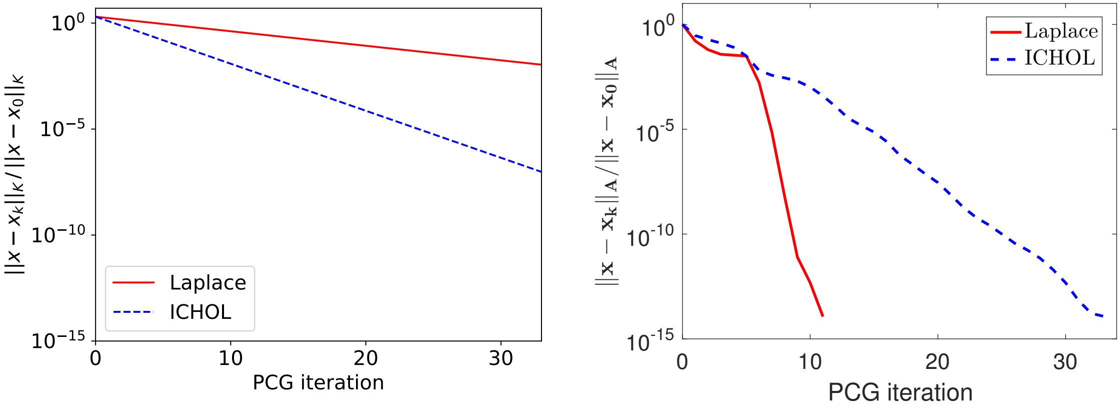

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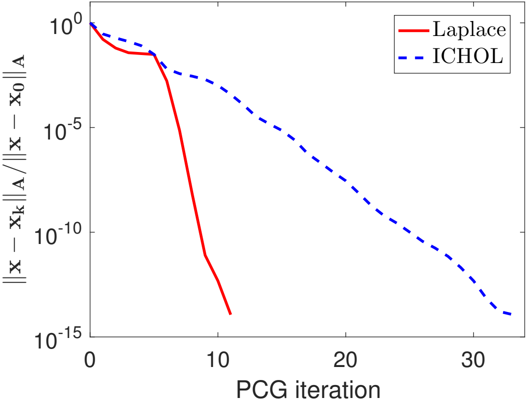
Energy norm of the error

$$\|\mathbf{x} - \mathbf{x}_k\|_{\mathbf{K}}^2 = \|\mathbf{r}_0\|^2 \sum_{l=1}^{N} \omega_l \frac{\left(\varphi_k^{CG}(\lambda_l)\right)^2}{\lambda_l}, \quad k = 1, 2, \ldots$$

- first residual (right-hand side, initial guess)

$$\mathbf{r}_0 = \mathbf{b} - \mathbf{K}\mathbf{x}_0$$
$$\omega_l = (\mathbf{r}_0, \phi_l)$$

- distribution of eigenvalues λ_l
- rounding errors (finite precision arithmetic)



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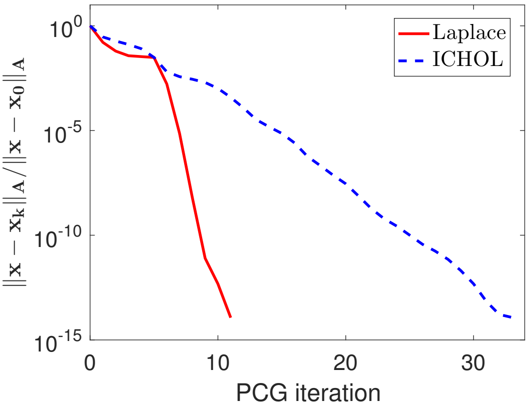

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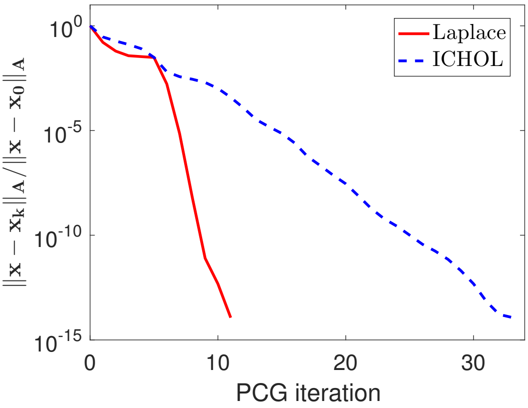

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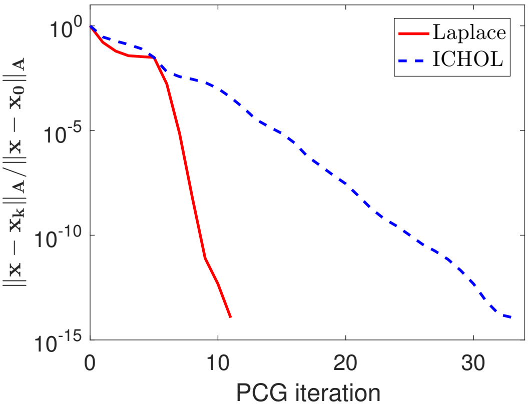

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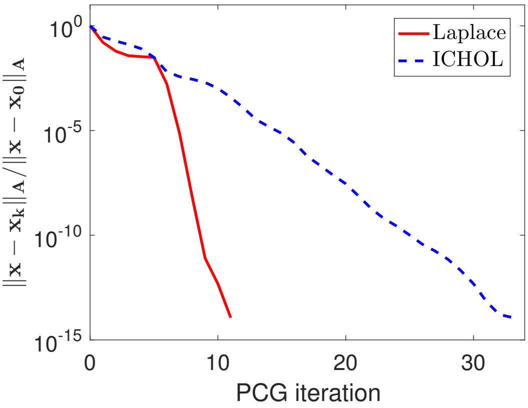

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Literature

Nielsen, Tveito, Hackbusch

2009 Preconditioning by inverting the Laplacian; an analysis of the eigenvalues

Gergelits, Mardal, Nielsen, Strakoš

2019 Laplacian preconditioning of elliptic PDEs: Localization of the eigenvalues of the discretized operator.
2020 Generalized spectrum of second order differential operators
2022 Numerical approximation of the spectrum of self-adjoint operators in operator preconditioning

Ladecký, Pultarová, Zeman

2020 Guaranteed two-sided bounds on all eigenvalues of preconditioned diffusion and elasticity problems solved by the finite element method
2021 Two-sided guaranteed bounds to individual eigenvalues of preconditioned finite element and finite difference problems

Generalized eigenvalue problem

- linear system matrix

$$\mathbf{K}$$

- eigenvalue problem

$$\mathbf{K}\phi_k = \lambda_k\, \phi_k, \quad k = 1, \ldots, N$$

- preconditioned linear system matrix

$$\left(\mathbf{K}^{\mathsf{ref}}\right)^{-1}\mathbf{K}$$

- generalized eigenvalue problem

$$\mathbf{K}\phi_k = \lambda_k\, \mathbf{K}^{\mathsf{ref}}\phi_k, \quad k = 1, \ldots, N$$

Eigenvalue bounds

- for every function φ_k having its support inside the patch $\mathcal{P}_k$

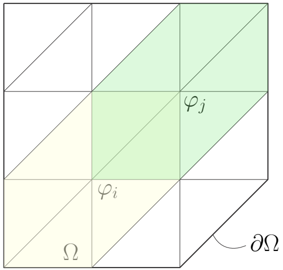
$$\lambda_k^{\mathrm{L}} = \operatorname*{ess\,inf}_{\boldsymbol{x}\in\mathcal{P}_k} \lambda_{\min}\left((\mathbf{A}^{\mathsf{ref}}(\boldsymbol{x}))^{-1}\mathbf{A}(\boldsymbol{x})\right)$$

$$\lambda_k^{\mathrm{U}} = \operatorname*{ess\,sup}_{\boldsymbol{x}\in\mathcal{P}_k} \lambda_{\max}\left((\mathbf{A}^{\mathsf{ref}}(\boldsymbol{x}))^{-1}\mathbf{A}(\boldsymbol{x})\right)$$

- sort the two series non-decreasingly,

$$\{\lambda_1^{\mathrm{L}}, \lambda_2^{\mathrm{L}}, \dots, \lambda_N^{\mathrm{L}}\} \rightarrow \lambda_{r(1)}^{L} \leq \lambda_{r(2)}^{L} \leq \dots \leq \lambda_{r(N)}^{L}$$

$$\{\lambda_1^{\mathrm{U}}, \lambda_2^{\mathrm{U}}, \dots, \lambda_N^{\mathrm{U}}\} \rightarrow \lambda_{s(1)}^{U} \leq \lambda_{s(2)}^{U} \leq \dots \leq \lambda_{s(N)}^{U}$$



Supports of φ_i and φ_j.

Generalized Rayleigh quotient bounds

Let $\mathbf{A}(\boldsymbol{x}), \mathbf{A}^{\mathsf{ref}}(\boldsymbol{x}) \in \mathbb{R}^{d\times d}$ be symmetric positive definite, then constants $0 < c_1 \leq c_2 < \infty$ bound the generalised Rayleigh quotient

$$c_1 \leq \frac{\boldsymbol{w}^T \mathbf{A}(\boldsymbol{x}) \boldsymbol{w}}{\boldsymbol{w}^T \mathbf{A}^{\mathsf{ref}}(\boldsymbol{x}) \boldsymbol{w}} \leq c_2, \quad \boldsymbol{x} \in \Omega, \text{ and } \boldsymbol{w} \in \mathbb{R}^d, \ \boldsymbol{w} \neq 0. \tag{1}$$

Then for $u \in H_0^1(\Omega)$, by setting $\boldsymbol{w} = \nabla u$ and integrating over Ω, we get

$$c_1 \leq \frac{\int_\Omega \nabla u \cdot \mathbf{A} \nabla u \,\mathrm{d}\boldsymbol{x}}{\int_\Omega \nabla u \cdot \mathbf{A}^{\mathsf{ref}} \nabla u \,\mathrm{d}\boldsymbol{x}} \leq c_2.$$

Using $u = \sum_{i=1}^{N} \mathsf{v}_i \varphi_i$, we get

$$c_1 \leq \frac{\int_\Omega \nabla u \cdot \mathbf{A} \nabla u \,\mathrm{d}\boldsymbol{x}}{\int_\Omega \nabla u \cdot \mathbf{A}^{\mathsf{ref}} \nabla u \,\mathrm{d}\boldsymbol{x}} = \frac{\mathbf{v}^T \mathbf{K} \mathbf{v}}{\mathbf{v}^T \mathbf{K}^{\mathsf{ref}} \mathbf{v}} \leq c_2, \quad \mathbf{v} \in \mathbb{R}^N, \ \mathbf{v} \neq \mathbf{0}. \tag{2}$$

Courant–Fischer min-max theorem*

If $\mathbf{K}, \mathbf{K}^{\text{ref}} \in \mathbb{R}^{N\times N}$ are symmetric positive definite, then

$$\lambda_j = \max_{S,\, \dim S = N-j+1} \; \min_{\mathbf{v}\in S,\, \mathbf{v}\neq \mathbf{0}} \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{K}^{\text{ref}}\mathbf{v}},$$

where S denotes a subspace of $\mathbb{R}^N$.

For $j = 1$ we have

$$\lambda_1 \quad = \quad \max_{S,\, \dim S = N} \; \min_{\mathbf{v}\in S,\, \mathbf{v}\neq 0} \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{K}^{\text{ref}}\mathbf{v}} = \min_{\mathbf{v}\in \mathbb{R}^N,\, \mathbf{v}\neq 0} \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{K}^{\text{ref}}\mathbf{v}}.$$

The next inequality follows from (1) and (2), such that

$$c_1 \leq \frac{\int_\Omega \nabla u \cdot \mathbf{A} \nabla u \,\mathrm{d}\boldsymbol{x}}{\int_\Omega \nabla u \cdot \mathbf{A}^{\text{ref}} \nabla u \,\mathrm{d}\boldsymbol{x}} = \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{K}^{\text{ref}}\mathbf{v}}, \quad \mathbf{v} \in \mathbb{R}^N,\, \mathbf{v} \neq \mathbf{0}.$$

* e.g. Theorem 8.1.2 in G. H. Golub, Ch. F. Van Loan: Matrix Computations.

Generalized eigenvalues of material data

- material data

$$c_1 \leq \frac{\boldsymbol{w}^T \mathbf{A}(\boldsymbol{x})\boldsymbol{w}}{\boldsymbol{w}^T \mathbf{A}^{\mathsf{ref}}(\boldsymbol{x})\boldsymbol{w}} \leq c_2, \quad \boldsymbol{x} \in \Omega, \text{ and } \boldsymbol{w} \in \mathbb{R}^d, \ \boldsymbol{w} \neq 0$$

- lower bound

$$\lambda_1^{\mathrm{L}} = \operatorname*{ess\,inf}_{\boldsymbol{x}\in\Omega} \ \lambda_{\min}\left(\left(\mathbf{A}^{\mathsf{ref}}(\boldsymbol{x})\right)^{-1}\mathbf{A}(\boldsymbol{x})\right) \leq \min_{\mathsf{v}\in\mathbb{R}^N,\, \mathsf{v}\neq 0} \frac{\mathsf{v}^T\mathsf{K}\mathsf{v}}{\mathsf{v}^T\mathsf{K}^{\mathsf{ref}}\mathsf{v}} = \lambda_1$$

- localization

$$\lambda_{r(1)}^{\mathrm{L}} = \operatorname*{ess\,inf}_{\boldsymbol{x}\in\mathcal{P}_{r(1)}} \ \lambda_{\min}\left(\left(\mathbf{A}^{\mathsf{ref}}(\boldsymbol{x})\right)^{-1}\mathbf{A}(\boldsymbol{x})\right)$$

Courant–Fischer min-max theorem†

If $\mathbf{K}, \mathbf{K}^{\text{ref}} \in \mathbb{R}^{N\times N}$ are symmetric positive definite, then

$$\lambda_j = \max_{S,\, \dim S = N-j+1} \ \min_{\mathbf{v}\in S,\, \mathbf{v}\neq \mathbf{0}} \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{K}^{\text{ref}}\mathbf{v}},$$

where S denotes a subspace of $\mathbb{R}^N$.

For $j = 1$ we have

$$\lambda_1 = \max_{S,\, \dim S = N} \ \min_{\mathbf{v}\in S,\, \mathbf{v}\neq 0} \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{K}^{\text{ref}}\mathbf{v}} = \min_{\mathbf{v}\in\mathbb{R}^N,\, \mathbf{v}\neq 0} \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{K}^{\text{ref}}\mathbf{v}}.$$

The next inequality follows from (1) and (2), such that

$$\lambda^{\mathrm{L}}_{r(1)} = \min_{\mathcal{P}_k\subset\Omega} \lambda^{\mathrm{L}}_k \leq \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{K}^{\text{ref}}\mathbf{v}} = \frac{\int_\Omega \nabla u \cdot \mathbf{A}\nabla u \,\mathrm{d}\boldsymbol{x}}{\int_\Omega \nabla u \cdot \mathbf{A}^{\text{ref}}\nabla u \,\mathrm{d}\boldsymbol{x}}, \quad \mathbf{v}\in\mathbb{R}^N,\ \mathbf{v}\neq 0.$$

† e.g. Theorem 8.1.2 in G. H. Golub, Ch. F. Van Loan: Matrix Computations.

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Courant–Fischer min-max theorem

If $\mathbf{K}, \mathbf{K}^{\text{ref}} \in \mathbb{R}^{N\times N}$ are symmetric positive definite, then

$$\lambda_j = \max_{S,\,\dim S = N-j+1} \; \min_{\mathbf{v}\in S,\,\mathbf{v}\neq 0} \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{K}^{\text{ref}}\mathbf{v}},$$

where S denotes a subspace of $\mathbb{R}^N$.

For $j = 2$ we have

$$\lambda_2 \;=\; \max_{S,\,\dim S = N-1} \; \min_{\mathbf{v}\in S,\,\mathbf{v}\neq 0} \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{K}^{\text{ref}}\mathbf{v}} \geq \min_{\mathbf{v}\in\mathbb{R}^N,\,\mathbf{v}\neq 0,\,\mathbf{v}_{r(1)}=0} \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{K}^{\text{ref}}\mathbf{v}}$$

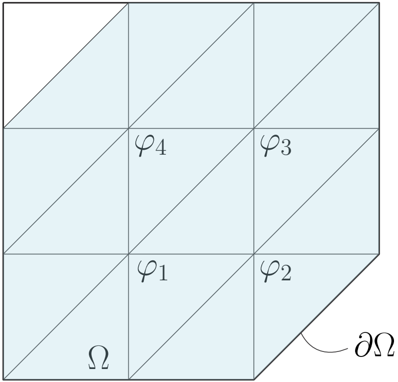
The next inequality follows from (1) and (2),

$$\lambda^{\mathrm{L}}_{r(2)} = \min_{\mathcal{P}_k\subset\mathcal{D}} \lambda^{\mathrm{L}}_k \leq \frac{\mathbf{v}^T\mathbf{K}\mathbf{v}}{\mathbf{v}^T\mathbf{K}^{\text{ref}}\mathbf{v}} = \frac{\int_{\mathcal{D}} \nabla u\cdot\mathbf{A}\nabla u\,\mathrm{d}\boldsymbol{x}}{\int_{\mathcal{D}} \nabla u\cdot\mathbf{A}^{\text{ref}}\nabla u\,\mathrm{d}\boldsymbol{x}}, \qquad \mathbf{v}\in\mathbb{R}^N,\ \mathbf{v}\neq 0,\ \mathbf{v}_{r(1)} = 0$$

where (due to $\mathbf{v}_{r(1)} = 0$) $\mathcal{D}$ contains only the supports of φ_k, $k \neq r(1)$.

Geometric interpretation

- Lower bounds:
  - $\lambda^{\mathrm{L}}_{r(1)}$ found in x_1
  - $\lambda^{\mathrm{L}}_{r(2)}$ found in x_2
  - $\lambda^{\mathrm{L}}_{r(3)}$ found in x_3
  - $\lambda^{\mathrm{L}}_{r(4)}$ found in x_3



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Geometric interpretation

- Lower bounds:
  - $\lambda^{\mathrm{L}}_{r(1)}$ found in $\boldsymbol{x}_1$
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  - $\lambda^{\mathrm{L}}_{r(3)}$ found in $\boldsymbol{x}_3$
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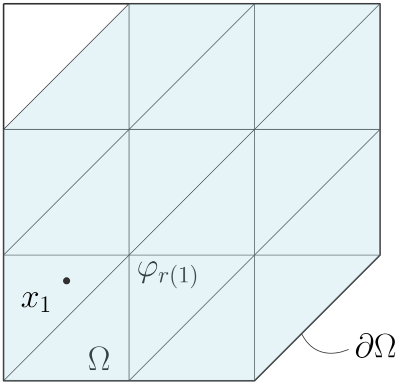

Geometric interpretation

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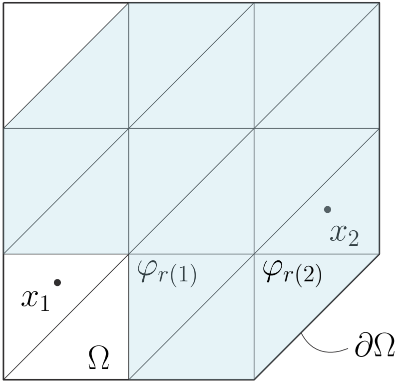

Geometric interpretation

- Lower bounds:
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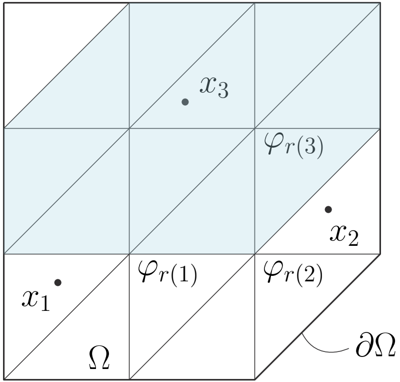

Geometric interpretation

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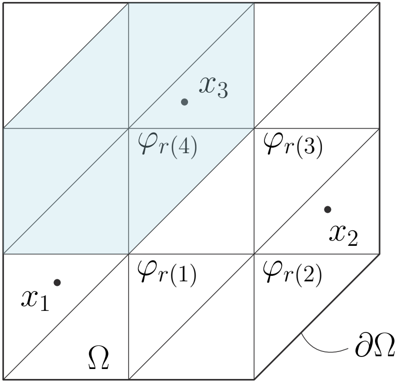


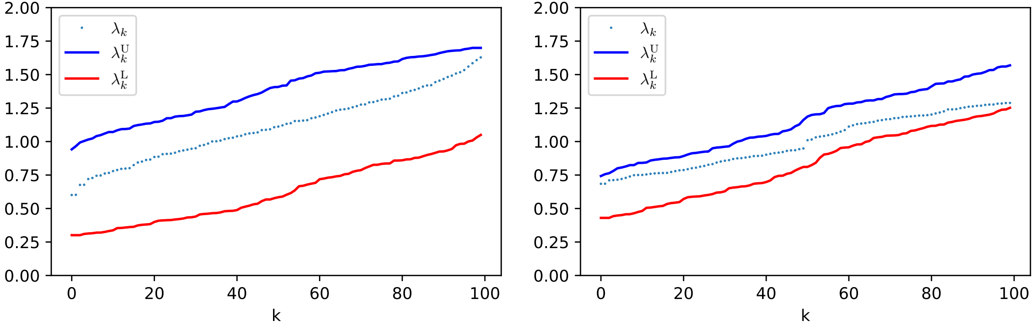
Example 2: Continuous data

- material data:

$$\mathbf{A}(\boldsymbol{x}) = \begin{pmatrix} 1 & 0.3 \\ 0.3 & 1 \end{pmatrix} + \begin{pmatrix} 0.3\sin(x_2) & 0.1\cos(x_1) \\ 0.1\cos(x_1) & 0.3\sin(x_2) \end{pmatrix}$$

- reference data:

$$\mathbf{A}_1^{\text{ref}}(\boldsymbol{x}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{A}_2^{\text{ref}}(\boldsymbol{x}) = \begin{pmatrix} 1 & 0.3 \\ 0.3 & 1 \end{pmatrix}$$



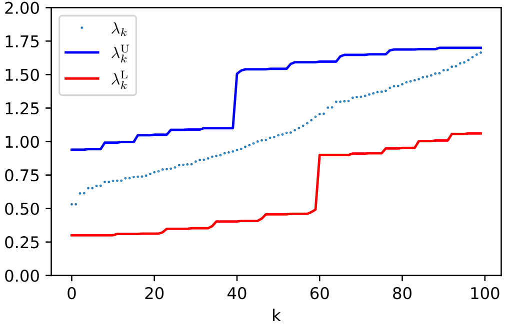
Example 2: Discontinuous data

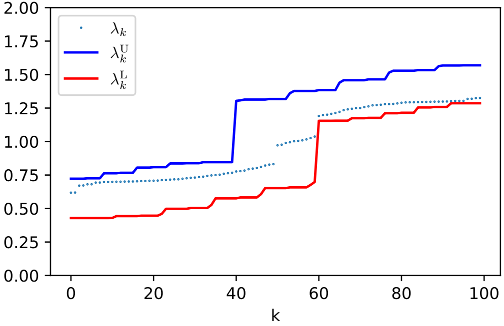
- material data:

$$\mathbf{A}(\boldsymbol{x}) = \begin{pmatrix} 1 & 0.3 \\ 0.3 & 1 \end{pmatrix} + \begin{pmatrix} 0.3\,\mathrm{sgn}(x_2) & 0.1\cos(x_1) \\ 0.1\cos(x_1) & 0.3\,\mathrm{sgn}(x_2) \end{pmatrix}$$

- reference data:

$$\mathbf{A}_1^{\text{ref}}(\boldsymbol{x}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{A}_2^{\text{ref}}(\boldsymbol{x}) = \begin{pmatrix} 1 & 0.3 \\ 0.3 & 1 \end{pmatrix}$$





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Homogeneous subdomain

- scalar multiple

$$\boldsymbol{A}^{ref}(\boldsymbol{x}) = a\boldsymbol{A}(\boldsymbol{x}) \quad \boldsymbol{x} \in \mathcal{P}_k$$

- bounds

$$\lambda_k^{\mathrm{L}} = \operatorname*{ess\,inf}_{\boldsymbol{x}\in\mathcal{P}_k} \lambda_{\min}\left((\mathbf{A}^{\text{ref}}(\boldsymbol{x}))^{-1}\mathbf{A}(\boldsymbol{x})\right)$$

$$\lambda_k^{\mathrm{U}} = \operatorname*{ess\,sup}_{\boldsymbol{x}\in\mathcal{P}_k} \lambda_{\max}\left((\mathbf{A}^{\text{ref}}(\boldsymbol{x}))^{-1}\mathbf{A}(\boldsymbol{x})\right)$$

$$\overbrace{\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}^{-1}}^{(\mathbf{A}^{\text{ref}})^{-1}} \overbrace{\begin{pmatrix}2 & 0\\ 0 & 2\end{pmatrix}}^{\mathbf{A}} \longrightarrow 2 \quad 2$$

$$\overbrace{\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}^{-1}}^{(\mathbf{A}^{\text{ref}})^{-1}} \overbrace{\begin{pmatrix}0.5 & 0\\ 0 & 0.5\end{pmatrix}}^{\mathbf{A}} \longrightarrow 0.5 \quad 0.5$$

Homogeneous subdomain

- scalar multiple

$$A^{ref}(\boldsymbol{x}) = a\boldsymbol{A}(\boldsymbol{x}) \quad \boldsymbol{x} \in \mathcal{P}_k$$

- bounds

$$\lambda_k^{\mathrm{L}} = \operatorname*{ess\,inf}_{\boldsymbol{x}\in\mathcal{P}_k} \lambda_{\min}\left((\mathbf{A}^{\mathsf{ref}}(\boldsymbol{x}))^{-1}\mathbf{A}(\boldsymbol{x})\right)$$

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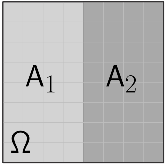
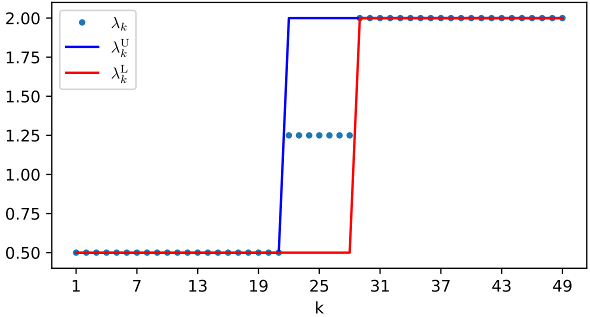
Example 3: Scalar multiple

- $\boldsymbol{A}^{ref} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$





Example 3: Scalar multiple

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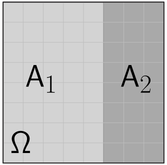

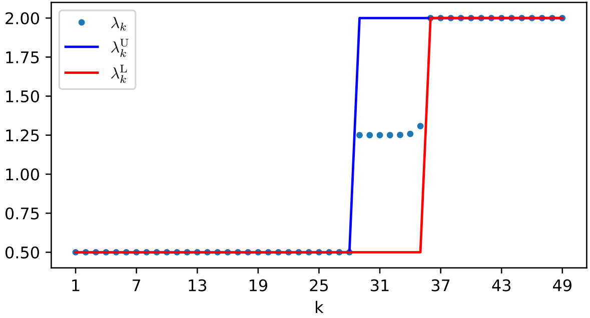

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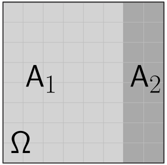
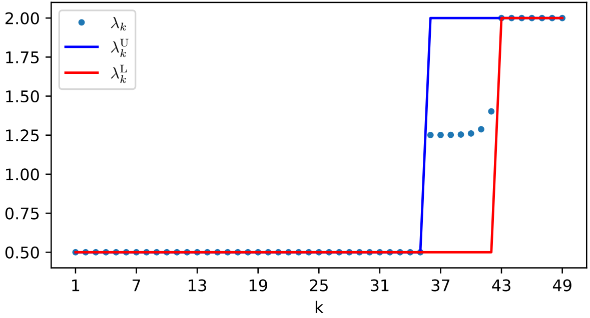
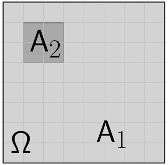
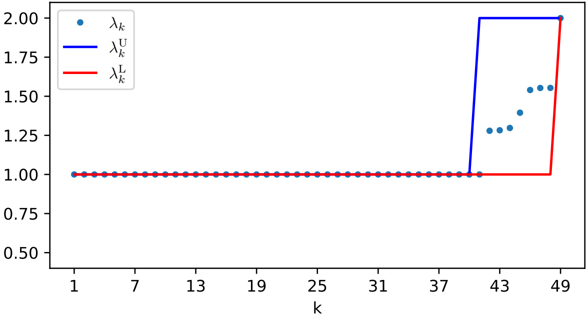




Example 4: Interfaces

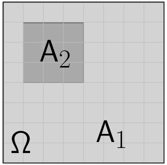
- $\boldsymbol{A}^{ref} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$

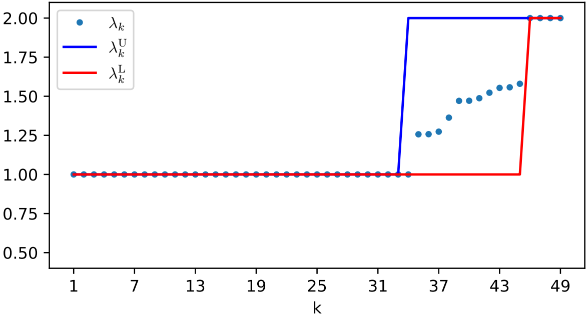




Example 4: Interfaces

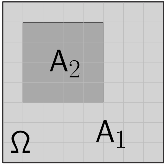
- $\boldsymbol{A}^{ref} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$

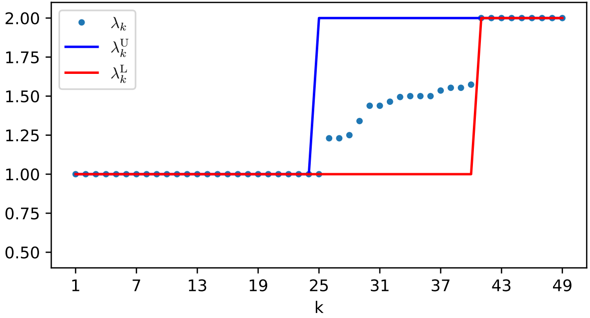




Example 4: Interfaces

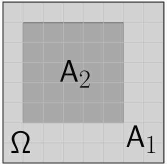
- $\boldsymbol{A}^{ref} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$

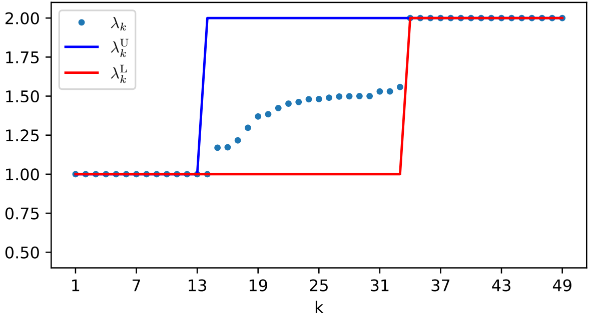




Example 4: Interfaces

- $\boldsymbol{A}^{ref} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$





Homogeneous subdomain

- scalar multiple

$$\boldsymbol{A}^{ref}(\boldsymbol{x}) \neq a\boldsymbol{A}(\boldsymbol{x}) \qquad \boldsymbol{x} \in \mathcal{P}_k$$

- bounds

$$\lambda_k^{\mathrm{L}} = \operatorname*{ess\,inf}_{\boldsymbol{x}\in\mathcal{P}_k} \lambda_{\min}\left((\mathbf{A}^{\mathsf{ref}}(\boldsymbol{x}))^{-1}\mathbf{A}(\boldsymbol{x})\right)$$

$$\lambda_k^{\mathrm{U}} = \operatorname*{ess\,sup}_{\boldsymbol{x}\in\mathcal{P}_k} \lambda_{\max}\left((\mathbf{A}^{\mathsf{ref}}(\boldsymbol{x}))^{-1}\mathbf{A}(\boldsymbol{x})\right)$$

$$\overbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}^{-1}}^{(\mathbf{A}^{\mathsf{ref}})^{-1}} \overbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1.5 \end{pmatrix}}^{\mathbf{A}} \longrightarrow 1.5 \quad 2$$

$$\overbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}^{-1}}^{(\mathbf{A}^{\mathsf{ref}})^{-1}} \overbrace{\begin{pmatrix} 2 & 0 \\ 0 & 1.8 \end{pmatrix}}^{\mathbf{A}} \longrightarrow 1.8 \quad 2$$

Homogeneous subdomain

- scalar multiple

$$\boldsymbol{A}^{ref}(\boldsymbol{x}) \neq a\boldsymbol{A}(\boldsymbol{x}) \qquad \boldsymbol{x} \in \mathcal{P}_k$$

- bounds

$$\lambda_k^{\mathrm{L}} = \operatorname*{ess\,inf}_{\boldsymbol{x}\in\mathcal{P}_k} \lambda_{\min}\left((\mathbf{A}^{\mathsf{ref}}(\boldsymbol{x}))^{-1}\mathbf{A}(\boldsymbol{x})\right)$$

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$$\overbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}^{-1}}^{(\mathbf{A}^{\mathsf{ref}})^{-1}} \overbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1.5 \end{pmatrix}}^{\mathbf{A}} \longrightarrow 1.5 \quad 2$$

$$\overbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}^{-1}}^{(\mathbf{A}^{\mathsf{ref}})^{-1}} \overbrace{\begin{pmatrix} 2 & 0 \\ 0 & 1.8 \end{pmatrix}}^{\mathbf{A}} \longrightarrow 1.8 \quad 2$$

Homogeneous subdomain

- scalar multiple

$$\boldsymbol{A}^{ref}(\boldsymbol{x}) \neq a\boldsymbol{A}(\boldsymbol{x}) \qquad \boldsymbol{x} \in \mathcal{P}_k$$

- bounds

$$\lambda_k^{\mathrm{L}} = \operatorname*{ess\,inf}_{\boldsymbol{x}\in\mathcal{P}_k} \lambda_{\min}\left((\mathbf{A}^{\mathsf{ref}}(\boldsymbol{x}))^{-1}\mathbf{A}(\boldsymbol{x})\right)$$

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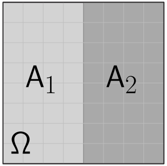
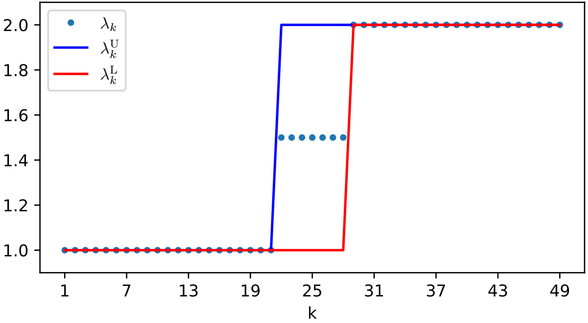
$$\overbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}^{-1}}^{(\mathbf{A}^{\mathsf{ref}})^{-1}} \overbrace{\begin{pmatrix} 2 & 0 \\ 0 & 1.8 \end{pmatrix}}^{\mathbf{A}} \longrightarrow 1.8 \quad 2$$

Example 4

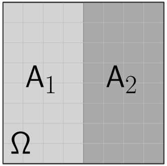
- $\boldsymbol{A}^{ref} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$

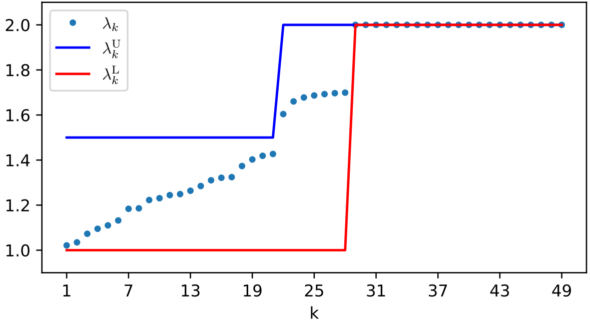




Example 4

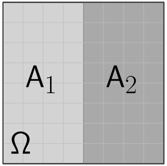
- $\boldsymbol{A}^{ref} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1.5 \end{pmatrix} \quad \boldsymbol{A}_2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$

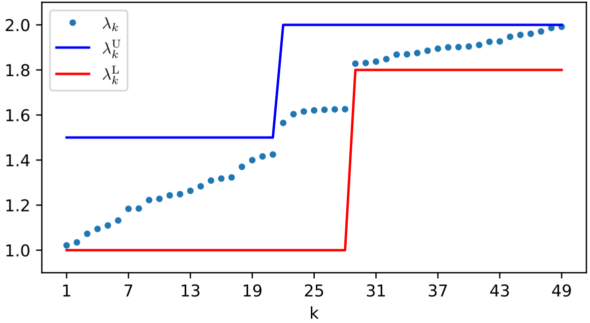




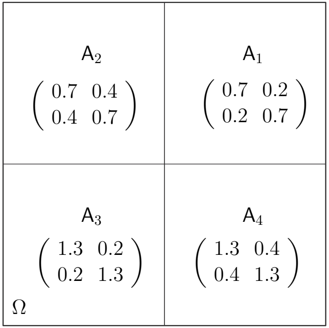
Example 4

- $\boldsymbol{A}^{ref} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \boldsymbol{A}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1.5 \end{pmatrix} \quad \boldsymbol{A}_2 = \begin{pmatrix} 2 & 0 \\ 0 & 1.8 \end{pmatrix}$

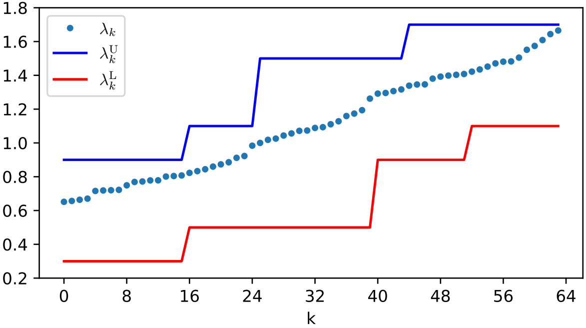




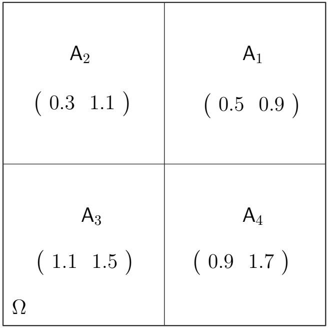
Example 5: Optimization



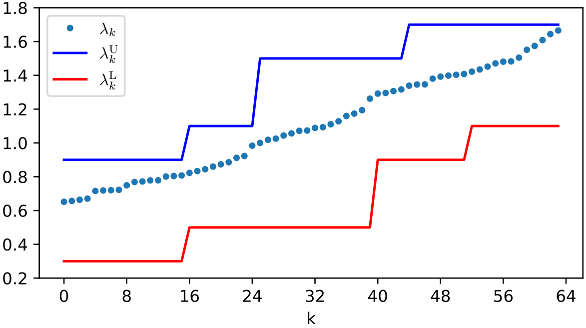
$$\mathbf{A}^{\text{ref}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



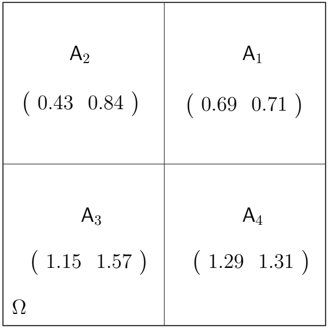
Example 5: Optimization



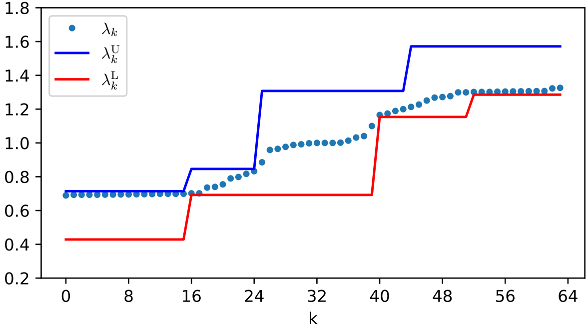
$$\mathbf{A}^{\text{ref}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



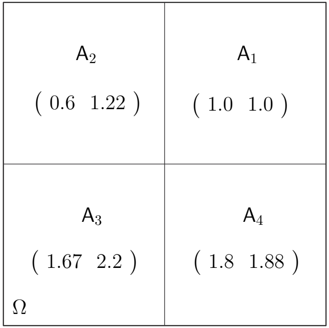
Example 5: Optimization



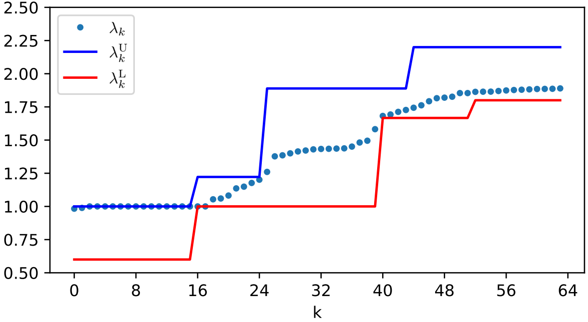
$$\mathbf{A}^{\mathrm{ref}} = \begin{pmatrix} 1 & 0.3 \\ 0.3 & 1 \end{pmatrix}$$



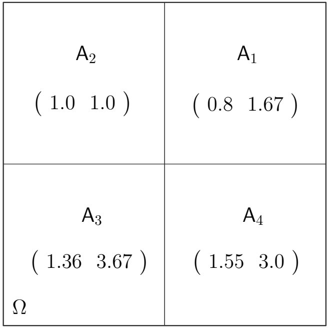
Example 5: Optimization



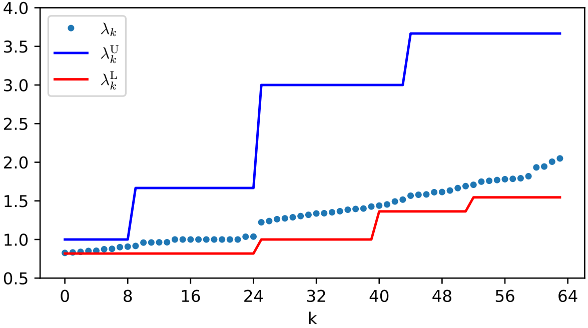
$$\mathbf{A}^{\mathsf{ref}} = \mathbf{A}_1 = \begin{pmatrix} 0.7 & 0.2 \\ 0.2 & 0.7 \end{pmatrix}$$



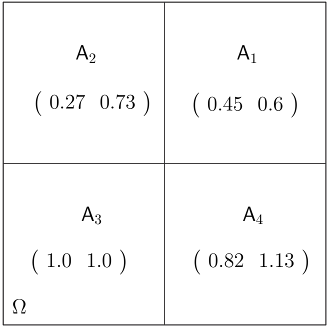
Example 5: Optimization



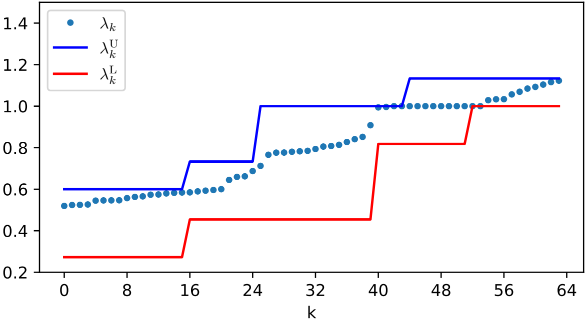
$$\mathbf{A}^{\text{ref}} = \mathbf{A}_2 = \begin{pmatrix} 0.7 & 0.4 \\ 0.4 & 0.7 \end{pmatrix}$$

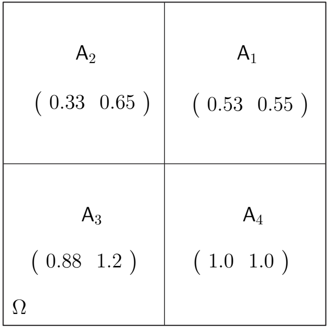


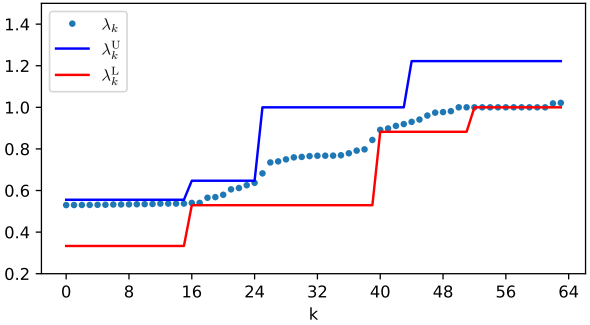
Example 5: Optimization



$$\mathbf{A}^{\text{ref}} = \mathbf{A}_3 = \begin{pmatrix} 1.3 & 0.2 \\ 0.2 & 1.3 \end{pmatrix}$$







$$\mathbf{A}^{\text{ref}} = \mathbf{A}_4 = \begin{pmatrix} 1.3 & 0.4 \\ 0.4 & 1.3 \end{pmatrix}$$

Small-strain elasticity

- governing equation

$$-\boldsymbol{\partial}^{\mathsf{T}}\mathbf{C}(\boldsymbol{x})\boldsymbol{\partial}\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{F}(\boldsymbol{x}) \quad \boldsymbol{x} \in \Omega$$

- original system matrix

$$\mathsf{K} = \int_\Omega \boldsymbol{\partial}\boldsymbol{v}^T\mathbf{C}\boldsymbol{\partial}\boldsymbol{u}\,\mathrm{d}\boldsymbol{x}$$

- reference system matrix

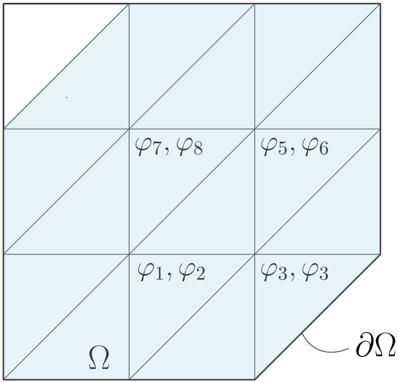
$$\mathsf{K}^{\mathsf{ref}} = \int_\Omega \boldsymbol{\partial}\boldsymbol{v}^T\mathbf{C}^{\mathsf{ref}}\boldsymbol{\partial}\boldsymbol{u}\,\mathrm{d}\boldsymbol{x}$$

- approximation

$$u_\alpha(\boldsymbol{x}) \approx u_\alpha^N(\boldsymbol{x}) = \sum_{I=1}^{N} u_\alpha^N(\boldsymbol{x}_\mathrm{n}^I)\varphi^I(\boldsymbol{x})$$

Geometric interpretation

- Lower bounds:
  - $\lambda^{\mathrm{L}}_{r(1)}$ found in x_1
  - $\lambda^{\mathrm{L}}_{r(2)}$ found in x_1
  - $\lambda^{\mathrm{L}}_{r(3)}$ found in x_2
  - $\lambda^{\mathrm{L}}_{r(4)}$ found in x_2
  - $\lambda^{\mathrm{L}}_{r(5)}$ found in x_3
  - $\lambda^{\mathrm{L}}_{r(6)}$ found in x_3
  - $\lambda^{\mathrm{L}}_{r(7)}$ found in x_3
  - $\lambda^{\mathrm{L}}_{r(8)}$ found in x_3



Geometric interpretation

- Lower bounds:
  - $\lambda^{\mathrm{L}}_{r(1)}$ found in $\boldsymbol{x}_1$
  - $\lambda^{\mathrm{L}}_{r(2)}$ found in $\boldsymbol{x}_1$
  - $\lambda^{\mathrm{L}}_{r(3)}$ found in $\boldsymbol{x}_2$
  - $\lambda^{\mathrm{L}}_{r(4)}$ found in $\boldsymbol{x}_2$
  - $\lambda^{\mathrm{L}}_{r(5)}$ found in $\boldsymbol{x}_3$
  - $\lambda^{\mathrm{L}}_{r(6)}$ found in $\boldsymbol{x}_3$
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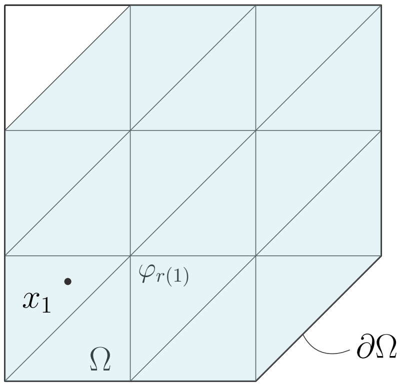
  - $\lambda^{\mathrm{L}}_{r(8)}$ found in $\boldsymbol{x}_3$



Geometric interpretation

- Lower bounds:
  - $\lambda^{\mathrm{L}}_{r(1)}$ found in $\boldsymbol{x}_1$
  - $\lambda^{\mathrm{L}}_{r(2)}$ found in $\boldsymbol{x}_1$
  - $\lambda^{\mathrm{L}}_{r(3)}$ found in $\boldsymbol{x}_2$
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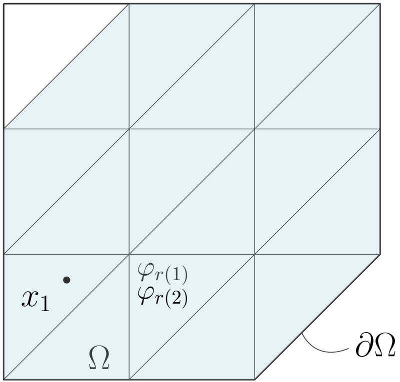
  - $\lambda^{\mathrm{L}}_{r(6)}$ found in $\boldsymbol{x}_3$
  - $\lambda^{\mathrm{L}}_{r(7)}$ found in $\boldsymbol{x}_3$
  - $\lambda^{\mathrm{L}}_{r(8)}$ found in $\boldsymbol{x}_3$



Geometric interpretation

- Lower bounds:
  - $\lambda^{\mathrm{L}}_{r(1)}$ found in $\boldsymbol{x}_1$
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  - $\lambda^{\mathrm{L}}_{r(3)}$ found in $\boldsymbol{x}_2$
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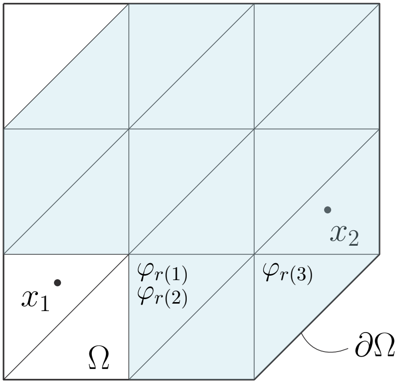
  - $\lambda^{\mathrm{L}}_{r(7)}$ found in $\boldsymbol{x}_3$
  - $\lambda^{\mathrm{L}}_{r(8)}$ found in $\boldsymbol{x}_3$



Geometric interpretation

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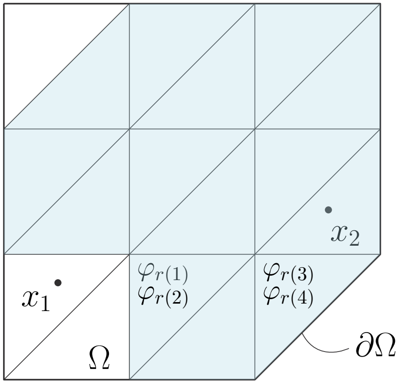

Geometric interpretation

- Lower bounds:
  - $\lambda^{\mathrm{L}}_{r(1)}$ found in $\boldsymbol{x}_1$
  - $\lambda^{\mathrm{L}}_{r(2)}$ found in $\boldsymbol{x}_1$
  - $\lambda^{\mathrm{L}}_{r(3)}$ found in $\boldsymbol{x}_2$
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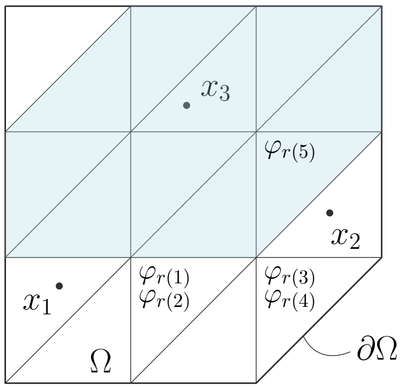
  - $\lambda^{\mathrm{L}}_{r(8)}$ found in $\boldsymbol{x}_3$



Geometric interpretation

- Lower bounds:
  - $\lambda^{\mathrm{L}}_{r(1)}$ found in $\boldsymbol{x}_1$
  - $\lambda^{\mathrm{L}}_{r(2)}$ found in $\boldsymbol{x}_1$
  - $\lambda^{\mathrm{L}}_{r(3)}$ found in $\boldsymbol{x}_2$
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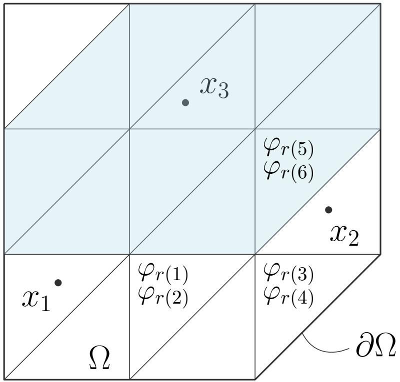
  - $\lambda^{\mathrm{L}}_{r(8)}$ found in $\boldsymbol{x}_3$



Geometric interpretation

- Lower bounds:
  - $\lambda^{\mathrm{L}}_{r(1)}$ found in $\boldsymbol{x}_1$
  - $\lambda^{\mathrm{L}}_{r(2)}$ found in $\boldsymbol{x}_1$
  - $\lambda^{\mathrm{L}}_{r(3)}$ found in $\boldsymbol{x}_2$
  - $\lambda^{\mathrm{L}}_{r(4)}$ found in $\boldsymbol{x}_2$
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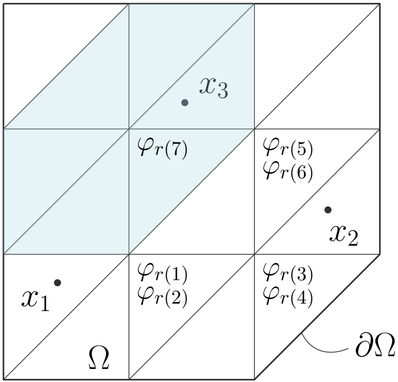

Geometric interpretation

- Lower bounds:
  - $\lambda^{\mathrm{L}}_{r(1)}$ found in $\boldsymbol{x}_1$
  - $\lambda^{\mathrm{L}}_{r(2)}$ found in $\boldsymbol{x}_1$
  - $\lambda^{\mathrm{L}}_{r(3)}$ found in $\boldsymbol{x}_2$
  - $\lambda^{\mathrm{L}}_{r(4)}$ found in $\boldsymbol{x}_2$
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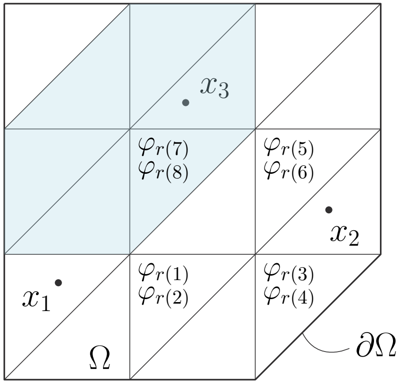
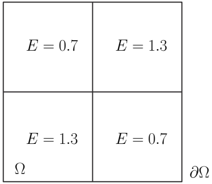
  - $\lambda^{\mathrm{L}}_{r(8)}$ found in $\boldsymbol{x}_3$

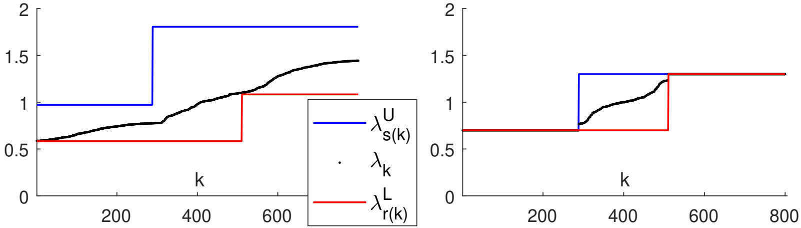


Example 6: Elasticity

$$\boldsymbol{C}(\boldsymbol{x}) = \frac{E(\boldsymbol{x})}{(1+\nu)(1-2\nu)} \begin{pmatrix} 1-\nu & \nu & 0 \\ \nu & 1-\nu & 0 \\ 0 & 0 & 0.5-\nu) \end{pmatrix}, \quad \nu = 0.2.$$



$\mathbf{C}_1^{\text{ref}} : \{E = 1, \nu_1 = 0\}$ and $\mathbf{C}_2^{\text{ref}} : \{E = 1, \nu_1 = 0.2\}$



Material data in quadrature points

- quadrature

$$\int_{\Omega} \boldsymbol{\partial}\tilde{\boldsymbol{v}}(\boldsymbol{x})^{\mathsf{T}}\mathbf{C}^{\mathsf{ref}}(\boldsymbol{x})\boldsymbol{\partial}\boldsymbol{u}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \approx \sum_{Q=1}^{N_{\mathrm{Q}}} \boldsymbol{\partial}\tilde{\boldsymbol{v}}(\boldsymbol{x}_{\mathrm{q}}^{Q})^{\mathsf{T}}\mathbf{C}^{\mathsf{ref}}(\boldsymbol{x}_{\mathrm{q}}^{Q})\boldsymbol{\partial}\boldsymbol{u}(\boldsymbol{x}_{\mathrm{q}}^{Q})\, w^{Q}$$

- bounds over quadrature points

$$\lambda_k^{\mathrm{L}} = \min_{\boldsymbol{x}_{\mathrm{q}}^{Q} \in \operatorname{supp} \varphi^k} \lambda_{\min}\left((\mathbf{C}^{\mathsf{ref}}(\boldsymbol{x}_{\mathrm{q}}^{Q}))^{-1}\mathbf{C}(\boldsymbol{x}_{\mathrm{q}}^{Q}) \right), \quad k = 1, \ldots, dN$$

$$\lambda_k^{\mathrm{U}} = \max_{\boldsymbol{x}_{\mathrm{q}}^{Q} \in \operatorname{supp} \varphi^k} \lambda_{\max}\left((\mathbf{C}^{\mathsf{ref}}(\boldsymbol{x}_{\mathrm{q}}^{Q}))^{-1}\mathbf{C}(\boldsymbol{x}_{\mathrm{q}}^{Q}) \right), \quad k = 1, \ldots, dN$$

Implementation per elements

- compute bounds for every element

$$c_1 \leq \frac{\boldsymbol{w}^T \mathbf{A}(\boldsymbol{x})\boldsymbol{w}}{\boldsymbol{w}^T \mathbf{A}^{\mathsf{ref}}(\boldsymbol{x})\boldsymbol{w}} \leq c_2, \quad \boldsymbol{x} \in \Omega^e, \text{ and } \boldsymbol{w} \in \mathbb{R}^d, \ \boldsymbol{w} \neq 0, e = 1, \ldots, N_\mathrm{e}$$

- bounds on local matrices

$$c_1 \leq \frac{\mathbf{v}^T \mathbf{K}_e \mathbf{v}}{\mathbf{v}^T \mathbf{K}_e^{\mathsf{ref}} \mathbf{v}} = \frac{\int_{\Omega^e} \nabla u \cdot \mathbf{A} \nabla u \,\mathrm{d}\boldsymbol{x}}{\int_{\Omega^e} \nabla u \cdot \mathbf{A}^{\mathsf{ref}} \nabla u \,\mathrm{d}\boldsymbol{x}} \leq c_2$$

- local matrices $\mathbf{K}_e \in \mathbb{R}^{N \times N}$ and $\mathbf{K}_e^{\mathsf{ref}} \in \mathbb{R}^{N \times N}$

$$\mathbf{K} = \sum_{e=1}^{N_\mathrm{e}} \mathbf{K}_e, \quad \mathbf{K}^{\mathsf{ref}} = \sum_{e=1}^{N_\mathrm{e}} \mathbf{K}_e^{\mathsf{ref}}$$

Bounds from local matrices

- lower bound on the first eigenvalue

$$\mathbf{v}^T \mathbf{K} \mathbf{v} \geq \lambda_1^{\mathrm{L}} \mathbf{v}^T \mathbf{K}^{\mathsf{ref}} \mathbf{v}, \quad \mathbf{v} \in \mathbb{R}^N, \mathbf{v} \neq \mathbf{0}$$

- equivalently in the sum form

$$\sum_{e=1}^{N_\mathrm{e}} \mathbf{v}^T \mathbf{K}_e \mathbf{v} \geq \lambda_1^{\mathrm{L}} \sum_{e=1}^{N_\mathrm{e}} \mathbf{v}^T \mathbf{K}_e^{\mathsf{ref}} \mathbf{v}, \quad \mathbf{v} \in \mathbb{R}^N, \mathbf{v} \neq \mathbf{0}$$

- **sufficient** condition

$$\mathbf{v}^T \mathbf{K}_e \mathbf{v} \geq \lambda_1^{\mathrm{L}} \mathbf{v}^T \mathbf{K}_e^{\mathsf{ref}} \mathbf{v}, \quad \mathbf{v} \in \mathbb{R}^N, \mathbf{v} \neq \mathbf{0}, e = 1, \ldots, N_\mathrm{e}$$

Courant–Fischer min-max theorem

- Courant-Fischer min-max principle

$$\lambda_2 = \max_{S,\, \dim S = N-1} \min_{\mathbf{v} \in S,\, \mathbf{v} \neq 0} \frac{\mathbf{v}^T \mathbf{K} \mathbf{v}}{\mathbf{v}^T \mathbf{K}^{\mathrm{ref}} \mathbf{v}} \geq \min_{\mathbf{v} \in \mathbb{R}^N,\, \mathbf{v} \neq 0,\, \mathbf{v}_{r(1)} = 0} \frac{\mathbf{v}^T \mathbf{K} \mathbf{v}}{\mathbf{v}^T \mathbf{K}^{\mathrm{ref}} \mathbf{v}}$$

- any $\lambda_2^{\mathrm{L}} \in \mathbb{R}$ such that

$$\mathbf{v}^T \mathbf{K} \mathbf{v} \geq \lambda_2^{\mathrm{L}}\, \mathbf{v}^T \mathbf{K}^{\mathrm{ref}} \mathbf{v}, \qquad \mathbf{v} \in \mathbb{R}^N,\ \mathbf{v}_{r(1)} = 0$$

  is a lower bound to λ_2.
- **sufficient** condition

$$\mathbf{v}^T \mathbf{K}_e \mathbf{v} \geq \lambda_2^{\mathrm{L}}\, \mathbf{v}^T \mathbf{K}_e^{\mathrm{ref}} \mathbf{v}, \quad e = 1, \ldots, N_{\mathrm{e}}, \quad \mathbf{v} \in \mathbb{R}^N, \mathbf{v} \neq \mathbf{0}, \mathbf{v}_{r(1)} = 0$$

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Generalized bounds

- locally assembled system matrices

$$\mathbf{K} = \sum_{e=1}^{N_\mathrm{e}} \mathbf{K}_e \qquad \mathbf{K}^{\mathrm{ref}} = \sum_{e=1}^{N_\mathrm{e}} \mathbf{K}_e^{\mathrm{ref}}$$

- can be applied to:
  - finite difference
  - stochastic Galerkin FE method
  - algebraic multilevel preconditioning
  - discontinuous Galerkin

Note that symmetric positive semi-definite $\mathbf{K}_e \in \mathbb{R}^{N \times N}$ and $\mathbf{K}_e^{\mathrm{ref}} \in \mathbb{R}^{N \times N}$ must have the same kernels.

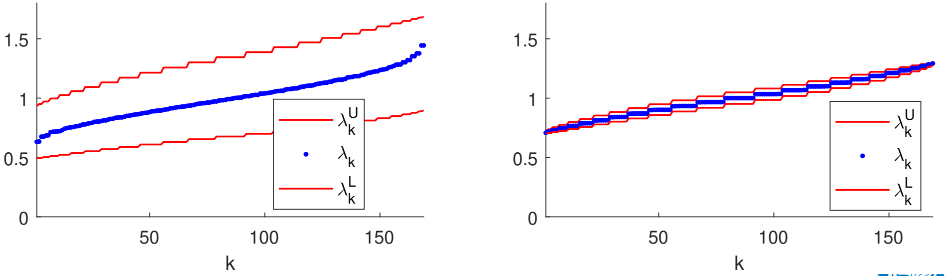
Example 7: Finite difference 1

- material data:

$$\mathbf{A}(\boldsymbol{x}) = \left(1 + 0.3\cos\left((x_1 + x_2)\frac{\pi}{2}\right)\right)\begin{pmatrix} 1 & 0.3 \\ 0.3 & 1 \end{pmatrix}$$

- reference data:

$$\mathbf{A}_1^{\text{ref}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \text{and} \quad \mathbf{A}_2^{\text{ref}} = \begin{pmatrix} 1 & 0.3 \\ 0.3 & 1 \end{pmatrix}$$



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Preconditioned conjugate gradients

- preconditioned system

$$(\mathbf{K}^{\text{ref}})^{-1}\mathbf{K}\mathbf{u} = (\mathbf{K}^{\text{ref}})^{-1}\mathbf{b}$$

- additional system

$$\mathbf{K}^{\text{ref}}\mathbf{z}_k = \mathbf{r}_k$$

procedure $\mathrm{PCG}(\boldsymbol{u}_0, \mathbf{K}, \mathbf{b}, \mathbf{M}, tol, it_{\max})$

$\quad \mathbf{r}_0 := \mathbf{b} - \mathbf{K}\boldsymbol{u}_0$

$\quad \mathbf{z}_0 := \mathbf{M}^{-1}\mathbf{r}_0$

$\quad nr_0 := \|\mathbf{r}_0\|$ ▷ initial residual

$\quad \mathbf{p}_0 := \mathbf{z}_0$

$\quad$ **while** $k \leq it_{max}$ **do** ▷ $k = 0, 1, \ldots, it_{max}$

$\quad\quad \mathbf{Kp}_k = \mathbf{Kp}_k$

$\quad\quad \alpha_k = \dfrac{\mathbf{r}_k^\top \mathbf{z}_k}{\mathbf{p}_k^\top \mathbf{K}\mathbf{p}_k}$

$\quad\quad \delta\tilde{\boldsymbol{u}}_{k+1} = \delta\tilde{\boldsymbol{u}}_k + \alpha_k \mathbf{p}_k$

$\quad\quad \mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k \mathbf{Kp}_k$

$\quad\quad \mathbf{z}_{k+1} = \mathbf{M}^{-1}\mathbf{r}_{k+1}$

$\quad\quad nr_{k+1} = \|\mathbf{r}_{k+1}\|$

$\quad\quad$ **if** $\dfrac{nr_{k+1}}{nr_0} < tol$ **then**

$\quad\quad\quad$ **return** $\boldsymbol{u}_{k+1}$

$\quad\quad \beta_k = \dfrac{\mathbf{r}_{k+1}^\top \mathbf{z}_{k+1}}{\mathbf{r}_k^\top \mathbf{z}_k}$

$\quad\quad \mathbf{p}_{k+1} = \mathbf{z}_{k+1} + \beta_k \mathbf{p}_k$

$\quad\quad k = k + 1$

$\quad$ **return** $\boldsymbol{u}_k$

Periodic homogenization

- governing equation

$$-\nabla \cdot \mathbf{A}(\boldsymbol{x})\nabla u(\boldsymbol{x}) = 0 \quad \boldsymbol{x} \in \mathcal{Y}$$

periodic B.C.

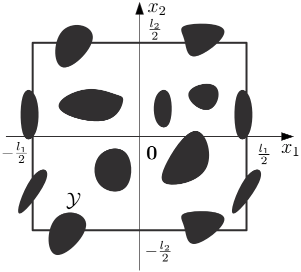
- overall gradient field

$$\nabla u(\boldsymbol{x}) = \boldsymbol{e} + \nabla \tilde{u}(\boldsymbol{x}) \quad \boldsymbol{x} \in \mathcal{Y}$$

$$\boldsymbol{e} = \frac{1}{|\mathcal{Y}|}\int_{\mathcal{Y}} \nabla u(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \in \mathbb{R}^d$$

- homogenized (constant) material data

$$\mathbf{A}_{\mathrm{H}}\boldsymbol{e} = \frac{1}{|\mathcal{Y}|}\int_{\mathcal{Y}} \mathbf{A}(\boldsymbol{x})(\boldsymbol{e} + \nabla \tilde{u}(\boldsymbol{x}))\,\mathrm{d}\boldsymbol{x}$$



A rectangular cell with outlined periodic microstructure.

Periodic homogenization

- governing equation

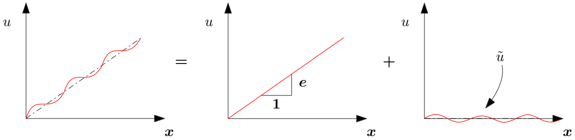
$$-\nabla \cdot \mathbf{A}(\boldsymbol{x})\nabla u(\boldsymbol{x}) = 0 \quad \boldsymbol{x} \in \mathcal{Y}$$

periodic B.C.

- overall gradient field

$$\nabla u(\boldsymbol{x}) = \boldsymbol{e} + \nabla \tilde{u}(\boldsymbol{x}) \quad \boldsymbol{x} \in \mathcal{Y}$$

$$\boldsymbol{e} = \frac{1}{|\mathcal{Y}|}\int_{\mathcal{Y}} \nabla u(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \in \mathbb{R}^d$$



- homogenized (constant) material data

$$\mathbf{A}_{\mathrm{H}}\boldsymbol{e} = \frac{1}{|\mathcal{Y}|}\int_{\mathcal{Y}} \mathbf{A}(\boldsymbol{x})(\boldsymbol{e} + \nabla \tilde{u}(\boldsymbol{x}))\,\mathrm{d}\boldsymbol{x}$$

Periodic homogenization

- governing equation

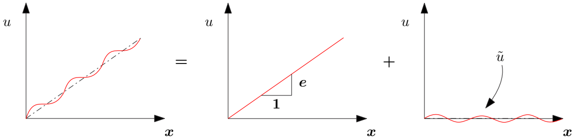
$$-\nabla \cdot \mathbf{A}(\boldsymbol{x})\nabla u(\boldsymbol{x}) = 0 \quad \boldsymbol{x} \in \mathcal{Y}$$

periodic B.C.

- overall gradient field

$$\nabla u(\boldsymbol{x}) = \boldsymbol{e} + \nabla \tilde{u}(\boldsymbol{x}) \quad \boldsymbol{x} \in \mathcal{Y}$$

$$\boldsymbol{e} = \frac{1}{|\mathcal{Y}|} \int_{\mathcal{Y}} \nabla u(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} \in \mathbb{R}^d$$



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- governing equation

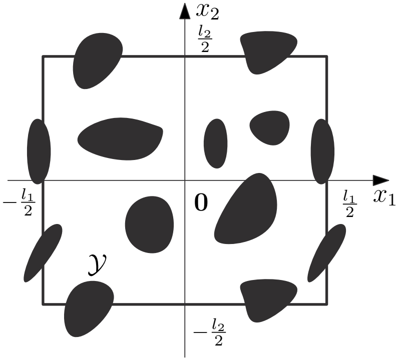
$$-\nabla \cdot \mathbf{A}(\boldsymbol{x})(\boldsymbol{e} + \nabla \tilde{u}(\boldsymbol{x})) = 0 \quad \boldsymbol{x} \in \mathcal{Y}$$

- weak form

$$\int_{\mathcal{Y}} \nabla \tilde{v}(\boldsymbol{x})^{\mathsf{T}} \mathbf{A}(\boldsymbol{x}) \nabla \tilde{u}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \int_{\mathcal{Y}} \nabla \tilde{v}(\boldsymbol{x})^{\mathsf{T}} \mathbf{A}(\boldsymbol{x}) \boldsymbol{e} \, \mathrm{d}\boldsymbol{x} \quad \tilde{v} \in \mathcal{V}$$

- system matrix

$$\mathbf{K}[j,i] = \int_{\mathcal{Y}} \nabla \varphi_j(\boldsymbol{x})^{\mathsf{T}} \mathbf{A} \nabla \varphi_i(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}$$



$$\mathcal{V} = \left\{ \tilde{v} : H^1_{per}(\mathcal{Y}), \int_{\mathcal{Y}} \tilde{v}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = 0 \right\}$$

Periodic homogenization

- governing equation

$$-\nabla \cdot \mathbf{A}(\boldsymbol{x})(\boldsymbol{e} + \nabla \tilde{u}(\boldsymbol{x})) = 0 \quad \boldsymbol{x} \in \mathcal{Y}$$

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$$\int_{\mathcal{Y}} \nabla \tilde{v}(\boldsymbol{x})^{\mathsf{T}} \mathbf{A}(\boldsymbol{x}) \nabla \tilde{u}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \int_{\mathcal{Y}} \nabla \tilde{v}(\boldsymbol{x})^{\mathsf{T}} \mathbf{A}(\boldsymbol{x}) \boldsymbol{e} \, \mathrm{d}\boldsymbol{x} \quad \tilde{v} \in \mathcal{V}$$

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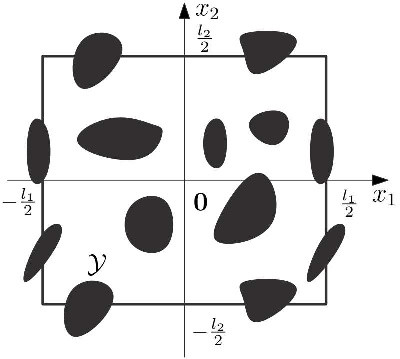

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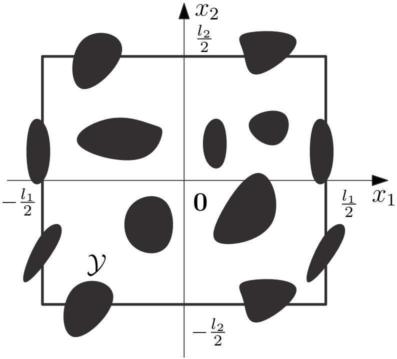


$\mathcal{V} = \left\{ \tilde{v} : H^1_{per}(\mathcal{Y}), \int_{\mathcal{Y}} \tilde{v}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = 0 \right\}$

Fourier-Galerkin method

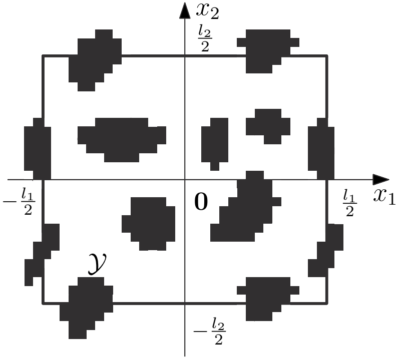
- regular (pixel/voxel) data structure
- Fourier-basis

$$\tilde{u}(\boldsymbol{x}) \approx \sum_{i=0}^{N} \widehat{u}_i \varphi_i^{FG}(\boldsymbol{x}) = \sum_{i=0}^{N} \widehat{u}_i \exp(2\pi \mathrm{i} \boldsymbol{k}_i \boldsymbol{x})$$

$$\nabla \tilde{u}(\boldsymbol{x}) \approx \sum_{i=0}^{N} \widehat{u}_i \nabla \varphi_i^{FG}(\boldsymbol{x}) = \sum_{i=0}^{N} 2\pi \mathrm{i} \boldsymbol{k}_i \, \widehat{u}_i \, \exp(2\pi \mathrm{i} \boldsymbol{k}_i \boldsymbol{x})$$

- linear system with Fourier coefficient

$$\mathbf{F}^{\mathsf{H}} \widehat{\mathbf{K}} \mathbf{F} \tilde{\mathbf{u}} = \mathbf{b} \qquad \widehat{\mathbf{u}} = \mathbf{F} \tilde{\mathbf{u}}$$



Fourier-Galerkin method: Homogeneous reference data

- closed-form expression

$$\widehat{\mathbf{K}}^{\mathsf{ref}}[j,i] = \int_{\mathcal{Y}} \nabla\varphi_j^{FG}(\boldsymbol{x})^{\mathsf{T}}\mathbf{A}^{\mathsf{ref}}\nabla\varphi_i^{FG}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \begin{cases} \boldsymbol{k}_j^{\mathsf{T}}\mathbf{A}^{\mathsf{ref}}\boldsymbol{k}_i & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases}$$

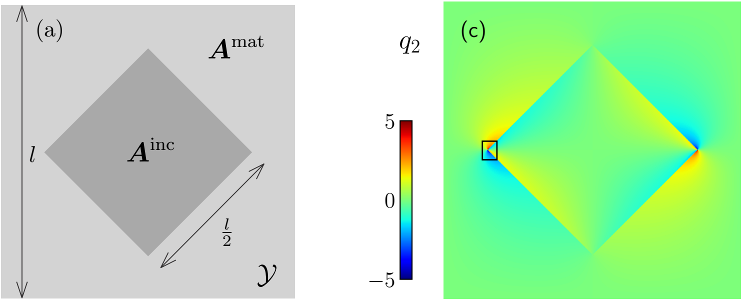
- $\widehat{\mathbf{K}}^{\mathsf{ref}}$ is block diagonal in the Fourier space

$$\left(\mathbf{K}^{\mathsf{ref}}\right)^{-1} = \mathbf{F}^{\mathsf{H}}\left(\widehat{\mathbf{K}}^{\mathsf{ref}}\right)^{-1}\mathbf{F}$$

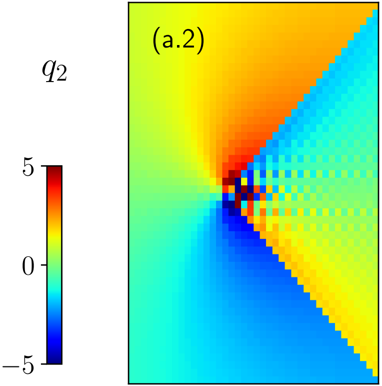
- accelerated by FFT

$$\underbrace{\mathcal{F}^{-1}\left(\widehat{\mathbf{K}}^{\mathsf{ref}}\right)^{-1}\mathcal{F}}_{(\mathbf{K}^{\mathsf{ref}})^{-1}}\mathbf{K}\tilde{\mathbf{u}} = \underbrace{\mathcal{F}^{-1}\left(\widehat{\mathbf{K}}^{\mathsf{ref}}\right)^{-1}\mathcal{F}}_{(\mathbf{K}^{\mathsf{ref}})^{-1}}\mathbf{b}$$

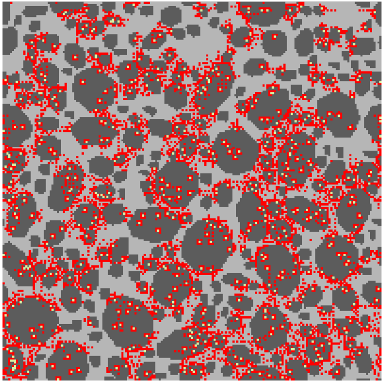
Fourier-Galerkin method: Heat conduction

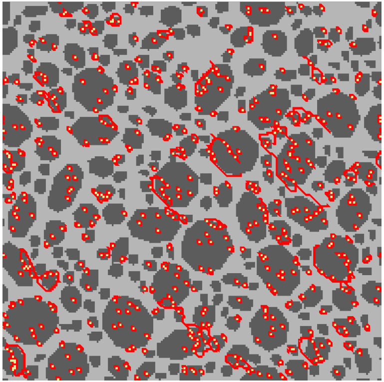


Oscillations



Damage fields in concrete



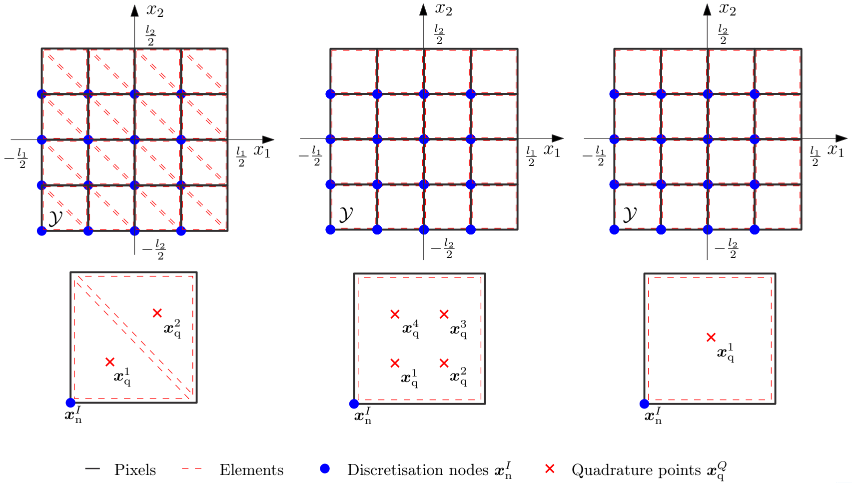


Aggregates Cement paste ASR gel pockets Damaged pixels

Fourier basis

linear FE basis.

Finite element method: discretisation grids



Finite element method: Assembly of $\widehat{\mathbf{K}}^{\text{ref}}$

- no (simple) closed-form expression

$$\widehat{\mathbf{K}}^{\text{ref}}[j,i] = \int_{\mathcal{Y}} \nabla\varphi_j^{FE}(\boldsymbol{x})^{\mathsf{T}} \mathbf{A}^{\text{ref}} \nabla\varphi_i^{FE}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \neq \begin{cases} \boldsymbol{k}_j^{\mathsf{T}} \mathbf{A}^{\text{ref}} \boldsymbol{k}_i & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases}$$

- $\widehat{\mathbf{K}}^{\text{ref}}$ is diagonal

$$\left(\mathbf{K}^{\text{ref}}\right)^{-1} = \mathbf{F}_d^{\mathsf{H}} \left(\widehat{\mathbf{K}}^{\text{ref}}\right)^{-1} \mathbf{F}_d.$$

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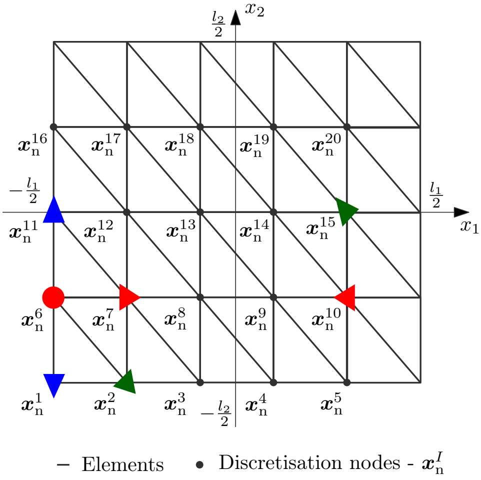
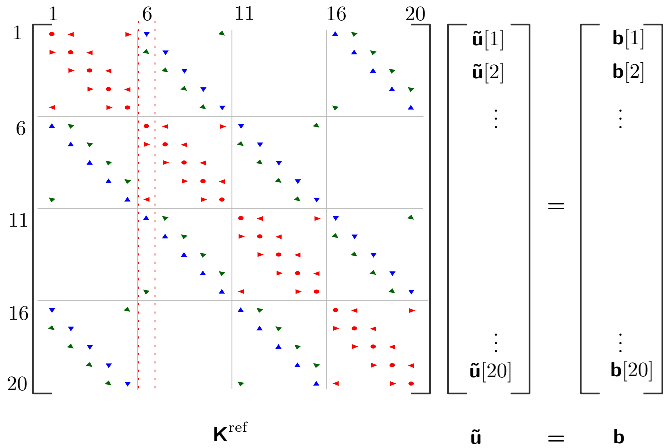


x_2
$\frac{l_2}{2}$
x_{n}^{16} x_{n}^{17} x_{n}^{18} x_{n}^{19} x_{n}^{20}
$-\frac{l_1}{2}$
$\frac{l_1}{2}$
x_1
x_{n}^{11} x_{n}^{12} x_{n}^{13} x_{n}^{14} x_{n}^{15}
x_{n}^{6} x_{n}^{7} x_{n}^{8} x_{n}^{9} x_{n}^{10}
x_{n}^{1} x_{n}^{2} x_{n}^{3} $-\frac{l_2}{2}$ x_{n}^{4} x_{n}^{5}
– Elements
• Discretisation nodes - x_{n}^{I}



1 6 11 16 20
1
6
11
16
20
$\tilde{\mathbf{u}}[1]$
$\tilde{\mathbf{u}}[2]$
$\tilde{\mathbf{u}}[20]$
=
$\mathbf{b}[1]$
$\mathbf{b}[2]$
$\mathbf{b}[20]$
$\mathbf{K}^{\text{ref}}$ $\tilde{\mathbf{u}}$ = $\mathbf{b}$

Finite element method: Assembly of $\widehat{\mathbf{K}}^{\mathrm{ref}}$

- $\widehat{\mathbf{K}}^{\mathrm{ref}}$ is diagonal

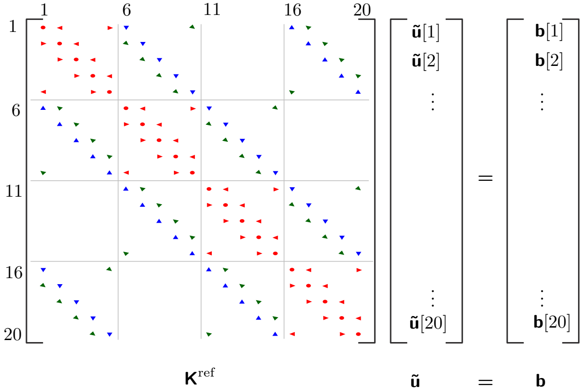
$$(\mathbf{K}^{\mathrm{ref}})^{-1} = \mathbf{F}_d^{\mathrm{H}} (\widehat{\mathbf{K}}^{\mathrm{ref}})^{-1} \mathbf{F}_d.$$

- unit impulse

$$\widehat{\mathbf{K}}^{\mathrm{ref}}[:,1] = \widehat{\mathbf{K}}^{\mathrm{ref}} \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

- diagonal

$$\mathrm{diag}(\widehat{\mathbf{K}}^{\mathrm{ref}}) = \mathcal{F}(\widehat{\mathbf{K}}^{\mathrm{ref}}[:,1])$$



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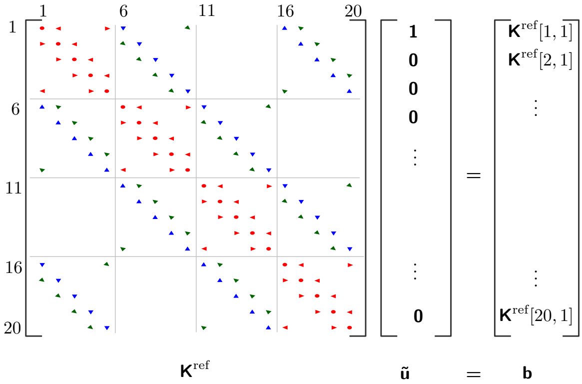

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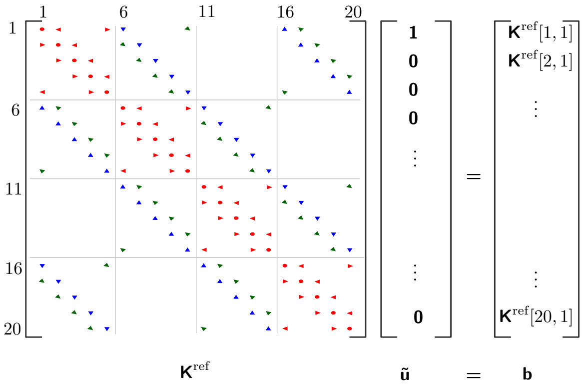
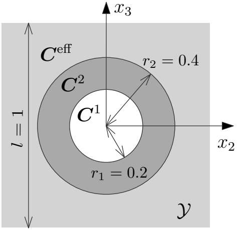
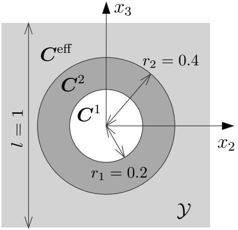
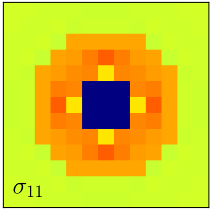


Example 9: Grid size independence – elasticity



Example 9: Grid size independence – elasticity





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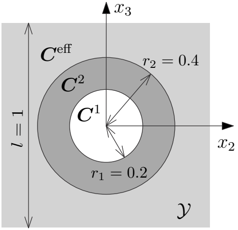

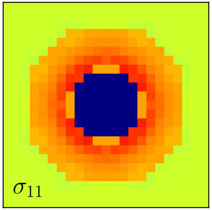

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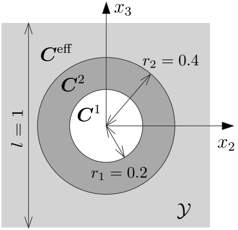

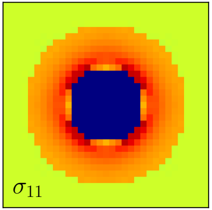

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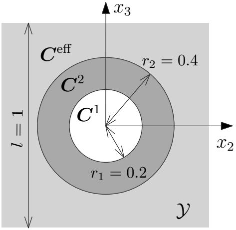

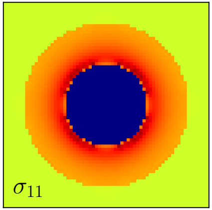

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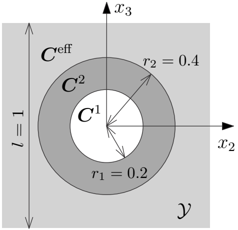
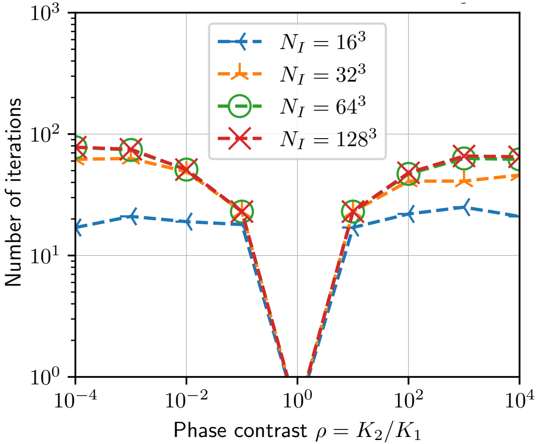
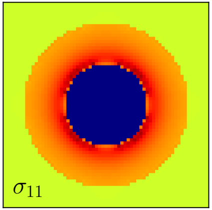
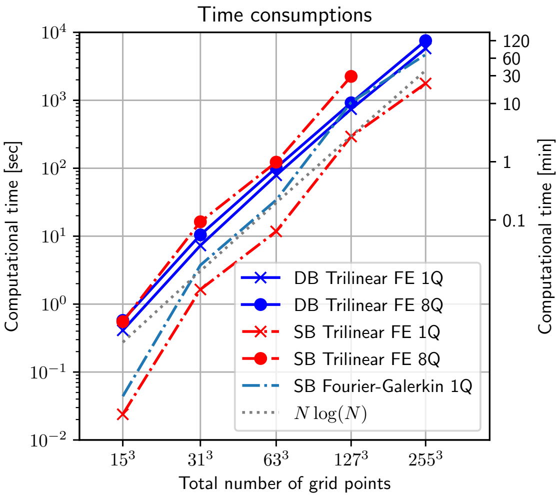




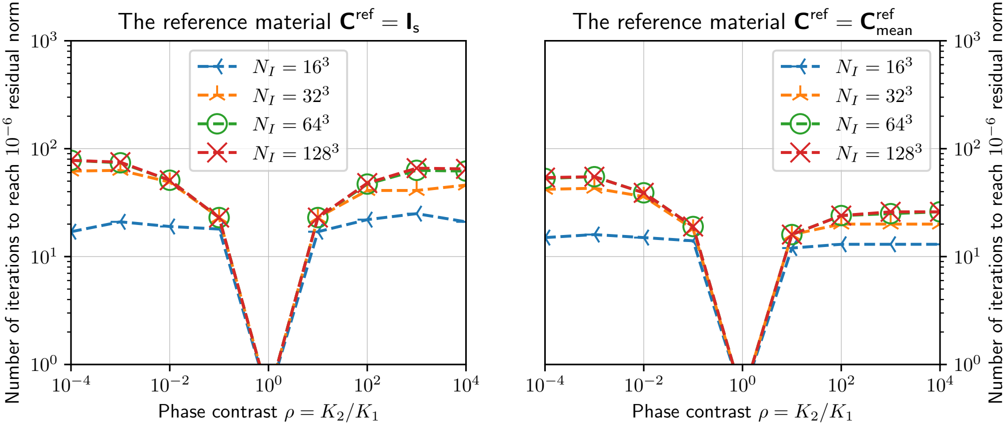


Example 9: Scaling

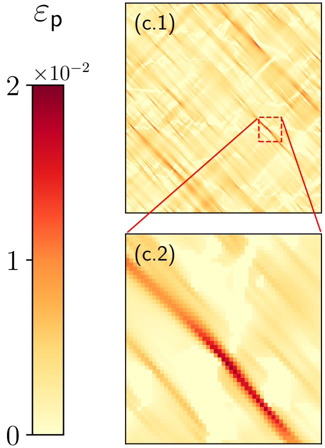


DB -displacement-based formulation, SB-strain-based formulation

Example 9: Choice of reference material

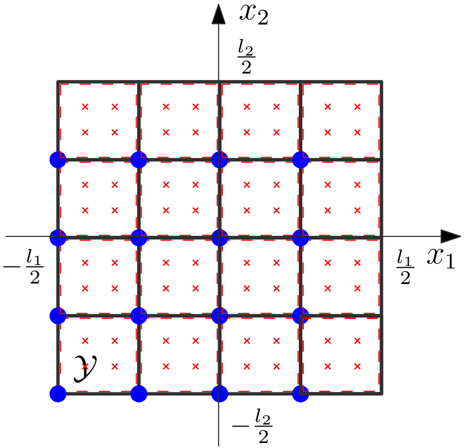


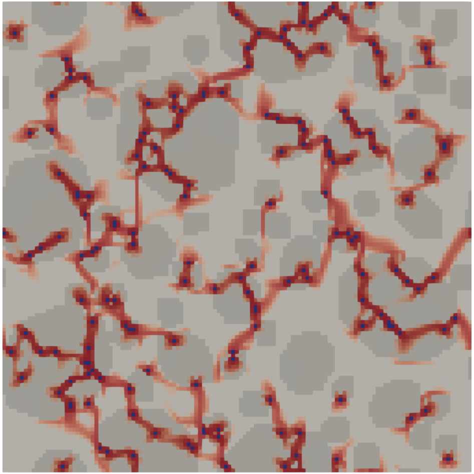
Example 10: Choice of reference material



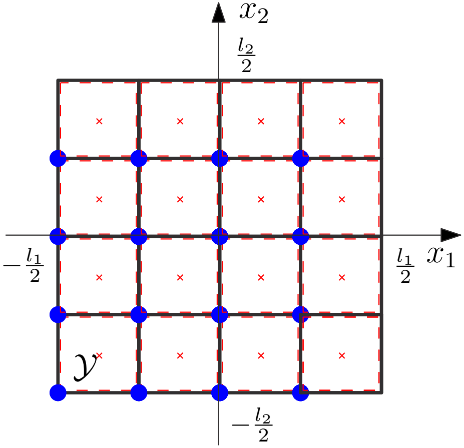
	$\mathbf{C}^{\mathrm{ref}}$	Fourier	linear FE	bilinear FE
Newton		11	9	10
(P)CG	$\mathbf{I}$	1012	861	761
	$\mathbf{I_s}$	781	609	540
	$\mathbf{C}^{\mathrm{ref}}_{\mathrm{mean}}$	585	457	407

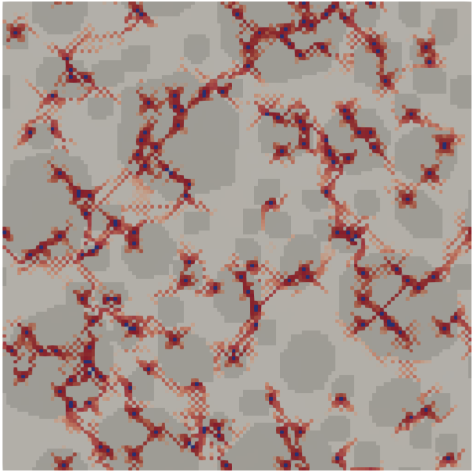
Example 11: Damage in concrete – bilinear FE



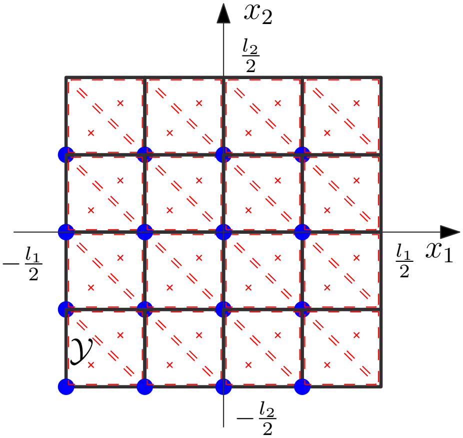


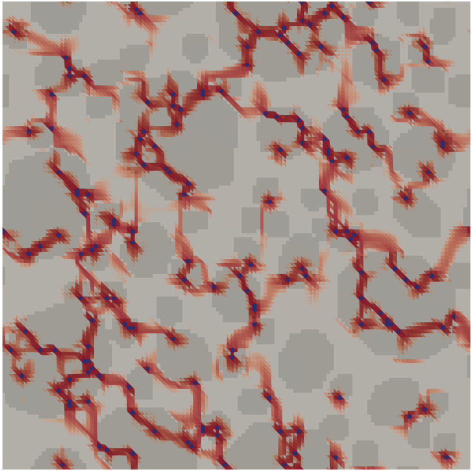
Example 11: Damage in concrete – under-integrated bilinear FE



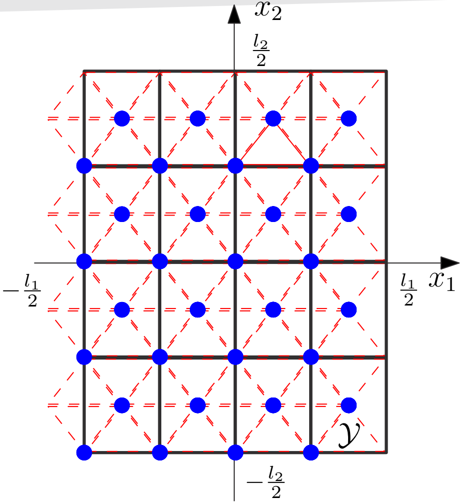


Example 11: Damage in concrete – linear FE





Example 11: Damage in concrete – isotropic mesh



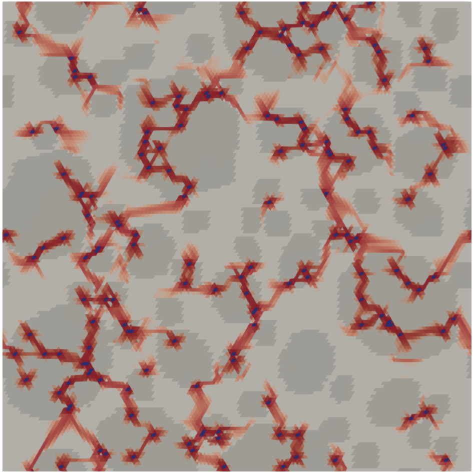


Table of contents

The take-home message

The discrete Green's (Laplace) operator preconditioning makes condition number independent of mesh size. Additionally, the distribution of eigenvalues can be estimated and optimized.

Collaborations

- Eigenvalues bounds


- FFT-based FE solvers

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE


UNI FREIBURG

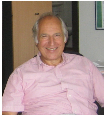


μSpectre

- Fourier-Galerkin

CAROLO-WILHELMINA BRAUNSCHWEIG





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Outlook & Support

Outlook:

- improve eigenvalues bounds
- PCG convergence estimate for homogenization

Thanks for financial support:

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- CAAS: CZ.02.1.01/0.0/0.0/16_019/0000778-01 (Jirásek, Bobok)
- SGS: SGS21/003-, SGS20/002-, SGS19/002-, SGS18/005-/OHK1/1T/11

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