SIAM Conference on Parallel Processing for Scientific Computing 2026

Computational homogenization methods based on the FFT with superior accuracy

Institute of Engineering Mathematics

Flavia Gehrig, Matti Schneider ■ *March 6 2026*

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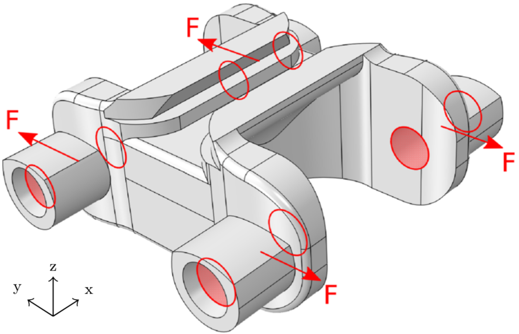
Computational homogenization: Small strain linear elasticity

Component (Macroscale)



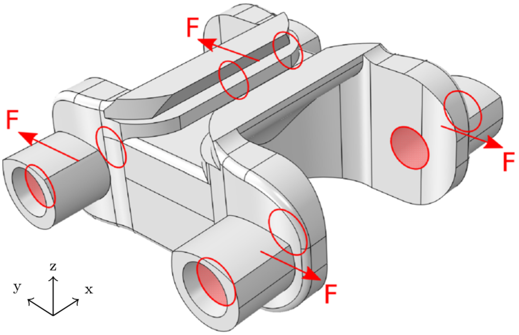
[Goldberg et al., 2017]

Quantities of interest

- Displacement $\boldsymbol{v}$
- Strain $\boldsymbol{\varepsilon} = \nabla^s \boldsymbol{v}$
- Stress $\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}$

Computational homogenization: Small strain linear elasticity

Component (Macroscale)



[Goldberg et al., 2017]

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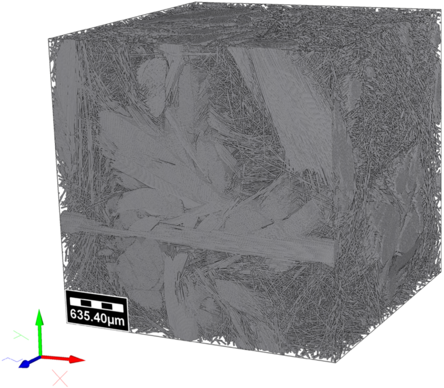
Computational homogenization: Small strain linear elasticity

Microstructure (Microscale)



[Schneider, 2017]

Challenge:

Heterogeneous microstructure

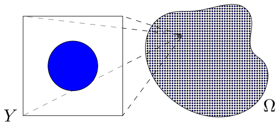
$\downarrow$

Heterogeneous stiffness $\mathbb{C}$

Computational homogenization: Small strain linear elasticity

given: $\boldsymbol{f}: \Omega \to \mathbb{R}^d$, BCs,

$\mathbb{C}: Y \to \mathcal{L}(\mathbb{R}^{d \times d})$

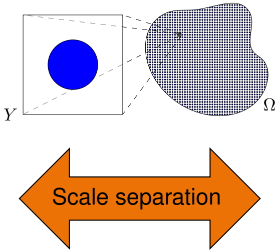


sought: $\boldsymbol{v}: \Omega \to \mathbb{R}^d$

Coupled problem:

$$\mathrm{div}\ [\mathbb{C}(\boldsymbol{x}) : \nabla^s \boldsymbol{v}(\boldsymbol{y})] = \boldsymbol{f} \quad \forall \boldsymbol{y} \in \Omega, \quad \boldsymbol{x} \in Y$$

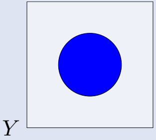
Computational homogenization: Small strain linear elasticity



Computational homogenization: Small strain linear elasticity

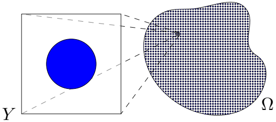
$\boldsymbol{E}$

Microscopic problem



$$\mathrm{div}\ [\mathbb{C}(\boldsymbol{x}) : (\boldsymbol{E} + \nabla^s \boldsymbol{u}(\boldsymbol{x}))] = \mathbf{0} \quad \forall \boldsymbol{x} \in Y,$$

with $\boldsymbol{u} : Y \to \mathbb{R}^d, \quad \mathbb{C} : Y \to \mathcal{L}(\mathbb{R}^{d\times d})$



Scale separation

Computational homogenization: Small strain linear elasticity

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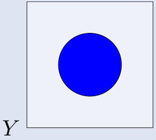
$\boldsymbol{E}$

Microscopic problem



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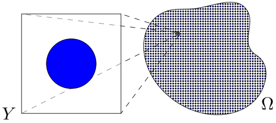
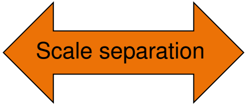


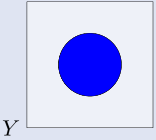


$\mathbb{C}^{\text{eff}}$

Computational homogenization: Small strain linear elasticity

$\boldsymbol{E}$

Microscopic problem



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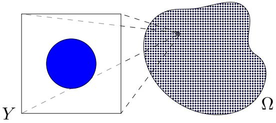
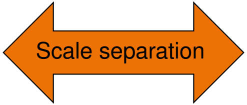
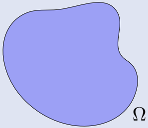




Macroscopic problem



$$\operatorname{div}\left[\mathbb{C}^{\text{eff}} : \nabla^s \boldsymbol{v}(\boldsymbol{y})\right] = \boldsymbol{f} \quad \forall \boldsymbol{y} \in \Omega,$$

with $\boldsymbol{v} : \Omega \to \mathbb{R}^d$

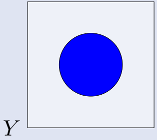
$\mathbb{C}^{\text{eff}}$

Computational homogenization: Small strain linear elasticity

Computational micromechanics

$\boldsymbol{E}$

Microscopic problem



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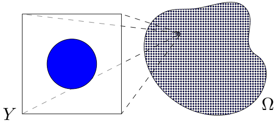
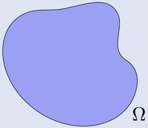


Scale separation

Macroscopic problem



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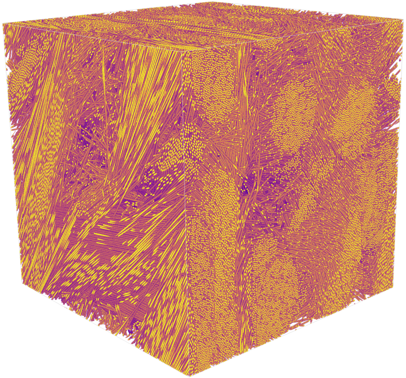
$\mathbb{C}^{\text{eff}}$

Computational micromechanics

Microscopic problem

$$\operatorname{div}\left[\mathbb{C} : (\boldsymbol{E} + \nabla^s \boldsymbol{u})\right] = \boldsymbol{0}$$

Complex microstructures



[Goerthofer et al., 2020]

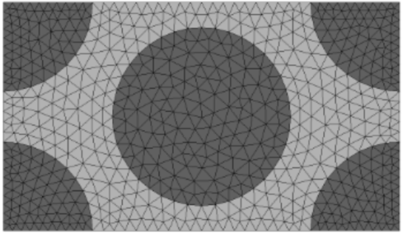
Computational micromechanics

Microscopic problem

$$\operatorname{div}\left[\mathbb{C} : (\boldsymbol{E} + \nabla^s \boldsymbol{u})\right] = \boldsymbol{0}$$

Complex microstructures

$\rightarrow$ Meshing



[Tomková et al., 2008]

Computational micromechanics

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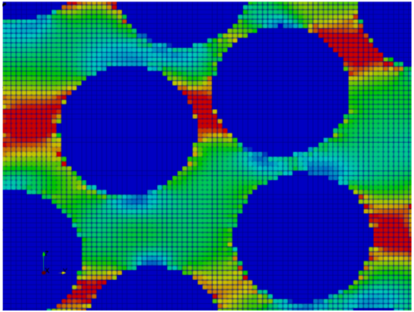
Microscopic problem

$$\operatorname{div}\left[\mathbb{C} : (\boldsymbol{E} + \nabla^s \boldsymbol{u})\right] = \boldsymbol{0}$$

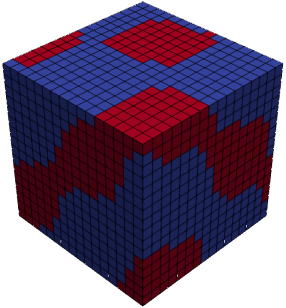
Complex microstructures

$\rightarrow$ Meshing vs. voxelizing



FFT-based computational micromechanics

[Moulinec and Suquet, 1994; Moulinec and Suquet, 1998]



Voxel segmented microstructure

FFT-based computational micromechanics

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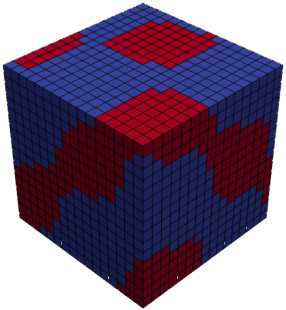
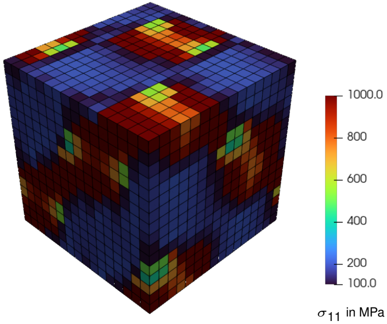


Voxel segmented microstructure

→ **FFT-based computational micromechanics** →



Local fields

Microscopic problem

$$\operatorname{div}\left[\mathbb{C} : (\boldsymbol{E} + \nabla^s \boldsymbol{u})\right] = \boldsymbol{0}$$

⇕

Lippmann–Schwinger equation

Kröner, 1972; Zeller and Dederichs, 1973

$$\boldsymbol{u} = \boldsymbol{u} - \mathbb{G}^0 \operatorname{div} \left[\mathbb{C} : (\boldsymbol{E} + \nabla^s \boldsymbol{u})\right]$$

with $\mathbb{G}^0 = (\operatorname{div} \mathbb{C}_0 : \nabla^s)^{-1}$

FFT-based computational micromechanics

[Moulinec and Suquet, 1994; Moulinec and Suquet, 1998]

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Microscopic problem

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$\Leftrightarrow$

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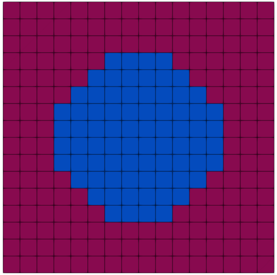
$\rightarrow$ local in Fourier space

FFT-based computational micromechanics

[Moulinec and Suquet, 1994; Moulinec and Suquet, 1998]



Lippmann–Schwinger equation

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FFT-based computational micromechanics

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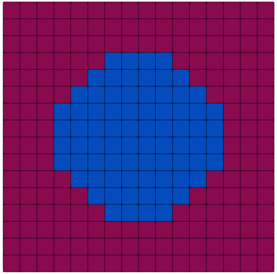

Basic scheme

$$\boldsymbol{u}^{k+1} = \boldsymbol{u}^k - \mathbb{G}^0 \mathrm{div} \left[\mathbb{C} : (\boldsymbol{E} + \nabla^s \boldsymbol{u}^k) \right]$$

FFT-based computational micromechanics

[Moulinec and Suquet, 1994; Moulinec and Suquet, 1998]

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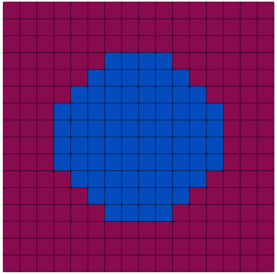

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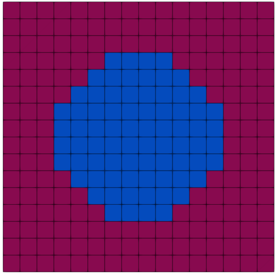
$$\mathcal{F}(r^k)$$



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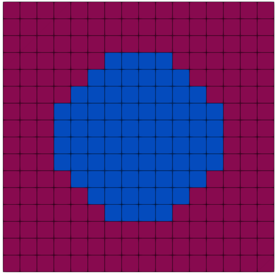
$$\mathcal{F}(\mathbb{G}^0)\mathcal{F}(r^k)$$

FFT-based computational micromechanics

[Moulinec and Suquet, 1994; Moulinec and Suquet, 1998]



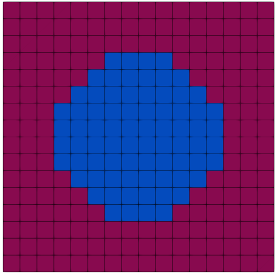
Basic scheme

$$\boldsymbol{u}^{k+1} = \boldsymbol{u}^k - \mathbb{G}^0 \mathrm{div}\left[\mathbb{C} : (\boldsymbol{E} + \nabla^s \boldsymbol{u}^k)\right]$$

$$\mathcal{F}^{-1}(\mathcal{F}(\mathbb{G}^0)\mathcal{F}(r^k))$$

FFT-based computational micromechanics

[Moulinec and Suquet, 1994; Moulinec and Suquet, 1998] [Kabel et al., 2014; Mishra et al., 2016]



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$$\boldsymbol{u}^{k+1} = \boldsymbol{u}^{k} - \mathcal{F}^{-1}(\mathcal{F}(\mathbb{G}^0)\mathcal{F}(r^k))$$

$\rightarrow$ FFT as preconditioner!

[Moulinec and Suquet, 1994; Moulinec and Suquet, 1998]   [Kabel et al., 2014; Mishra et al., 2016]

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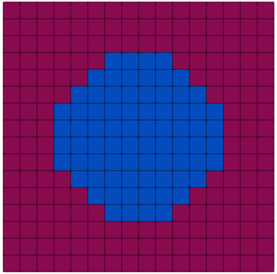

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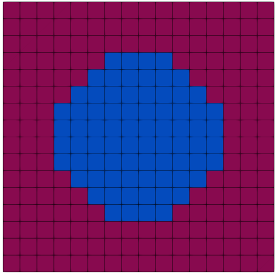
Discretizations   Solvers

FFT-based computational micromechanics

[Moulinec and Suquet, 1994; Moulinec and Suquet, 1998] [Kabel et al., 2014; Mishra et al., 2016]



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$\rightarrow$ FFT as preconditioner!

Discretizations
[Brisard and Dormieux, 2010; Willot, 2015]
[Schneider et al., 2017, 2016]

Solvers
[Zeman et al., 2010; Schneider, 2019]
[Wicht et al., 2020]

FFT-based computational micromechanics

[Moulinec and Suquet, 1994; Moulinec and Suquet, 1998] [Kabel et al., 2014; Mishra et al., 2016]

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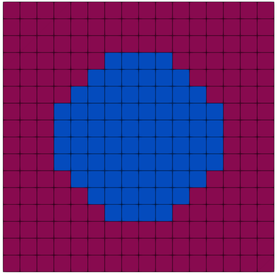

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Discretizations
[Brisard and Dormieux, 2010; Willot, 2015]
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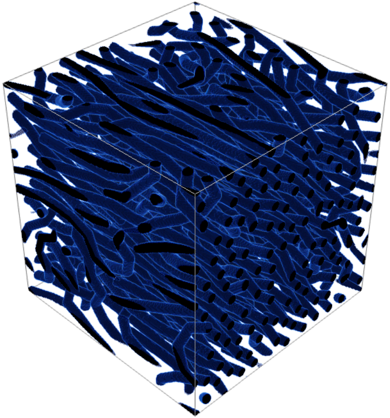
Solvers
[Zeman et al., 2010; Schneider, 2019]
[Wicht et al., 2020]

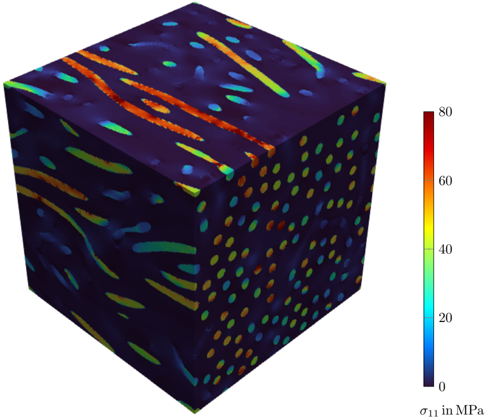
Non-periodic boundary conditions
[Gélébart, 2020; Sancho et al., 2023]
[Risthaus and Schneider, 2024]

FFT-based computational micromechanics



- 256^3 voxels
- Periodic boundary conditions

FFT-based computational micromechanics



- RAM: $256^3 \cdot 3 \cdot 4 \cdot 8$bytes $=$ 1.6GB
- Runtime on 8 threads: 2.3 min

Accuracy versus efficiency: Traditionally

FFT-based computational homogenization

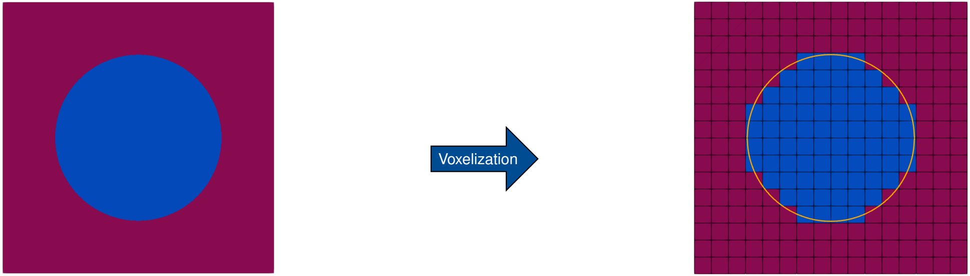
Efficiency

- FFT
- No matrix assembly
- Parallelization straight forward

Accuracy

- Suboptimal error convergence rates

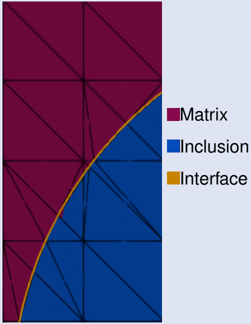
Reason for lack in accuracy



Ragged interface

Discretization from FEM community

X-FEM/GFEM **Moës et al., 1999; Strouboulis et al., 2000**

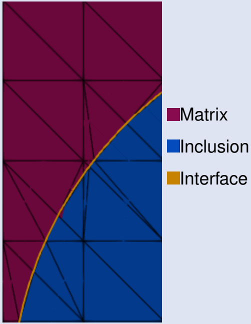


- Optimal error convergence rates

Discretization from FEM community

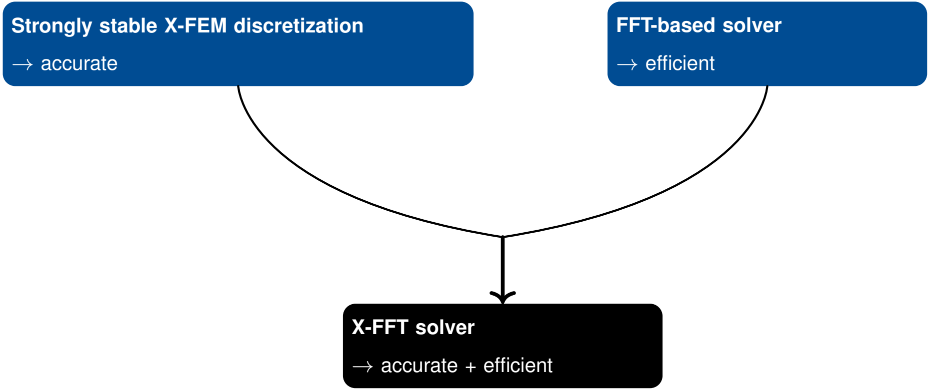
Strongly stable X-FEM/GFEM

Babuška et al., 2017



- Optimal error convergence rates
- Mesh-independent bound on condition number for 2D thermal homogenization problems

X-FFT solver



Strongly stable X-FEM discretization
→ accurate
FFT-based solver
→ efficient
X-FFT solver
→ accurate + efficient

X-FFT solver

Strongly stable X-FEM discretization

$\longrightarrow$ accurate

FFT-based solver

$\longrightarrow$ efficient

X-FFT solver

$\longrightarrow$ accurate + efficient

- 2D thermal conductivity
  [Gehrig and Schneider, 2025a,b]
- 3D linear elasticity
  [Gehrig and Schneider, 2026]

FEM ansatz for the displacement fluctuation

[Belytschko and Black, 1999; Moës et al., 1999]

$$\boldsymbol{u}(\boldsymbol{x}) = \sum_{i \in I} \boldsymbol{N}^i_{\mathrm{FE}}(\boldsymbol{x}) \boldsymbol{u}^i_{\mathrm{FE}}$$

X-FEM ansatz for the displacement fluctuation

[Belytschko and Black, 1999; Moës et al., 1999]

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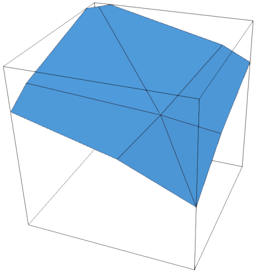
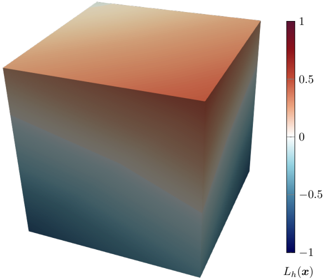
$$\boldsymbol{u}(\boldsymbol{x}) = \sum_{i \in I} \boldsymbol{N}^i_{\mathrm{FE}}(\boldsymbol{x}) \boldsymbol{u}^i_{\mathrm{FE}} + \sum_{j \in J} \rho(\boldsymbol{x}) \boldsymbol{N}^j_{\mathrm{FE}}(\boldsymbol{x}) \boldsymbol{u}^j_X$$

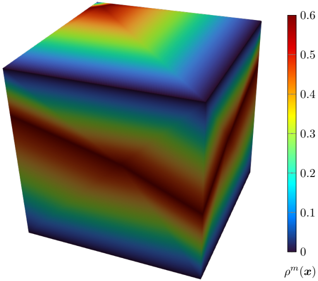
X-FEM enrichment



Interface



Level set representation



Modified abs enrichment

[Moës et al., 2003]

X-FFT preconditioning

[Gehrig and Schneider, 2025a]

Linear system $\underline{\underline{A}}\,\underline{u} = \underline{b}$ with $\underline{\underline{A}} = \begin{bmatrix} \underline{\underline{A_{11}}} & \underline{\underline{A_{12}}} \\ \underline{\underline{A_{21}}} & \underline{\underline{A_{22}}} \end{bmatrix}$

X-FFT preconditioning

[Gehrig and Schneider, 2025a]

Linear system $\underline{\underline{A}}\,\underline{u} = \underline{b}$ with $\underline{\underline{A}} = \begin{bmatrix} \underline{\underline{A_{11}}} & \underline{\underline{A_{12}}} \\ \underline{\underline{A_{21}}} & \underline{\underline{A_{22}}} \end{bmatrix}$

FE part:

Green's operator $\underline{\underline{G}}^0$

[Schneider et al., 2016; Leuschner and Fritzen, 2018; Ladecký et al., 2023]

$$\text{cond}\left((\underline{\underline{G}}^0)^{\frac{1}{2}}\,\underline{\underline{A_{11}}}\,(\underline{\underline{G}}^0)^{\frac{1}{2}}\right) \leq c_1$$

X-FFT preconditioning

[Gehrig and Schneider, 2025a]

Linear system $\underline{\underline{A}}\,\underline{u} = \underline{b}$ with $\underline{\underline{A}} = \begin{bmatrix} \underline{\underline{A}}_{11} & \underline{\underline{A}}_{12} \\ \underline{\underline{A}}_{21} & \underline{\underline{A}}_{22} \end{bmatrix}$

FE part:

Green's operator $\underline{\underline{G}}^0$

[Schneider et al., 2016; Leuschner and Fritzen, 2018; Ladecký et al., 2023]

$$\text{cond}\left((\underline{\underline{G}}^0)^{\frac{1}{2}} \underline{\underline{A}}_{11} (\underline{\underline{G}}^0)^{\frac{1}{2}} \right) \leq c_1$$

Enriched part:

Diagonal preconditioner $\underline{\underline{D}}^0$

[Babuška and Banerjee, 2012; Babuška et al., 2017]

$$\text{cond}\left(\begin{bmatrix} \underline{\underline{G}}^0 & \\ & \underline{\underline{D}}^0 \end{bmatrix}^{\frac{1}{2}} \underline{\underline{A}} \begin{bmatrix} \underline{\underline{G}}^0 & \\ & \underline{\underline{D}}^0 \end{bmatrix}^{\frac{1}{2}} \right) \leq c_2$$

Implementation

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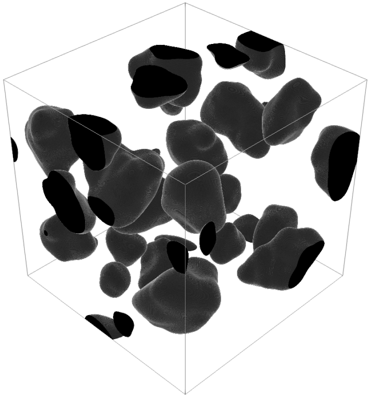
Software

- PyFFTW (FFTW3 [Frigo and Johnson, 2005])
- Python with Cython extensions
- Parallelization with OpenMP

Computational investigations: Rock-cement microstructure

[Gehrig and Schneider, 2026]

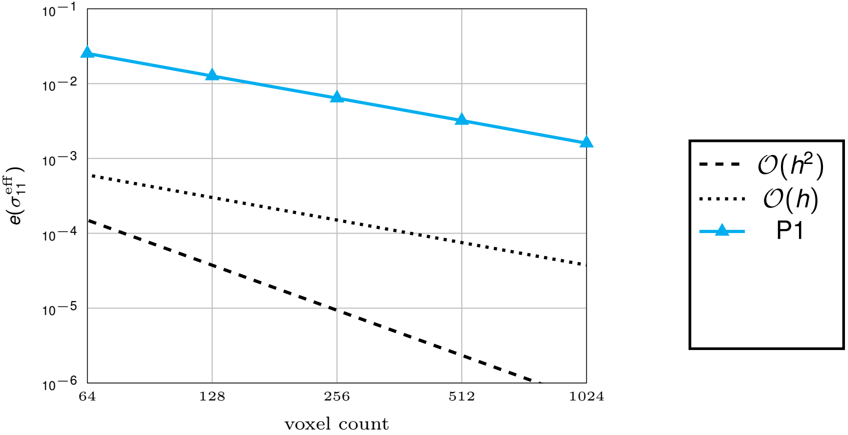


[Gehrig and Schneider, 2026]

- Displacement-based linear CG solver
- Periodic boundary conditions
- Prescribe effective strain $\bar{\varepsilon}_{11} = 0.1\%$

Error in effective stress

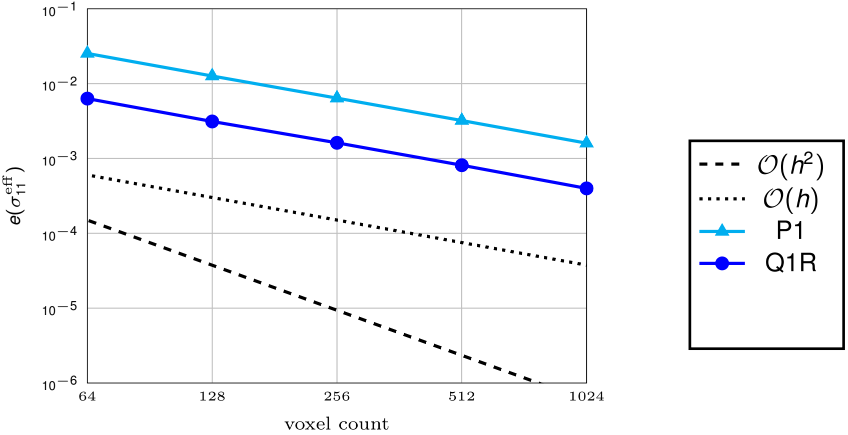
[Gehrig and Schneider, 2026; Lendvai and Schneider, 2024; Willot, 2015]



[Gehrig and Schneider, 2026]

Error in effective stress

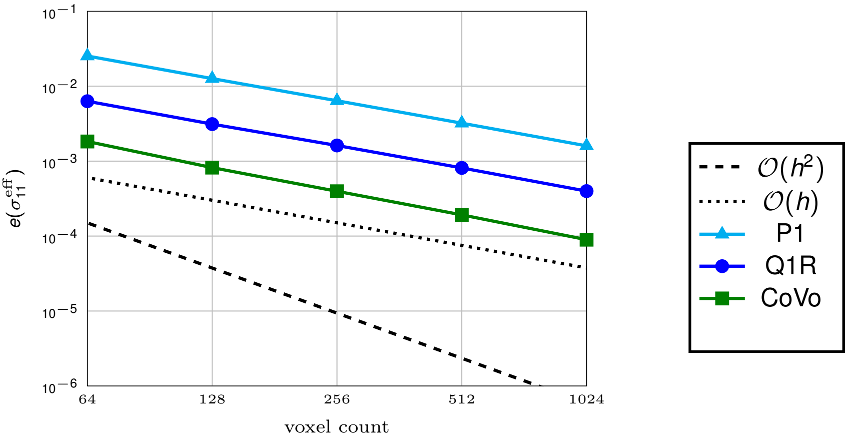
[Gehrig and Schneider, 2026; Lendvai and Schneider, 2024; Willot, 2015]



[Gehrig and Schneider, 2026]

Error in effective stress

[Gehrig and Schneider, 2026; Lendvai and Schneider, 2024; Willot, 2015]



[Gehrig and Schneider, 2026]

Error in effective stress

[Gehrig and Schneider, 2026; Lendvai and Schneider, 2024; Willot, 2015]

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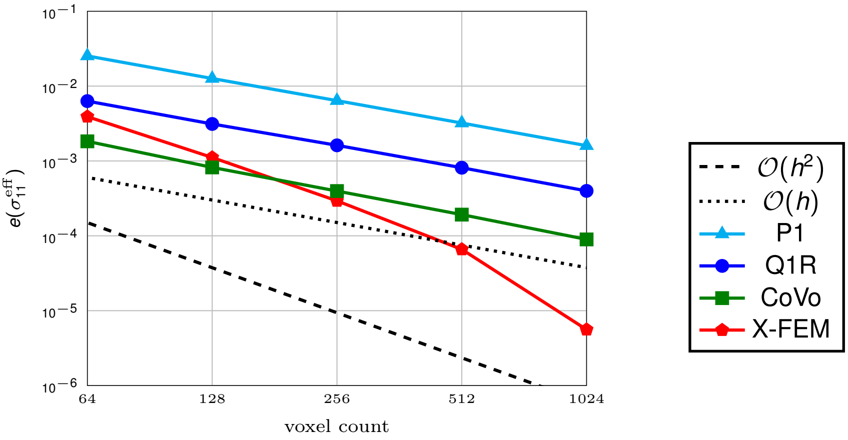
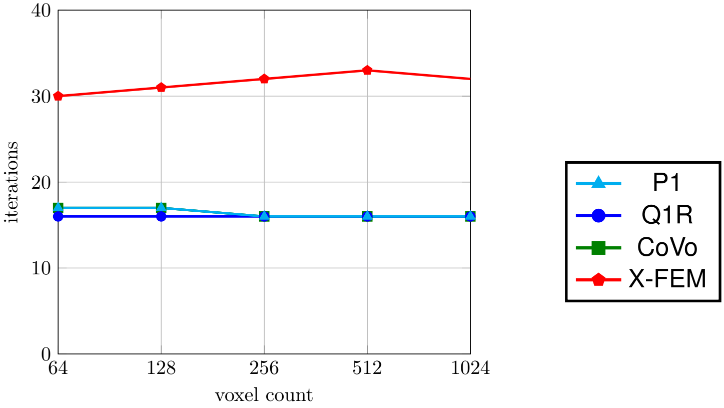


[Gehrig and Schneider, 2026]

Iteration count until convergence

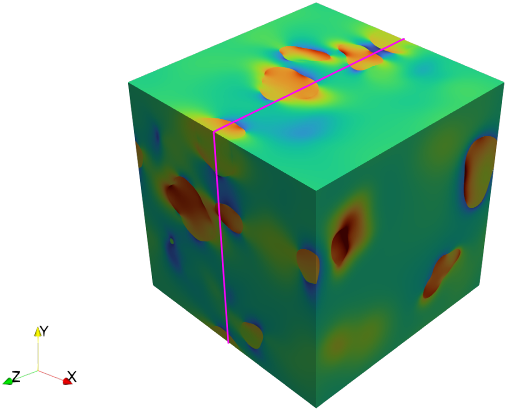
[Gehrig and Schneider, 2026; Lendvai and Schneider, 2024; Willot, 2015]



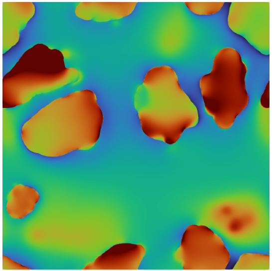
[Gehrig and Schneider, 2026]

Local stress field: Reference

[Gehrig and Schneider, 2026]



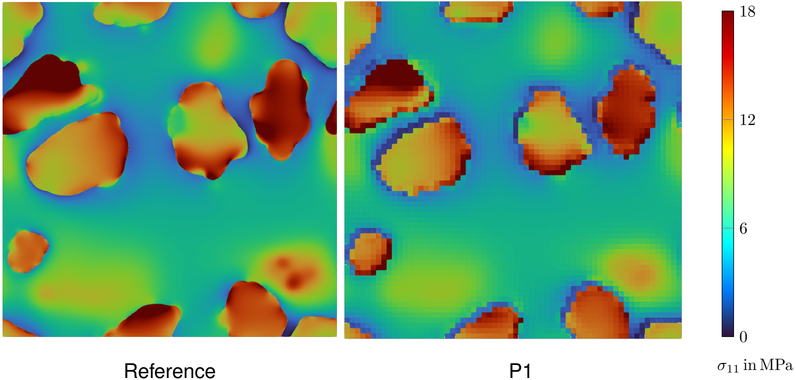
Full field



Slice in y-z plane

Local stress field

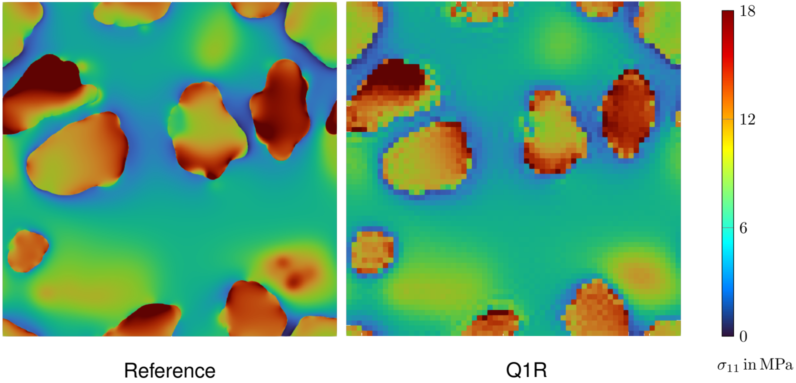
[Gehrig and Schneider, 2026]



Reference P1

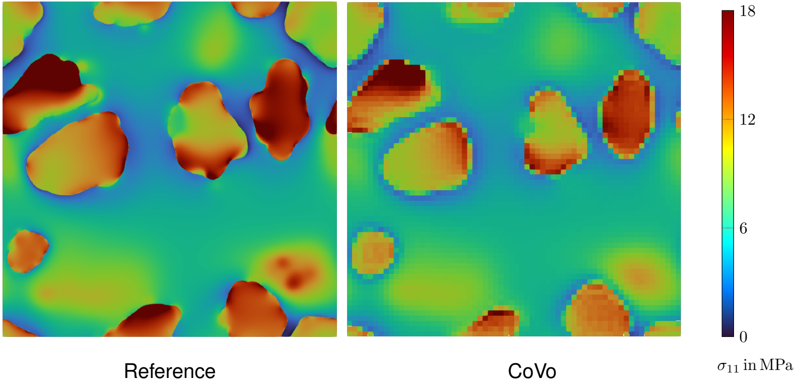
Local stress field

[Gehrig and Schneider, 2026]



Local stress field

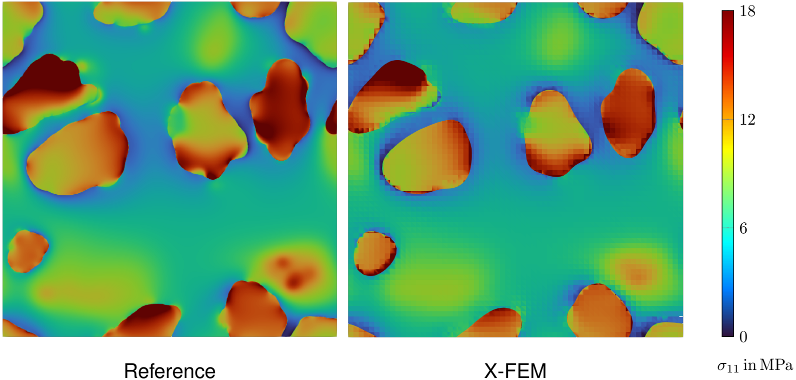
[Gehrig and Schneider, 2026]



Reference CoVo

Local stress field

[Gehrig and Schneider, 2026]



Reference X-FEM

Conclusion: X-FFT solver for 3D linear elasticity

[Gehrig and Schneider, 2026]

Efficiency

- FFT
- No matrix assembly
- Parallelization straightforward

Accuracy

Conclusion: X-FFT solver for 3D linear elasticity

[Gehrig and Schneider, 2026]

Efficiency

- FFT
- No matrix assembly
- Parallelization straightforward

Accuracy

- Optimal error convergence rates

Conclusion: FFT-based computational micromechanics

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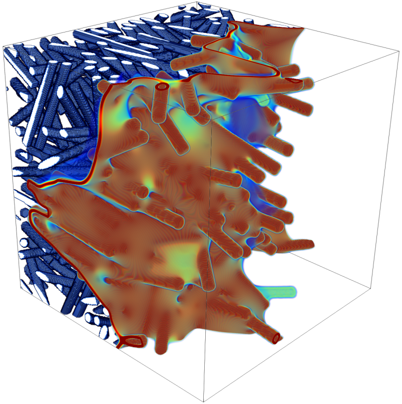
Applicability

- Beyond homogeneous coefficients
- Beyond simple discretizations
- Beyond periodic BCs
- Beyond regular grids
- Beyond linear problems



[Ernesti and Schneider, 2021]

Thank you for your attention!

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Prof. Dr. Matti Schneider

matti.schneider@uni-due.de

M.Sc. Flavia Gehrig

flavia.gehrig@uni-due.de

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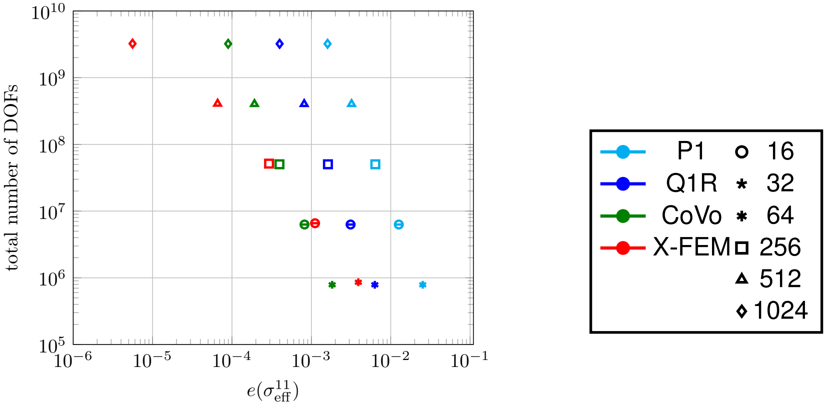
Appendix: Degrees of freedom (DOFs)

[Gehrig and Schneider, 2026]



[Gehrig and Schneider, 2026]