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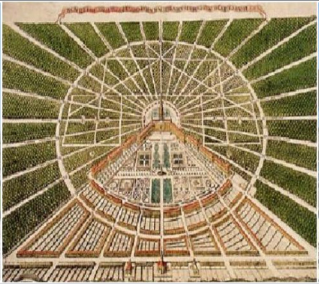
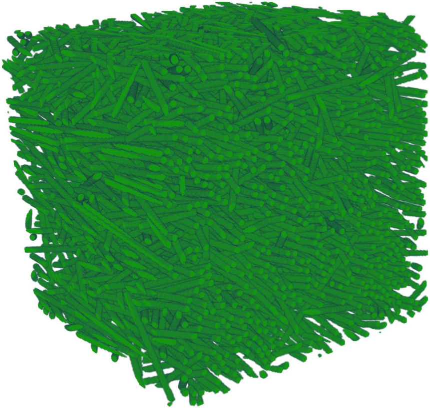
Matti Schneider

Polarization methods

Introduction to FFT-based numerical methods for the homogenization of random materials

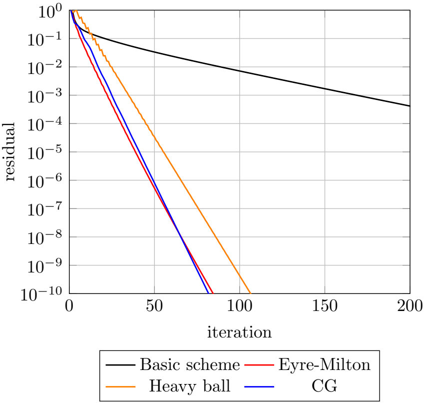


Practical performance - setup



- glass-fiber reinforced PA, 256^3
- $\phi = 20\%$, $r_a = 30$, $A = \mathrm{diag}(0.8, 0.1, 0.1)$
- generated by SAM [MS, Comput Mech, 2017]
- $E_{\mathrm{Fiber}} = 72$ GPa, $\nu_{\mathrm{Fiber}} = 0.22$, $E_{\mathrm{PA}} = 2.1$ GPa, $\nu_{\mathrm{PA}} = 0.3$
- uniaxial extension in e_1

Power of polarization schemes



- Eyre-Milton matches CG
- Eyre-Milton requires **two** strain fields
- **Polarization methods**?!

Overview

1. Polarization methods
2. Evaluating the Cayley operator
3. Connection to optimization
4. Adaptive parameter selection
5. Summary and conclusions

Overview

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3. Connection to optimization
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The Eyre-Milton equation

Lippmann-Schwinger equation

$$\varepsilon = \bar{\varepsilon} - \Gamma^0 : \left[S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$\varepsilon + \Gamma^0 : \left[S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right] = \bar{\varepsilon}$$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$\varepsilon + \Gamma^0 : \left[S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right] = \bar{\varepsilon}$$

- $\sigma = S(\cdot, \varepsilon)$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$\varepsilon + \Gamma^0 : \left[\sigma - \mathbb{C}^0 : \varepsilon\right] = \bar{\varepsilon}$$

- $\sigma = S(\cdot, \varepsilon)$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$\varepsilon + \Gamma^0 : \left[\sigma - \mathbb{C}^0 : \varepsilon\right] = \bar{\varepsilon}$$

- $\sigma = S(\cdot, \varepsilon)$
- $\tau = \sigma - \mathbb{C}^0 : \varepsilon$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$\varepsilon + \Gamma^0 : \tau = \bar{\varepsilon}$$

- $\sigma = S(\cdot, \varepsilon)$
- $\tau = \sigma - \mathbb{C}^0 : \varepsilon$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$\varepsilon + \Gamma^0 : \tau = \bar{\varepsilon}$$

- $\sigma = S(\cdot, \varepsilon)$
- $\tau = \sigma - \mathbb{C}^0 : \varepsilon$
- $P = \sigma + \mathbb{C}^0 : \varepsilon$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$\varepsilon + \Gamma^0 : \tau = \bar{\varepsilon}$$

- $\sigma = S(\cdot, \varepsilon)$
- $\tau = \sigma - \mathbb{C}^0 : \varepsilon$
- $P = \sigma + \mathbb{C}^0 : \varepsilon$
- $P - \tau = \ldots$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$\varepsilon + \Gamma^0 : \tau = \bar{\varepsilon}$$

- $\sigma = S(\cdot, \varepsilon)$
- $\tau = \sigma - \mathbb{C}^0 : \varepsilon$
- $P = \sigma + \mathbb{C}^0 : \varepsilon$
- $P - \tau = \sigma + \mathbb{C}^0 : \varepsilon - \sigma + \mathbb{C}^0 : \varepsilon$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$\varepsilon + \Gamma^0 : \tau = \bar{\varepsilon}$$

- $\sigma = S(\cdot, \varepsilon)$
- $\tau = \sigma - \mathbb{C}^0 : \varepsilon$
- $P = \sigma + \mathbb{C}^0 : \varepsilon$
- $P - \tau = 2\,\mathbb{C}^0 : \varepsilon$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$2\,\mathbb{C}^0 : \varepsilon + 2\,\mathbb{C}^0 : \Gamma^0 : \tau = 2\,\mathbb{C}^0 : \bar{\varepsilon}$$

- $\sigma = \mathsf{S}(\cdot, \varepsilon)$
- $\tau = \sigma - \mathbb{C}^0 : \varepsilon$
- $P = \sigma + \mathbb{C}^0 : \varepsilon$
- $P - \tau = 2\,\mathbb{C}^0 : \varepsilon$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$P - \tau + 2\,\mathbb{C}^0 : \Gamma^0 : \tau = 2\,\mathbb{C}^0 : \bar{\varepsilon}$$

- $\sigma = S(\cdot, \varepsilon)$
- $\tau = \sigma - \mathbb{C}^0 : \varepsilon$
- $P = \sigma + \mathbb{C}^0 : \varepsilon$
- $P - \tau = 2\,\mathbb{C}^0 : \varepsilon$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$P - [\mathrm{Id} - 2\,\mathbb{C}^0 : \Gamma^0] : \tau = 2\,\mathbb{C}^0 : \bar{\varepsilon}$$

- $\sigma = \mathsf{S}(\cdot, \varepsilon)$
- $\tau = \sigma - \mathbb{C}^0 : \varepsilon$
- $P = \sigma + \mathbb{C}^0 : \varepsilon$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$P - [\mathrm{Id} - 2\,\mathbb{C}^0 : \Gamma^0] : \tau = 2\,\mathbb{C}^0 : \bar{\varepsilon}$$

- $\sigma = \mathsf{S}(\cdot, \varepsilon)$
- $\tau = \sigma - \mathbb{C}^0 : \varepsilon = Z^0(P)$ with $Z^0 = (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}$
- $P = \sigma + \mathbb{C}^0 : \varepsilon$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$P - [\mathrm{Id} - 2\,\mathbb{C}^0 : \Gamma^0] : Z^0(P) = 2\,\mathbb{C}^0 : \bar{\varepsilon}$$

- $\sigma = \mathsf{S}(\cdot, \varepsilon)$
- $\tau = \sigma - \mathbb{C}^0 : \varepsilon = Z^0(P)$ with $Z^0 = (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}$
- $P = \sigma + \mathbb{C}^0 : \varepsilon$

The Eyre-Milton equation

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$$P - [\mathrm{Id} - 2\,\mathbb{C}^0 : \Gamma^0] : Z^0(P) = 2\,\mathbb{C}^0 : \bar{\varepsilon}$$

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- $\tau = \sigma - \mathbb{C}^0 : \varepsilon = Z^0(P)$ with $Z^0 = (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}$
- $Y^0 = \mathrm{Id} - 2\,\mathbb{C}^0 : \Gamma^0$

The Eyre-Milton equation

Lippmann-Schwinger equation

$$P - Y^0 : Z^0(P) = 2\,\mathbb{C}^0 : \bar{\varepsilon}$$

- $\sigma = \mathsf{S}(\cdot, \varepsilon)$
- $\tau = \sigma - \mathbb{C}^0 : \varepsilon = Z^0(P)$ with $Z^0 = (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}$
- $Y^0 = \mathrm{Id} - 2\,\mathbb{C}^0 : \Gamma^0$

The Eyre-Milton equation II

ε solves the Lippmann-Schwinger equation

$$\varepsilon = \bar{\varepsilon} - \Gamma^0 : \left[S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

if and only if $P = S(\cdot, \varepsilon) + \mathbb{C}^0 : \varepsilon$ solves the **Eyre-Milton equation**

$$P = 2\, \mathbb{C}^0 : \bar{\varepsilon} + Y^0 : Z^0(P)$$

with

$$Y^0 = \mathrm{Id} - 2\, \mathbb{C}^0 : \Gamma^0 \quad \text{and} \quad Z^0 = (S - \mathbb{C}^0)(S + \mathbb{C}^0)^{-1}$$

The Eyre-Milton equation II

ε solves the Lippmann-Schwinger equation

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$$P = 2\, \mathbb{C}^0 : \bar{\varepsilon} + Y^0 : Z^0(P)$$

with

$$Y^0 = \mathrm{Id} - 2\, \mathbb{C}^0 : \Gamma^0 \quad \text{and} \quad Z^0 = (S - \mathbb{C}^0)(S + \mathbb{C}^0)^{-1}$$

▹ constant

The Eyre-Milton equation II

ε solves the Lippmann-Schwinger equation

$$\varepsilon = \bar{\varepsilon} - \Gamma^0 : \left[S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

if and only if $P = S(\cdot, \varepsilon) + \mathbb{C}^0 : \varepsilon$ solves the **Eyre-Milton equation**

$$P = 2\,\mathbb{C}^0 : \bar{\varepsilon} + Y^0 : Z^0(P)$$

with

$$\hat{Y}^0 = \mathrm{Id} - 2\,\mathbb{C}^0 : \hat{\Gamma}^0 \quad \text{and} \quad Z^0 = (S - \mathbb{C}^0)(S + \mathbb{C}^0)^{-1}$$

▹ local in Fourier space

The Eyre-Milton equation II

ε solves the Lippmann-Schwinger equation

$$\varepsilon = \bar{\varepsilon} - \Gamma^0 : \left[S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

if and only if $P = S(\cdot, \varepsilon) + \mathbb{C}^0 : \varepsilon$ solves the **Eyre-Milton equation**

$$P = 2\, \mathbb{C}^0 : \bar{\varepsilon} + Y^0 : Z^0(P)$$

with

$$Y^0 = \mathrm{Id} - 2\, \mathbb{C}^0 : \Gamma^0 \quad \text{and} \quad Z^0 = (S - \mathbb{C}^0)(S + \mathbb{C}^0)^{-1}$$

▹ local in real space

The Eyre-Milton equation II

ε solves the Lippmann-Schwinger equation

$$\varepsilon = \bar{\varepsilon} - \Gamma^0 : \left[S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

if and only if $P = S(\cdot, \varepsilon) + \mathbb{C}^0 : \varepsilon$ solves the **Eyre-Milton equation**

$$P = 2\, \mathbb{C}^0 : \bar{\varepsilon} + Y^0 : Z^0(P)$$

with

$$Y^0 = \mathrm{Id} - 2\, \mathbb{C}^0 : \Gamma^0 \quad \text{and} \quad Z^0 = (S - \mathbb{C}^0)(S + \mathbb{C}^0)^{-1}$$

▹ unknown explicit on left-hand side

The Eyre-Milton method

Basic scheme

$$\varepsilon^{k+1} = \bar{\varepsilon} - \Gamma^0 : \left[S(\cdot, \varepsilon^k) - \mathbb{C}^0 : \varepsilon^k \right]$$

Eyre-Milton scheme ↗ [D. J. Eyre and G. W. Milton, The European Physical Journal - Applied Physics, 1999]

$$P^{k+1} = 2\,\mathbb{C}^0 : \bar{\varepsilon} + Y^0 : Z^0(P^k), \quad Y^0 = \mathrm{Id} - 2\,\mathbb{C}^0 : \Gamma^0 \quad Z^0 = (S - \mathbb{C}^0)(S + \mathbb{C}^0)^{-1}$$

Polarization methods

Basic scheme

$$\varepsilon^{k+1} = \bar{\varepsilon} - \Gamma^0 : \left[S(\cdot, \varepsilon^k) - \mathbb{C}^0 : \varepsilon^k \right]$$

Polarization scheme

$$P^{k+1} = \gamma\, P^k + (1-\gamma)\left(2\, \mathbb{C}^0 : \bar{\varepsilon} + Y^0 : Z^0(P^k)\right)$$

- damping factor $\gamma \in [0, 1)$
- $\gamma = 0$ ↗ [D. J. Eyre and G. W. Milton, The European Physical Journal - Applied Physics, 1999]
- $\gamma = 1/2$ ↗ [J. C. Michel, H. Moulinec, and P. Suquet, International Journal for Numerical Methods in Engineering, 2001]
- general γ & $\gamma = 1/4$ ↗ [V. Monchiet and G. Bonnet, International Journal for Numerical Methods in Engineering, 2012]

Damping basic scheme?

$$\varepsilon^{k+1} = \bar{\varepsilon} - \Gamma^0 : \left[S(\cdot, \varepsilon^k) - \mathbb{C}^0 : \varepsilon^k \right]$$

Damping basic scheme?

$$\varepsilon^{k+1} = \varepsilon^k - s^k \, \Gamma : S(\cdot, \varepsilon^k)$$

Damping basic scheme?

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$$\varepsilon^{k+1} = \gamma\,\varepsilon^k + (1-\gamma)\left[\varepsilon^k - s^k\,\Gamma : \mathsf{S}(\cdot, \varepsilon^k)\right]$$

Damping basic scheme?

$$\varepsilon^{k+1} = \gamma\,\varepsilon^k + (1-\gamma)\varepsilon^k - (1-\gamma)s^k\,\Gamma : \mathsf{S}(\cdot, \varepsilon^k)$$

Damping basic scheme?

$$\varepsilon^{k+1} = \varepsilon^k - (1-\gamma)s^k\,\Gamma : \mathsf{S}(\cdot, \varepsilon^k)$$

Damping basic scheme?

$$\varepsilon^{k+1} = \varepsilon^k - (1-\gamma) s^k \, \Gamma : S(\cdot, \varepsilon^k)$$

- damping $\equiv$ changing step size, i.e., $\mathbb{C}^0$

Questions

Polarization scheme

$$P^{k+1} = \gamma\, P^k + (1-\gamma)\left(2\,\mathbb{C}^0 : \bar{\varepsilon} + Y^0 : Z^0(P^k)\right)$$

- Convergence? How to choose γ and $\mathbb{C}^0$?
- Convergence criterion?
- Implementation?
- Connection to optimization?

Convergence

$$\alpha_- \leq \lambda \leq \alpha_+ \quad \forall x, \xi \, \forall \lambda \in \mathtt{Eig}\left(\frac{\partial S}{\partial \varepsilon}(x, \xi)\right)$$

implies

$$\|P^{k+1} - P^*\|_{L^2} \leq \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right) \|P^k - P^*\|_{L^2}, \quad \kappa = \alpha_+ / \alpha_-$$

for

$$\alpha_0 = \sqrt{\alpha_- \alpha_+} \quad \text{and} \quad \gamma = 0$$

$\Rightarrow$ # iterations $\propto \sqrt{\kappa}$

[P. Giselsson and S. Boyd, IEEE transactions on automatic control, 2017]

[MS, D. Wicht, and T. Böhlke, Computational Mechanics, 2019]

Convergence criterion

- if $P^k = \sigma^k + \mathbb{C}^0 : \varepsilon^k$,
  then $\operatorname{div} \sigma^k \neq 0$ **and** $\varepsilon^k \neq \bar{\varepsilon} + \nabla^s u$
- holds: ↗ [MS, D. Wicht, and T. Böhlke, Computational Mechanics, 2019]

$$\frac{\|P^{k+1} - P^k\|_{L^2}^2}{4(1-\gamma)^2} = \|\Gamma : \sigma^k\|_{L^2}^2 + \alpha_0^2 \left\| \varepsilon^k - \Gamma : \varepsilon^k - \left\langle \varepsilon^k \right\rangle_Q \right\|_{L^2}^2 + \alpha_0^2 \left\| \left\langle \varepsilon^k \right\rangle_Q - \bar{\varepsilon} \right\|_{L^2}^2$$

Convergence criterion

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- if $P^k = \sigma^k + \mathbb{C}^0 : \varepsilon^k$,
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equilibrium

Convergence criterion

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- if $P^k = \sigma^k + \mathbb{C}^0 : \varepsilon^k$,
  then $\operatorname{div} \sigma^k \neq 0$ **and** $\varepsilon^k \neq \bar{\varepsilon} + \nabla^s u$
- holds: ↗ [MS, D. Wicht, and T. Böhlke, Computational Mechanics, 2019]

$$\frac{\|P^{k+1} - P^k\|_{L^2}^2}{4(1-\gamma)^2} = \|\Gamma : \sigma^k\|_{L^2}^2 + \alpha_0^2 \left\| \varepsilon^k - \Gamma : \varepsilon^k - \left\langle \varepsilon^k \right\rangle_Q \right\|_{L^2}^2 + \alpha_0^2 \left\| \left\langle \varepsilon^k \right\rangle_Q - \bar{\varepsilon} \right\|_{L^2}^2$$

compatibility

Convergence criterion

- if $P^k = \sigma^k + \mathbb{C}^0 : \varepsilon^k$,
  then $\operatorname{div} \sigma^k \neq 0$ **and** $\varepsilon^k \neq \bar{\varepsilon} + \nabla^s u$
- holds: ↗ [MS, D. Wicht, and T. Böhlke, Computational Mechanics, 2019]

$$\frac{\|P^{k+1} - P^k\|_{L^2}^2}{4(1-\gamma)^2} = \|\Gamma : \sigma^k\|_{L^2}^2 + \alpha_0^2 \left\|\varepsilon^k - \Gamma : \varepsilon^k - \left\langle \varepsilon^k \right\rangle_Q\right\|_{L^2}^2 + \alpha_0^2 \left\|\left\langle \varepsilon^k \right\rangle_Q - \bar{\varepsilon}\right\|_{L^2}^2$$

prescribed strain

Convergence criterion

- if $P^k = \sigma^k + \mathbb{C}^0 : \varepsilon^k$,
  then $\operatorname{div} \sigma^k \neq 0$ **and** $\varepsilon^k \neq \bar{\varepsilon} + \nabla^s u$
- holds: ↗ [MS, D. Wicht, and T. Böhlke, Computational Mechanics, 2019]

$$\frac{\|P^{k+1} - P^k\|^2_{L^2}}{4(1-\gamma)^2} = \|\Gamma : \sigma^k\|^2_{L^2} + \alpha_0^2 \left\| \varepsilon^k - \Gamma : \varepsilon^k - \left\langle \varepsilon^k \right\rangle_Q \right\|^2_{L^2} + \alpha_0^2 \left\| \left\langle \varepsilon^k \right\rangle_Q - \bar{\varepsilon} \right\|^2_{L^2}$$

- use

$$\frac{\|P^{k+1} - P^k\|_{L^2}}{2(1-\gamma)\|\bar{\sigma}^k\|} \overset{!}{\leq} \texttt{tol}$$

Implementations

- two different implementations
- each with distinct advantages

Implementation # 1

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Algorithm 1 Eyre-Milton scheme $(\bar{\varepsilon}, \texttt{maxit}, \texttt{tol}, \alpha_0, \gamma)$

$P \leftarrow \mathsf{S}(\cdot, \varepsilon^0) + \mathbb{C}^0 : \varepsilon^0$ ▷ $\varepsilon^0 \equiv \bar{\varepsilon}$ or via extrapolation

$\texttt{res} \leftarrow 1$

$k \leftarrow 0$

while $k < \texttt{maxit}$ **and** $\texttt{res} > \texttt{tol}$ **do**

  $k \leftarrow k + 1$

  $R \leftarrow P$

  $P \leftarrow (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}(P)$ ▷ compute $\bar{\sigma}$

  $P \leftarrow 2\mathbb{C}^0 : \bar{\varepsilon} + (\mathrm{Id} - 2\Gamma) : P$ ▷ use FFT & favorite discretization

  $\texttt{res} \leftarrow 0.5\|P - R\|/\|\bar{\sigma}\|$

  $P \leftarrow \gamma R + (1 - \gamma) P$

end while

$\varepsilon \leftarrow (\mathsf{S} + \mathbb{C}^0)^{-1}(P)$

return $\varepsilon, \bar{\sigma}, \texttt{res}$ ▷ Requires two polarization fields

↗ [D. J. Eyre and G. W. Milton, The European Physical Journal - Applied Physics, 1999]

Alternative formulation

$$
\begin{aligned}
\varepsilon^{k+1/2} &= \bar{\varepsilon} - \Gamma^0 : (\sigma^k - \mathbb{C}^0 : e^k) && \triangleright \text{ basic step} \\
\varepsilon^k &= (1-2\gamma)\, e^k + 2(1-\gamma)\, \varepsilon^{k+1/2} && \\
\mathsf{S}(\cdot, e^{k+1}) + \mathbb{C}^0 : e^{k+1} &= \sigma^k + \mathbb{C}^0 : \varepsilon^k && \triangleright \text{ implicit solve} \\
\sigma^{k+1} &= \sigma^k + \mathbb{C}^0 : (\varepsilon^k - e^{k+1}) &&
\end{aligned}
$$

↗ [J. C. Michel, H. Moulinec, and P. Suquet, International Journal for Numerical Methods in Engineering, 2001]

↗ [V. Monchiet and G. Bonnet, International Journal for Numerical Methods in Engineering, 2012]

↗ [H. Moulinec and F. Silva, International Journal for Numerical Methods in Engineering, 2014]

- identical iterates as γ-damped Eyre-Milton
- derivation ↗ bonus slides

Alternative formulation

$$\begin{aligned} \varepsilon^{k+1/2} &= \bar{\varepsilon} - \Gamma^0 : (\sigma^k - \mathbb{C}^0 : e^k) && \triangleright \text{ basic step} \\ \varepsilon^k &= (1-2\gamma)\, e^k + 2(1-\gamma)\, \varepsilon^{k+1/2} \\ \mathsf{S}(\cdot, e^{k+1}) + \mathbb{C}^0 : e^{k+1} &= \sigma^k + \mathbb{C}^0 : \varepsilon^k && \triangleright \text{ implicit solve} \\ \sigma^{k+1} &= \sigma^k + \mathbb{C}^0 : (\varepsilon^k - e^{k+1}) \end{aligned}$$

↗ [J. C. Michel, H. Moulinec, and P. Suquet, International Journal for Numerical Methods in Engineering, 2001]

↗ [H. Moulinec and F. Silva, International Journal for Numerical Methods in Engineering, 2014]

- convergence criterion? use

$$\|\mathbb{C}^0 : (\varepsilon^{k+1/2} - e^k)\|_{L^2} \overset{!}{\leq} \mathtt{tol}\, \|\bar{\sigma}^k\|$$

↗ [MS, International Journal for Numerical Methods in Engineering, 2021]

Implementation # 2

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Algorithm 2 ADMM $(\bar{\varepsilon}, \texttt{maxit}, \texttt{tol}, \alpha_0, \gamma)$

$e \leftarrow \varepsilon^0$ ▹ $\varepsilon^0 \equiv \bar{\varepsilon}$ or via extrapolation

$\sigma \leftarrow \mathsf{S}(\cdot, \varepsilon^0)$

$\texttt{res} \leftarrow 1$

$k \leftarrow 0$

while $k < \texttt{maxit}$ **and** $\texttt{res} > \texttt{tol}$ **do**

  $k \leftarrow k + 1$

  $\bar{\sigma} \leftarrow \langle \sigma \rangle_Q$

  $\varepsilon \leftarrow \sigma - \mathbb{C}^0 : e$

  $\varepsilon \leftarrow \bar{\varepsilon} - 1/\alpha_0 \, \Gamma : \varepsilon$ ▹ use FFT & favorite discretization

  $\texttt{res} \leftarrow \alpha_0 \, \|\varepsilon - e\|_{L^2} / \|\bar{\sigma}\|$

  $\varepsilon \leftarrow (1 - 2\gamma) e + 2(1 - \gamma)\varepsilon$

  $\begin{bmatrix} e \\ \sigma \end{bmatrix} \leftarrow \begin{bmatrix} (\mathsf{S} + \mathbb{C}^0)^{-1}(\sigma + \mathbb{C}^0 : \varepsilon) \\ \sigma + \mathbb{C}^0 : (\varepsilon - e) \end{bmatrix}$

end while

return $e, \bar{\sigma}, \texttt{res}$ ▹ Requires three fields

[J. C. Michel, H. Moulinec, and P. Suquet, International Journal for Numerical Methods in Engineering, 2001]

[MS, International Journal for Numerical Methods in Engineering, 2021]

Summary part 1

- polarization schemes are powerful & need little memory
- two (equivalent) implementations on two/three fields
- critical issue:

$$\begin{aligned} P &\leftarrow (S - \mathbb{C}^0)(S + \mathbb{C}^0)^{-1}(P) && \text{(Implementation \# 1)} \\ e &\leftarrow (S + \mathbb{C}^0)^{-1}(\sigma + \mathbb{C}^0 : \varepsilon) && \text{(Implementation \# 2)} \end{aligned}$$

How to **invert** the stress function?

Overview

The Cayley operator

$$P \mapsto Z^0(P) \equiv (\mathbb{S} - \mathbb{C}^0)(\mathbb{S} + \mathbb{C}^0)^{-1}(P)$$

- analogous to Cayley transform $z \mapsto (z-1)/(z+1)$, $z = x + i\,y$
- performance of polarization schemes hinges on Z^0

Linear elasticity

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$$P \mapsto Z^0(P) \equiv (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}(P)$$

- $\mathsf{S}(x, \varepsilon) = \mathbb{C}(x) : \varepsilon$

Linear elasticity

$$P \mapsto Z^0(P) \equiv (\mathbb{C} - \mathbb{C}^0)(\mathbb{C} + \mathbb{C}^0)^{-1}(P)$$

- $\mathsf{S}(x, \varepsilon) = \mathbb{C}(x) : \varepsilon$

Linear elasticity

$$P \mapsto Z^0(P) \equiv (\mathbb{C} - \mathbb{C}^0)(\mathbb{C} + \mathbb{C}^0)^{-1}(P)$$

- $\mathsf{S}(x, \varepsilon) = \mathbb{C}(x) : \varepsilon$
- precompute $(\mathbb{C} - \mathbb{C}^0)(\mathbb{C} + \mathbb{C}^0)^{-1}$ and cache

Linear elasticity

$$P \mapsto Z^0(P) \equiv (\mathbb{C} - \mathbb{C}^0)(\mathbb{C} + \mathbb{C}^0)^{-1}(P)$$

- $\mathsf{S}(x, \varepsilon) = \mathbb{C}(x) : \varepsilon$
- precompute $(\mathbb{C} - \mathbb{C}^0)(\mathbb{C} + \mathbb{C}^0)^{-1}$ and cache
- classical strategy of Eyre & Milton

Beyond linear elasticity

$$P \mapsto Z^0(P) \equiv (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}(P)$$

Beyond linear elasticity

$$P \mapsto Z^0(P) \equiv (\mathbb{S} - \mathbb{C}^0)(\mathbb{S} + \mathbb{C}^0)^{-1}(P)$$

- digression:

$$P = \sigma + \mathbb{C}^0 : \varepsilon \quad \longrightarrow \quad \begin{bmatrix} \sigma \\ \varepsilon \end{bmatrix} \quad \longrightarrow \quad \tau = \sigma - \mathbb{C}^0 : \varepsilon$$

Beyond linear elasticity

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$$P \mapsto Z^0(P) \equiv (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}(P)$$

- digression:

$$P = \sigma + \mathbb{C}^0 : \varepsilon \quad \longrightarrow \quad \begin{bmatrix} \sigma \\ \varepsilon \end{bmatrix} \quad \longrightarrow \quad \tau = \sigma - \mathbb{C}^0 : \varepsilon$$

"disassemble" P

Beyond linear elasticity

$$P \mapsto Z^0(P) \equiv (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}(P)$$

- digression:

$$P = \sigma + \mathbb{C}^0 : \varepsilon \quad \longrightarrow \quad \begin{bmatrix} \sigma \\ \varepsilon \end{bmatrix} \quad \longrightarrow \quad \tau = \sigma - \mathbb{C}^0 : \varepsilon$$

"disassemble" P:

1. solve $\quad \mathsf{S}(\cdot, \varepsilon) + \mathbb{C}^0 : \varepsilon = P$

Beyond linear elasticity

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"disassemble" P:

1. solve $\mathsf{S}(\cdot, \varepsilon) + \mathbb{C}^0 : \varepsilon = P$
2. compute $\sigma = P - \mathbb{C}^0 : \varepsilon$

Beyond linear elasticity

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$$P \mapsto Z^0(P) \equiv (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}(P)$$

- digression:

$$P = \sigma + \mathbb{C}^0 : \varepsilon \quad \longrightarrow \quad \varepsilon \quad \longrightarrow \quad \sigma \quad \longrightarrow \quad \tau = \sigma - \mathbb{C}^0 : \varepsilon$$

"disassemble" P:

1. solve $\quad \mathsf{S}(\cdot, \varepsilon) + \mathbb{C}^0 : \varepsilon = P$
2. compute $\quad \sigma = P - \mathbb{C}^0 : \varepsilon$

Beyond linear elasticity

$$P \mapsto Z^0(P) \equiv (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}(P)$$

- digression:

$$P = \sigma + \mathbb{C}^0 : \varepsilon \quad \longrightarrow \quad \varepsilon \quad \longrightarrow \quad \sigma \quad \longrightarrow \quad \tau = \sigma - \mathbb{C}^0 : \varepsilon$$

"disassemble" P:

1. solve $\mathsf{S}(\cdot, \varepsilon) + \mathbb{C}^0 : \varepsilon = P$ ▹ nonlinear, inverse solve
2. compute $\sigma = P - \mathbb{C}^0 : \varepsilon$

Beyond linear elasticity

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$$P \mapsto Z^0(P) \equiv (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}(P)$$

- digression:

$$P = \sigma + \mathbb{C}^0 : \varepsilon \quad \longrightarrow \quad \begin{bmatrix} \sigma \\ \varepsilon \end{bmatrix} \quad \longrightarrow \quad \tau = \sigma - \mathbb{C}^0 : \varepsilon$$

"disassemble" P

Beyond linear elasticity

$$P \mapsto Z^0(P) \equiv (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}(P)$$

- digression:

$$P = \sigma + \mathbb{C}^0 : \varepsilon \quad \longrightarrow \quad \begin{bmatrix} \sigma \\ \varepsilon \end{bmatrix} \quad \longrightarrow \quad \tau = \sigma - \mathbb{C}^0 : \varepsilon$$

"disassemble" P:

1. solve $\quad \sigma + \mathbb{C}^0 : \mathsf{S}^{-1}(\cdot, \sigma) = \quad P$ ▹ compute σ from "strain"

Beyond linear elasticity

$$P \mapsto Z^0(P) \equiv (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}(P)$$

- digression:

$$P = \sigma + \mathbb{C}^0 : \varepsilon \quad \longrightarrow \quad \begin{bmatrix} \sigma \\ \varepsilon \end{bmatrix} \quad \longrightarrow \quad \tau = \sigma - \mathbb{C}^0 : \varepsilon$$

"disassemble" P:

1. solve $\sigma + \mathbb{C}^0 : \mathsf{S}^{-1}(\cdot, \sigma) = \quad P$
2. compute $\varepsilon = \mathbb{D}^0 : (P - \sigma)$ $\quad \triangleright\ \mathbb{D}^0 = (\mathbb{C}^0)^{-1}$

Beyond linear elasticity

$$P \mapsto Z^0(P) \equiv (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}(P)$$

- digression:

$$P = \sigma + \mathbb{C}^0 : \varepsilon \quad \longrightarrow \quad \sigma \quad \longrightarrow \quad \varepsilon \quad \longrightarrow \quad \tau = \sigma - \mathbb{C}^0 : \varepsilon$$

"disassemble" P:

1. solve $\sigma + \mathbb{C}^0 : \mathsf{S}^{-1}(\cdot, \sigma) = P$
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Beyond linear elasticity

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"disassemble" P:

1. solve $\mathsf{S}^{-1}(\cdot, \sigma) + \mathbb{D}^0 : \sigma = \mathbb{D}^0 : P$
2. compute $\varepsilon = \mathbb{D}^0 : (P - \sigma)$ $\quad \triangleright\ \mathbb{D}^0 = (\mathbb{C}^0)^{-1}$

Beyond linear elasticity

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$$P \mapsto Z^0(P) \equiv (\mathsf{S} - \mathbb{C}^0)(\mathsf{S} + \mathbb{C}^0)^{-1}(P)$$

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"disassemble" P:

1. solve $\mathsf{S}^{-1}(\cdot, \sigma) + \mathbb{D}^0 : \sigma = \mathbb{D}^0 : P$ ▹ compute σ from "strain"
2. compute $\varepsilon = \mathbb{D}^0 : (P - \sigma)$ ▹ $\mathbb{D}^0 = (\mathbb{C}^0)^{-1}$

Hook-type materials

$$\begin{aligned} \sigma &= \mathbb{C} : (\varepsilon - \varepsilon^{\mathtt{in}}) \\ 0 &= g(\sigma, z, \dot{z}) \qquad \triangleright\ z = (\varepsilon^{\mathtt{in}}, \tilde{z}) \end{aligned}$$

Hook-type materials

$$
\begin{aligned}
\sigma &= \mathbb{C} : (\varepsilon - \varepsilon^{\mathrm{in}}) && \triangleright \text{ Hooke's law} \\
0 &= g(\sigma, z, \dot{z}) && \triangleright\ z = (\varepsilon^{\mathrm{in}}, \tilde{z})
\end{aligned}
$$

- inelastic strain $\varepsilon^{\mathrm{in}}$
- evolution depends only on stress
- examples: viscoelasticity, elastoplasticity, elastoviscoplasticity, crystal plasticity, . . .

Hook-type materials & polarization

$$
\begin{aligned}
\sigma &= \mathbb{C} : (\varepsilon - \varepsilon^{\mathtt{in}}) \\
0 &= g(\sigma, z, \dot{z}) \qquad \triangleright\ z = (\varepsilon^{\mathtt{in}}, \tilde{z})
\end{aligned}
$$

- classically: ε given, σ sought

Hook-type materials & polarization

$$
\begin{aligned}
\sigma &= \mathbb{C} : (\varepsilon - \varepsilon^{\mathrm{in}}) \\
0 &= g(\sigma, z, \dot{z}) \qquad \triangleright\ z = (\varepsilon^{\mathrm{in}}, \tilde{z})
\end{aligned}
$$

- polarization: $P = \sigma + \mathbb{C}^0 : \varepsilon$ given, σ sought

Hook-type materials & polarization

$$\begin{aligned} \sigma &= \mathbb{C} : (\varepsilon - \varepsilon^{\mathtt{in}}) \\ 0 &= g(\sigma, z, \dot{z}) \qquad \triangleright\ z = (\varepsilon^{\mathtt{in}}, \tilde{z}) \end{aligned}$$

- polarization: $P = \sigma + \mathbb{C}^0 : \varepsilon$ given, σ sought

$$\sigma = \mathbb{C} : (\varepsilon - \varepsilon^{\mathtt{in}}), \quad \varepsilon = \mathbb{D}^0 : (P - \sigma)$$

Hook-type materials & polarization

$$\begin{aligned} \sigma &= \mathbb{C} : (\varepsilon - \varepsilon^{\mathtt{in}}) \\ 0 &= g(\sigma, z, \dot{z}) \qquad \triangleright\ z = (\varepsilon^{\mathtt{in}}, \tilde{z}) \end{aligned}$$

- polarization: $P = \sigma + \mathbb{C}^0 : \varepsilon$ given, σ sought

$$\sigma = \mathbb{C} : (\mathbb{D}^0 : (P - \sigma) - \varepsilon^{\mathtt{in}})$$

Hook-type materials & polarization

$$\begin{aligned} \sigma &= \mathbb{C} : (\varepsilon - \varepsilon^{\mathtt{in}}) \\ 0 &= g(\sigma, z, \dot{z}) \qquad \triangleright\ z = (\varepsilon^{\mathtt{in}}, \tilde{z}) \end{aligned}$$

- polarization: $P = \sigma + \mathbb{C}^0 : \varepsilon$ given, σ sought

$$\sigma + \mathbb{C} : \mathbb{D}^0 : \sigma = \mathbb{C} : (\mathbb{D}^0 : P - \varepsilon^{\mathtt{in}})$$

Hook-type materials & polarization

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$$\begin{aligned} \sigma &= \mathbb{C} : (\varepsilon - \varepsilon^{\mathtt{in}}) \\ 0 &= g(\sigma, z, \dot{z}) \qquad \triangleright\ z = (\varepsilon^{\mathtt{in}}, \tilde{z}) \end{aligned}$$

- polarization: $P = \sigma + \mathbb{C}^0 : \varepsilon$ given, σ sought

$$\mathbb{D} : \sigma + \mathbb{D}^0 : \sigma = \mathbb{D}^0 : P - \varepsilon^{\mathtt{in}} \qquad \triangleright\ \mathbb{D} \equiv \mathbb{C}^{-1}$$

Hook-type materials & polarization

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$$\begin{aligned} \sigma &= \mathbb{C} : (\varepsilon - \varepsilon^{\mathtt{in}}) \\ 0 &= g(\sigma, z, \dot{z}) \qquad \triangleright\, z = (\varepsilon^{\mathtt{in}}, \tilde{z}) \end{aligned}$$

- polarization: $P = \sigma + \mathbb{C}^0 : \varepsilon$ given, σ sought

$$(\mathbb{D} + \mathbb{D}^0) : \sigma = \mathbb{D}^0 : P - \varepsilon^{\mathtt{in}}$$

Hook-type materials & polarization

$$
\begin{aligned}
\sigma &= \mathbb{C} : (\varepsilon - \varepsilon^{\mathtt{in}}) \\
0 &= g(\sigma, z, \dot{z}) \qquad \triangleright\ z = (\varepsilon^{\mathtt{in}}, \tilde{z})
\end{aligned}
$$

- polarization: $P = \sigma + \mathbb{C}^0 : \varepsilon$ given, σ sought

$$\sigma = (\mathbb{D} + \mathbb{D}^0)^{-1}(\mathbb{D}^0 : P - \varepsilon^{\mathtt{in}})$$

Hook-type materials & polarization

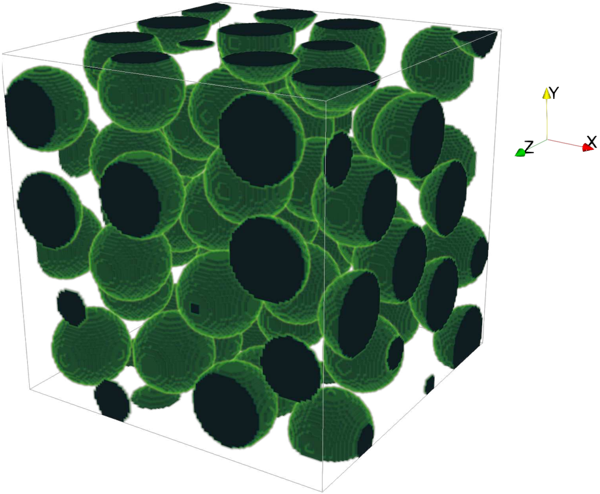
$$\begin{aligned} \sigma &= \mathbb{C} : (\varepsilon - \varepsilon^{\mathtt{in}}) \\ 0 &= g(\sigma, z, \dot{z}) \qquad \triangleright\; z = (\varepsilon^{\mathtt{in}}, \tilde{z}) \end{aligned}$$

- polarization: $P = \sigma + \mathbb{C}^0 : \varepsilon$ given, σ sought

$$\sigma = (\mathbb{D} + \mathbb{D}^0)^{-1} (\mathbb{D}^0 : P - \varepsilon^{\mathtt{in}})$$

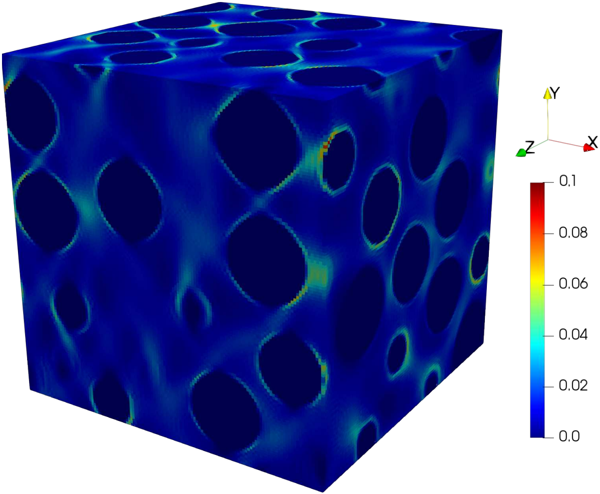
- solving for σ **implicitly** $\equiv$ computing σ **explicitly**

Practical performance - setup



- MMC
- Si particles
- Al matrix, vM plastic, power-law hardening

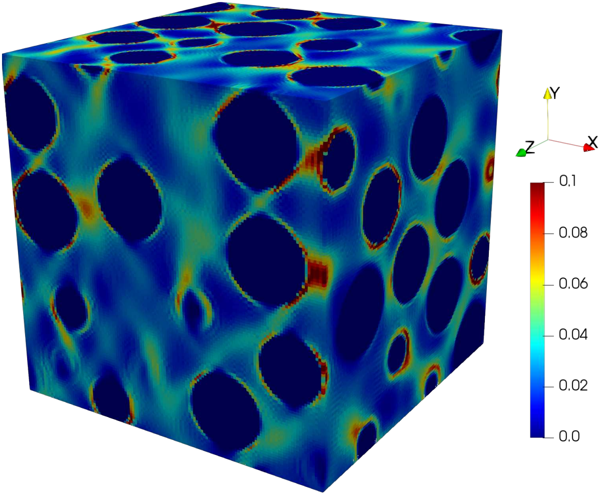
Practical performance - fields



- MMC
- Si particles
- Al matrix,
  vM plastic,
  power-law
  hardening

plastic strain @ 1% strain

Practical performance - fields



- MMC
- Si particles
- Al matrix, vM plastic, power-law hardening

plastic strain @ 2% strain

Practical performance - fields

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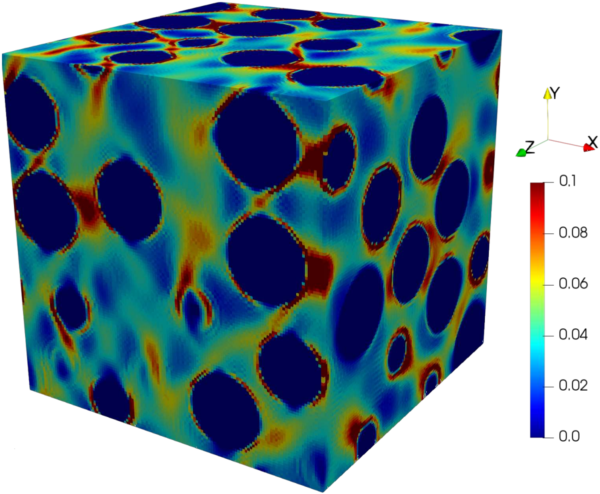

- MMC
- Si particles
- Al matrix, vM plastic, power-law hardening

plastic strain @ 3% strain

Practical performance - iterations

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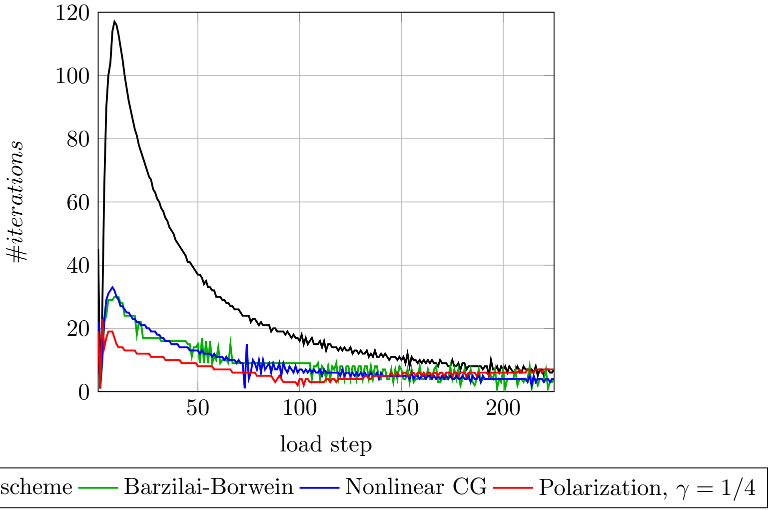

Practical performance - iterations

	16^3	32^3	64^3	128^3
Basic Scheme	24.62	23.41	24.8	25.98
Barzilai-Borwein	9.95	9.42	9.40	9.36
$\gamma = 0$	7.69	7.4	7.31	8.74
$\gamma = 1/2$	7.0	7.08	6.51	6.83
$\gamma = 1/4$	10.94	10.37	9.47	9.84
Heavy-ball method	29.15	35.72	33.79	34.73
Nonlinear CG	9.91	9.24	9.11	9.05

$\nearrow$ average iterations for 225 load steps

Summary part II

performance of polarization schemes $\Longleftrightarrow$ efficiency of computing Z^0

Compute Z^0 cheaply for:

- linear elasticity ↗ [D. J. Eyre and G. W. Milton, The European Physical Journal - Applied Physics, 1999]
- Hooke-type materials ↗ [MS, D. Wicht, and T. Böhlke, Computational Mechanics, 2019]
- Norton model ↗ [J. C. Michel, H. Moulinec, and P. Suquet, International Journal for Numerical Methods in Engineering, 2001]
- simple damage models
- ...

nuisance vs. publication potential :p

Overview

1. Polarization methods
2. Evaluating the Cayley operator
3. Connection to optimization
4. Adaptive parameter selection
5. Summary and conclusions

Optimization

Goal:

$$f(x) \longrightarrow \min_{x \in X}$$

continuous gradient descent

$$\dot{x} = -\nabla f(x)$$

Optimization

Goal:

$$f(x) \longrightarrow \min_{x \in X}$$

explicit gradient descent

$$\frac{x^{k+1} - x^k}{s} = -\nabla f(x^k)$$

Optimization

Goal:

$$f(x) \longrightarrow \min_{x \in X}$$

explicit gradient descent

$$\frac{x^{k+1} - x^k}{s} = -\nabla f(x^k)$$

$\nearrow$ unstable for $s \gg 1$

Optimization

Goal:

$$f(x) \longrightarrow \min_{x \in X}$$

implicit gradient descent

$$\frac{x^{k+1} - x^k}{s} = -\nabla f(x^{k+1})$$

Optimization

Goal:

$$f(x) \longrightarrow \min_{x \in X}$$

implicit gradient descent

$$\frac{x^{k+1} - x^k}{s} = -\nabla f(x^{k+1})$$

$\nearrow$ stable for any $s > 0$

Optimization

Goal:

$$f(x) \longrightarrow \min_{x \in X}$$

implicit gradient descent

$$\frac{x^{k+1} - x^k}{s} = -\nabla f(x^{k+1})$$

↗ stable for any $s > 0$
↗ numerically infeasible

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$\frac{x^{k+1/2} - x^k}{s/2} = -\nabla g(x^{k+1/2}) - \nabla h(x^k)$$
$$\frac{x^{k+1} - x^{k+1/2}}{s/2} = -\nabla g(x^{k+1/2}) - \nabla h(x^{k+1})$$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$\frac{x^{k+1/2} - x^k}{s/2} = -\nabla g(x^{k+1/2}) - \nabla h(x^k)$$

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$\nearrow$ stable for any $s > 0$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$\frac{x^{k+1/2} - x^k}{s/2} = -\nabla g(x^{k+1/2}) - \nabla h(x^k)$$

$$\frac{x^{k+1} - x^{k+1/2}}{s/2} = -\nabla g(x^{k+1/2}) - \nabla h(x^{k+1})$$

- $\lambda \equiv s/2$

Composite optimization

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Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$\frac{x^{k+1/2} - x^k}{\lambda} = -\nabla g(x^{k+1/2}) - \nabla h(x^k)$$

$$\frac{x^{k+1} - x^{k+1/2}}{\lambda} = -\nabla g(x^{k+1/2}) - \nabla h(x^{k+1})$$

- $\lambda \equiv s/2$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$\begin{aligned} x^{k+1/2} - x^k &= -\lambda\, \nabla g(x^{k+1/2}) - \lambda\, \nabla h(x^k) \\ x^{k+1} - x^{k+1/2} &= -\lambda\, \nabla g(x^{k+1/2}) - \lambda\, \nabla h(x^{k+1}) \end{aligned}$$

- $\lambda \equiv s/2$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$\begin{aligned} x^{k+1/2} + \lambda \nabla g(x^{k+1/2}) &= x^k - \lambda \nabla h(x^k) \\ x^{k+1} + \lambda \nabla h(x^{k+1}) &= x^{k+1/2} - \lambda \nabla g(x^{k+1/2}) \end{aligned}$$

- $\lambda \equiv s/2$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$(\mathrm{Id} + \lambda \nabla g)(x^{k+1/2}) = (\mathrm{Id} - \lambda \nabla h)(x^k)$$
$$(\mathrm{Id} + \lambda \nabla h)(x^{k+1}) = (\mathrm{Id} - \lambda \nabla g)(x^{k+1/2})$$

- $\lambda \equiv s/2$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$\begin{aligned} x^{k+1/2} &= (\mathrm{Id} + \lambda \nabla g)^{-1}(\mathrm{Id} - \lambda \nabla h)(x^k) \\ x^{k+1} &= (\mathrm{Id} + \lambda \nabla h)^{-1}(\mathrm{Id} - \lambda \nabla g)(x^{k+1/2}) \end{aligned}$$

- $\lambda \equiv s/2$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$x^{k+1} = (\mathrm{Id} + \lambda \nabla h)^{-1} (\mathrm{Id} - \lambda \nabla g)(\mathrm{Id} + \lambda \nabla g)^{-1} (\mathrm{Id} - \lambda \nabla h)(x^k)$$

- $\lambda \equiv s/2$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$x^{k+1} = (\mathrm{Id} + \lambda \nabla h)^{-1} (\mathrm{Id} - \lambda \nabla g)(\mathrm{Id} + \lambda \nabla g)^{-1} (\mathrm{Id} - \lambda \nabla h)(x^k)$$

- $\lambda \equiv s/2$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$(\mathrm{Id} + \lambda\, \nabla h)(x^{k+1}) = (\mathrm{Id} - \lambda\, \nabla g)(\mathrm{Id} + \lambda\, \nabla g)^{-1}(\mathrm{Id} - \lambda\, \nabla h)(x^k)$$

- $\lambda \equiv s/2$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$(\mathrm{Id} + \lambda \nabla h)(x^{k+1}) = (\mathrm{Id} - \lambda \nabla g)(\mathrm{Id} + \lambda \nabla g)^{-1}(\mathrm{Id} - \lambda \nabla h)(x^k)$$

- $\lambda \equiv s/2$
- $y^k = (\mathrm{Id} + \lambda \nabla h)(x^k)$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$y^{k+1} = (\mathrm{Id} - \lambda \nabla g)(\mathrm{Id} + \lambda \nabla g)^{-1}(\mathrm{Id} - \lambda \nabla h)(x^k)$$

- $\lambda \equiv s/2$
- $y^k = (\mathrm{Id} + \lambda \nabla h)(x^k)$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$y^{k+1} = (\mathrm{Id} - \lambda \nabla g)(\mathrm{Id} + \lambda \nabla g)^{-1}(\mathrm{Id} - \lambda \nabla h)(\mathrm{Id} + \lambda \nabla h)^{-1}(y^k)$$

- $\lambda \equiv s/2$
- $y^k = (\mathrm{Id} + \lambda \nabla h)(x^k)$

Composite optimization

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Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$y^{k+1} = (\mathrm{Id} - \lambda \nabla g)(\mathrm{Id} + \lambda \nabla g)^{-1} (\mathrm{Id} - \lambda \nabla h)(\mathrm{Id} + \lambda \nabla h)^{-1} (y^k)$$

- $\lambda \equiv s/2$
- $y^k = (\mathrm{Id} + \lambda \nabla h)(x^k)$

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$y^{k+1} = (\mathrm{Id} - \lambda \nabla g)(\mathrm{Id} + \lambda \nabla g)^{-1}(\mathrm{Id} - \lambda \nabla h)(\mathrm{Id} + \lambda \nabla h)^{-1}(y^k)$$

- $\lambda \equiv s/2$
- $y^k = (\mathrm{Id} + \lambda \nabla h)(x^k)$
- Peaceman-Rachford splitting

↗ [D. W. Peaceman and H. H. Rachford, Journal of the Society for Industrial and Applied Mathematics, 1955]

Composite optimization

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

semi-implicit gradient descent

$$y^{k+1} = \gamma\, y^k + (1-\gamma)(\mathrm{Id} - \lambda\, \nabla g)(\mathrm{Id} + \lambda\, \nabla g)^{-1}(\mathrm{Id} - \lambda\, \nabla h)(\mathrm{Id} + \lambda\, \nabla h)^{-1}(y^k)$$

- $\lambda \equiv s/2$
- $y^k = (\mathrm{Id} + \lambda\, \nabla h)(x^k)$
- Douglas-Rachford splitting, $\gamma \in [0, 1)$

↗ [J. Douglas and H. H. Rachford, Transactions of the American Mathematical Society, 1956]

Application to hyperelasticity

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

- X as for basic scheme
- $h(\varepsilon) = \langle w(\cdot, \varepsilon) \rangle_Q$
- g encodes compatibility constraint

$$g(\varepsilon) = \begin{cases} 0, & \varepsilon = \bar{\varepsilon} + \nabla^s u \quad \text{for some periodic} \quad u : Q \to \mathbb{R}^d \\ +\infty, & \text{otherwise} \end{cases}$$

Application to hyperelasticity

Goal:

$$g(x) + h(x) \longrightarrow \min_{x \in X}$$

- X as for basic scheme
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$$g(\varepsilon) = \begin{cases} 0, & \varepsilon = \bar{\varepsilon} + \nabla^s u \quad \text{for some periodic} \quad u : Q \to \mathbb{R}^d \\ +\infty, & \text{otherwise} \end{cases}$$

- ↗ leads to Eyre-Milton scheme with $P^k = y^k/\lambda$ and $\mathbb{C}^0 = 1/\lambda \ \mathrm{Id}$

↗ [MS, D. Wicht, and T. Böhlke, Computational Mechanics, 2019]

Synopsis part III

- both the basic and the polarization scheme are **gradient methods**
- basic is explicit ↗ step-size restriction
- polarization methods are semi-implicit ↗ larger step sizes feasible

$$\frac{1}{\lambda^{\texttt{pol}}} \equiv \sqrt{\alpha_- \alpha_+} \leq \frac{\alpha_- + \alpha_+}{2} \equiv \frac{1}{s^{\texttt{basic}}}$$

- import knowledge from optimization
- Eyre-Milton $\Longleftrightarrow$ Douglas-Rachford splitting
- Michel-Moulinec-Suquet $\Longleftrightarrow$ Alternating-direction method of multipliers (ADMM)

Overview

1. Polarization methods

2. Evaluating the Cayley operator

3. Connection to optimization

4. Adaptive parameter selection

5. Summary and conclusions

Why?

- had benefits for primal solvers
- no eigenvalue decomposition
- optimal ref. material for polarization:

$$\alpha_0 = \sqrt{\alpha_- \alpha_+} \quad \text{for} \quad \alpha_- \leq \lambda \leq \alpha_+ \quad \forall x, \xi \, \forall \lambda \in \mathtt{Eig}\left(\frac{\partial S}{\partial \varepsilon}(x, \xi)\right)$$

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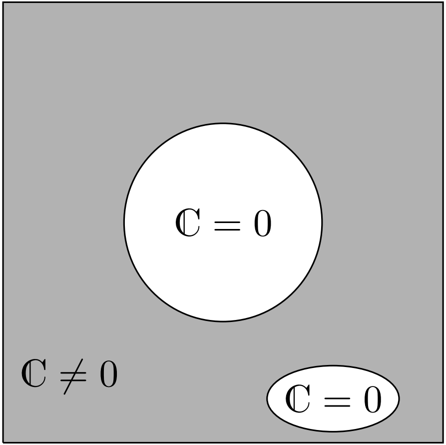
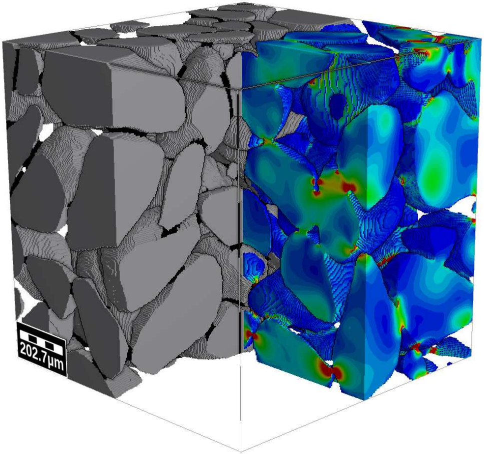
makes **no sense** for $\alpha_- = 0 \nearrow$ porous materials

Porous materials - schematic



Porous materials - for real



bound sand grains

[M. Schneider, T. Hofmann et al, International Journal of Solids and Structures, 2018]

Porous materials - the problem

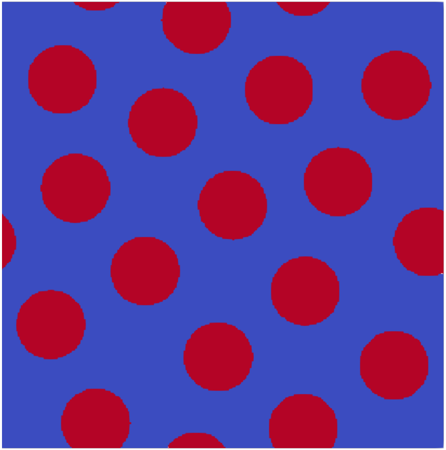
- whether or not the solvers converge
  depends on the **discretization** used

[F. Willot, B. Abdallah, and Y.-P. Pellegrini, International Journal for Numerical Methods in Engineering, 2014]

[MS, F. Ospald, and M. Kabel, International Journal for Numerical Methods in Engineering, 2016]

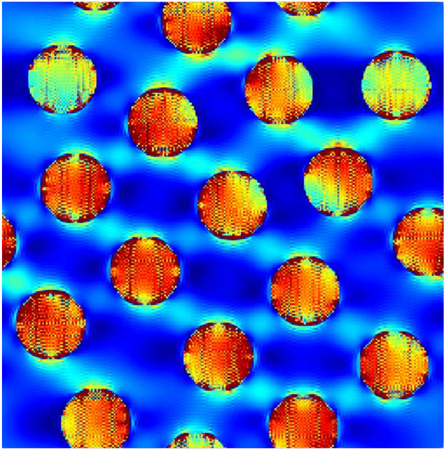
[MS, International Journal for Numerical Methods in Engineering, 2020]

Minimal example - geometry



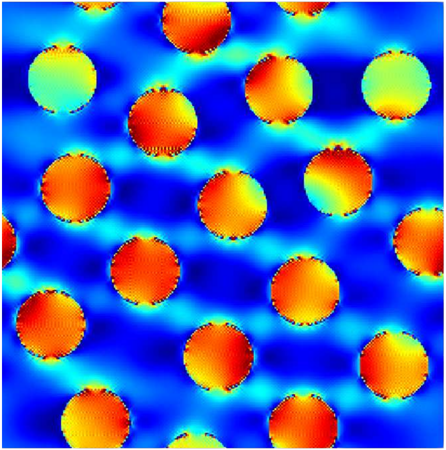
30% pores, 256^2, quartz sand, $E = 66.9$ GPa and $\nu = 0.25$
5% strain in x

Minimal example - Moulinec-Suquet



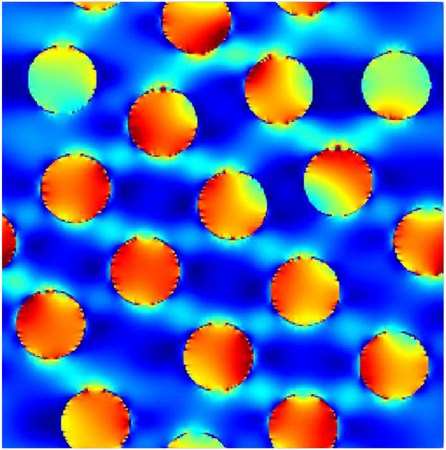
$||\varepsilon||$

Minimal example - rotated staggered



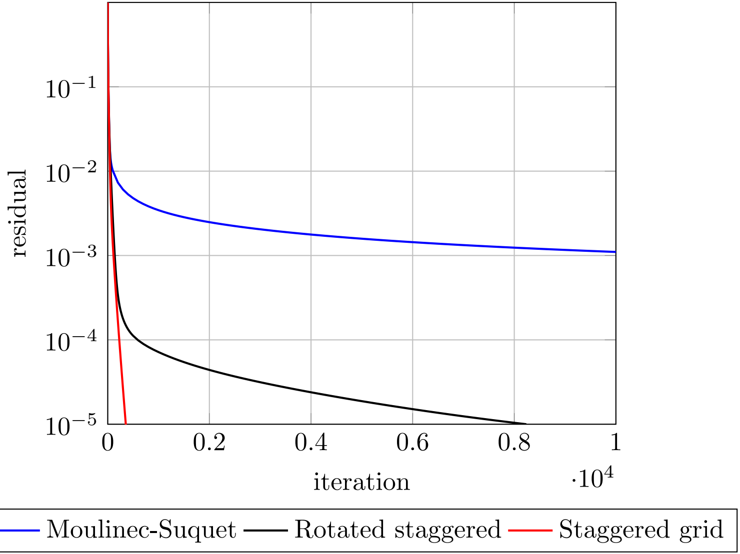
$||\varepsilon||$

Minimal example - staggered grid

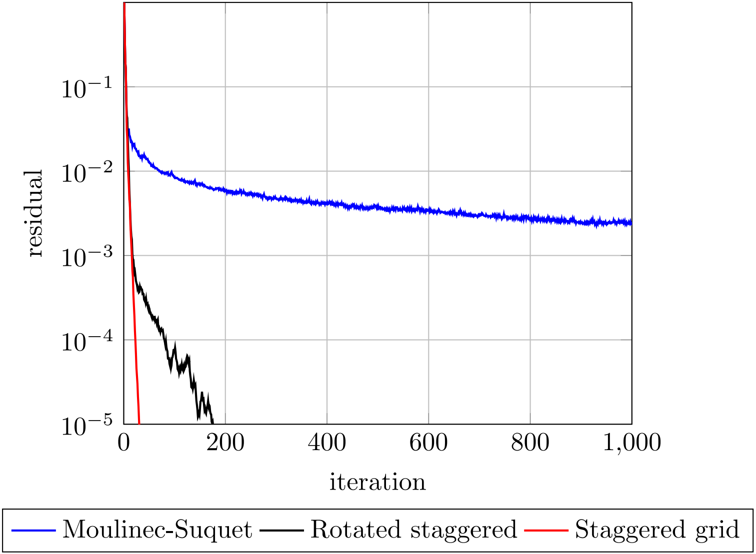


$||\varepsilon||$

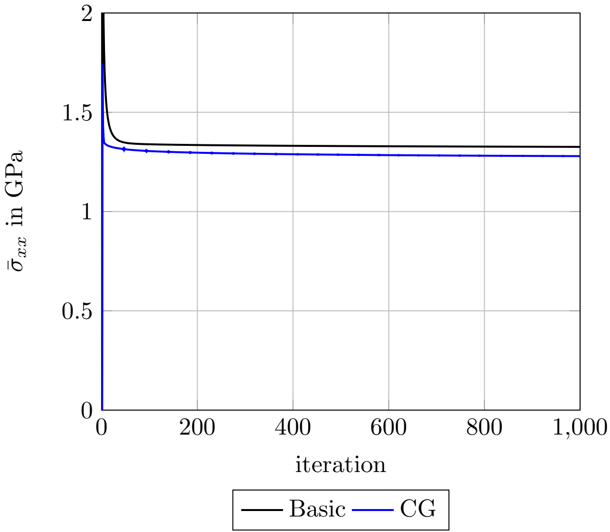
Minimal example - basic



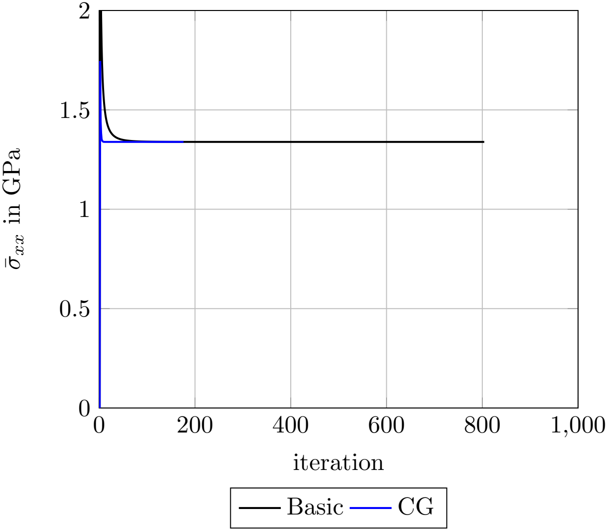
Minimal example - CG



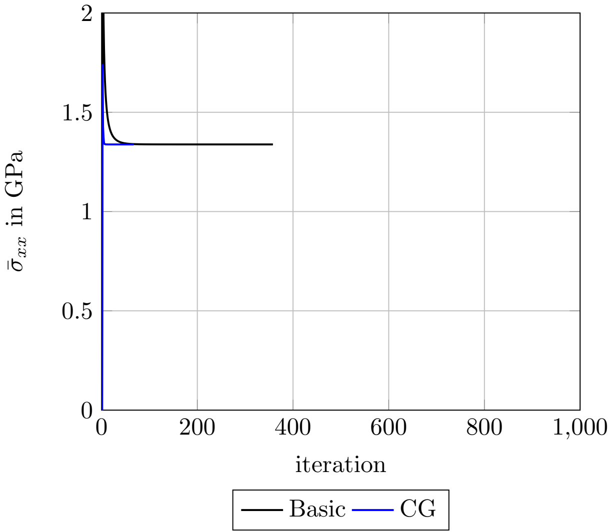
Minimal example - Moulinec-Suquet



Minimal example - Rotated staggered



Minimal example - Staggered grid



Upshot for porous microstructures

- Fourier-type discretizations **numerically unstable**
- prefer finite differences / FEM

Adaptive parameters & polarization

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KIT Karlsruhe Institute of Technology

two flavors:

- Eyre-Milton

$$P^{k+1} = \gamma\, P^k + (1-\gamma)\left[2\,\mathbb{C}^0 : \bar{\varepsilon} + Y^0 : Z^0(P^k), \quad P^k = \sigma^k + \mathbb{C}^0 : e^k\right]$$

- Michel-Moulinec-Suquet

$$\begin{aligned}
\varepsilon^{k+1/2} &= \bar{\varepsilon} - \Gamma^0 : (\sigma^k - \mathbb{C}^0 : e^k) \\
\varepsilon^k &= (1-2\gamma)\, e^k + 2(1-\gamma)\,\varepsilon^{k+1/2} \\
\mathsf{S}(\cdot, e^{k+1}) + \mathbb{C}^0 : e^k &= \sigma^k + \mathbb{C}^0 : \varepsilon^k \\
\sigma^{k+1} &= \sigma^k + \mathbb{C}^0 : (\varepsilon^k - e^k)
\end{aligned}$$

Adaptive parameters & polarization

two flavors:

- Eyre-Milton ↗ less suitable for adaptivity

$$P^{k+1} = \gamma\, P^k + (1-\gamma)\left[2\, \mathbb{C}^0 : \bar{\varepsilon} + Y^0 : Z^0(P^k), \quad P^k = \sigma^k + \mathbb{C}^0 : e^k\right]$$

- Michel-Moulinec-Suquet

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Adaptive parameters & polarization

- Michel-Moulinec-Suquet

$$
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\sigma^{k+1} &= \sigma^k + \mathbb{C}^0 : (\varepsilon^k - e^k)
\end{aligned}
$$

- many possibilities ↗ [MS, International Journal for Numerical Methods in Engineering, 2021]
- simplest one:

$$
\alpha^k = \frac{\|\sigma^k\|_{L^2}}{\|e^k\|_{L^2}}
$$

↗ [D. A. Lorenz and Q. Tran-Dinh, Computational Optimization and Applications, 2019]

Implementation # 2 - adaptive

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KIT Karlsruhe Institute of Technology

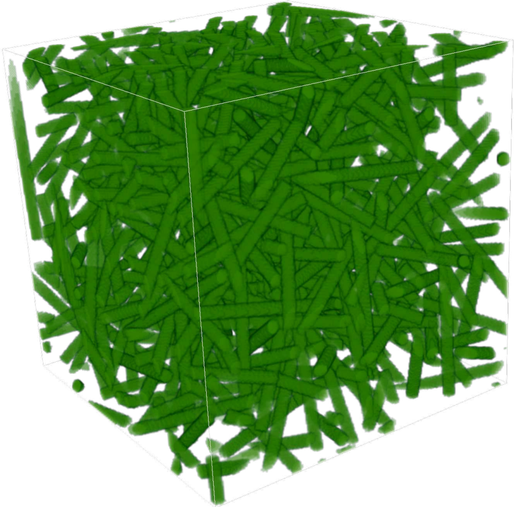
Algorithm 3 ADMM $(\bar{\varepsilon}, \texttt{maxit}, \texttt{tol}, \alpha_0 = \alpha_0^{\texttt{init}}, \gamma)$

$e \leftarrow \varepsilon^0$ ▷ $\varepsilon^0 \equiv \bar{\varepsilon}$ or via extrapolation
$\sigma \leftarrow \mathsf{S}(\cdot, \varepsilon^0)$
$\texttt{res} \leftarrow 1$
$k \leftarrow 0$
while $k < \texttt{maxit}$ **and** $\texttt{res} > \texttt{tol}$ **do**
    $k \leftarrow k + 1$
    $\bar{\sigma} \leftarrow \langle \sigma \rangle_Q$
    $\alpha_0 \leftarrow \|\sigma\|_{L^2} / \|e\|_{L^2}$
    $\varepsilon \leftarrow \sigma - \mathbb{C}^0 : e$
    $\varepsilon \leftarrow \bar{\varepsilon} - 1/\alpha_0 \, \Gamma : \varepsilon$ ▷ use FFT & favorite discretization
    $\texttt{res} \leftarrow \alpha_0 \, \|\varepsilon - e\|_{L^2} / \|\bar{\sigma}\|$
    $\varepsilon \leftarrow (1 - 2\gamma) e + 2(1 - \gamma)\varepsilon$
    $\begin{bmatrix} e \\ \sigma \end{bmatrix} \leftarrow \begin{bmatrix} (\mathsf{S} + \mathbb{C}^0)^{-1}(\sigma + \mathbb{C}^0 : \varepsilon) \\ \sigma + \mathbb{C}^0 : (\varepsilon - e) \end{bmatrix}$
end while
return $e, \bar{\sigma}, \texttt{res}$ ▷ Requires three fields

[J. C. Michel, H. Moulinec, and P. Suquet, International Journal for Numerical Methods in Engineering, 2001]

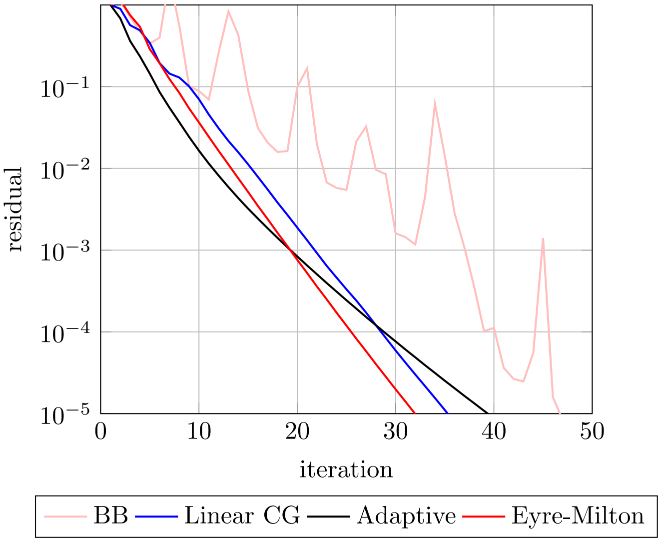
[MS, International Journal for Numerical Methods in Engineering, 2021]

Performance - setup

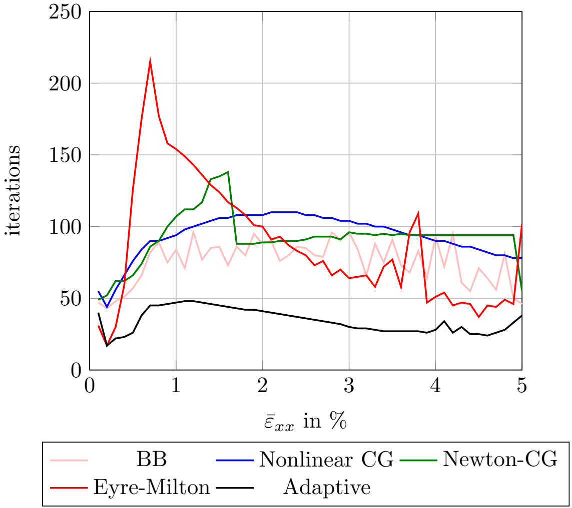


PA6, 15% short glass fibers

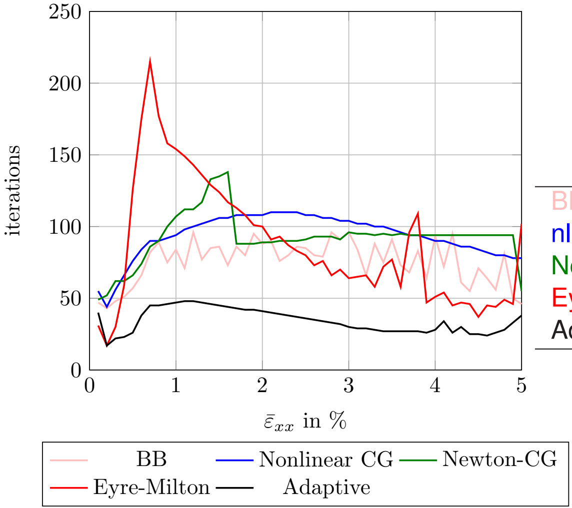
Performance - linear



Performance - vM plastic

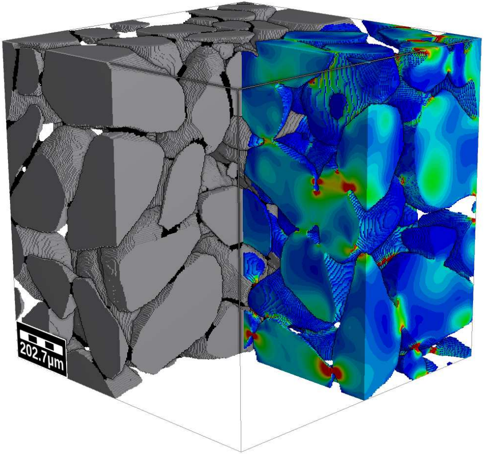


Performance - vM plastic



	it (time in s)
BB	75.48 (3320.7)
nl CG	93.42 (4995.0)
Newton	92.18 (4402.6)
Eyre-Milton	87.18 (4358.6)
Adaptive	34.26 (1770.6)

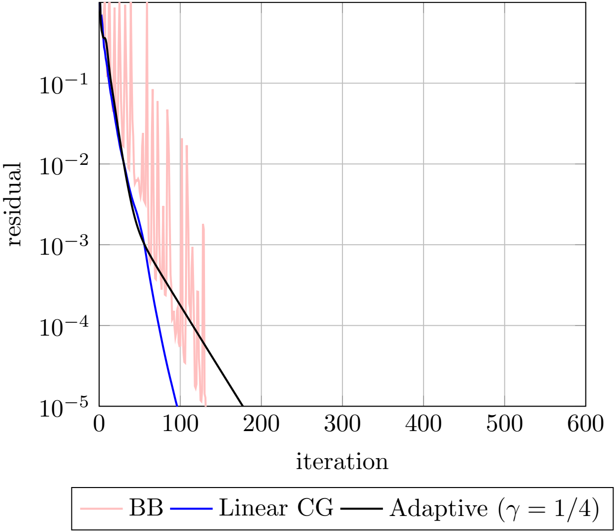
Porous materials - for real



bound sand grains

[M. Schneider, T. Hofmann et al, International Journal of Solids and Structures, 2018]

Performance - grains @ staggered



Synopsis part IV

- porous? ↗ discretization!
- adaptive polarization schemes @ MMS implementation
- simple and effective

Overview

1. Polarization methods
2. Evaluating the Cayley operator
3. Connection to optimization
4. Adaptive parameter selection
5. Summary and conclusions

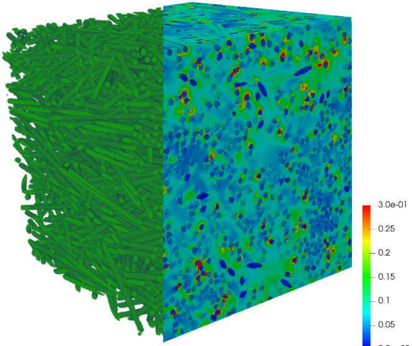
Summary

- polarization schemes specific to FFT-based methods
- extremely powerful
- not for beginners
- recommendations:

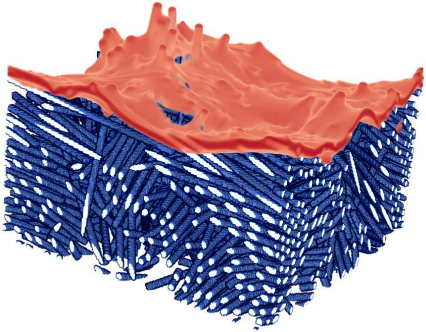
material law	finite material contrast	with pores
linear	linear CG	linear CG
cheap	BB	BB
	polarization	Nonlinear CG
expensive	Newton-CG	Newton-CG
	Nonlinear CG	Nonlinear CG

↗ [MS, "A review of nonlinear FFT-based computational homogenization methods", Acta Mechanica, 2021]

The end



[**MS**, IJNME, 2019]



[Ernesti-**MS**-Böhlke, CMAME, 2020]

matti.schneider@kit.edu