

14–18 march 2022, Champs-sur-Marne (France)

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

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Abstract

Analysis at the macroscopic scale of a structure that exhibits heterogeneities at the microscopic scale requires a first homogenization step that allows the heterogeneous constitutive material to be replaced with an equivalent, homogeneous material.

Approximate homogenization schemes (based on mean field/effective field approaches) as well as rigorous bounds have been around for several decades; they are extremely versatile and can address all kinds of material non-linearities. However, they rely on a rather crude description of the microstructure. For applications where a better account of the finest details of the microstructure is desirable, the solution to the so-called corrector problem (that delivers the homogenized properties) must be computed by means of full-field simulations. Such simulations are complex, and classical discretization strategies (e.g., interface-fitting finite elements) are ill-suited to the task.

During the 1990s, Hervé Moulinec and Pierre Suquet introduced a new numerical method for solving the corrector problem. This method is based on the discretization of an integral equation that is equivalent to the original boundary-value problem. Observing that the resulting linear system has a very simple structure (block-diagonal plus block-circulant), Moulinec and Suquet used the fast Fourier transform (FFT) to compute the matrix-vector products that are required to find the solution efficiently.

During the last decade, the resulting method has gained in popularity (the initial Moulinec Suquet paper is cited 134 times over the 1998–2009 period and 619 times over the 2010–2020 period — source: Scopus). Significant advances have been made on various topics: theoretical analysis of the convergence, discretization strategies, innovative linear and non-linear solvers, etc.

Nowadays, FFT-based homogenization methods have become state-of-the-art techniques in materials science and are used for industry with increasing frequency. A 5-day introductory course to FFT-based homogenization methods was held on 14-18 march 2022 at Univ Gustave Eiffel, Champs sur Marne, France. The intent of this workshop was to provide an accessible introduction to FFT-based computational homogenization methods and also have a glimpse at the current research frontier.

The workshop was open to research students (M2 onwards) as well as researchers from both academia and industrial R&D. Each of the nine sessions of this workshop was composed of a theoretical lecture followed by hands-on applications (mostly on computers).

We are happy to share in the present document our slides of the nine lectures.

March 2022,

S. Brisard, M. Schneider and F. Willot

License

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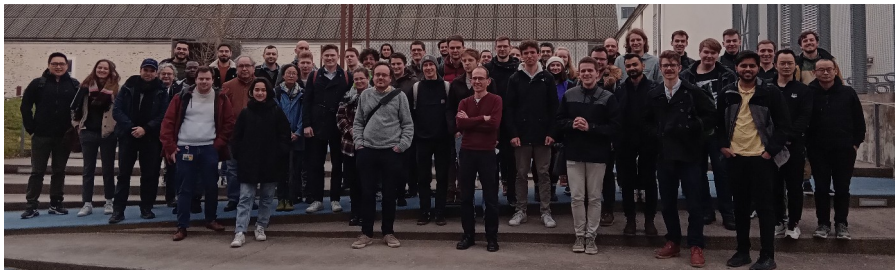
Acknowledgements

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F. Ernesti was deeply involved in the creation of the material for the tutorial sessions.

S. Gajek and L. Risthaus helped the participants during the tutorial sessions.

This workshop would not have taken place without the help of: B. Mchiouar-Slimani, N. Lambre, C. Réter, E. Séchan and A. Filoreau.



Finally, we thank all participants for their attention!

Introduction to FFT-based numerical methods for
the homogenization of random materials (14–18 march 2022)

Introduction

Sébastien Brisard, Felix Ernesti, Matti Schneider, François Willot

Before we start (1/3)



Université
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Deutsch-Französische
Hochschule

Acknowledgements

The financial support of Université Franco-Allemande Deutsch-Französische Hochschule is gratefully acknowledged.



Download slides

<https://fft-workshop-22.sciencesconf.org/>



Interruptions are most welcome

**Do ask questions if you need to
Let us know if we are too slow or too fast**

Before we start (2/3)

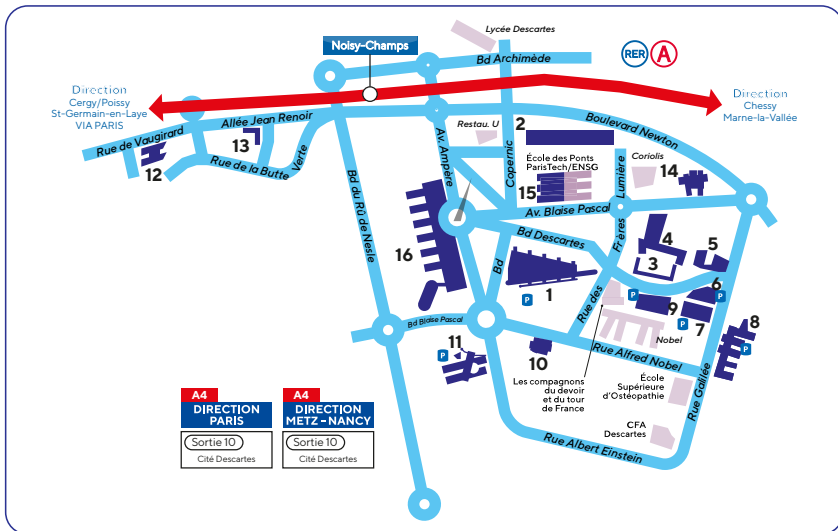
Navigating Univ Gustave Eiffel

- All lectures in the G. Percec building (4)
- Tutorial sessions in the Copernic building (1)
- Lunch at the Bienvenüe building (2);
food trucks all around the campus
- We offer lunch on thursday
- We will provide coffee for morning breaks
(but we are running on a very low budget!)

Wednesday is special

- Morning lectures at Mines ParisTech
- Afternoon: guided tour of the School of Mines Mineralogy Museum

CITÉ DESCARTES



Before we start (3/3)

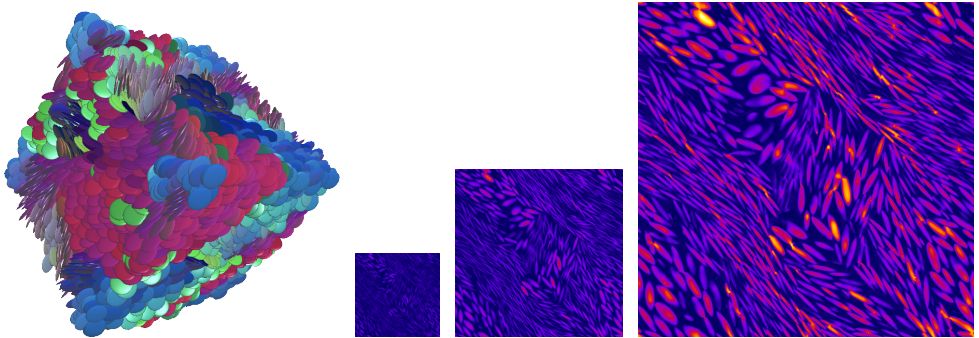
We share our codes!

- This workshop: <https://fft-workshop-22.sciencesconf.org/>
- Morphhom (Fortran):
<https://people.cmm.minesparis.psl.eu/users/willoot/morphhom/>
- Janus: <https://github.com/sbrisard/janus> (Python)
- Scapin: <https://github.com/sbrisard/Scapin.jl> (Julia)

A very unfortunate name

- Bad: “FFT-based methods”
- Better: “Lippmann–Schwinger solvers”
- Any ideas?

To wet your appetite...



- 10,000 spheroidal inclusions: $f = 60\%$, $c/a = 1/8$
- Moderate contrast $\mu_i/\mu_m = 100$
- Response to macroscopic shear strain
- Simulations on 256^3 , 512^3 and 1024^3 grids
(1.5×10^6 , 0.8×10^9 , 6.4×10^9 unknowns!)

The bird's eye view (1/3)

Numerical computation of the response of heterogeneous materials to macroscopic solicitations

- Grid-based: no need for conforming mesh, CT images OK (sort of)
- Straightforward implementation (including parallelization)
- Matrix-free implementation
- Matrix-vector product uses the DFT (hence FFT)
- Versatile: cont. mechanics, conductivity, Darcy flow, etc.
- Coupling with other grid-based techniques (phase fields)
- See also review by Schneider [1]

[1] M. Schneider, *Acta Mechanica* **2021**, 232, 2051–2100.

The bird's eye view (2/3)

Start from the initial, boundary value problem

$$\left\{ \begin{array}{l} \mathbf{div} \boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon} \\ \boldsymbol{\varepsilon} = \mathbf{sym} \mathbf{grad} \mathbf{u} \\ \text{Periodic BCs, } \bar{\boldsymbol{\varepsilon}} \end{array} \right.$$

We don't really care about the displacement!

Reformulate as an equivalent integral equation

$$\boldsymbol{\varepsilon} + \Gamma_0 [(\mathbf{C} - \mathbf{C}_0) : \boldsymbol{\varepsilon}] = \bar{\boldsymbol{\varepsilon}}$$

Lippmann–Schwinger (LS) equation

Discretize (how?) and unleash iterative linear solvers

$$(D + C) \cdot x = b \quad \left\{ \begin{array}{l} D : \text{block-diagonal} \\ C : \text{block-circulant} \end{array} \right.$$

The bird's eye view (3/3)

Historical (non-exhaustive) outline

- Seminal papers: Moulinec, Suquet (and Michel) [1–3]
- Early contribution from Eyre and Milton [4]
- New contributions started in late 2000: [5–7]
- Other groups joined soon afterwards: Fraunhofer ITWM (Germany), CEA (France), Eindhoven University (The Netherlands)...
- Small but vibrant community
- Mini-symposium at each Ecocomas Congress

- [1] H. Moulinec, P. Suquet, *Comptes rendus de l'Académie des sciences. Série II Mécanique physique chimie astronomie* **1994**, 318, 1417–1423.
- [2] H. Moulinec, P. Suquet, *Computer Methods in Applied Mechanics and Engineering* **1998**, 157, 69–94.
- [3] J. C. Michel, H. Moulinec, P. Suquet, *International Journal for Numerical Methods in Engineering* **2001**, 52, 139–160.
- [4] D. J. Eyre, G. W. Milton, *The European Physical Journal - Applied Physics* **1999**, 6, 41–47.
- [5] F. Willot, Y.-P. Pellegrini, Fast Fourier Transform Computations and Build-up of Plastic Deformation in 2D, Elastic-Perfectly Plastic, Pixelwise Disordered Porous Media, arXiv e-print 0802.2488, **2008**.
- [6] J. Zeman et al., *Journal of Computational Physics* **2010**, 229, 8065–8071.
- [7] S. Brisard, L. Dormieux, *Computational Materials Science* **2010**, 49, 663–671.

Outline of the week (1/2)

Tutorial sessions (FE)

- Develop your own code!
- Make sure your computer is properly set up

Block 1: spatial discretization (SB)

- Introduction: the Green operator and the LS equation
- Consistent discretization of the LS equation
- Asymptotically consistent discretizations of the LS equation

Convergence wrt grid-size!

Outline of the week (2/2)

Block 2: solvers (MS)

- Treating inelastic problems with the basic scheme
- Faster primal solvers
- Polarization methods

Convergence wrt number of iterations!

Block 3: extensions & applications (FW)

- The RVE method
- Other physics, multiphysical couplings
- FFT methods for Stokes flow in porous media

Convergence wrt size and number of realizations!

Enjoy this week!

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Introduction to FFT-based numerical methods for the
homogenization of random materials (14–18 march 2022)



Introduction: the Green operator and the Lippmann–Schwinger equation

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Laboratoire Navier, École des Ponts, Univ. Gustave Eiffel, CNRS, Marne-la-Vallée, France



Outline of the session on spatial discretization

- Lecture 1 — Introduction: the Green operator and the Lippmann–Schwinger (LS) equation
- Lecture 2 — Consistent discretization of the LS equation
- Lecture 3 — Asymptotically consistent discretizations of the LS equation

Outline of Lecture 1

- Homogenization in a nutshell
- The “corrector” problem
- Formal definition of the Green operator
- The Lippmann–Schwinger (LS) equation
- The “basic” scheme
- Fourier series in a nutshell
- Derivation of the periodic Green operator (homogeneous material)

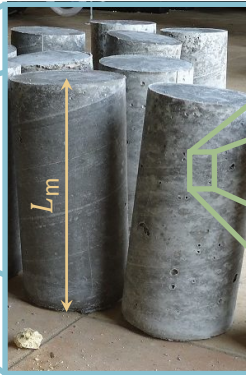
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Random homogenization



Macroscopic scale



Mesoscopic scale



Microscopic scale

Separation of scales

$$L_\mu \ll L_m \ll L_M$$

Source: [Structurae](#), [BGEA Labo](#) and [Aménagements Déco Lafarge](#)

What is homogenization?

Homogenization is the process of replacing the complex **microstructure** (cementitious matrix + aggregates) with an “equivalent”, **homogeneous material**.

The goal is to establish the (quantitative) rule that relates the **geometry** and **mechanical properties** of the constituents to the **macroscopic mechanical properties**.

At the scale of the structure (the pylons of the cable-stayed bridge), material heterogeneities (aggregates, ...) are **ignored**.

The response of the structure is computed as if it was **homogeneous**.

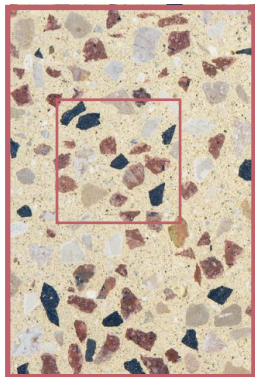
Effective (macroscopic) linear elastic properties

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{C}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}) \quad \Rightarrow \quad \langle \boldsymbol{\sigma} \rangle = \mathbf{C}^{\text{eff}} : \langle \boldsymbol{\varepsilon} \rangle$$

Effective properties are found at the mesoscopic scale, experimentally or from an upscaling prediction

From random to periodic homogenization

A conceptual gap that will be discussed by F. Willot (Lecture 7)



Some structures are indeed periodic

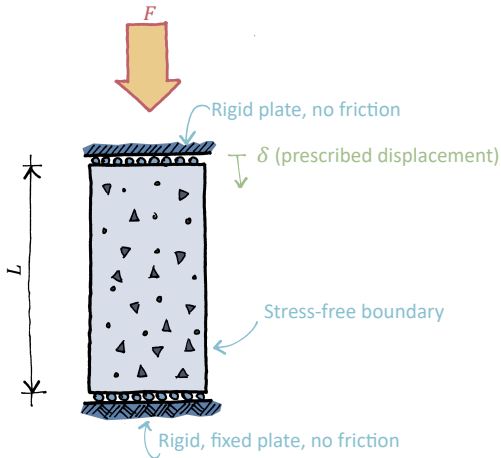


Waffle slab (source: [Holedeck](#))

Outline of Lecture 1

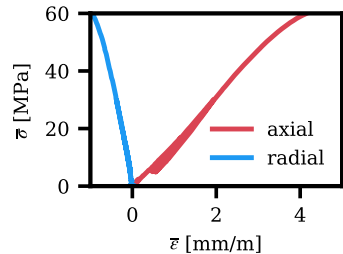
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Experimental characterization (top-down approach)



Macroscopic variables

- Macro. stress: F/A
- Macro. strain: δ/L



Compression test on a concrete sample
(Courtesy S. Bahafid, S. Ghabezloo)

Upscaling prediction (bottom-up approach)

“Corrector” problem reproduces physical experiment in-silico!

The unit-cell

$$\Omega = (0, L_1) \times \cdots \times (0, L_d)$$

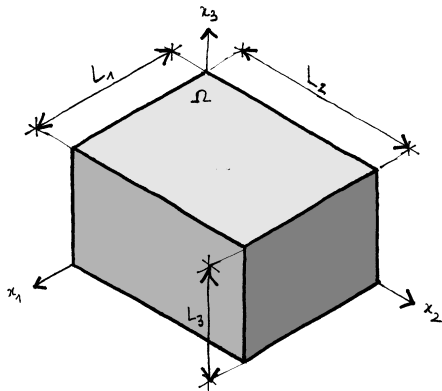
Field equations

$$\left\{ \begin{array}{l} \text{div } \boldsymbol{\sigma} = 0 \\ \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon} \\ \boldsymbol{\varepsilon} = \text{sym grad } \mathbf{u} \end{array} \right.$$

Periodic boundary conditions

$$\left\{ \begin{array}{l} \mathbf{u}(\mathbf{x}) - \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{x} \text{ is } \Omega\text{-periodic} \\ \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) \text{ is } \Omega\text{-skew-periodic} \end{array} \right. \Leftrightarrow \left\{ \begin{array}{l} \mathbf{u}(\mathbf{x} + L_i \mathbf{e}_i) = \mathbf{u}(\mathbf{x}) + L_i \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{e}_i \\ \boldsymbol{\sigma}(\mathbf{x} + L_i \mathbf{e}_i) \cdot \mathbf{e}_i = \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{e}_i \end{array} \right.$$

(no summation on i)



Post-processing the effective stiffness

Macroscopic strain is **prescribed!**

$$\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}$$

The corrector problem is **linear!**

There exists \mathbf{L} such that $\langle \boldsymbol{\sigma} \rangle = \mathbf{L} : \bar{\boldsymbol{\varepsilon}} = \mathbf{L} : \langle \boldsymbol{\varepsilon} \rangle \Rightarrow \mathbf{L} = \mathbf{C}^{\text{eff}}$

The homogenization workflow

- Solve corrector problem for **6 independent load cases**

$$\bar{\boldsymbol{\varepsilon}} = \text{sym}(\mathbf{e}_i \otimes \mathbf{e}_j)$$

- Find the components of the effective stiffness

$$C_{ijkl} = \langle \sigma_{ij} \rangle$$

Introducing eigenstresses

$$\left\{ \begin{array}{l} \mathbf{div} \boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma}(\mathbf{x} + L_i \mathbf{e}_i) \cdot \mathbf{e}_i = \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{e}_i \\ \boldsymbol{\varepsilon} = \mathbf{sym} \mathbf{grad} \mathbf{u} \\ \mathbf{u}(\mathbf{x} + L_i \mathbf{e}_i) = \mathbf{u}(\mathbf{x}) + L_i \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{e}_i \\ \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \end{array} \right.$$

Loading parameters

- $\bar{\boldsymbol{\varepsilon}} \in \mathcal{T}$: symmetric, second-order tensor
- $\boldsymbol{\varpi} \in \mathcal{T}(\Omega)$: symmetric, second-order tensor **field**
(with square-integrable coefficients)

Eigenstresses?

- A very cheap extension
- Useful for: thermoelasticity, poroelasticity, elastoplasticity, ...

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Displacements are of no importance

For homogenization purposes, only σ and ε matter!

The subspace of self-equilibrated stresses

$$\sigma \in \mathcal{S}(\Omega) \Leftrightarrow \begin{cases} \mathbf{div} \sigma = 0 \\ \sigma(\mathbf{x} + L_i \mathbf{e}_i) \cdot \mathbf{e}_i = \sigma(\mathbf{x}) \cdot \mathbf{e}_i \end{cases}$$

The subspace of compatible strains

$$\varepsilon \in \mathcal{E}(\Omega) \Leftrightarrow \text{there exists } \mathbf{u} \text{ such that } \begin{cases} \varepsilon = \mathbf{sym} \operatorname{grad} \mathbf{u} \\ \mathbf{u}(\mathbf{x} + L_i \mathbf{e}_i) = \mathbf{u}(\mathbf{x}) \end{cases}$$

Equivalent formulation of the corrector problem

$$\text{Find } \sigma \in \mathcal{S}(\Omega) \text{ and } \varepsilon \in \bar{\varepsilon} + \mathcal{E}(\Omega) \text{ such that } \sigma = \mathbf{C} : \varepsilon + \boldsymbol{\omega} \quad (\text{v1})$$

$$\text{Find } \varepsilon \in \bar{\varepsilon} + \mathcal{E}(\Omega) \text{ such that } \mathbf{C} : \varepsilon + \boldsymbol{\omega} \in \mathcal{S}(\Omega) \quad (\text{v2})$$

Abstracting the corrector problem

The abstract prestressed corrector problem

$$\mathcal{P}(\mathbf{C}, \boldsymbol{\varpi}, \bar{\boldsymbol{\varepsilon}}) \quad \left\{ \begin{array}{l} \text{Given } \bar{\boldsymbol{\varepsilon}} \in \mathcal{T} \text{ and } \boldsymbol{\varpi} \in \mathcal{T}(\Omega) \\ \text{Find } \boldsymbol{\varepsilon} \in \bar{\boldsymbol{\varepsilon}} + \mathcal{E}(\Omega) \text{ such that } \mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \in \mathcal{S}(\Omega) \end{array} \right.$$

Axioms

1. **Linearity:** $\mathcal{S}(\Omega)$ and $\mathcal{E}(\Omega)$ are vector subspaces of $\mathcal{T}(\Omega)$
2. $\mathcal{S}(\Omega)$ contains the **constant stress fields**
3. **Strain control:** for all $\boldsymbol{\varepsilon} \in \mathcal{E}(\Omega)$, $\langle \boldsymbol{\varepsilon} \rangle = 0$
4. **Hill–Mandel lemma:** $\langle \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \rangle = 0$ for all $\boldsymbol{\sigma} \in \mathcal{S}(\Omega)$ and $\boldsymbol{\varepsilon} \in \mathcal{E}(\Omega)$
5. **Well-posedness:** $\mathcal{P}(\mathbf{C}, \boldsymbol{\varpi}, \bar{\boldsymbol{\varepsilon}})$ always has a unique solution
(ellipticity condition on \mathbf{C})

The Green operator for strains

$$\mathcal{P}(\mathbf{C}, \boldsymbol{\varpi}, \bar{\boldsymbol{\varepsilon}}) \quad \left\{ \begin{array}{l} \text{Given } \bar{\boldsymbol{\varepsilon}} \in \mathcal{T} \text{ and } \boldsymbol{\varpi} \in \mathcal{T}(\Omega) \\ \text{Find } \boldsymbol{\varepsilon} \in \bar{\boldsymbol{\varepsilon}} + \mathcal{E}(\Omega) \text{ such that } \mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \in \mathcal{S}(\Omega) \end{array} \right.$$

Definition [1–3]

The Green operator Γ associated with the (**possibly heterogeneous**) material \mathbf{C} is the mapping $\Gamma: \mathcal{T}(\Omega) \rightarrow \mathcal{E}(\Omega)$ such that

$$\boldsymbol{\varepsilon} = -\Gamma(\boldsymbol{\varpi}) \text{ is the solution to } \mathcal{P}(\mathbf{C}, \boldsymbol{\varpi}, \bar{\boldsymbol{\varepsilon}} = \mathbf{0})$$

Straightforward properties

- Γ is a **linear operator**
- $\langle \Gamma(\boldsymbol{\varpi}) \rangle = \mathbf{0}$ for all $\boldsymbol{\varpi} \in \mathcal{T}(\Omega)$
- The solution to $\mathcal{P}(\mathbf{C}, \boldsymbol{\varpi}, \bar{\boldsymbol{\varepsilon}} \neq \mathbf{0})$ is $\boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} - \Gamma(\boldsymbol{\varpi})$ **when \mathbf{C} is homogeneous!**

[1] J. Korringa, *Journal of Mathematical Physics* **1973**, *14*, 509–513.

[2] R. Zeller, P. H. Dederichs, *Physica Status Solidi (B)* **1973**, *55*, 831–842.

[3] E. Kröner in *Topics in Applied Continuum Mechanics*, (Eds.: J. L. Zeman, F. Ziegler), Springer Verlag Wien, Vienna, **1974**, pp. 22–38.

Properties of the Γ operator

- $\Gamma(\boldsymbol{\sigma}) = \mathbf{0}$ for all $\boldsymbol{\sigma} \in \mathcal{S}(\Omega)$
- $\langle \boldsymbol{\varpi}_1 : \Gamma(\boldsymbol{\varpi}_2) \rangle = \langle \Gamma(\boldsymbol{\varpi}_1) : \boldsymbol{\varpi}_2 \rangle$ for all $\boldsymbol{\varpi}_1, \boldsymbol{\varpi}_2 \in \mathcal{T}(\Omega)$
- $\Gamma[\mathbf{C} : \Gamma(\boldsymbol{\varpi})] = \Gamma(\boldsymbol{\varpi})$ for all $\boldsymbol{\varpi} \in \mathcal{T}(\Omega)$

TODO: write proof

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The Lippmann–Schwinger equation (1/2)

Introduce a homogeneous reference material \mathbf{C}_0 with Green operator Γ_0

Stress-polarization

$$\boldsymbol{\tau} = \boldsymbol{\sigma} - \mathbf{C}_0 : \boldsymbol{\varepsilon} = (\mathbf{C} - \mathbf{C}_0) : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \quad \Rightarrow \quad \mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} = \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau}$$

Equivalent formulations of the corrector problem

Find $\boldsymbol{\varepsilon} \in \bar{\boldsymbol{\varepsilon}} + \mathcal{E}(\Omega)$ such that $\mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \in \mathcal{S}(\Omega)$

$$\text{Find } \begin{cases} \boldsymbol{\varepsilon} \in \bar{\boldsymbol{\varepsilon}} + \mathcal{E}(\Omega) \\ \boldsymbol{\tau} \in \mathcal{T}(\Omega) \end{cases} \quad \text{such that} \quad \begin{cases} \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau} \in \mathcal{S}(\Omega) \\ \boldsymbol{\tau} = (\mathbf{C} - \mathbf{C}_0) : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \end{cases}$$

$$\text{Find } \boldsymbol{\varepsilon}, \boldsymbol{\tau} \in \mathcal{T}(\Omega) \text{ such that } \begin{cases} \boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} - \Gamma_0(\boldsymbol{\tau}) \\ \boldsymbol{\tau} = (\mathbf{C} - \mathbf{C}_0) : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \end{cases}$$

The Lippmann–Schwinger equation (2/2)

Equivalent formulation of the corrector problem

$$\text{Find } \boldsymbol{\varepsilon}, \boldsymbol{\tau} \in \mathcal{T}(\Omega) \text{ such that } \begin{cases} \boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} - \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \\ \boldsymbol{\tau} = \boldsymbol{\sigma} - \mathbf{C}_0 : \boldsymbol{\varepsilon} = (\mathbf{C} - \mathbf{C}_0) : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \end{cases}$$

Strain-based form of LS equation [1–3]

$$\text{Find } \boldsymbol{\varepsilon} \in \mathcal{T}(\Omega) \text{ such that } \begin{cases} \boldsymbol{\varepsilon} + \boldsymbol{\Gamma}_0(\boldsymbol{\sigma} - \mathbf{C}_0 : \boldsymbol{\varepsilon}) = \bar{\boldsymbol{\varepsilon}} \\ \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon} + \boldsymbol{\varpi} \end{cases}$$

[1] J. Koringa, *Journal of Mathematical Physics* **1973**, 14, 509–513.

[2] R. Zeller, P. H. Dederichs, *Physica Status Solidi (B)* **1973**, 55, 831–842.

[3] E. Kröner in *Topics in Applied Continuum Mechanics*, (Eds.: J. L. Zeman, F. Ziegler), Springer Verlag Wien, Vienna, **1974**, pp. 22–38.

Non-linearities

To be further discussed during the week!

Non-linear elasticity [1]

Find $\boldsymbol{\varepsilon} \in \mathcal{T}(\Omega)$ such that

$$\begin{cases} \boldsymbol{\varepsilon} + \boldsymbol{\Gamma}_0(\boldsymbol{\sigma} - \mathbf{C}_0 : \boldsymbol{\varepsilon}) = \bar{\boldsymbol{\varepsilon}} \\ \boldsymbol{\sigma} = \mathcal{F}(\boldsymbol{\varepsilon}) \end{cases}$$

Generalized standard materials

Use successive linearizations *à la* Newton–Raphson [2]
or **condensed pseudo-potentials** [3, 4]

Geometric non-linearities

Similar formulation with the \mathbf{F}, \mathbf{P} (Piola I) pair [5]

- [1] H. Moulinec, P. Suquet, *Comptes rendus de l'Académie des sciences. Série II Mécanique physique chimie astronomie* **1994**, 318, 1417–1423.
- [2] L. Gélébart, R. Mondon-Cancel, *Computational Materials Science* **2013**, 77, 430–439.
- [3] N. Lahellec, P. Suquet, *Journal of the Mechanics and Physics of Solids* **2007**, 55, 1932–1963.
- [4] M. Schneider, D. Wicht, T. Böhlke, *Computational Mechanics* **2019**, 64, 1073–1095.
- [5] M. Kabel, T. Böhlke, M. Schneider, *Computational Mechanics* **2014**, 54, 1497–1514.

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LS as a fixed-point problem

Find $\boldsymbol{\varepsilon} \in \mathcal{T}(\Omega)$ such that $\boldsymbol{\varepsilon} + \boldsymbol{\Gamma}_0[(\mathbf{C} - \mathbf{C}_0) : \boldsymbol{\varepsilon}] = \bar{\boldsymbol{\varepsilon}}$

Standard linear problem

$$\begin{aligned}(I + H) \cdot x = b &\Leftrightarrow x = (I - H + H^2 - H^3 + \dots) \cdot b \\ &= b - H \cdot [b - H \cdot (b - H \dots)]\end{aligned}$$

Fixed-point iterations

$$x_0 = b \quad \text{and} \quad x_{n+1} = b - H \cdot x_n$$

Conditional convergence

Converges if $\|H\| < 1!$

The “basic” scheme [1, 2]

Fixed-point iterations for the LS equation

$$\boldsymbol{\varepsilon}_0 = \bar{\boldsymbol{\varepsilon}} \quad \text{and} \quad \begin{cases} \boldsymbol{\sigma}_n = \mathcal{F}(\boldsymbol{\varepsilon}_n) \\ \boldsymbol{\varepsilon}_{n+1} = \bar{\boldsymbol{\varepsilon}} - \Gamma_0(\boldsymbol{\sigma}_n - \mathbf{C}_0 : \boldsymbol{\varepsilon}_n) \end{cases}$$

Only conditionally convergent! [3, 4]

A classical simplification [1, 2]

$$\boldsymbol{\varepsilon}_0 = \bar{\boldsymbol{\varepsilon}} \quad \text{and} \quad \begin{cases} \boldsymbol{\sigma}_n = \mathcal{F}(\boldsymbol{\varepsilon}_n) \\ \boldsymbol{\varepsilon}_{n+1} = \boldsymbol{\varepsilon}_n - \Gamma_0(\boldsymbol{\sigma}_n) \end{cases}$$

TODO: write proof!

- [1] H. Moulinec, P. Suquet, *Comptes rendus de l'Académie des sciences. Série II Mécanique physique chimie astronomie* **1994**, 318, 1417–1423.
- [2] H. Moulinec, P. Suquet, *Computer Methods in Applied Mechanics and Engineering* **1998**, 157, 69–94.
- [3] J. C. Michel, H. Moulinec, P. Suquet, *International Journal for Numerical Methods in Engineering* **2001**, 52, 139–160.
- [4] H. Moulinec, P. Suquet, G. W. Milton, *International Journal for Numerical Methods in Engineering* **2018**, 114, 1103–1130.

Time to take a step back...

Reference material?

- For the LS equation to be of use, Γ_0 must be known
- Reference material must be homogeneous! (see next slides)

Solve first, then discretize?

- In principle, fixed-point iterations is a viable solution procedure
- But unknowns are fields that require spatial discretization

Discretize first, then solve?

- Spatial discretization (e.g. Galerkin) leads to a linear system [1, 2]
- Use any (matrix-free) linear solver [3, 4]
- Allows convergence analysis wrt discretization parameter [1, 2, 5]

[1] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, 217–220, 197–212.

[2] J. Vondřejc, J. Zeman, I. Marek, *Computers & Mathematics with Applications* **2014**, 68, 156–173.

[3] J. Zeman et al., *Journal of Computational Physics* **2010**, 229, 8065–8071.

[4] S. Brisard, L. Dormieux, *Computational Materials Science* **2010**, 49, 663–671.

[5] M. Schneider, *Mathematical Methods in the Applied Sciences* **2015**, 38, 2761–2778.

Outline of Lecture 1

- Homogenization in a nutshell
- The “corrector” problem
- Formal definition of the Green operator
- The Lippmann–Schwinger (LS) equation
- The “basic” scheme
- **Fourier series in a nutshell**
- Derivation of the periodic Green operator (homogeneous material)

Fourier series in a nutshell (1/2)

Input data is a periodic function;
output data is an infinite, discrete set of numbers

Multi-indices (tuples)

- $m = (m_1, \dots, m_d), n = (n_1, \dots, n_d)$: frequency indices
- $p = (p_1, \dots, p_d), q = (q_1, \dots, q_d)$: cell indices (pixels, voxels)

Discrete wave vectors over unit-cell $\Omega = (0, L_1) \times \dots \times (0, L_d)$

$$\mathbf{k}_n = \frac{2\pi n_1}{L_1} \mathbf{e}_1 + \dots + \frac{2\pi n_d}{L_d} \mathbf{e}_d$$

Fourier coefficients of a periodic function

$$\tilde{f}_n \stackrel{\text{def}}{=} \frac{1}{|\Omega|} \int_{\mathbf{x} \in \Omega} f(\mathbf{x}) e^{-i\mathbf{k}_n \cdot \mathbf{x}} dx_1 \dots dx_d$$

Extends to tensor fields!

Fourier series in a nutshell (2/2)

Basic properties

$$\langle \mathbf{T} \rangle = \tilde{\mathbf{T}}_0 \quad \widetilde{\mathbf{grad} \mathbf{T}}_n = \tilde{\mathbf{T}}_n \otimes i\mathbf{k}_n \quad \widetilde{\mathbf{div} \mathbf{T}}_n = \tilde{\mathbf{T}}_n \cdot i\mathbf{k}_n$$

Inversion (under mild regularity conditions)

$$f(\mathbf{x}) = \sum_{n \in \mathbb{Z}^d} \tilde{f}_n e^{i\mathbf{k}_n \cdot \mathbf{x}}$$

Plancherel theorem and Parseval's identity

$$\langle f^* g \rangle = \sum_{n \in \mathbb{Z}^d} \tilde{f}_n^* \tilde{g}_n \quad \langle |f|^2 \rangle = \sum_{n \in \mathbb{Z}^d} |\tilde{f}_n|^2$$

Circular convolution theorem

$$\widetilde{f \star g}_n = \tilde{f}_n \tilde{g}_n \quad \text{with} \quad f \star g(\mathbf{x}) \stackrel{\text{def}}{=} \frac{1}{|\Omega|} \int_{\mathbf{y} \in \Omega} f(\mathbf{x} - \mathbf{y}) g(\mathbf{y}) dy_1 \dots dy_d$$

Outline of Lecture 1

- Homogenization in a nutshell
- The “corrector” problem
- Formal definition of the Green operator
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- The “basic” scheme
- Fourier series in a nutshell
- Derivation of the periodic Green operator (homogeneous material)

What should we expect?

Γ_0 is a translation-invariant, linear operator

Integral representation of the Γ_0 linear operator

$$\boldsymbol{\varepsilon} = -\Gamma_0(\boldsymbol{\tau}) \quad \boldsymbol{\varepsilon}(\mathbf{x}) = -\frac{1}{|\Omega|} \int_{\Omega} \mathbf{Q}_0(\mathbf{x}, \mathbf{y}) : \boldsymbol{\tau}(\mathbf{y}) \, dy_1 \dots dy_d$$

Translation invariance

$$\boldsymbol{\varepsilon}(\mathbf{x}) = -\frac{1}{|\Omega|} \int_{\Omega} \mathbf{Q}_0(\mathbf{x} - \mathbf{y}) : \boldsymbol{\tau}(\mathbf{y}) \, dy_1 \dots dy_d$$

Circular convolution theorem

$$\tilde{\boldsymbol{\varepsilon}}_n = -\tilde{\mathbf{Q}}_{0,n} : \tilde{\boldsymbol{\tau}}_n$$

Note

$$\tilde{\boldsymbol{\varepsilon}}_0 = \mathbf{0} \quad \text{since} \quad \langle \boldsymbol{\varepsilon} \rangle = \mathbf{0}$$

Fourier expansion of Green operator (1/3)

Use Fourier expansions of all mechanical fields

$$\begin{Bmatrix} \mathbf{u}(\mathbf{x}) \\ \boldsymbol{\varepsilon}(\mathbf{x}) \\ \boldsymbol{\sigma}(\mathbf{x}) \\ \boldsymbol{\tau}(\mathbf{x}) \end{Bmatrix} = \sum_{n \in \mathbb{Z}^d} \begin{Bmatrix} \tilde{\mathbf{u}}_n \\ \tilde{\boldsymbol{\varepsilon}}_n \\ \tilde{\boldsymbol{\sigma}}_n \\ \tilde{\boldsymbol{\tau}}_n \end{Bmatrix} e^{i\mathbf{k}_n \cdot \mathbf{x}}$$

Fourier coefficients of the Green operator

$$\tilde{\boldsymbol{\varepsilon}}_n = -\hat{\Gamma}_0^\infty(\mathbf{k}_n) : \tilde{\boldsymbol{\tau}}_n \quad \text{with} \quad \hat{\Gamma}_0^\infty(\mathbf{k}) = \mathbf{I} : [\mathbf{k} \otimes (\mathbf{k} \cdot \mathbf{C}_0 \cdot \mathbf{k})^{-1} \otimes \mathbf{k}] : \mathbf{I}$$

$$I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$

$\hat{\Gamma}_0^\infty(\mathbf{k})$ does not depend on $\|\mathbf{k}\|$!

Fourier expansion of Green operator (2/3)

Rewrite BVP in Fourier space

$$\mathbf{div} \boldsymbol{\sigma} = \mathbf{0} \quad \longrightarrow \quad \tilde{\boldsymbol{\sigma}}_n \cdot i\mathbf{k}_n = \mathbf{0} \quad (1)$$

$$\boldsymbol{\sigma} = \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau} \quad \longrightarrow \quad \tilde{\boldsymbol{\sigma}}_n = \mathbf{C}_0 : \tilde{\boldsymbol{\varepsilon}}_n + \tilde{\boldsymbol{\tau}}_n \quad (2)$$

$$\boldsymbol{\varepsilon} = \mathbf{sym} \mathbf{grad} \mathbf{u} \quad \longrightarrow \quad \tilde{\boldsymbol{\varepsilon}}_n = \mathbf{sym}(\tilde{\mathbf{u}}_n \otimes i\mathbf{k}_n) \quad (3)$$

$(\mathbf{C}_0 = \text{const. is crucial!})$

Combine (2) and (3)

$$\left. \begin{array}{l} \tilde{\boldsymbol{\sigma}}_n = \mathbf{C}_0 : \tilde{\boldsymbol{\varepsilon}}_n + \tilde{\boldsymbol{\tau}}_n \\ \tilde{\boldsymbol{\varepsilon}}_n = \mathbf{sym}(\tilde{\mathbf{u}}_n \otimes i\mathbf{k}_n) \end{array} \right\} \Rightarrow \tilde{\boldsymbol{\sigma}}_n = (\mathbf{C}_0 \cdot i\mathbf{k}_n) \cdot \tilde{\mathbf{u}}_n + \tilde{\boldsymbol{\tau}}_n$$

Plug into (1)

$$\tilde{\boldsymbol{\sigma}}_n \cdot i\mathbf{k}_n = \mathbf{0} \Rightarrow (\mathbf{k}_n \cdot \mathbf{C}_0 \cdot \mathbf{k}_n) \cdot \tilde{\mathbf{u}}_n = i\tilde{\boldsymbol{\tau}}_n \cdot \mathbf{k}_n$$

Fourier expansion of Green operator (3/3)

General expression of displacement

$$\begin{aligned}\tilde{\mathbf{u}}_n &= i(\mathbf{k}_n \cdot \mathbf{C}_0 \cdot \mathbf{k}_n)^{-1} \cdot \tilde{\boldsymbol{\tau}}_n \cdot \mathbf{k}_n \\ &= i[(\mathbf{k}_n \cdot \mathbf{C}_0 \cdot \mathbf{k}_n)^{-1} \otimes \mathbf{k}_n] : \tilde{\boldsymbol{\tau}}_n \\ &= i[(\mathbf{k}_n \cdot \mathbf{C}_0 \cdot \mathbf{k}_n)^{-1} \otimes \mathbf{k}_n] : (\mathbf{I} : \tilde{\boldsymbol{\tau}}_n) \\ &= i\{[(\mathbf{k}_n \cdot \mathbf{C}_0 \cdot \mathbf{k}_n)^{-1} \otimes \mathbf{k}_n] : \mathbf{I}\} : \tilde{\boldsymbol{\tau}}_n\end{aligned}$$

General expression of strain

$$\tilde{\boldsymbol{\varepsilon}}_n = \mathbf{sym}(i\mathbf{k}_n \otimes \tilde{\mathbf{u}}_n) = \mathbf{I} : (i\mathbf{k}_n \otimes \tilde{\mathbf{u}}_n) = -\hat{\boldsymbol{\Gamma}}_0^\infty(\mathbf{k}_n) : \tilde{\boldsymbol{\tau}}_n$$

with

$$\hat{\boldsymbol{\Gamma}}_0^\infty(\mathbf{k}) = \mathbf{I} : [\mathbf{k} \otimes (\mathbf{k} \cdot \mathbf{C}_0 \cdot \mathbf{k})^{-1} \otimes \mathbf{k}] : \mathbf{I}$$

Isotropic reference material

$$\mathbf{C}_0 = 2\mu_0 \left(\frac{1 + \nu_0}{1 - 2\nu_0} \mathbf{J} + \mathbf{K} \right) \quad \mathbf{J} = \frac{1}{3} \boldsymbol{\delta} \otimes \boldsymbol{\delta} \quad \mathbf{K} = \mathbf{I} - \mathbf{J}$$

$$\|\mathbf{t}\| = 1 : \quad \mathbf{t} \cdot \mathbf{C}_0 \cdot \mathbf{t} = \mu_0 \left(\boldsymbol{\delta} + \frac{1}{1 - 2\nu_0} \mathbf{t} \otimes \mathbf{t} \right)$$

$$(\mathbf{t} \cdot \mathbf{C}_0 \cdot \mathbf{t})^{-1} = \frac{1}{\mu_0} \left[\boldsymbol{\delta} - \frac{1}{2(1 - \nu_0)} \mathbf{t} \otimes \mathbf{t} \right]$$

Remember that $\mathbf{p} = \mathbf{t} \otimes \mathbf{t}$ and $\mathbf{q} = \boldsymbol{\delta} - \mathbf{t} \otimes \mathbf{t}$ are orthogonal projectors

$$\mathbf{p} : \mathbf{p} = \mathbf{p} \quad \mathbf{q} : \mathbf{q} = \mathbf{q} \quad \mathbf{p} : \mathbf{q} = \mathbf{q} : \mathbf{p} = 0$$

$$\left\{ \hat{\Gamma}_{0,ijhl}^{\infty}(\mathbf{k}) = \frac{\delta_{ih} t_j t_l + \delta_{il} t_j t_h + \delta_{jh} t_i t_l + \delta_{jl} t_i t_h}{4\mu_0} - \frac{t_i t_j t_h t_l}{2\mu_0(1 - \nu_0)} \right.$$

$$\left. \mathbf{t} = \mathbf{k} / \|\mathbf{k}\| \right.$$

Applies to 3D and plane strain elasticity!

The Green operator in the real space

Integral expression of the Green operator

$$\boldsymbol{\varepsilon} = -\boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \quad \boldsymbol{\varepsilon}(\mathbf{x}) = -\frac{1}{|\Omega|} \int_{\Omega} \mathbf{Q}_0(\mathbf{x} - \mathbf{y}) : \boldsymbol{\tau}(\mathbf{y}) \, dy_1 \dots dy_d$$

Formal expression using Fourier series

$$\mathbf{Q}_0(\mathbf{r}) = \sum_{n \in \mathbb{Z}^d} \underbrace{\{\mathbf{I} : [\mathbf{k}_n \otimes (\mathbf{k}_n \cdot \mathbf{C}_0 \cdot \mathbf{k}_n)^{-1} \otimes \mathbf{k}_n] : \mathbf{I}\}}_{\hat{\boldsymbol{\Gamma}}_0^\infty(\mathbf{k}_n)} e^{i\mathbf{k}_n \cdot \mathbf{r}}$$

Formal expression using Poisson summation formula [1]

$$\mathbf{Q}_0(\mathbf{r}) = \sum_{n \in \mathbb{Z}^d} \boldsymbol{\Gamma}_0^\infty(\mathbf{r} + n_1 L_1 \mathbf{e}_1 + \dots + n_d L_d \mathbf{e}_d)$$

Non convergent series – Use at your own risk!

[1] M. Zecevic, R. A. Lebensohn, *International Journal for Numerical Methods in Engineering* **2021**, 122, 7536–7552.

Conclusion

Summary of Lecture 1

- The “corrector” problem
- Formal definition of the Green operator
- The Lippmann–Schwinger (LS) equation
- The “basic scheme” and the need for spatial discretization
- Derivation of the Green operator

In Lecture 2

Consistent Galerkin discretization of the LS equation

Thank you for your attention!

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`https://cv.archives-ouvertes.fr/sbrisard`

`https://sbrisard.github.io`



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Consistent discretization of the LS equation

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Université
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Outline of Lecture 2

- Weak form of the LS equation
- Galerkin discretization of the LS equation
- The discretized operators
- Applying the discrete Green operator
- Towards linear LS solvers
- The last piece of the jigsaw

Bibliographic notes

- The contents of this lecture is largely based on refs. [1, 2]
- I used the book by Ern and Guermond [3] for the proofs

[1] S. Brisard, L. Dormieux, *Computational Materials Science* **2010**, 49, 663–671.

[2] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, 217–220, 197–212.

[3] A. Ern, J.-L. Guermond, *Theory and Practice of Finite Elements*, Springer-Verlag, New York, **2004**.

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The stress-polarization based LS equation

Remember: equivalent formulation of the corrector problem

$$\text{Find } \boldsymbol{\varepsilon}, \boldsymbol{\tau} \in \mathcal{T}(\Omega) \text{ such that } \begin{cases} \boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} - \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \\ \boldsymbol{\tau} = \boldsymbol{\sigma} - \mathbf{C}_0 : \boldsymbol{\varepsilon} = (\mathbf{C} - \mathbf{C}_0) : \boldsymbol{\varepsilon} + \boldsymbol{\omega} \end{cases}$$

Polarization-based form of LS equation [1]

$$\text{Find } \boldsymbol{\tau} \in \mathcal{T}(\Omega) \text{ such that } (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} + \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) = \bar{\boldsymbol{\varepsilon}} + (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\omega}$$

Getting rid of eigenstresses

$$\text{Find } \boldsymbol{\tau} \in \mathcal{T}(\Omega) \text{ such that } (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} + \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) = \bar{\boldsymbol{\varepsilon}} \\ \bar{\boldsymbol{\varepsilon}} \in \mathcal{T}(\Omega) \quad \text{possibly heterogeneous!}$$

[1] J. Willis, *Journal of the Mechanics and Physics of Solids* **1977**, 25, 185–202.

Weak form of the LS equation

1. Start from strong form

Find $\boldsymbol{\tau} \in \mathcal{T}(\Omega)$ such that, for all $\mathbf{x} \in \Omega$:

$$[\mathbf{C}(\mathbf{x}) - \mathbf{C}_0(\mathbf{x})]^{-1} : \boldsymbol{\tau}(\mathbf{x}) + \boldsymbol{\Gamma}_0(\boldsymbol{\tau})(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}}(\mathbf{x})$$

2. Multiply by arbitrary test function

Find $\boldsymbol{\tau} \in \mathcal{T}(\Omega)$ such that, for all $\mathbf{x} \in \Omega$ and $\boldsymbol{\theta} \in \mathcal{T}(\Omega)$:

$$\boldsymbol{\theta}(\mathbf{x}) : [\mathbf{C}(\mathbf{x}) - \mathbf{C}_0(\mathbf{x})]^{-1} : \boldsymbol{\tau}(\mathbf{x}) + \boldsymbol{\theta}(\mathbf{x}) : \boldsymbol{\Gamma}_0(\boldsymbol{\tau})(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}}(\mathbf{x}) : \boldsymbol{\theta}(\mathbf{x})$$

3. Take volume average over Ω

Find $\boldsymbol{\tau} \in \mathcal{T}(\Omega)$ such that, for all $\boldsymbol{\theta} \in \mathcal{T}(\Omega)$

$$\langle \boldsymbol{\theta} : (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} \rangle + \langle \boldsymbol{\theta} : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \rangle = \langle \bar{\boldsymbol{\varepsilon}} : \boldsymbol{\theta} \rangle$$

Outline of Lecture 2

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Galerkin discretization of the LS equation

The initial variational problem

Find $\boldsymbol{\tau} \in \mathcal{T}(\Omega)$ such that, for all $\boldsymbol{\theta} \in \mathcal{T}(\Omega)$

$$\underbrace{\langle \boldsymbol{\theta} : (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} \rangle + \langle \boldsymbol{\theta} : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \rangle}_{a(\boldsymbol{\tau}, \boldsymbol{\theta})} = \underbrace{\langle \bar{\boldsymbol{\varepsilon}} : \boldsymbol{\theta} \rangle}_{\ell(\boldsymbol{\theta})}$$

The approximation space

- $\mathcal{T}^N(\Omega) \subset \mathcal{T}(\Omega)$: finite dimension subspace
- N : discretization parameter (to be defined)

The discretized variational problem

Find $\boldsymbol{\tau}^N \in \mathcal{T}^N(\Omega)$ such that, for all $\boldsymbol{\theta}^N \in \mathcal{T}^N(\Omega)$

$$\langle \boldsymbol{\theta}^N : (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}^N \rangle + \langle \boldsymbol{\theta}^N : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^N) \rangle = \langle \bar{\boldsymbol{\varepsilon}} : \boldsymbol{\theta}^N \rangle$$

The approximation subspace (1/2)

Discretization over a grid

- **Regular grid** of size $N = (N_1, \dots, N_d)$ over unit-cell Ω
- Grid spacing: $h_i = L_i/N_i$, total number of cells: $\mathcal{N} = N_1 \dots N_d$

Numbering of cells

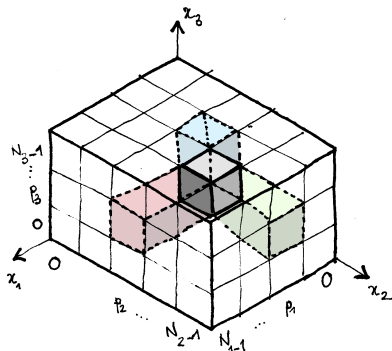
$$\mathcal{P} = \{0, \dots, N_1 - 1\} \times \dots \times \{0, \dots, N_d - 1\}$$

Cell average

$$\langle Q \rangle_p \stackrel{\text{def}}{=} \frac{1}{h_1 \dots h_d} \int_{\mathbf{x} \in \Omega_p} Q(\mathbf{x}) \, dx_1 \dots dx_d$$

Average over whole unit-cell

$$\langle Q \rangle = \frac{1}{\mathcal{N}} \sum_{p \in \mathcal{P}} \langle Q \rangle_p$$



The approximation subspace (2/2)

Definition of $\mathcal{T}^N(\Omega)$

Space of **cell-wise constant**, 2^{nd} -order, symmetric tensors

$$\text{number of dofs} = \dim \mathcal{T}^N = \frac{1}{2} \mathcal{N} d(d+1)$$

Trial and test functions defined by their cell-values

$$\boldsymbol{\tau}^N(\mathbf{x}) = \boldsymbol{\tau}_p^N \quad \text{and} \quad \boldsymbol{\theta}^N(\mathbf{x}) = \boldsymbol{\theta}_p^N \quad (\mathbf{x} \in \Omega_p)$$

Cell-averages of trial and test functions

$$\langle \boldsymbol{\tau}^N \rangle_p = \boldsymbol{\tau}_p^N \quad \text{and} \quad \langle \boldsymbol{\theta}^N \rangle_p = \boldsymbol{\theta}_p^N$$

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- The last piece of the jigsaw

Evaluating ℓ over $\mathcal{T}^N(\Omega)$

$$\ell(\boldsymbol{\theta}) = \langle \bar{\boldsymbol{\varepsilon}} : \boldsymbol{\theta} \rangle$$

$$\ell(\boldsymbol{\theta}^N) = \frac{1}{\mathcal{N}} \sum_{p \in \mathcal{P}} \langle \boldsymbol{\theta}^N : \bar{\boldsymbol{\varepsilon}} \rangle_p = \frac{1}{\mathcal{N}} \sum_{p \in \mathcal{P}} \boldsymbol{\theta}_p^N : \langle \bar{\boldsymbol{\varepsilon}} \rangle_p = \frac{1}{\mathcal{N}} \sum_{p \in \mathcal{P}} \boldsymbol{\theta}_p^N : \bar{\boldsymbol{\varepsilon}}_p^N$$

$$\bar{\boldsymbol{\varepsilon}}_p^N \stackrel{\text{def}}{=} \langle \bar{\boldsymbol{\varepsilon}} \rangle_p = \bar{\boldsymbol{\varepsilon}} + \langle (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\omega} \rangle_p$$

$\bar{\boldsymbol{\varepsilon}}^N$ can be seen as a cell-wise constant tensor field!

$$\ell(\boldsymbol{\theta}^N) = \langle \bar{\boldsymbol{\varepsilon}}^N : \boldsymbol{\theta}^N \rangle$$

Evaluating a over $\mathcal{T}^N(\Omega)$ (1/3)

$$a(\boldsymbol{\tau}, \boldsymbol{\theta}) = \langle \boldsymbol{\theta} : (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} \rangle + \langle \boldsymbol{\theta} : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \rangle$$

$$\begin{aligned} \langle \boldsymbol{\theta}^N : (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}^N \rangle &= \frac{1}{\mathcal{N}} \sum_{p \in \mathcal{P}} \langle \boldsymbol{\theta}^N : (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}^N \rangle_p \\ &= \frac{1}{\mathcal{N}} \sum_{p \in \mathcal{P}} \boldsymbol{\theta}_p^N : \langle (\mathbf{C} - \mathbf{C}_0)^{-1} \rangle_p : \boldsymbol{\tau}_p^N \\ &= \frac{1}{\mathcal{N}} \sum_{p \in \mathcal{P}} \boldsymbol{\theta}_p^N : (\mathbf{C}_p^N - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}_p^N \end{aligned}$$

$$\mathbf{C}_p^N \stackrel{\text{def}}{=} \mathbf{C}_0 + [\langle (\mathbf{C} - \mathbf{C}_0)^{-1} \rangle_p]^{-1}$$

$$\langle \boldsymbol{\theta}^N : (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}^N \rangle = \langle \boldsymbol{\theta}^N : (\mathbf{C}^N - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}^N \rangle$$

Evaluating a over $\mathcal{T}^N(\Omega)$ (2/3)

$$a(\boldsymbol{\tau}, \boldsymbol{\theta}) = \langle \boldsymbol{\theta} : (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} \rangle + \langle \boldsymbol{\theta} : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}) \rangle$$

$$\langle \boldsymbol{\theta}^N : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^N) \rangle = \frac{1}{\mathcal{N}} \sum_{p \in \mathcal{P}} \langle \boldsymbol{\theta}^N : \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^N) \rangle_p = \frac{1}{\mathcal{N}} \sum_{p \in \mathcal{P}} \boldsymbol{\theta}_p^N : \langle \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^N) \rangle_p$$

Introducing the discrete Green operator

- Let $\boldsymbol{\eta}_p^N = \langle \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^N) \rangle_p$: cell-values of $\boldsymbol{\eta}^N \in \mathcal{T}^N(\Omega)$
- The mapping $\boldsymbol{\tau}^N \mapsto \boldsymbol{\eta}^N$ is an **endomorphism** over $\mathcal{T}^N(\Omega)$
- This endomorphism is the **discrete Green operator** $\boldsymbol{\Gamma}_0^N$

Evaluating a over $\mathcal{T}^N(\Omega)$ (3/3)

Formal definition of the discrete Green operator

$$\Gamma_0^N : \begin{cases} \mathcal{T}^N(\Omega) \longrightarrow \mathcal{T}^N(\Omega) \\ \boldsymbol{\tau}^N \mapsto \boldsymbol{\eta}^N \end{cases} \quad \text{such that} \quad \boldsymbol{\eta}_p^N = \langle \Gamma_0(\boldsymbol{\tau}^N) \rangle_p$$

Cell-average of (the opposite of) the strain induced by a cell-wise constant eigenstress

Going back to the bilinear form

$$\begin{aligned} \langle \boldsymbol{\theta}^N : \Gamma_0(\boldsymbol{\tau}^N) \rangle &= \frac{1}{\mathcal{N}} \sum_{p \in \mathcal{P}} \boldsymbol{\theta}_p^N : \langle \Gamma_0(\boldsymbol{\tau}^N) \rangle_p = \frac{1}{\mathcal{N}} \sum_{p \in \mathcal{P}} \boldsymbol{\theta}_p^N : \boldsymbol{\eta}_p^N \\ &= \frac{1}{\mathcal{N}} \sum_{p \in \mathcal{P}} \langle \boldsymbol{\theta}^N : \boldsymbol{\eta}^N \rangle_p = \langle \boldsymbol{\theta}^N : \boldsymbol{\eta}^N \rangle = \langle \boldsymbol{\theta}^N : \Gamma_0^N(\boldsymbol{\eta}^N) \rangle \end{aligned}$$

The discrete LS equation

Exact evaluation of the linear and bilinear forms

$$\begin{aligned}\ell(\boldsymbol{\theta}^N) &= \langle \bar{\boldsymbol{\varepsilon}}^N : \boldsymbol{\theta}^N \rangle \\ a(\boldsymbol{\tau}^N, \boldsymbol{\theta}^N) &= \langle \boldsymbol{\theta}^N : (\mathbf{C}^N - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}^N \rangle + \langle \boldsymbol{\theta}^N : \boldsymbol{\Gamma}_0^N(\boldsymbol{\eta}^N) \rangle\end{aligned}$$

Discrete variational problem

Find $\boldsymbol{\tau}^N \in \mathcal{T}^N(\Omega)$ such that, for all $\boldsymbol{\theta}^N \in \mathcal{T}^N(\Omega)$

$$\langle \boldsymbol{\theta}^N : (\mathbf{C}^N - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}^N \rangle + \langle \boldsymbol{\theta}^N : \boldsymbol{\Gamma}_0^N(\boldsymbol{\eta}^N) \rangle = \langle \bar{\boldsymbol{\varepsilon}}^N : \boldsymbol{\theta}^N \rangle$$

The associated linear system

$$(\mathbf{C}^N - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}^N + \boldsymbol{\Gamma}_0^N(\boldsymbol{\tau}^N) = \bar{\boldsymbol{\varepsilon}}^N$$

Outline of Lecture 2

- Weak form of the LS equation
- Galerkin discretization of the LS equation
- The discretized operators
- **Applying the discrete Green operator**
- Towards linear LS solvers
- The last piece of the jigsaw

Announcing the Fast Fourier Transform

Formal definition of the discrete Green operator

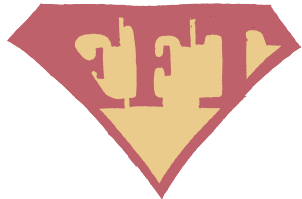
$$\Gamma_0^N : \begin{cases} \mathcal{J}^N(\Omega) \longrightarrow \mathcal{J}^N(\Omega) \\ \boldsymbol{\tau}^N \mapsto \boldsymbol{\eta}^N \end{cases} \quad \text{such that} \quad \boldsymbol{\eta}_p^N = \langle \Gamma_0(\boldsymbol{\tau}^N) \rangle_p$$

Translation-invariance

$$\langle \Gamma_0(\boldsymbol{\tau}^N) \rangle_p = \sum_{q \in \mathcal{P}} \Gamma_{0,p,q}^N : \boldsymbol{\tau}_q^N = \sum_{q \in \mathcal{P}} \Gamma_{0,p-q}^N : \boldsymbol{\tau}_q^N$$

$\Gamma_{0,p} : \boldsymbol{\tau}_0$ is the (opposite of the) average strain in cell p
induced by the eigenstress $\boldsymbol{\tau}_0$ in the $(0, \dots, 0)$ cell.

This looks like a job for
the Fast Fourier Transform!



On the discrete Fourier transform (1/2)

Input and output data are finite sets of numbers

$(x_p)_p$ and $(\hat{x}_n)_n$ with $0 \leq p_i, n_i < N_i$ and $i = 1, \dots, d$

Definition

$$\hat{x}_n \stackrel{\text{def}}{=} \sum_{p \in \mathcal{P}} x_p U_{np}^{N,*} \quad \text{with} \quad U_n^N \stackrel{\text{def}}{=} \exp\left[2i\pi\left(\frac{n_1}{N_1} + \dots + \frac{n_d}{N_d}\right)\right]$$

Output is a discrete, **periodic** series: $\hat{x}_{n+mN} = \hat{x}_n$

Implementation: fast Fourier transform (FFT)

$\mathcal{O}(N \log N)$ rather than $\mathcal{O}(N^2)$

Note

$\begin{cases} n + p \\ np \end{cases}$ should be understood as the tuple $\begin{cases} (n_1 + p_1, \dots, n_d + p_d) \\ (n_1 p_1, \dots, n_d p_d) \end{cases}$

On the discrete Fourier transform (2/2)

Inversion

$$x_p = \frac{1}{\mathcal{N}} \sum_{n \in \mathcal{P}} \hat{x}_n U_{np}^{\mathcal{N}}$$

Input can also be seen as a discrete,
periodic series ($x_{p+qN} \stackrel{\text{def}}{=} x_p$).

Plancherel theorem

$$\sum_{p \in \mathcal{P}} x_p^* y_p = \frac{1}{\mathcal{N}} \sum_{n \in \mathcal{P}} \hat{x}_n^* \hat{y}_n$$

Circular convolution theorem

$$\widehat{x \star y}_n = \hat{x}_n \hat{y}_n \quad \text{with} \quad (x \star y)_p \stackrel{\text{def}}{=} \sum_{q \in \mathcal{P}} x_{p-q} y_q$$

DFTs and the discrete Green operator

Definition of the discrete Green operator

$$\boldsymbol{\eta}^N = \boldsymbol{\Gamma}_0^N(\boldsymbol{\tau}^N) \quad \text{such that} \quad \eta_p^N = \langle \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^N) \rangle_p$$

Translation-invariant expression

$$\langle \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^N) \rangle_p = \sum_{q \in \mathcal{P}} \boldsymbol{\Gamma}_{0,p-q}^N : \boldsymbol{\tau}_q^N$$

Introduce DFT

$$\hat{\boldsymbol{\Gamma}}_{0,n}^N = \text{DFT}_n(\boldsymbol{\Gamma}_{0,\bullet}^N)$$

Use circular convolution theorem

$$\boldsymbol{\eta}^N = \text{DFT}^{-1}(\hat{\boldsymbol{\Gamma}}_0^N : \hat{\boldsymbol{\tau}}^N) = \text{DFT}^{-1}[\hat{\boldsymbol{\Gamma}}_0^N : \text{DFT}(\boldsymbol{\tau}^N)]$$

Note that we still don't know the $\hat{\boldsymbol{\Gamma}}_{0,\bullet}^N$!!!

Pseudo-implementation (1/2)

```
class DiscreteGreenOperator:
    def __init__(self, mu0, nu0, grid_shape):
        self.mu0 = mu0 # Elastic constants of
        self.nu0 = nu0 # reference material
        self.C0 = ... # Stiffness as a matrix
        self.grid_shape = grid_shape
        self.dim = len(grid_shape)
        self.spatial_axes = tuple(range(self.dim))

    def cell_indices(self):
        ranges = map(range, self.spatial_axes)
        return itertools.product(*ranges)

# ... To be continued...
```

Pseudo-implementation (2/2)

```
class DiscreteGreenOperator:
    # ... Continued...

    def fourier_mode(self, n):
        # Return n-th Fourier mode as a matrix
        #
        # !!! WE STILL NEED TO DERIVE THESE GUYS !!!
        #

    def apply(self, tau):
        tau_hat = np.fftn(tau, axes=self.spatial_axes)
        eta_hat = np.empty_like(tau_hat)
        for n in self.cell_indices():
            eta_hat[n] = self.fourier_mode(n) @ tau_hat[n]
        return np.ifftn(eta_hat, axes=self.spatial_axes)
```

Outline of Lecture 2

- Weak form of the LS equation
- Galerkin discretization of the LS equation
- The discretized operators
- Applying the discrete Green operator
- Towards linear LS solvers
- The last piece of the jigsaw

What we have shown so far

The discretized LS equation

$$(\mathbf{C}^N - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}^N + \boldsymbol{\Gamma}_0^N(\boldsymbol{\tau}^N) = \bar{\boldsymbol{\epsilon}}^N$$

$$\bar{\boldsymbol{\epsilon}}_p^N = \bar{\boldsymbol{\epsilon}} + \langle (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\omega} \rangle_p$$

$$\mathbf{C}_p^N = \mathbf{C}_0 + [\langle (\mathbf{C} - \mathbf{C}_0)^{-1} \rangle_p]^{-1}$$

$$\boldsymbol{\Gamma}_0^N(\boldsymbol{\tau}^N) = \text{DFT}^{-1}[\hat{\boldsymbol{\Gamma}}_0^N : \text{DFT}(\boldsymbol{\tau}^N)]$$

Notes

- Convergence wrt grid-size can be proved (using rudimentary FE tools!)
- This linear system must be implemented!

The Kelvin–Mandel representation

2nd order, symmetric, tensors

$$[\mathbf{s}] = [s_{11}, s_{22}, s_{33}, \sqrt{2}s_{23}, \sqrt{2}s_{31}, \sqrt{2}s_{12}]^T$$

4th order tensors with minor symmetries

$$[\mathbf{T}] = \begin{bmatrix} T_{1111} & T_{1122} & T_{1133} & \sqrt{2}T_{1123} & \sqrt{2}T_{1131} & \sqrt{2}T_{1112} \\ T_{2211} & T_{2222} & T_{2233} & \sqrt{2}T_{2223} & \sqrt{2}T_{2231} & \sqrt{2}T_{2212} \\ T_{3311} & T_{3322} & T_{3333} & \sqrt{2}T_{3323} & \sqrt{2}T_{3331} & \sqrt{2}T_{3312} \\ \sqrt{2}T_{2311} & \sqrt{2}T_{2322} & \sqrt{2}T_{2333} & 2T_{2323} & 2T_{2331} & 2T_{2312} \\ \sqrt{2}T_{3111} & \sqrt{2}T_{3122} & \sqrt{2}T_{3133} & 2T_{3123} & 2T_{3131} & 2T_{3112} \\ \sqrt{2}T_{1211} & \sqrt{2}T_{1222} & \sqrt{2}T_{1233} & 2T_{1223} & 2T_{1231} & 2T_{1212} \end{bmatrix}$$

Some properties

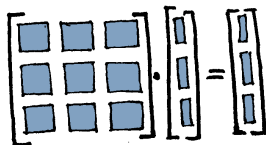
$$\mathbf{s}_1 : \mathbf{s}_2 = [\mathbf{s}_1]^T \cdot [\mathbf{s}_2] \quad [\mathbf{T} : \mathbf{s}] = [\mathbf{T}] \cdot [\mathbf{s}] \quad [\mathbf{T}^{-1}] = [\mathbf{T}]^{-1}$$

The structure of the linear system

$$(\mathbf{C}^N - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}^N + \boldsymbol{\Gamma}_0^N(\boldsymbol{\tau}^N) = \bar{\boldsymbol{\epsilon}}^N \quad \Leftrightarrow \quad A \cdot x = b$$

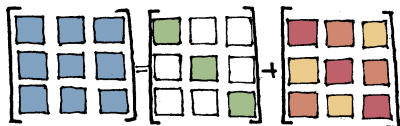
- $s = d(d + 1)/2$
- x and b are defined by $s \times 1$ blocks

$$x_p = [\boldsymbol{\tau}_p] \quad \text{and} \quad b_p = [\bar{\boldsymbol{\epsilon}}_p^N]$$



- A is defined by $s \times s$ blocks

$$A_{pq} = \underbrace{\delta_{pq}[\mathbf{C}^N - \mathbf{C}_0]^{-1}}_{\text{block-diagonal}} + \underbrace{[\boldsymbol{\Gamma}_{0,p-q}^N]}_{\text{block-circulant}}$$



**Storage would in principle be possible!
(but we don't do that)**

On iterative (matrix-free) linear solvers

$$A \cdot x = b$$

```
import scipy.sparse.linalg

class MyOperator(scipy.sparse.linalg.LinearOperator):
    def __init__(self, ...):
        pass

    def _matvec(self, x):
        # Compute  $y = Ax$ 
        return y

A = MyOperator()
b = ...
x, info = scipy.sparse.linalg.cg(A, b)
```

Pseudo-implementation (1/2)

```
class LippmannSchwingerOperator(LinearOperator):
    def __init__(self, C, Gamma0):
        self.C = np.copy(C)
        self.Gamma0 = Gamma0
        dim = Gamma0.dim
        sym = (dim * (dim + 1)) // 2
        self.tau_shape = Gamma0.grid_shape + (sym,)

    # ... To be continued...
```

Pseudo-implementation (2/2)

```
class LippmannSchwingerOperator(LinearOperator):
    # ... Continued...

    def polarization_to_strain(self, tau):
        eta = np.empty_like(tau)
        C0 = self.Gamma0.C0
        for p in self.Gamma0.cell_indices():
            eta[p] = np.linalg.solve(self.C[p]-C0, tau[p])
        return eta

    def _matvec(self, x):
        tau = x.reshape(self.tau_shape)
        eta1 = self.polarization_to_strain(tau)
        eta2 = self.Gamma0.apply(tau)
        return eta1 + eta2
```

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Fourier coefficients of cell-wise constant functions

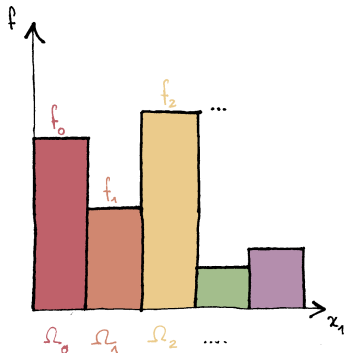
Cell-wise constant functions

$$\mathbf{x} \in \Omega_p : f(\mathbf{x}) = f_p$$

Fourier coefficients

$$\tilde{f}_n = \frac{W_n^N U_{n/2}^{N,*}}{\mathcal{N}} \hat{f}_n$$

$$W_n^N = \text{sinc} \frac{\pi n_1}{N_1} \dots \text{sinc} \frac{\pi n_d}{N_d}$$



- \tilde{f}_n : Fourier coefficients of the **periodic function** f (**infinite** series)
- \hat{f}_n : discrete Fourier transform of the **cell values** f_p (**finite** series)

Cell-averages in Fourier space

Let f be *any* Ω -periodic function.

$$\langle f \rangle_p = \sum_{n \in \mathcal{P}} \left[\sum_{m \in \mathbb{Z}^d} (-1)^m W_{n+mN}^N \tilde{f}_{n+mN} \right] U_{n(p+1/2)}^N$$

Let g be a cell-wise constant function. From Plancherel's theorem

$$\langle f g^* \rangle = \sum_{n \in \mathbb{Z}^d} \tilde{f}_n \tilde{g}_n^* = \frac{1}{N} \sum_{n \in \mathbb{Z}^d} W_n^N U_{n/2}^N \tilde{f}_n \hat{g}_n^* = \frac{1}{N} \sum_{n \in \mathcal{P}} \sum_{m \in \mathbb{Z}^d} W_{n+mN}^N \underbrace{U_{(n+mN)/2}^N}_{=(-1)^m U_{n/2}^N} \tilde{f}_{n+mN} \underbrace{\hat{g}_{n+mN}^*}_{=\hat{g}_n^*}$$

Therefore

$$\frac{1}{h_1 \dots h_d} \int_{\Omega} f g^* = \sum_{n \in \mathcal{P}} \left(\sum_{m \in \mathbb{Z}^d} (-1)^m W_{n+mN} \tilde{f}_{n+mN} \right) \hat{g}_n^* U_{n/2}^N$$

Let g be the indicator function of Ω_p ($p \in \mathcal{P}$): $g_q = \delta_{pq}$. Then

$$\hat{g}_n = \sum_{q \in \mathcal{P}} \delta_{pq} U_{nq}^{N*} = U_{np}^{N*}$$

Expression of the discrete Green op. (1/2)

Remember expression of **continuous** Green operator

$$\Gamma_0(\boldsymbol{\tau})(\mathbf{x}) = \sum_{n \in \mathbb{Z}^d} \tilde{\Gamma}_0(\mathbf{k}_n) : \tilde{\boldsymbol{\tau}}_n e^{i\mathbf{k}_n \cdot \mathbf{x}}$$

Remember definition of **discrete** Green operator

$$\boldsymbol{\tau}^N \in \mathcal{T}^N(\Omega) \mapsto \boldsymbol{\eta}^N = \Gamma_0^N(\boldsymbol{\tau}^N) \in \mathcal{T}^N(\Omega) \quad \text{such that} \quad \boldsymbol{\eta}_p^N = \langle \Gamma_0(\boldsymbol{\tau}^N) \rangle_p$$

Average strain induced by cell-wise constant eigenstress

$$\tilde{\boldsymbol{\eta}}_n = \tilde{\Gamma}_0(\mathbf{k}_n) : \tilde{\boldsymbol{\tau}}_n^N = \frac{W_n^N U_{n/2}^{N,*}}{\mathcal{N}} \tilde{\Gamma}_0(\mathbf{k}_n) : \hat{\boldsymbol{\tau}}_n^N \quad \text{with} \quad \boldsymbol{\eta} = \Gamma_0(\boldsymbol{\tau}^N)$$

$$\langle \boldsymbol{\eta} \rangle_p = \frac{1}{\mathcal{N}} \sum_{n \in \mathcal{P}} \left[\sum_{m \in \mathbb{Z}^d} (W_{n+mN}^N)^2 \tilde{\Gamma}_0(\mathbf{k}_{n+mN}) : \underbrace{\hat{\boldsymbol{\tau}}_{n+mN}^N}_{=\hat{\boldsymbol{\tau}}_n^N} \right] U_{np}^N$$

Expression of the discrete Green op. (2/2)

What we have shown so far

$$\langle \Gamma_0(\boldsymbol{\tau}^N) \rangle_p = \frac{1}{\mathcal{N}} \sum_{n \in \mathcal{P}} \left[\sum_{m \in \mathbb{Z}^d} (W_{n+mN}^N)^2 \hat{\Gamma}_0^\infty(\mathbf{k}_{n+mN}) \right] : \hat{\boldsymbol{\tau}}_n^N U_{np}^N$$

Introduce the following quantity

$$\hat{\Gamma}_{0,n}^N = \sum_{m \in \mathbb{Z}^d} (W_{n+mN}^N)^2 \hat{\Gamma}_0^\infty(\mathbf{k}_{n+mN})$$

Then

$$\langle \Gamma_0(\boldsymbol{\tau}) \rangle_p = \frac{1}{\mathcal{N}} \sum_{n \in \mathcal{P}} \hat{\Gamma}_{0,n}^N : \hat{\boldsymbol{\tau}}_n^N U_{np}^N$$

Recognize an inverse DFT

$$\Gamma_0^N(\boldsymbol{\tau}^N) = \text{DFT}^{-1}(\hat{\Gamma}_0^N : \hat{\boldsymbol{\tau}}^N)$$

Conclusion

Summary of Lecture 2

- Galerkin discretization of the LS equation
- The **consistent** discretized operators
- Using the FFT to apply the discrete Green operator
- Using matrix-free solvers

$$\hat{\Gamma}_{0,n}^N = \sum_{m \in \mathbb{Z}^d} (W_{n+mN}^N)^2 \hat{\Gamma}_0^\infty(\mathbf{k}_{n+mN})$$

Conclusion

- I must confess something...
- In lecture 3: asymptotically consistent discretizations (aka “variational crimes”)

Thank you for your attention!

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`https://cv.archives-ouvertes.fr/sbrisard`

`https://sbrisard.github.io`



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Asymptotically consistent discretizations of the LS equation

Sébastien Brisard

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In the previous episode...

The discretized LS equation

$$(\mathbf{C}^N - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}^N + \boldsymbol{\Gamma}_0^N(\boldsymbol{\tau}^N) = \bar{\boldsymbol{\epsilon}}^N$$

Exact discretization of the operators

$$\bar{\boldsymbol{\epsilon}}_p^N = \bar{\boldsymbol{\epsilon}} + \langle (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\omega} \rangle_p \quad \boldsymbol{\Gamma}_0^N(\boldsymbol{\tau}^N) = \text{DFT}^{-1}[\hat{\boldsymbol{\Gamma}}_0^N : \text{DFT}(\boldsymbol{\tau}^N)]$$

$$\mathbf{C}_p^N = \mathbf{C}_0 + [\langle (\mathbf{C} - \mathbf{C}_0)^{-1} \rangle_p]^{-1} \quad \hat{\boldsymbol{\Gamma}}_{0,n}^N = \sum_{m \in \mathbb{Z}^d} (W_{n+mN}^N)^2 \hat{\boldsymbol{\Gamma}}_0^\infty(\mathbf{k}_{n+mN})$$

$$\mathbf{k}_n = \frac{2\pi n_1}{L_1} \mathbf{e}_1 + \cdots + \frac{2\pi n_d}{L_d} \mathbf{e}_d \quad W_n^N = \text{sinc} \frac{\pi n_1}{N_1} \cdots \text{sinc} \frac{\pi n_d}{N_d}$$

Outline of Lecture 3

- Consistent discretization... so what?
- On asymptotically consistent discretizations
- Asymptotically consistent discretizations of the microstructure
- Asymptotically consistent discretizations of the Green operator
- Comparison of some discretizations

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Consistent discretization... so what? (1/2)

Consistent equivalent stiffness of heterogeneous cells

$$\mathbf{C}_p^N = \mathbf{C}_0 + [\langle (\mathbf{C} - \mathbf{C}_0)^{-1} \rangle_p]^{-1}$$

“The Brisard–Dormieux mixing rule is necessary to ensure that the computed effective properties constitute a bound on the effective stiffness [1], and thus tend to increase the error.”

Kabel, Merkert, and Schneider [2]

[1] S. Brisard, L. Dormieux, *Computational Materials Science* **2010**, 49, 663–671.

[2] M. Kabel, D. Merkert, M. Schneider, *Computer Methods in Applied Mechanics and Engineering* **2015**, 294, 168–188.

Consistent discretization... so what? (2/2)

Consistent discrete Green operator

$$\hat{\Gamma}_{0,n}^N = \sum_{m \in \mathbb{Z}^d} (W_{n+mN}^N)^2 \hat{\Gamma}_0^\infty(\mathbf{k}_{n+mN})$$

$$\mathbf{k}_n = \frac{2\pi n_1}{L_1} \mathbf{e}_1 + \dots + \frac{2\pi n_d}{L_d} \mathbf{e}_d \quad W_n^N = \text{sinc} \frac{\pi n_1}{N_1} \dots \text{sinc} \frac{\pi n_d}{N_d}$$

“The second disadvantage of the discretization concerns the practical computation of the operator Γ_0^N . Although explicit expressions for the Fourier coefficients of the operator Γ_0^N are available, **the involved series converges rather slowly** in three spatial dimensions [1].”

Schneider [2]

[1] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, 217–220, 197–212.

[2] M. Schneider, *Acta Mechanica* **2021**, 232, 2051–2100.

These are fair comments!

Looking back at the history

- “FFT-based methods” [1, 2] predate the Galerkin setting [3]!
- It all started with the derivation of rigorous **bounds** [4, 5]
- “What if the reference material is not stiffer or softer than all phases?”
- The Galerkin setting allowed to prove convergence (w.r.t. grid-size) for **any** reference material!
- General setting can be extended to **any** flavour of “FFT-based method”: asymptotically consistent discretizations [6]

- [1] H. Moulinec, P. Suquet, *Comptes rendus de l'Académie des sciences. Série II Mécanique physique chimie astronomie* **1994**, 318, 1417–1423.
- [2] H. Moulinec, P. Suquet, *Computer Methods in Applied Mechanics and Engineering* **1998**, 157, 69–94.
- [3] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, 217–220, 197–212.
- [4] Z. Hashin, S. Shtrikman, *Journal of the Mechanics and Physics of Solids* **1962**, 10, 335–342.
- [5] S. Brisard, L. Dormieux, *Computational Materials Science* **2010**, 49, 663–671.
- [6] A. Ern, J.-L. Guermond, *Theory and Practice of Finite Elements*, Springer-Verlag, New York, **2004**.

Outline of Lecture 3

- Consistent discretization... so what?
- **On asymptotically consistent discretizations**
- Asymptotically consistent discretizations of the microstructure
- Asymptotically consistent discretizations of the Green operator
- Comparison of some discretizations

What is a variational crime?

The initial problem

Find $u \in V$ such that, for all $v \in V$: $a(u, v) = \ell(v)$

Exhaustive exploration of V is not possible!

Consistent discretization

Find $u^h \in V^h$ such that, for all $v^h \in V^h$: $a(u^h, v^h) = \ell(v^h)$

$V^h \subset V$ and $\dim V^h < \infty$: **exhaustive exploration is possible!**

Exact evaluation of the bilinear and linear forms!

Asymptotically consistent discretization

Find $u^h \in V^h$ such that, for all $v^h \in V^h$: $a^h(u^h, v^h) = \ell^h(v^h)$

Approximations of linear and bilinear forms must be asymptotically consistent [1]

[1] A. Ern, J.-L. Guermond, *Theory and Practice of Finite Elements*, Springer-Verlag, New York, 2004.

We are all criminals

Examples of variational crimes (FEM)

- The bilinear form

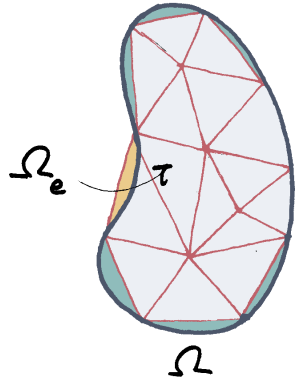
$$a(\mathbf{u}, \mathbf{v}) = \int_{\Omega} \boldsymbol{\epsilon}(\mathbf{u}) : \mathbf{C} : \boldsymbol{\epsilon}(\mathbf{v})$$

- Geometry

$$\bigcup_e \Omega_e \neq \Omega$$

- Quadrature

$$\int_{\Omega_e} \boldsymbol{\epsilon}(\mathbf{u}) : \mathbf{C} : \boldsymbol{\epsilon}(\mathbf{v}) \simeq \sum_g w_g \boldsymbol{\epsilon}(\mathbf{u})(\mathbf{x}_g) : \mathbf{C}(\mathbf{x}_g) : \boldsymbol{\epsilon}(\mathbf{v})(\mathbf{x}_g)$$



Non-consistent vs. asymptotically consistent discretizations

- Additional error induced by lack of consistency must be of the same order as the inherent discretization error!
- See ref. [1] for a mathematical definition!
- Owing to the framework set in ref. [2], asymptotic consistency is the most important property you need to ensure to prove convergence (wrt grid-size) of your new fancy discretization scheme!

[1] A. Ern, J.-L. Guermond, *Theory and Practice of Finite Elements*, Springer-Verlag, New York, **2004**.

[2] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, 217–220, 197–212.

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Handling heterogeneous cells (1/2)

Consistent mixing rule [1, 2]

$$\mathbf{C}_p^N = \mathbf{C}_0 + \left[\langle (\mathbf{C} - \mathbf{C}_0)^{-1} \rangle_p \right]^{-1}$$

This rule is sub-optimal! [3]

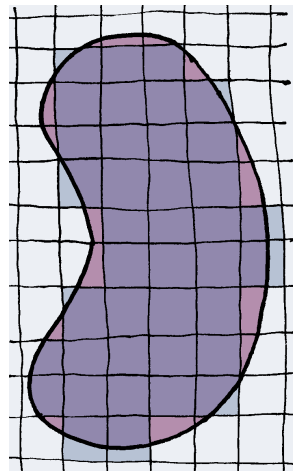
Alternative, non-consistent rules

- “Black-or-white”

$$\mathbf{C}_p^N = \mathbf{C}(\mathbf{x}_p) = \text{stiffness at cell center}$$

- Voigt, Reuss [4, 3]

These rule omit information on local orientation of the interface!

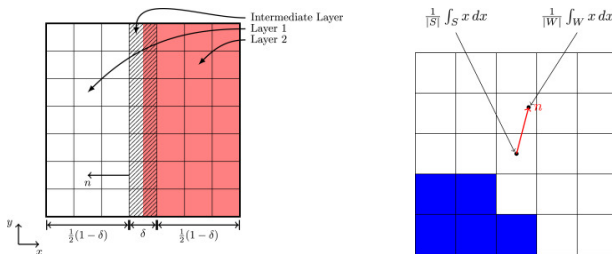


- [1] S. Brisard, L. Dormieux, *Computational Materials Science* **2010**, 49, 663–671.
- [2] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, 217–220, 197–212.
- [3] M. Kabel, D. Merkert, M. Schneider, *Computer Methods in Applied Mechanics and Engineering* **2015**, 294, 168–188.
- [4] J. Sanahuja, C. Toulemonde, *Cement and Concrete Research* **2011**, 41, 1320–1329.

Handling heterogeneous cells (2/2)

Laminate approximation [1]

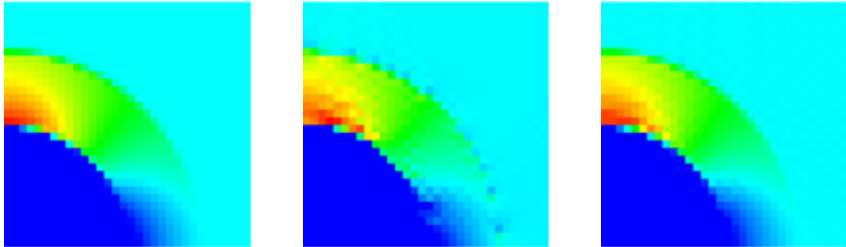
- Require sub-voxel microstructural information
- Approximate local normal
- Note: slightly different definition of consistency in this paper



Reproduced from [1]

[1] M. Kabel, D. Merkert, M. Schneider, *Computer Methods in Applied Mechanics and Engineering* **2015**, 294, 168–188.

Mixing rules in action



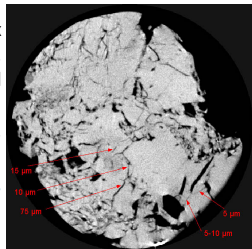
Analytical solution (left), black-or-white rule (middle), laminate rule (right) — Reproduced from [1]

[1] M. Kabel, D. Merkert, M. Schneider, *Computer Methods in Applied Mechanics and Engineering* **2015**, 294, 168–188.

On the partial volume effect

100 μm slice through fractured limestone from the lower Ismay member of the Paradox Formation. Scan field of view is 21.5 mm, and individual pixels are 42 μm on a side. After scanning the entire volume, the sample was cut and fractures were measured in thin section. Fractures are visible despite being considerably thinner than the pixel width, because of partial volume effects. Sample and measurements courtesy of Dr. Brenda Kirkland, University of Texas at Austin.

(Reproduced from <https://www.ctlab.geo.utexas.edu/about-ct/artifacts-and-partial-volume-effects/>)



**“Gray” voxels, even in two-phase (black and white) materials!
Mechanical properties?**

Assigning stiffness to gray voxels

- Requires chemical composition (ill-posed problem) [1]
- Use mixing rule based on volume fraction only?
- Normal from neighbouring voxels?

[1] S. Scheiner et al., *Biomaterials* **2009**, 30, 2411–2419.

Outline of Lecture 3

- Consistent discretization... so what?
- On asymptotically consistent discretizations
- Asymptotically consistent discretizations of the microstructure
- Asymptotically consistent discretizations of the Green operator
- Comparison of some discretizations

The need for non-consistent discrete Green operators

The consistent discrete Green operator

$$\hat{\Gamma}_{0,n}^N = \sum_{m \in \mathbb{Z}^d} (W_{n+mN}^N)^2 \hat{\Gamma}_0^\infty(\mathbf{k}_{n+mN}) \quad \text{with} \quad W_n^N = \text{sinc} \frac{\pi n_1}{N_1} \cdots \text{sinc} \frac{\pi n_d}{N_d}$$

Very slow convergence!

Non-consistent discrete Green operators

- “Approximate” in some sense the consistent operator
- Must be computed efficiently
- Keep the nice, block-diagonal structure!

$$\Gamma_0^{N,\text{nc}}(\boldsymbol{\tau}^N) = \text{DFT}^{-1}[\hat{\Gamma}_0^{N,\text{nc}} : \text{DFT}(\boldsymbol{\tau}^N)]$$

A classical (though not too deep) trap... ...most of my students fall into!

When the spatial resolution is low and when the number N_j of discretization point is even, a special attention must be paid to the highest frequencies

$$\xi_j = \pm \left(\frac{N_j}{2} - 1 \right) \frac{1}{T_j}, \quad j = 1 \text{ or } 2.$$

In most FFT packages, the Fourier expansion at these frequencies consists of either $\cos(\xi_j x_j)$ or $\exp(-i\xi_j x_j)$, instead of the correct expression consisting of the two terms $\exp(-i\xi_j x_j)$ and $\exp(i\xi_j x_j)$. Therefore, even when the stress σ is correctly approached by its Fourier expansion in step a) of the algorithm (10), the result of step d) may not approach accurately the Fourier expansion of the strain ε at these particular frequencies. This is because \hat{F}^0 is neither even nor odd with respect to each individual component ξ_j . Oscillations were observed when (4) was used with relatively small values of N_j (lower than 128). This problem was fixed by using a different expression of \hat{F}^0 in algorithm (10) at these frequencies.

$$\hat{F}^0 = (\mathbf{c}^0)^{-1}.$$

In other terms, the stress σ is forced to $\mathbf{0}$ by the algorithm at these frequencies when convergence is reached.

Reproduced from Ref. [1]

[1] H. Moulinec, P. Suquet, *Computer Methods in Applied Mechanics and Engineering* **1998**, 157, 69–94.

The classical trap continued

DFT of a series of **real** numbers

$$\hat{x}_n = \hat{x}_{N-n}^*$$

Symmetry property of discrete Green operators

Discrete Green operators must map real fields onto real fields

$$\hat{\Gamma}_{0,n}^{N,nc} = \hat{\Gamma}_{0,N-n}^{N,nc,*}$$

**The consistent discrete Green operator
has this property by construction!**

The “fftfreq” function

Definition

$$Z_n^N = \begin{cases} n & \text{if } 2n < N \\ n - N & \text{if } 2n \geq N \end{cases}$$

$N=4$

n	0	1	2	3
-----	---	---	---	---

Z_n^N	0	1	-2	-1
---------	---	---	----	----

Important property

$$Z_{N-n}^N = \begin{cases} -Z_n^N & \text{if } 2n \neq N \\ Z_n^N & \text{if } 2n = N \end{cases}$$

$N=5$

n	0	1	2	3	4
-----	---	---	---	---	---

Z_n^N	0	1	2	-2	-1
---------	---	---	---	----	----

$$Z_{N-n,N} = \begin{cases} N-n & \text{if } 2(N-n) < N \\ N-n-N & \text{if } 2(N-n) \geq N \end{cases} = \begin{cases} N-n & \text{if } 2n > N \\ -n & \text{if } 2n \leq N \end{cases} = \begin{cases} -n & \text{if } 2n > N \\ -n & \text{if } 2n = N \\ -(n-N) & \text{if } 2n < N \end{cases}$$

Extension to tuples

$$N = (N_1, \dots, N_d) \text{ and } n = (n_1, \dots, n_d) : \quad Z_n^N = (Z_{n_1}^{N_1}, \dots, Z_{n_d}^{N_d})$$

Truncating high frequencies

The original discretization of Moulinec and Suquet [1, 2]

$$\hat{\mathbf{r}}_{0,n}^{N,MS} \stackrel{\text{def}}{=} \hat{\mathbf{r}}_0^\infty(\mathbf{k}_{z_n^N})$$

Symmetry property?

- If none of the n_i is equal to $2N_i$

$$\hat{\mathbf{r}}_{0,N-n}^{N,MS} = \hat{\mathbf{r}}_0^\infty(\mathbf{k}_{z_{N-n}^N}) = \hat{\mathbf{r}}_0^\infty(\mathbf{k}_{-z_n^N}) = \hat{\mathbf{r}}_0^\infty(\mathbf{k}_{-z_n^N}) = \hat{\mathbf{r}}_{0,n}^{N,MS}$$

- If all the n_i are equal to $2N_i$, then

$$\hat{\mathbf{r}}_{0,N-n}^{N,MS} = \hat{\mathbf{r}}_{0,n}^{N,MS}$$

- If some (but not all) of the n_i are equal to $2N_i$, then we are in trouble

$$\hat{\mathbf{r}}_{0,n}^{N,MS} = \mathbf{C}_0^{-1} \quad \text{or} \quad \hat{\mathbf{r}}_{0,n}^{N,MS} = \mathbf{0}$$

[1] H. Moulinec, P. Suquet, *Comptes rendus de l'Académie des sciences. Série II Mécanique physique chimie astronomie* **1994**, 318, 1417–1423.

[2] H. Moulinec, P. Suquet, *Computer Methods in Applied Mechanics and Engineering* **1998**, 157, 69–94.

Smoothly filtering out high frequencies

Using a “cosine window” [1]

$$\hat{\mathbf{r}}_{0,n}^{N,\text{BD}} = \sum_{m \in \{-1,0\}^d} (C_{n+mN}^N)^2 \hat{\mathbf{r}}_0^\infty(\mathbf{k}_{n+mN}) \quad \text{with} \quad C_n^N = \cos \frac{\pi n_1}{2N_1} \cdots \cos \frac{\pi n_d}{2N_d}$$

Symmetry property?

Yes!

Connection with band-limited discretizations

- A radically different approach
- Discretization in the Fourier space rather than the real space
- See e.g. refs [2–4]

[1] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, 217–220, 197–212.

[2] J. Zeman et al., *Journal of Computational Physics* **2010**, 229, 8065–8071.

[3] J. Vondřejc, J. Zeman, I. Marek, *Computers & Mathematics with Applications* **2014**, 68, 156–173.

[4] J. Vondřejc, J. Zeman, I. Marek, *Computer Methods in Applied Mechanics and Engineering* **2015**, 297, 258–291.

Discretization in the real space

Remember definition of discrete Green operator

$$\boldsymbol{\tau}^N \in \mathcal{T}^N(\Omega) \mapsto \boldsymbol{\eta}^N = \boldsymbol{\Gamma}_0^N(\boldsymbol{\tau}^N) \in \mathcal{T}^N(\Omega) \quad \text{such that} \quad \boldsymbol{\eta}_p^N = \langle \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^N) \rangle_p$$

$\boldsymbol{\eta}^N$ is the cell-average of $\boldsymbol{\eta} = \boldsymbol{\Gamma}_0(\boldsymbol{\tau}^N)$,
which itself solves an elasticity problem

The discrete Green operator as the solution to a BVP

$$\left\{ \begin{array}{l} \mathbf{div} \boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma} = \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau}^N \\ \boldsymbol{\varepsilon} = \mathbf{sym} \mathbf{grad} \mathbf{u} \\ \mathbf{u} \text{ is } \Omega\text{-periodic!} \end{array} \right.$$

Discretize this problem and derive explicit solution
that defines a discrete Green operator.

Finite differences and DFT (1/2)

The 1d case, forward differences

$(x_p)_{0 \leq p < N}$ is given: $\Delta^+ x_p = x_{p+1} - x_p$

$$\begin{aligned}\widehat{\Delta^+ x}_n &= \sum_p x_{p+1} \exp(-2i\pi np/N) - \hat{x}_n \\ &= \sum_p x_p \exp[-2i\pi n(p-1)/N] - \hat{x}_n \\ &= \exp(2i\pi n/N) \underbrace{\sum_p x_p \exp(-2i\pi np/N)}_{\hat{x}_n} - \hat{x}_n \\ &= [\exp(2i\pi n/N) - 1] \hat{x}_n \\ &= 2i \sin(\pi n/N) \exp(i\pi n/N) \hat{x}_n\end{aligned}$$

Finite differences and DFT (2/2)

The 1d case, forward differences

$$\widehat{\Delta^+} x_n = 2i \sin(\pi n/N) \exp(i\pi n/N) \hat{x}_n$$

The 1d case, backward differences

$$\widehat{\Delta^-} x_n = 2i \sin(\pi n/N) \exp(-i\pi n/N) \hat{x}_n$$

The multi-dimensional case

$$\widehat{\Delta_i^+} x_n = 2i \sin(\pi n_i/N_i) \exp(i\pi n_i/N_i) \hat{x}_n$$

$$\widehat{\Delta_i^-} x_n = 2i \sin(\pi n_i/N_i) \exp(-i\pi n_i/N_i) \hat{x}_n$$

The seminal work of Willot & Pellegrini [1]

Forward differences for gradients, backwards differences for divergences

$$\left\{ \begin{array}{l} \operatorname{div} \boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma} = \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau}^N \\ \boldsymbol{\varepsilon} = \mathbf{sym} \operatorname{grad} \mathbf{u} \end{array} \right. \rightarrow \left\{ \begin{array}{l} \hat{\boldsymbol{\sigma}}_n^N \cdot i\mathbf{b}_n^{N,*} = \mathbf{0} \\ \hat{\boldsymbol{\sigma}}_n^N = \mathbf{C}_0 : \hat{\boldsymbol{\varepsilon}}_n^N + \hat{\boldsymbol{\tau}}_n^N \\ \hat{\boldsymbol{\varepsilon}}_n^N = \frac{1}{2} [\hat{\mathbf{u}}_n^N \otimes (i\mathbf{b}_n^N) + (i\mathbf{b}_n^N) \otimes \hat{\mathbf{u}}_n^N] \end{array} \right.$$

$$\mathbf{b}_n^N = 2 \sin \frac{\pi n_1}{N_1} \exp \frac{i\pi n_1}{N_1} \mathbf{e}_1 + \dots + 2 \sin \frac{\pi n_d}{N_d} \exp \frac{i\pi n_d}{N_d} \mathbf{e}_d$$

see Lecture 1

$$\hat{\boldsymbol{\varepsilon}}_n^N = -\hat{\boldsymbol{\Gamma}}_{0,n}^{N,\text{WP08}} : \hat{\boldsymbol{\tau}} \quad \hat{\boldsymbol{\Gamma}}_{0,n}^{N,\text{WP08}} = \mathbf{I} : [\mathbf{b}_n^N \otimes (\mathbf{b}_n^{N,*} \cdot \mathbf{C}_0 \cdot \mathbf{b}_n^N)^{-1} \otimes \mathbf{b}_n^{N,*}] : \mathbf{I}$$

[1] F. Willot, Y.-P. Pellegrini, Fast Fourier Transform Computations and Build-up of Plastic Deformation in 2D, Elastic-Perfectly Plastic, Pixelwise Disordered Porous Media, arXiv e-print 0802.2488, 2008.

More sophisticated FD schemes (1/2)

“Rotated grids” [1]

$$\hat{\mathbf{r}}_{0,n}^{N, \text{Willot}15} = \hat{\mathbf{r}}_0^\infty(\mathbf{b}_n^N) \quad \mathbf{b}_n^N = \frac{2N_1}{L_1} \tan \frac{\pi n_1}{N_1} \mathbf{e}_1 + \dots + \frac{2N_d}{L_d} \tan \frac{\pi n_d}{N_d} \mathbf{e}_d$$

(proof of this operational formula can be found in ref. [2])

In the rest of this section, we derive a discrete scheme in 2D different from (22) and (23). In this scheme, the displacement field is evaluated at the 4 corners of the pixels and the strain and stress fields are evaluated at the centers of the pixels. We first express these fields in the 45°-rotated basis:

$$\mathbf{f}_1 = \frac{\mathbf{e}_1 + \mathbf{e}_2}{\sqrt{2}}, \quad \mathbf{f}_2 = \frac{\mathbf{e}_2 - \mathbf{e}_1}{\sqrt{2}} \quad (30)$$

by:

$$u_i = R_{ij} u_j, \quad \varepsilon_{ij} = R_{il} \varepsilon_{lj} R'_{ij}, \quad \sigma_{ij} = R_{il} \sigma_{lj} R'_{ij}, \quad R_{ij} = \frac{1 - 2\delta_{i1}\delta_{j2}}{\sqrt{2}} \quad (31)$$

where uppercase indices refer to components in the rotated grid. We discretize (1) in the rotated basis by the centered differences (see Fig. 1):

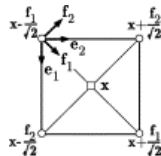
$$\sigma_{ij}(\mathbf{x}) = C_{ijkl}(\mathbf{x}) \varepsilon_{kl}(\mathbf{x}) \quad (32a)$$

$$\sigma_{11}(\mathbf{x}) - \sigma_{11}(\mathbf{x} - \sqrt{2}\mathbf{f}_1) + \sigma_{12}\left(\mathbf{x} + \frac{\mathbf{f}_2 - \mathbf{f}_1}{\sqrt{2}}\right) - \sigma_{12}\left(\mathbf{x} - \frac{\mathbf{f}_1 + \mathbf{f}_2}{\sqrt{2}}\right) = 0 \quad (32b)$$

$$\varepsilon_{KL}(\mathbf{x}) = \frac{1}{2\sqrt{2}} \left[u_K\left(\mathbf{x} + \frac{\mathbf{f}_L}{\sqrt{2}}\right) - u_K\left(\mathbf{x} - \frac{\mathbf{f}_L}{\sqrt{2}}\right) + u_L\left(\mathbf{x} + \frac{\mathbf{f}_K}{\sqrt{2}}\right) - u_L\left(\mathbf{x} - \frac{\mathbf{f}_K}{\sqrt{2}}\right) \right] \quad (32c)$$

where \mathbf{x} lie at the centers of the pixels and $\mathbf{x} \pm \mathbf{f}_i/\sqrt{2}$ lie at the corners.

(reproduced from ref. [1])

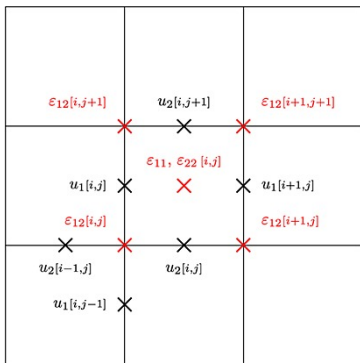


[1] F. Willot, *Comptes Rendus Mécanique* **2015**, 343, 232–245.

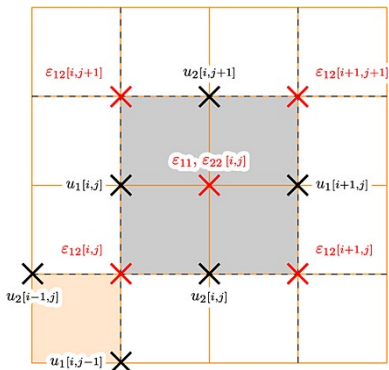
[2] S. Brisard, *International Journal for Numerical Methods in Engineering* **2017**, 109, 459–486.

More sophisticated FD schemes (2/2)

Staggered grids [1]



(a)



(b)

(reproduced from ref. [1])

[1] M. Schneider, F. Ospald, M. Kabel, *International Journal for Numerical Methods in Engineering* **2015**, n/a–n/a.

Finite element discretizations

The discrete Green operator is a standard BVP

$$\begin{cases} \operatorname{div} \boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma} = \mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\tau}^N \\ \boldsymbol{\varepsilon} = \operatorname{sym} \operatorname{grad} \mathbf{u} \end{cases} \quad \text{Use finite elements?}$$

On the resulting FE problem

- Homogeneous material
Cartesian grid } \Rightarrow homogeneous element stiffness matrix
- “Nearly” closed-form solution in Fourier space!

$$\hat{\Gamma}_{0,n}^{N,FE} = h_1 \cdots h_d \mathbf{I} : (\hat{\mathbf{b}}_n^N \otimes \hat{\mathbf{K}}_n^N \otimes \hat{\mathbf{b}}_n^{N,*}) : \mathbf{I}$$

- See refs. [1, 2]

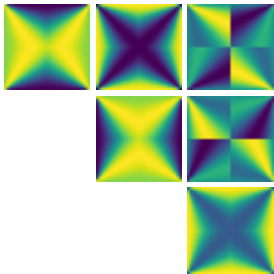
[1] M. Schneider, D. Merkert, M. Kabel, *International Journal for Numerical Methods in Engineering* **2017**, 109, 1461–1489.

[2] S. Brisard, *International Journal for Numerical Methods in Engineering* **2017**, 109, 459–486.

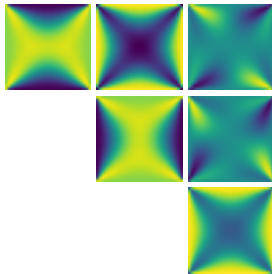
Outline of Lecture 3

- Consistent discretization... so what?
- On asymptotically consistent discretizations
- Asymptotically consistent discretizations of the microstructure
- Asymptotically consistent discretizations of the Green operator
- **Comparison of some discretizations**

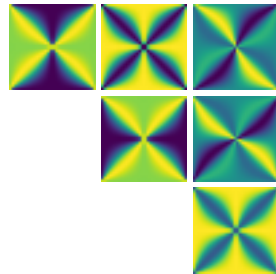
Comparison in Fourier space



Moulinec and Suquet [1]



Brisard and Dormieux [2]



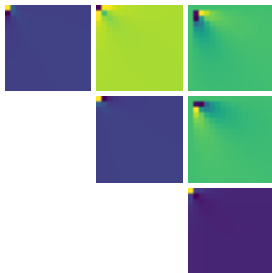
Willot [3]

- [1] H. Moulinec, P. Suquet, *Computer Methods in Applied Mechanics and Engineering* **1998**, 157, 69–94.
- [2] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, 217–220, 197–212.
- [3] F. Willot, *Comptes Rendus Mécanique* **2015**, 343, 232–245.

Comparison for impulse



Moulinec and Suquet [1]



Brisard and Dormieux [2]



Willot [3]

- [1] H. Moulinec, P. Suquet, *Computer Methods in Applied Mechanics and Engineering* **1998**, 157, 69–94.
- [2] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, 217–220, 197–212.
- [3] F. Willot, *Comptes Rendus Mécanique* **2015**, 343, 232–245.

Which operator should I use?

Moulinec and Suquet [1]

- Pros: cheap, no dependency on \mathbf{C}_0
- Cons: strong Gibbs

Willot [2] (recommended)

- Pros: quite cheap, no dependency on \mathbf{C}_0
- Cons: slight Gibbs

Brisard and Dormieux [3]

- Pros: virtually no Gibbs, “almost” delivers a bound
- Cons: costly, dependency on \mathbf{C}_0

Schneider, Merkert, and Kabel [4]

- Pros: no dependency on \mathbf{C}_0
- Cons: quite costly
- Gibbs?

[1] H. Moulinec, P. Suquet, *Computer Methods in Applied Mechanics and Engineering* **1998**, 157, 69–94.

[2] F. Willot, *Comptes Rendus Mécanique* **2015**, 343, 232–245.

[3] S. Brisard, L. Dormieux, *Computer Methods in Applied Mechanics and Engineering* **2012**, 217–220, 197–212.

[4] M. Schneider, D. Merkert, M. Kabel, *International Journal for Numerical Methods in Engineering* **2017**, 109, 1461–1489.

Conclusion (1/2)

Summary of Lecture 2

- Consistent discretization is useless (but for the sake of pedagogy)
- It paves the way to asymptotically consistent discretizations
- Many possible discretizations... pick your own!

Summary of this Block

- Homogenization requires the solution to the corrector problem
- This corrector problem can be transformed into a single integral equation: the Lippmann–Schwinger equation
- Upon Galerkin discretization, the discrete LS equation has a nice (block-diagonal plus block circulant) structure that calls for matrix-free implementation and the use of FFT
- Several strategies are possible to derive good asymptotically consistent discretizations

Conclusion (2/2)

Some personal thoughts

“FFT-based methods” = discretization scheme + a solver

A numerical code should be structured accordingly

continuous Green operators / discretization schemes / solvers

Ongoing projects

- Full rewrite of my code: `Scapin.jl`
<https://github.com/sbrisard/Scapin.jl>
- Open-book: *An introduction to Lippmann–Schwinger solvers*
<https://github.com/sbrisard/LS-intro>
(although Matti did an excellent job already, see Ref. [1])

[1] M. Schneider, *Acta Mechanica* **2021**, 232, 2051–2100.

Thank you for your attention!

`sebastien.brisard@univ-eiffel.fr`

`https://navier-lab.fr/en/equipe/brisard-sebastien`

`https://cv.archives-ouvertes.fr/sbrisard`

`https://sbrisard.github.io`

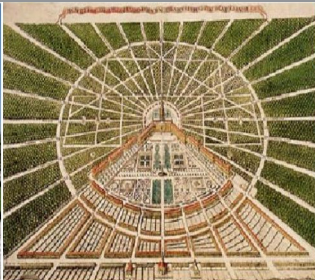


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Matti Schneider

Treating inelastic problems with the basic scheme

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



In memoriam



Prof. Dr. Wolfgang Seemann
31.3.1961 - 8.2.2022

Overview I

1. From inelasticity to elasticity

2. The nonlinear basic scheme

3. Gradient descent

Overview

1. From inelasticity to elasticity

2. The nonlinear basic scheme

3. Gradient descent

Linear elasticity

given:

- cell Q
- stiffness $\mathbb{C}(x)$
- strain $\bar{\varepsilon}$

sought:

- $u : Q \rightarrow \mathbb{R}^d$ (periodic)

$$\begin{aligned}\varepsilon &= \bar{\varepsilon} + \nabla^s u && \text{(compatibility)} \\ \sigma &= \mathbb{C} : \varepsilon && \text{(material law)} \\ \operatorname{div} \sigma &= 0 && \text{(equilibrium)}\end{aligned}$$

output:

- $\bar{\sigma} = \langle \sigma \rangle_Q$
- $\Rightarrow \bar{\sigma} = \mathbb{C}^{\text{eff}} : \bar{\varepsilon}$

Linear elasticity

given:

- cell Q
- stiffness $\mathbb{C}(x)$
- strain $\bar{\varepsilon}$

sought:

- $u : Q \rightarrow \mathbb{R}^d$ (periodic)

$$\varepsilon = \bar{\varepsilon} + \nabla^s u \quad (\text{compatibility})$$

$$\sigma = \mathbb{C} : \varepsilon \quad (\text{material law})$$

$$\operatorname{div} \sigma = 0 \quad (\text{equilibrium})$$

output:

- $\bar{\sigma} = \langle \sigma \rangle_Q$
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Linear elasticity

given:

- cell Q
- stiffness $\mathbb{C}(x)$
- strain $\bar{\varepsilon}$

sought:

- $u : Q \rightarrow \mathbb{R}^d$ (periodic)

$$\varepsilon = \bar{\varepsilon} + \nabla^s u \quad (\text{compatibility})$$

$$\sigma = \mathbb{C} : \varepsilon \quad (\text{material law})$$

$$\operatorname{div} \sigma = 0 \quad (\text{equilibrium})$$

output:

- $\bar{\sigma} = \langle \sigma \rangle_Q$
- $\Rightarrow \bar{\sigma} = \mathbb{C}^{\text{eff}} : \bar{\varepsilon}$

Linear elasticity - beyond?

given:

- cell Q
- stiffness $\mathbb{C}(x)$
- strain $\bar{\varepsilon}$

sought:

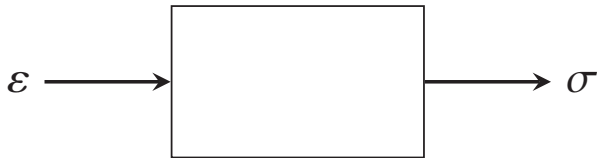
- $u : Q \rightarrow \mathbb{R}^d$ (periodic)

$$\begin{aligned}\varepsilon &= \bar{\varepsilon} + \nabla^s u && \text{(compatibility)} \\ \sigma &= \mathbb{C} : \varepsilon && \text{(material law)} \\ \operatorname{div} \sigma &= 0 && \text{(equilibrium)}\end{aligned}$$

output:

- $\bar{\sigma} = \langle \sigma \rangle_Q$
- $\Rightarrow \bar{\sigma} = \mathbb{C}^{\text{eff}} : \bar{\varepsilon}$

Inelasticity?



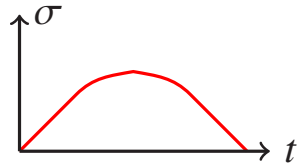
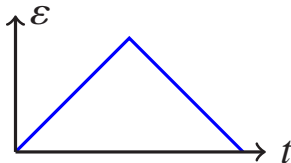
input:

- initial state
- strain history $\varepsilon : [t_{\text{start}}, t_{\text{end}}] \rightarrow \text{Sym}(d)$

output:

- stress history $\sigma : [t_{\text{start}}, t_{\text{end}}] \rightarrow \text{Sym}(d)$

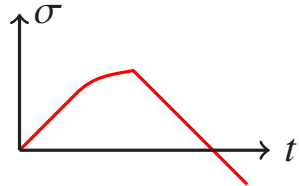
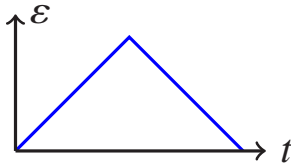
Inelasticity?



elasticity:

$$\sigma = f(\varepsilon)$$

Inelasticity?

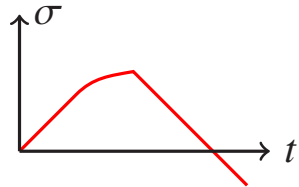
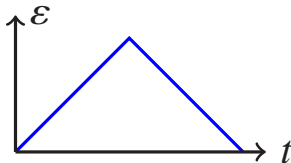


inelasticity:

$$\sigma = f(\varepsilon, z)$$

$$0 = g(\varepsilon, z, \dot{z})$$

Inelasticity?



inelasticity:

$$\sigma = f(\varepsilon, z)$$

$$0 = g(\varepsilon, z, \dot{z})$$

Example - vM plasticity

$$\begin{aligned}\sigma &= f(\varepsilon, z) \\ 0 &= g(\varepsilon, z, \dot{z})\end{aligned}$$

- $z = (\varepsilon^p, p)$
- Hooke's law

$$\sigma = \mathbb{C} : (\varepsilon - \varepsilon^p)$$

- evolution

$$\begin{aligned}\dot{\varepsilon}^p &= \dot{p} \sqrt{\frac{3}{2}} \frac{\text{dev } \sigma}{\|\text{dev } \sigma\|}, \\ \sqrt{\frac{3}{2}} \|\text{dev } \sigma\| &\leq \sigma_Y(p), \quad \dot{p} \geq 0, \quad \left(\sqrt{\frac{3}{2}} \|\text{dev } \sigma\| - \sigma_Y(p) \right) \dot{p} = 0\end{aligned}$$

Example - vM plasticity

$$\begin{aligned}\sigma &= f(\varepsilon, z) \\ 0 &= g(\varepsilon, z, \dot{z})\end{aligned}$$

- $z = (\varepsilon^p, p)$
- Hooke's law

$$\sigma = \mathbb{C} : (\varepsilon - \varepsilon^p)$$

- evolution

$$\dot{\varepsilon}^p = \dot{p} \sqrt{\frac{3}{2}} \frac{\text{dev } \sigma}{\|\text{dev } \sigma\|},$$

$$\dot{p} = \max \left(0, \dot{p} + \rho \left(\sqrt{\frac{3}{2}} \|\text{dev } \sigma\| - \sigma_Y(p) \right) \right), \quad \rho > 0$$

Linear elasticity - **beyond?**

given:

- cell Q
- **stiffness** $\mathbb{C}(x)$
- strain $\bar{\varepsilon}$

sought:

- $u : Q \rightarrow \mathbb{R}^d$ (periodic)

$$\varepsilon = \bar{\varepsilon} + \nabla^s u \quad (\text{compatibility})$$

$$\sigma = \mathbb{C} : \varepsilon \quad (\text{material law})$$

$$\operatorname{div} \sigma = 0 \quad (\text{equilibrium})$$

output:

- $\bar{\sigma} = \langle \sigma \rangle_Q$
- $\Rightarrow \bar{\sigma} = \mathbb{C}^{\text{eff}} : \bar{\varepsilon}$

Upscaling inelasticity

given:

- cell Q
- functions $f(x, \varepsilon, z)$ and $g(x, \varepsilon, z, \dot{z})$
- strain history $\bar{\varepsilon}(t)$
- initial condition $z_0(x)$

sought:

- $u : Q \times [t_{\text{start}}, t_{\text{end}}] \rightarrow \mathbb{R}^d$ (periodic) and $z : Q \times [t_{\text{start}}, t_{\text{end}}] \rightarrow \mathbb{R}^K$

$$\begin{aligned}\varepsilon &= \bar{\varepsilon} + \nabla^s u && \text{(compatibility)} \\ \sigma &= f(x, \varepsilon, z) && \text{(material law)} \\ 0 &= g(\varepsilon, z, \dot{z}), \quad z(x, t_{\text{start}}) = z_0(x) && \text{(internal evolution)} \\ \operatorname{div} \sigma &= 0 && \text{(equilibrium)}\end{aligned}$$

output:

- $\bar{\sigma}(t) = \langle \sigma(t, \cdot) \rangle_Q$

Upscaling inelasticity

given:

- cell Q
- functions $f(x, \varepsilon, z)$ and $g(x, \varepsilon, z, \dot{z})$
- strain history $\bar{\varepsilon}(t)$
- initial condition $z_0(x)$

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$$\varepsilon = \bar{\varepsilon} + \nabla^s u \quad (\text{compatibility})$$

$$\sigma = f(x, \varepsilon, z) \quad (\text{material law})$$

$$0 = g(\varepsilon, z, \dot{z}), \quad z(x, t_{\text{start}}) = z_0(x) \quad (\text{internal evolution})$$

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Upscaling inelasticity



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given:

- cell Q
- functions $f(x, \varepsilon, z)$ and $g(x, \varepsilon, z, \dot{z})$
- strain history $\bar{\varepsilon}(t)$
- initial condition $z_0(x)$
- **time discretization** $t_{\text{start}} = t_0 < t_1 < \dots < t_N = t_{\text{end}}$, e.g.,
 $\dot{z}(t_{n+1}) \approx (z_{n+1} - z_n)/(t_{n+1} - t_n)$

sought ($n \rightarrow n + 1$):

- $u_{n+1} : Q \rightarrow \mathbb{R}^d$ (periodic) and $z_{n+1} : Q \rightarrow \mathbb{R}^K$

$$0 = \operatorname{div} f(x, \bar{\varepsilon}_{n+1} + \nabla^s u_{n+1}, z_{n+1})$$

$$0 = g(\varepsilon_{n+1}, z_{n+1}, (z_{n+1} - z_n)/(t_{n+1} - t_n))$$

output:

- $\bar{\sigma}_{n+1} = \langle \sigma_{n+1} \rangle_Q$

Fix time step, drop $n + 1$

sought:

■ $u : Q \rightarrow \mathbb{R}^d$ (periodic) and $z : Q \rightarrow \mathbb{R}^K$

$$0 = \operatorname{div} f(x, \bar{\varepsilon} + \nabla^s u, z)$$

$$0 = g(\varepsilon, z, (z - z_n)/(t_{n+1} - t_n))$$

- PDE in u (d unknowns) ↗ non-local, sparse (after discretization)
- algebraic equation in z (K unknowns) ↗ local

Fix time step, drop $n + 1$

sought:

- $u : Q \rightarrow \mathbb{R}^d$ (periodic) and $z : Q \rightarrow \mathbb{R}^K$

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- PDE in u (d unknowns) ↗ non-local, sparse (after discretization)
- algebraic equation in z (K unknowns) ↗ local

Option I: solve full system

sought:

- $u : Q \rightarrow \mathbb{R}^d$ (periodic) and $z : Q \rightarrow \mathbb{R}^K$

$$0 = \operatorname{div} f(x, \bar{\varepsilon} + \nabla^s u, z)$$

$$0 = g(\varepsilon, z, (z - z_n)/(t_{n+1} - t_n))$$

- $d + K$ unknowns (at x)
- non-local, sparse (after discretization)

Option II: eliminate z

sought:

- $u : Q \rightarrow \mathbb{R}^d$ (periodic) and $z : Q \rightarrow \mathbb{R}^K$

$$0 = \operatorname{div} f(x, \bar{\varepsilon} + \nabla^s u, z)$$

$$0 = g(\varepsilon, z, (z - z_n)/(t_{n+1} - t_n))$$

- idea: write z as implicit function of ε

$$z \text{ solves } g(\varepsilon, z, (z - z_n)/(t_{n+1} - t_n)) = 0 \iff z = h_n(\varepsilon)$$

Option II: eliminate z

sought:

■ $u : Q \rightarrow \mathbb{R}^d$ (periodic) and $z : Q \rightarrow \mathbb{R}^K$

$$0 = \operatorname{div} f(x, \bar{\varepsilon} + \nabla^s u, h_n(\bar{\varepsilon} + \nabla^s u))$$

$$z = h_n(\bar{\varepsilon} + \nabla^s u)$$

- d unknowns (at x)
- non-local, sparse (after discretization)
- “static condensation”

Option II: eliminate z

sought:

- $u : Q \rightarrow \mathbb{R}^d$ (periodic) and $z : Q \rightarrow \mathbb{R}^K$

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- leads to a **pseudo-elastic** problem for u
- z obtained in post-processing
- basis of user material routines

Option II: eliminate z

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- leads to a **pseudo-elastic** problem for u
- z obtained in post-processing
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Digression Part I

- inelasticity ↗ time steps
- move from one time step to the next
- eliminate the internal variables, update later
- we are left with solving

$$\operatorname{div} S(x, \bar{\varepsilon} + \nabla^s u) = 0$$

with an **elastic** “stress function” S

$$S(x, \varepsilon) \equiv f(x, \varepsilon, h_n(\varepsilon))$$

Overview

1. From inelasticity to elasticity

2. The nonlinear basic scheme

3. Gradient descent

Linear elasticity

given:

- cell Q
- stiffness $\mathbb{C}(x)$
- strain $\bar{\varepsilon}$

sought:

- $u : Q \rightarrow \mathbb{R}^d$ (periodic)

$$\varepsilon = \bar{\varepsilon} + \nabla^s u \quad (\text{compatibility})$$

$$\sigma = \mathbb{C} : \varepsilon \quad (\text{material law})$$

$$\operatorname{div} \sigma = 0 \quad (\text{equilibrium})$$

output:

- $\bar{\sigma} = \langle \sigma \rangle_Q$
- $\Rightarrow \bar{\sigma} = \mathbb{C}^{\text{eff}} : \bar{\varepsilon}$

Non-Linear elasticity

given:

- cell Q
- stress function S
- strain $\bar{\varepsilon}$

sought:

- $u : Q \rightarrow \mathbb{R}^d$ (periodic)

$$\varepsilon = \bar{\varepsilon} + \nabla^s u \quad (\text{compatibility})$$

$$\sigma = S(x, \varepsilon) \quad (\text{material law})$$

$$\operatorname{div} \sigma = 0 \quad (\text{equilibrium})$$

output:

- $\bar{\sigma} = \langle \sigma \rangle_Q$

Lippmann-Schwinger reformulation



seek $u : Q \rightarrow \mathbb{R}^d$:

$$0 = -\operatorname{div} S(\cdot, \bar{\varepsilon} + \nabla^s u)$$

Lippmann-Schwinger reformulation

seek $u : Q \rightarrow \mathbb{R}^d$:

$$\operatorname{div} \mathbb{C}^0 : (\bar{\varepsilon} + \nabla^s u) = -\operatorname{div} \left[\mathbb{S}(\cdot, \bar{\varepsilon} + \nabla^s u) - \mathbb{C}^0 : (\bar{\varepsilon} + \nabla^s u) \right]$$

- reference material \mathbb{C}^0

Lippmann-Schwinger reformulation

seek $u : Q \rightarrow \mathbb{R}^d$:

$$\operatorname{div} \mathbb{C}^0 : \nabla^s u = -\operatorname{div} \left[\mathbb{S}(\cdot, \bar{\varepsilon} + \nabla^s u) - \mathbb{C}^0 : (\bar{\varepsilon} + \nabla^s u) \right]$$

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Lippmann-Schwinger reformulation



seek $u : Q \rightarrow \mathbb{R}^d$:

$$\operatorname{div} \mathbb{C}^0 : \nabla^s u = -\operatorname{div} \left[\mathbb{S}(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

- reference material \mathbb{C}^0
- total strain $\varepsilon = \bar{\varepsilon} + \nabla^s u$

Lippmann-Schwinger reformulation

seek $u : Q \rightarrow \mathbb{R}^d$:

$$u = -G^0 \operatorname{div} [S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon]$$

- reference material \mathbb{C}^0
- total strain $\varepsilon = \bar{\varepsilon} + \nabla^s u$
- $G^0 = (\operatorname{div} \mathbb{C}^0 : \nabla^s)^{-1}$

Lippmann-Schwinger reformulation



seek $u : Q \rightarrow \mathbb{R}^d$:

$$\nabla^s u = -\nabla^s G^0 \operatorname{div} [S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon]$$

- reference material \mathbb{C}^0
- total strain $\varepsilon = \bar{\varepsilon} + \nabla^s u$
- $G^0 = (\operatorname{div} \mathbb{C}^0 : \nabla^s)^{-1}$

Lippmann-Schwinger reformulation

seek $u : Q \rightarrow \mathbb{R}^d$:

$$\bar{\varepsilon} + \nabla^s u = \bar{\varepsilon} - \nabla^s G^0 \operatorname{div} [S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon]$$

- reference material \mathbb{C}^0
- total strain $\varepsilon = \bar{\varepsilon} + \nabla^s u$
- $G^0 = (\operatorname{div} \mathbb{C}^0 : \nabla^s)^{-1}$

Lippmann-Schwinger reformulation

seek $u : Q \rightarrow \mathbb{R}^d$:

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

- reference material \mathbb{C}^0
- total strain $\varepsilon = \bar{\varepsilon} + \nabla^s u$
- $\Gamma^0 = \nabla^s (\text{div } \mathbb{C}^0 : \nabla^s)^{-1} \text{div}$

Lippmann-Schwinger reformulation

seek $\varepsilon : Q \rightarrow \text{Sym}(d)$:

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

- reference material \mathbb{C}^0
- total strain $\varepsilon = \bar{\varepsilon} + \nabla^s u$
- $\Gamma^0 = \nabla^s (\text{div } \mathbb{C}^0 : \nabla^s)^{-1} \text{div}$

Nonlinear Lippmann-Schwinger equation



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seek $\varepsilon : Q \rightarrow \text{Sym}(d)$:

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

Nonlinear **basic scheme**

seek $\varepsilon^{k+1} : Q \rightarrow \text{Sym}(d)$:

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

Nonlinear basic scheme

seek $\varepsilon^{k+1} : Q \rightarrow \text{Sym}(d)$:

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

- conceived by Moulinec & Suquet

[H. Moulinec and P. Suquet, Comptes Rendus de l'Académie des Sciences, 1994]

[H. Moulinec and P. Suquet, CMAME, 1998]

- works with any discretization

Nonlinear basic scheme

seek $\varepsilon^{k+1} : Q \rightarrow \text{Sym}(d)$:

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

Questions:

- When does it converge?
- How to choose \mathbb{C}^0 ?

Nonlinear basic scheme

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- How to choose \mathbb{C}^0 ?

Overview

1. From inelasticity to elasticity

2. The nonlinear basic scheme

3. Gradient descent

Gradient descent

Goal:

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

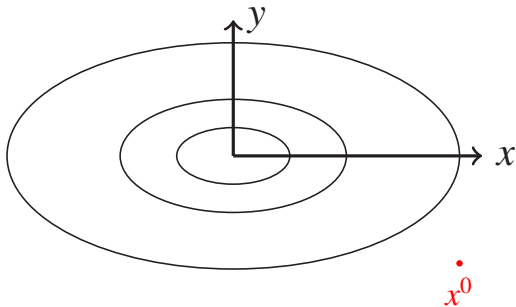
Critical point eq.:

$$\nabla f(x) \stackrel{!}{=} 0$$

Gradient descent:

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

s^k ... step size



Gradient descent

Goal:

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

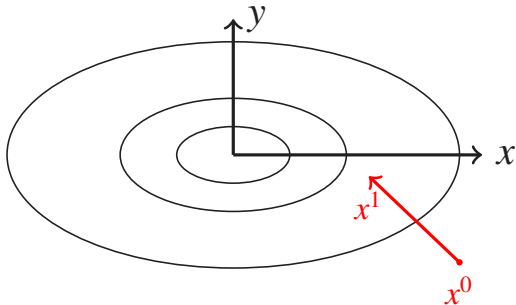
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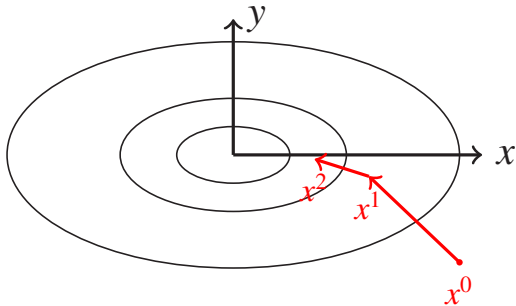
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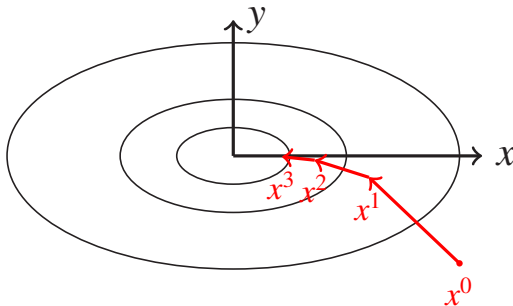
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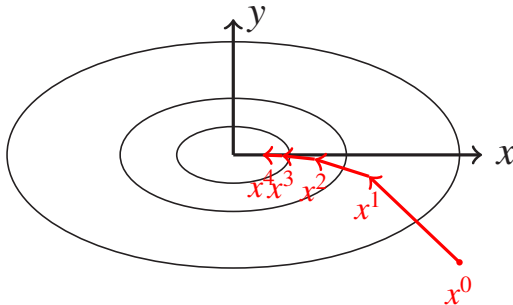
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s^k ... step size



Projected gradient descent

Goal:

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

Critical point eq.:

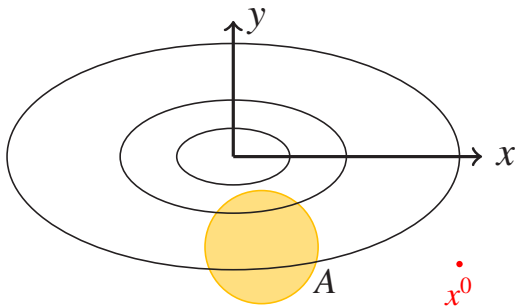
$$x \stackrel{!}{=} P_A(x - s \nabla f(x))$$

Gradient descent:

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

s^k ... step size

$$z = P_A(y) \text{ realizes } \min_{z \in A} \|y - z\|$$



Projected gradient descent

Goal:

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

Critical point eq.:

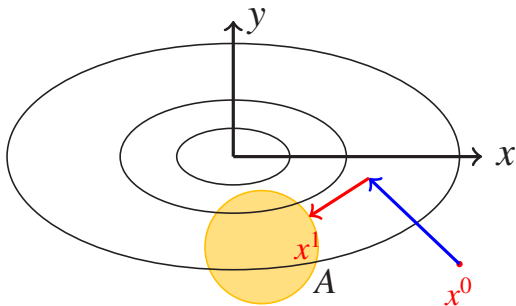
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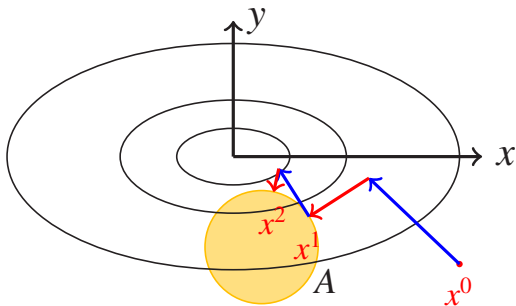
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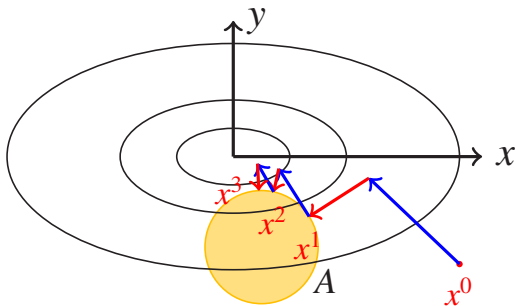
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s^k ... step size

$$z = P_A(y) \text{ realizes } \min_{z \in A} \|y - z\|$$



Application to hyperelasticity

- X contains $\varepsilon : Q \rightarrow \text{Sym}(d)$ with inner product

$$(\varepsilon_1, \varepsilon_2)_{L^2} = \langle \varepsilon_1 : \varepsilon_2 \rangle_Q$$

- $f(\varepsilon) = \langle w(\cdot, \varepsilon) \rangle_Q$ for elastic energy, $S = \partial w / \partial \varepsilon$
- constraint set

$$A = \left\{ \varepsilon \mid \varepsilon = \bar{\varepsilon} + \nabla^s u \quad \text{for some periodic } u : Q \rightarrow \mathbb{R}^d \right\}$$

- any critical point of $f(\varepsilon) \rightarrow \min_{\varepsilon \in A}$ satisfies

$$\text{div } S(\cdot, \varepsilon) = 0$$

for some u with $\varepsilon = \bar{\varepsilon} + \nabla^s u$

Projected gradient descent?

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

- $\nabla f(x) = ?$
- $P_A = ?$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \left. \frac{d}{ds} f(x + sv) \right|_{s=0} \quad \text{for all } v$$

our case:

$$f(\varepsilon) = \langle w(\cdot, \varepsilon) \rangle_Q$$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \left. \frac{d}{ds} f(x + sv) \right|_{s=0} \quad \text{for all } v$$

our case:

$$f(\varepsilon) = \frac{1}{|Q|} \int_Q w(x, \varepsilon) dx$$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \left. \frac{d}{ds} f(x + sv) \right|_{s=0} \quad \text{for all } v$$

our case:

$$f(\varepsilon + s\xi) = \frac{1}{|Q|} \int_Q w(x, \varepsilon + s\xi) dx$$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \left. \frac{d}{ds} f(x + sv) \right|_{s=0} \quad \text{for all } v$$

our case:

$$\left. \frac{d}{ds} f(\varepsilon + s\xi) \right|_{s=0} = \frac{d}{ds} \frac{1}{|Q|} \int_Q w(x, \varepsilon + s\xi) dx \Big|_{s=0}$$

Gradient?

implicit characterization:

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$$\left. \frac{d}{ds} f(\varepsilon + s\xi) \right|_{s=0} = \frac{1}{|Q|} \int_Q \frac{\partial w}{\partial \varepsilon}(x, \varepsilon) : \xi \, dx$$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \left. \frac{d}{ds} f(x + sv) \right|_{s=0} \quad \text{for all } v$$

our case:

$$(\nabla f(\varepsilon), \xi)_{L^2} = \frac{1}{|Q|} \int_Q \frac{\partial w}{\partial \varepsilon}(x, \varepsilon) : \xi \, dx$$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \left. \frac{d}{ds} f(x + sv) \right|_{s=0} \quad \text{for all } v$$

our case:

$$\frac{1}{|Q|} \int_Q \nabla f(\varepsilon) : \xi \, dx = \frac{1}{|Q|} \int_Q \frac{\partial w}{\partial \varepsilon}(x, \varepsilon) : \xi \, dx$$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \left. \frac{d}{ds} f(x + sv) \right|_{s=0} \quad \text{for all } v$$

our case:

$$\nabla f(\varepsilon) = \frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon)$$

Projector?

implicit characterization:

$$z = P_A(x) \quad \text{minimizes} \quad \|x - z\|_X^2 \quad \text{among} \quad z \in A$$

our case:

$$\xi = P_A(\varepsilon) \quad \text{minimizes} \quad \|\varepsilon - \xi\|_{L^2}^2 \quad \text{among} \quad \xi \in A$$

Projector?

implicit characterization:

$$z = P_A(x) \quad \text{minimizes} \quad \|x - z\|_X^2 \quad \text{among} \quad z \in A$$

our case:

$$\bar{\varepsilon} + \nabla^s u = P_A(\varepsilon) \quad \text{minimizes} \quad \|\varepsilon - \bar{\varepsilon} - \nabla^s u\|_{L^2}^2 \quad \text{among} \quad \bar{\varepsilon} + \nabla^s u \in A$$

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i.e.,

$$\left. \frac{d}{ds} \|\varepsilon - \bar{\varepsilon} - \nabla^s(u + sv)\|_{L^2}^2 \right|_{s=0} \stackrel{!}{=} 0 \quad \text{for all} \quad v : Q \rightarrow \mathbb{R}^d$$

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i.e.,

$$(\varepsilon - \bar{\varepsilon} - \nabla^s u, -2\nabla^s v)_{L^2} \stackrel{!}{=} 0 \quad \text{for all} \quad v : Q \rightarrow \mathbb{R}^d$$

Projector?

implicit characterization:

$$z = P_A(x) \quad \text{minimizes} \quad \|x - z\|_X^2 \quad \text{among} \quad z \in A$$

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i.e.,

$$\langle (\varepsilon - \bar{\varepsilon} - \nabla^s u) : \nabla^s v \rangle_Q \stackrel{!}{=} 0 \quad \text{for all} \quad v : Q \rightarrow \mathbb{R}^d$$

Projector?

implicit characterization:

$$z = P_A(x) \quad \text{minimizes} \quad \|x - z\|_X^2 \quad \text{among} \quad z \in A$$

our case:

$$\bar{\varepsilon} + \nabla^s u = P_A(\varepsilon) \quad \text{minimizes} \quad \|\varepsilon - \bar{\varepsilon} - \nabla^s u\|_{L^2}^2 \quad \text{among} \quad u : Q \rightarrow \mathbb{R}^d,$$

i.e.,

$$-\langle \operatorname{div} (\varepsilon - \bar{\varepsilon} - \nabla^s u) \cdot v \rangle_Q \stackrel{!}{=} 0 \quad \text{for all} \quad v : Q \rightarrow \mathbb{R}^d$$

Projector?

implicit characterization:

$$z = P_A(x) \quad \text{minimizes} \quad \|x - z\|_X^2 \quad \text{among} \quad z \in A$$

our case:

$$\bar{\varepsilon} + \nabla^s u = P_A(\varepsilon) \quad \text{minimizes} \quad \|\varepsilon - \bar{\varepsilon} - \nabla^s u\|_{L^2}^2 \quad \text{among} \quad u : Q \rightarrow \mathbb{R}^d,$$

i.e.,

$$-\operatorname{div} (\varepsilon - \bar{\varepsilon} - \nabla^s u) \stackrel{!}{=} 0$$

Projector?

implicit characterization:

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our case:

$$\bar{\varepsilon} + \nabla^s u = P_A(\varepsilon) \quad \text{minimizes} \quad \|\varepsilon - \bar{\varepsilon} - \nabla^s u\|_{L^2}^2 \quad \text{among} \quad u : Q \rightarrow \mathbb{R}^d,$$

i.e.,

$$\operatorname{div} \nabla^s u \stackrel{!}{=} \operatorname{div} (\varepsilon - \bar{\varepsilon})$$

Projector?

implicit characterization:

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i.e.,

$$\operatorname{div} \nabla^s u \stackrel{!}{=} \operatorname{div} \varepsilon$$

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our case:

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i.e.,

$$u = (\operatorname{div} \nabla^s)^{-1} \operatorname{div} \varepsilon$$

Projector?

implicit characterization:

$$z = P_A(x) \quad \text{minimizes} \quad \|x - z\|_X^2 \quad \text{among} \quad z \in A$$

our case:

$$\bar{\varepsilon} + \nabla^s (\operatorname{div} \nabla^s)^{-1} \operatorname{div} \varepsilon = P_A(\varepsilon)$$

Projector?

implicit characterization:

$$z = P_A(x) \quad \text{minimizes} \quad \|x - z\|_X^2 \quad \text{among} \quad z \in A$$

our case:

$$P_A(\varepsilon) = \bar{\varepsilon} + \Gamma : \varepsilon \quad \text{with} \quad \Gamma \equiv \nabla^s (\operatorname{div} \nabla^s)^{-1} \operatorname{div} .$$

Projected gradient descent?

$$\varepsilon^{k+1} = P_A(\varepsilon^k - s^k \nabla f(\varepsilon^k))$$

- $\nabla f(\varepsilon) = ?$
- $P_A(\varepsilon) = ?$

Projected gradient descent?



$$\varepsilon^{k+1} = P_A(\varepsilon^k - s^k \nabla f(\varepsilon^k))$$

- $\nabla f(\varepsilon) = \frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon)$
- $P_A(\varepsilon) = \bar{\varepsilon} + \Gamma : \varepsilon$ with $\Gamma \equiv \nabla^s (\operatorname{div} \nabla^s)^{-1} \operatorname{div}$

Projected gradient descent?



$$\varepsilon^{k+1} = P_A \left(\varepsilon^k - s^k \frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon^k) \right)$$

- $\nabla f(\varepsilon) = \frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon)$
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Projected gradient descent?

$$\boldsymbol{\varepsilon}^{k+1} = \bar{\boldsymbol{\varepsilon}} + \boldsymbol{\Gamma} : \left(\boldsymbol{\varepsilon}^k - s^k \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\cdot, \boldsymbol{\varepsilon}^k) \right)$$

- $\nabla f(\boldsymbol{\varepsilon}) = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\cdot, \boldsymbol{\varepsilon})$
- $P_A(\boldsymbol{\varepsilon}) = \bar{\boldsymbol{\varepsilon}} + \boldsymbol{\Gamma} : \boldsymbol{\varepsilon}$ with $\boldsymbol{\Gamma} \equiv \nabla^s (\operatorname{div} \nabla^s)^{-1} \operatorname{div}$

Projected gradient descent?

$$\varepsilon^{k+1} = \bar{\varepsilon} + \Gamma : \left(\varepsilon^k - s^k \frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon^k) \right) \quad \text{with} \quad \Gamma \equiv \nabla^s (\operatorname{div} \nabla^s)^{-1} \operatorname{div}$$

Projected gradient descent?

$$\varepsilon^{k+1} = \bar{\varepsilon} + s^k \Gamma : \left(\frac{1}{s^k} \varepsilon^k - \frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon^k) \right) \quad \text{with} \quad \Gamma \equiv \nabla^s (\operatorname{div} \nabla^s)^{-1} \operatorname{div}$$

Projected gradient descent?

$$\varepsilon^{k+1} = \bar{\varepsilon} - s^k \Gamma : \left(\frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon^k) - \frac{1}{s^k} \varepsilon^k \right) \quad \text{with} \quad \Gamma \equiv \nabla^s (\text{div } \nabla^s)^{-1} \text{div}$$

Projected gradient descent?

$$\varepsilon^{k+1} = \bar{\varepsilon} - s^k \Gamma : \left(\frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon^k) - \frac{1}{s^k} \varepsilon^k \right) \quad \text{with} \quad \Gamma \equiv \nabla^s (\operatorname{div} \nabla^s)^{-1} \operatorname{div}$$

- suppose $s^k \equiv s^0$
- define $\mathbb{C}^0 \equiv \frac{1}{s^0} \operatorname{Id}$
- associated $\Gamma^0 \equiv s^0 \Gamma$
- write $S = \partial w / \partial \varepsilon$

Projected gradient descent?

$$\varepsilon^{k+1} = \bar{\varepsilon} - s^k \Gamma : \left(\frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon^k) - \frac{1}{s^k} \varepsilon^k \right) \quad \text{with} \quad \Gamma \equiv \nabla^s (\operatorname{div} \nabla^s)^{-1} \operatorname{div}$$

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$$\varepsilon^{k+1} = \bar{\varepsilon} - s^k \Gamma : \left(\frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon^k) - \mathbf{C}^0 : \varepsilon^k \right) \quad \text{with} \quad \Gamma \equiv \nabla^s (\operatorname{div} \nabla^s)^{-1} \operatorname{div}$$

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Projected gradient descent?

$$\varepsilon^{k+1} = \bar{\varepsilon} - \Gamma^0 : \left(\mathbf{S}(\cdot, \varepsilon^k) - \mathbb{C}^0 : \varepsilon^k \right) \quad \text{with} \quad \Gamma \equiv \nabla^s (\operatorname{div} \nabla^s)^{-1} \operatorname{div}$$

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- write $\mathbf{S} = \partial w / \partial \varepsilon$

Projected gradient descent!

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

- hyperelastic basic scheme \equiv projected gradient descent

[M. Kabel, T. Böhlke, MS, Comput Mech, 2014]

So what?

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

- reference material \equiv inverse step size

$$\mathbb{C}^0 \equiv \frac{1}{s^0} \text{Id}$$

- s^0 large \Rightarrow instability
- s^0 small $\Rightarrow f(\varepsilon^{k+1}) < f(\varepsilon^k)$ (unless critical)

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- import knowledge from **optimization**, e.g., on convergence

↗ [MS, CMAME, 2017]

So what?

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

- α_+ -Lipschitz condition

$$\|S(x, \xi_1) - S(x, \xi_2)\| \leq \alpha_+ \|\xi_1 - \xi_2\| \quad \text{for all } x \in Q \quad \text{and} \quad \xi_1, \xi_2 \in \text{Sym}(d)$$

- monotone S (convex w)

$$(S(x, \xi_1) - S(x, \xi_2)) : (\xi_1 - \xi_2) \geq 0 \quad \text{for all } x \in Q \quad \text{and} \quad \xi_1, \xi_2 \in \text{Sym}(d)$$

- choose $\mathbb{C}^0 = \alpha_+ \text{Id}$ and obtain logarithmic convergence

$$f(\varepsilon^k) - \min f(\varepsilon^*) \leq \frac{2\alpha_+ \|\varepsilon^0 - \varepsilon^*\|^2}{k+4}$$

So what?

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- **strongly** α_- -monotone S (**strongly** α_- -convex w)

$$(S(x, \xi_1) - S(x, \xi_2)) : (\xi_1 - \xi_2) \geq \alpha_- \|\xi_1 - \xi_2\|^2 \quad \text{for all } x \in Q, \xi_1, \xi_2 \in \text{Sym}(d)$$

- choose $\mathbb{C}^0 = (\alpha_+ + \alpha_-)/2$ Id and obtain **linear** convergence

$$\|\varepsilon^{k+1} - \varepsilon^*\|_{L^2} \leq \left(\frac{\alpha_+ - \alpha_-}{\alpha_+ + \alpha_-} \right) \|\varepsilon^k - \varepsilon^*\|_{L^2}$$

So what?

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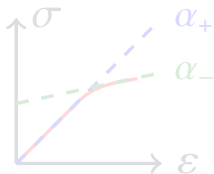
$$\|\varepsilon^{k+1} - \varepsilon^*\|_{L^2} \leq \left(\frac{\alpha_+ - \alpha_-}{\alpha_+ + \alpha_-} \right)^{k+1} \|\varepsilon^0 - \varepsilon^*\|_{L^2}$$

On the conditions

- if $S \in C^1$ in ε

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

$$\alpha_- \text{-strongly convex} \iff \lambda \geq \alpha_- \quad \forall x, \xi \quad \forall \lambda \in \text{Eig} \left(\frac{\partial S}{\partial \varepsilon}(x, \xi) \right)$$



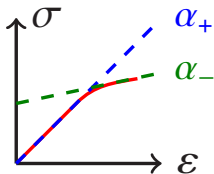
- maximum/minimum slopes of algo tangent
- estimated on-line
- theory does not cover porosity/softening

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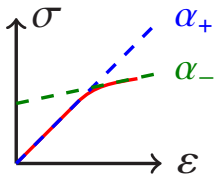
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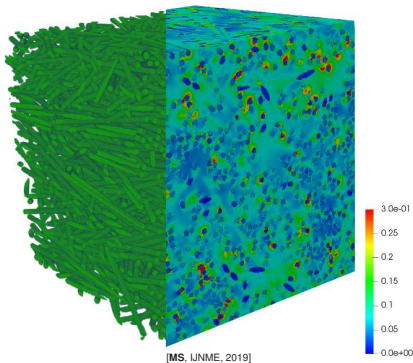


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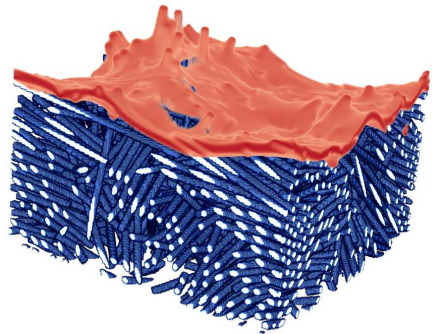
Digression Part III

- basic scheme \equiv projected gradient descent
- provides **intuition**
- import insights from optimization, e.g., Nesterov's book
- projected gradient descent ++ \equiv basic scheme ++ (tomorrow)

The end



[MS, IJNME, 2019]



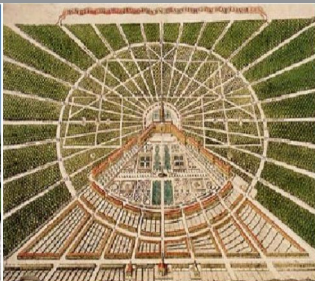
[Ernesti-MS-Böhle, CMAME, 2020]

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Matti Schneider

Faster primal solvers

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



Overview

1. Accelerated gradient methods

2. Newton - CG

3. Adaptive parameter selection

4. Summary and conclusions

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Previously ...

sought:

$$\langle w(\cdot, \varepsilon) \rangle_Q \longrightarrow \min_{\varepsilon = \bar{\varepsilon} + \nabla^s u} \iff \operatorname{div} S(\cdot, \bar{\varepsilon} + \nabla^s u) = 0, \quad S \equiv \frac{\partial w}{\partial \varepsilon}$$

basic scheme:

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

coincides with (projected) gradient descent

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

Convergence criterion?

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

know:

$$\varepsilon^k = \bar{\varepsilon} + \Gamma^0 : \mathbb{C}^0 : \varepsilon^k \quad (\Leftarrow P_A(P_A(x)) = P_A(x))$$

Convergence criterion?

$$\varepsilon^{k+1} = \varepsilon^k - \Gamma^0 : S(\cdot, \varepsilon^k)$$

know:

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Convergence criterion?

$$\varepsilon^{k+1} - \varepsilon^k = -\Gamma^0 : S(\cdot, \varepsilon^k)$$

Convergence criterion?

$$\varepsilon^{k+1} - \varepsilon^k = -\frac{1}{\alpha_0} \Gamma : S(\cdot, \varepsilon^k)$$

Convergence criterion?

$$\alpha_0 (\varepsilon^{k+1} - \varepsilon^k) = -\Gamma : S(\cdot, \varepsilon^k)$$

Convergence criterion?

$$\alpha_0 \|\varepsilon^{k+1} - \varepsilon^k\| = \|\Gamma : S(\cdot, \varepsilon^k)\|$$

Convergence criterion?

$$\frac{\alpha_0 \|\varepsilon^{k+1} - \varepsilon^k\|}{\|\bar{\sigma}^k\|} = \frac{\|\Gamma : S(\cdot, \varepsilon^k)\|}{\|\bar{\sigma}^k\|} \stackrel{!}{\leq} \text{tol}$$

Why?

- dimension-free
- independent of algorithm, i.e., α_0
- readily computable

Algorithm 1 Basic scheme ($\bar{\varepsilon}, \text{maxit}, \text{tol}, \alpha_0$)

- 1: $\varepsilon \leftarrow \varepsilon^0$ ▷ $\varepsilon^0 \equiv \bar{\varepsilon}$ or via extrapolation
 - 2: $\text{res} \leftarrow 1$
 - 3: $\bar{\sigma} \leftarrow 0$
 - 4: $k \leftarrow 0$
 - 5: **while** $k < \text{maxit}$ **and** $\text{res} > \text{tol}$ **do**
 - 6: $k \leftarrow k + 1$
 - 7: $\xi \leftarrow \varepsilon$
 - 8: $\varepsilon \leftarrow S(\cdot, \varepsilon) - \alpha_0 \varepsilon$ ▷ estimate α_{\pm}
 - 9: $\bar{\sigma} \leftarrow \langle \varepsilon \rangle_Q + \alpha_0 \bar{\sigma}$ ▷ $\langle \varepsilon \rangle_Q = \hat{\varepsilon}(0)$
 - 10: $\varepsilon \leftarrow \bar{\varepsilon} - 1/\alpha_0 \Gamma : \varepsilon$ ▷ use FFT & favorite discretization
 - 11: $\text{res} \leftarrow \alpha_0 \|\varepsilon - \xi\| / \|\bar{\sigma}\|$ ▷ update α_0 afterwards
 - 12: **end while**
 - 13: **return** $\varepsilon, \bar{\sigma}, \text{res}$ ▷ Requires two strain fields
-

[H. Moulinec and P. Suquet, Comptes Rendus de l'Académie des Sciences, 1994]

[H. Moulinec and P. Suquet, CMAME, 1998]

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

implies

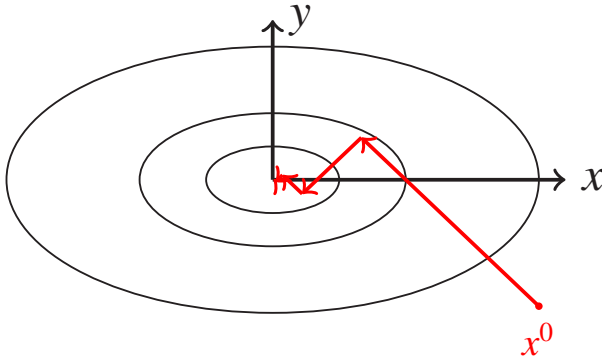
$$\|\varepsilon^{k+1} - \varepsilon^*\|_{L^2} \leq \left(\frac{\kappa - 1}{\kappa + 1} \right) \|\varepsilon^k - \varepsilon^*\|_{L^2}$$

for

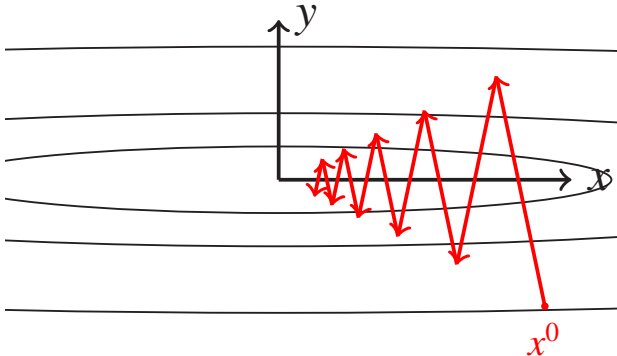
$$\alpha_0 = \frac{\alpha_- + \alpha_+}{2} \quad \text{and} \quad \kappa = \frac{\alpha_+}{\alpha_-}$$

\Rightarrow # iterations $\propto \kappa$

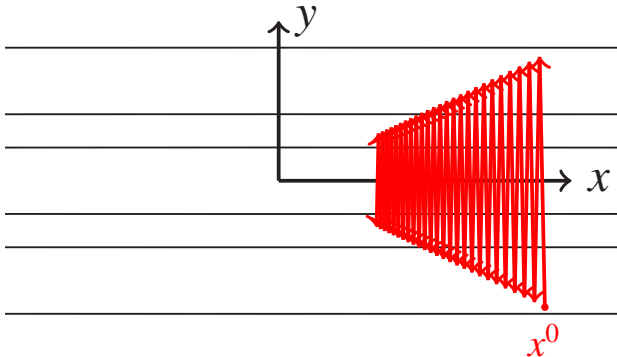
- What if $\kappa \gg 1$? ↗ $\kappa = 2$



- What if $\kappa \gg 1$? ↗ $\kappa = 10$



■ What if $\kappa \gg 1$? ↗ $\kappa = 100$



- augment (projected) gradient descent ↗ **heavy-ball method** (Polyak)

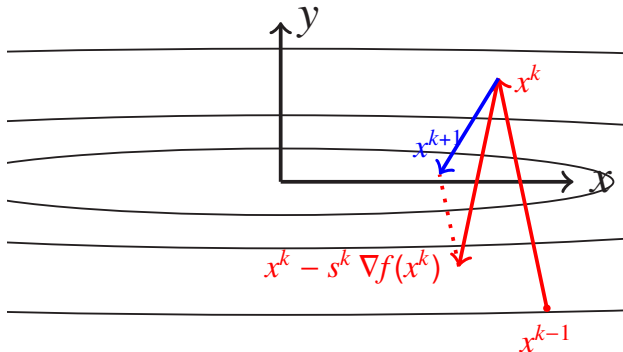
[B. Polyak, USSR Computational Mathematics and Mathematical Physics, 1964]

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

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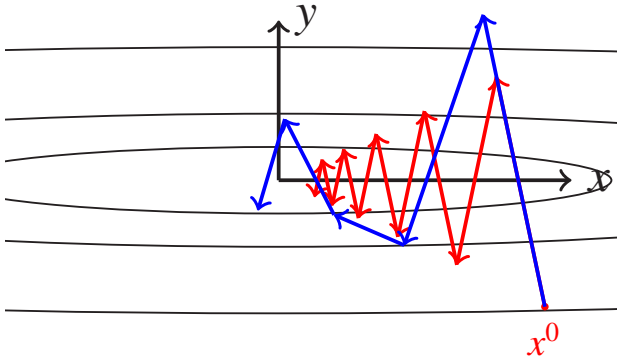
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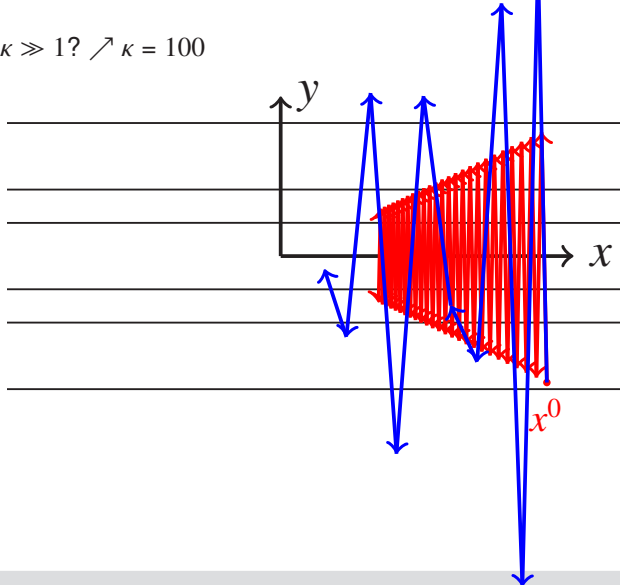
Gradient vs fast gradient

- What if $\kappa \gg 1$? ↗ $\kappa = 10$



Gradient vs fast gradient

- What if $\kappa \gg 1$? ↗ $\kappa = 100$



Heavy ball for micromechanics

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

with

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

best rate for (linear elasticity)

$$\alpha_0 = \left(\frac{\sqrt{\alpha_-} + \sqrt{\alpha_+}}{2} \right)^2 \quad \text{and} \quad \beta^k = \frac{\sqrt{k} - 1}{\sqrt{k} + 1} \quad \text{with} \quad \kappa = \frac{\alpha_+}{\alpha_-}$$

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

Heavy ball for micromechanics

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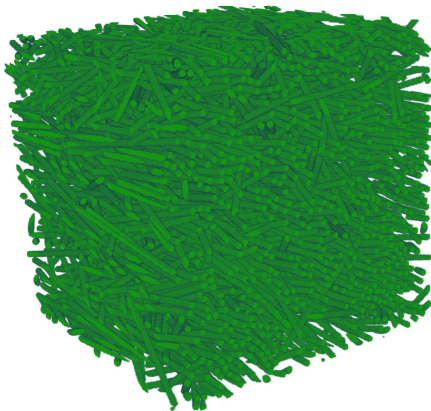
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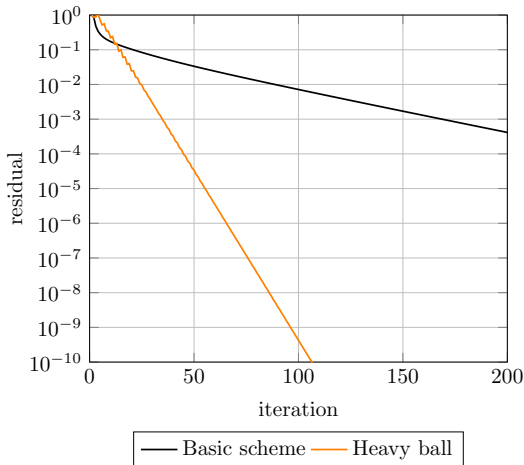
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Practical performance - setup



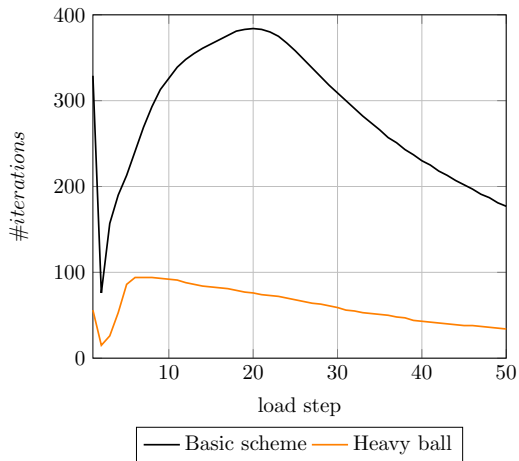
- glass-fiber reinforced PA, 256^3
 - $\phi = 20\%$, $r_a = 30$,
 $A = \text{diag}(0.8, 0.1, 0.1)$
 - generated by SAM
- [MS, Computational Mechanics, 2017]
- $E_{\text{Fiber}} = 72 \text{ GPa}$, $\nu_{\text{Fiber}} = 0.22$,
 $E_{\text{PA}} = 2.1 \text{ GPa}$, $\nu_{\text{PA}} = 0.3$
 - uniaxial extension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

[MS, International Journal for Numerical Methods in Engineering, 2019]



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Practical performance - vM plasticity



- von Mises elastoplastic matrix
- 5% uniaxial extension in x
- $tol = 10^{-5}$

	average it.	
	Basic	Heavy ball
128^3	284.08	64.64
256^3	382.7	61.58

[MS, International Journal for Numerical Methods in Engineering, 2019]

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

- rewriting (for implementation)

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

- rewriting (for residual)

$$\varepsilon^{k+1} - \varepsilon^k = -\Gamma^0 : S(\cdot, \varepsilon^k) + \beta_k (\varepsilon^k - \varepsilon^{k-1})$$

$$\|\varepsilon^{k+1} - \varepsilon^k\|^2 = \|\Gamma^0 : S(\cdot, \varepsilon^k)\|^2 - \frac{2\beta_k}{\alpha_0} \left(S(\cdot, \varepsilon^k), \varepsilon^k - \varepsilon^{k-1} \right)_{L^2} + \beta_k^2 \|\varepsilon^k - \varepsilon^{k-1}\|_{L^2}^2$$

Algorithm 2 Heavy Ball ($\bar{\varepsilon}$, maxit, tol, α_0, β)

- 1: $[\varepsilon, \xi] \leftarrow [\varepsilon^0, \varepsilon^0]$ ▷ $\varepsilon^0 \equiv \bar{\varepsilon}$ or via extrapolation
- 2: $[\text{res}, \bar{\sigma}, k, p] \leftarrow [1, 0, 0, 0]$
- 3: **while** $k < \text{maxit}$ **and** $\text{res} > \text{tol}$ **do**
- 4: $k \leftarrow k + 1$
- 5: $p_{\text{old}} \leftarrow p$
- 6:
$$\begin{bmatrix} \varepsilon \\ \xi \\ p \\ q \end{bmatrix} \leftarrow \begin{bmatrix} S(\cdot, \varepsilon) - \alpha_0 \varepsilon - \alpha_0 \beta (\varepsilon - \xi) \\ \varepsilon \\ \|\varepsilon - \xi\|^2 \\ (S(\cdot, \varepsilon), \varepsilon - \xi)_{L^2} \end{bmatrix}$$
 ▷ estimate α_{\pm}
- 7: $\bar{\sigma} \leftarrow \langle \varepsilon \rangle_Q + \alpha_0 \bar{\varepsilon}$ ▷ $\langle \varepsilon \rangle_Q = \hat{\varepsilon}(0)$
- 8: $\varepsilon \leftarrow \bar{\varepsilon} - 1/\alpha_0 \Gamma : \varepsilon$ ▷ use FFT & favorite discretization
- 9: $\text{res} \leftarrow (p + 2\beta q/\alpha_0 - \beta^2 p_{\text{old}})/\|\bar{\sigma}\|$ ▷ update α_0, β afterwards
- 10: **end while**
- 11: **return** $\varepsilon, \bar{\sigma}, \text{res}$ ▷ Requires two strain fields

[F. Ernesti and MS, CMAME, 2020]

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Linear conjugate gradient method

- goal: $\frac{1}{2}x^T Ax - b^T x \longrightarrow \min_x$
- utilize

$$d^k = -\nabla f(x^k) + \gamma^{k-1} d^{k-1}$$
$$x^{k+1} = x^k + \alpha^k d^k$$

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- ↗ Hestenes-Stiefel (1952)
- optimal Krylov method

Algorithm 3 Linear CG ($A, b, x^0, \maxit, \text{tol}$)

```
1:  $g \leftarrow Ax^0 - b$ 
2:  $d \leftarrow -g$ 
3:  $r \leftarrow \|g\|$ 
4:  $k \leftarrow 0$ 
5: while  $k < \maxit$  and  $r > \text{tol}$  do
6:    $k \leftarrow k + 1$ 
7:    $r_{\text{old}} \leftarrow r$ 
8:    $z \leftarrow Ad$ 
9:    $\alpha \leftarrow r^2 / d^T z$ 
10:   $x \leftarrow x + \alpha d$ 
11:   $g \leftarrow g + \alpha z$ 
12:   $r \leftarrow \|g\|$ 
13:   $\gamma \leftarrow r^2 / r_{\text{old}}^2$ 
14:   $d \leftarrow -g + \gamma d$ 
15: end while
16: return  $x, r$ 
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[M. Hestenes and E. Stiefel, Journal of Research of the National Bureau of Standards, 1952]

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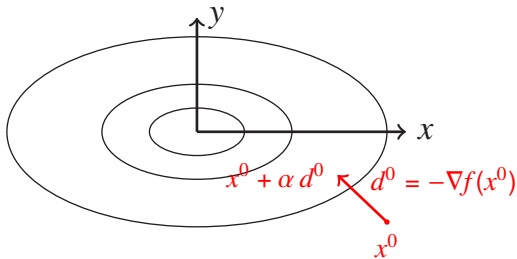
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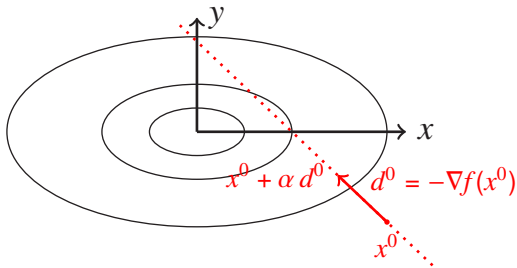
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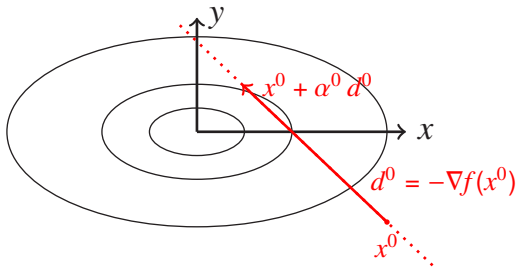
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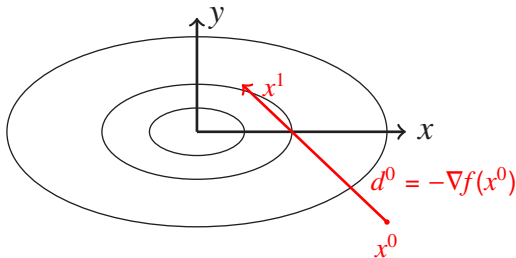
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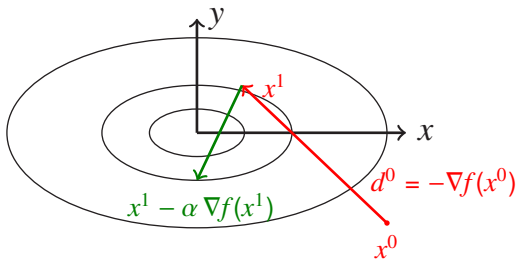
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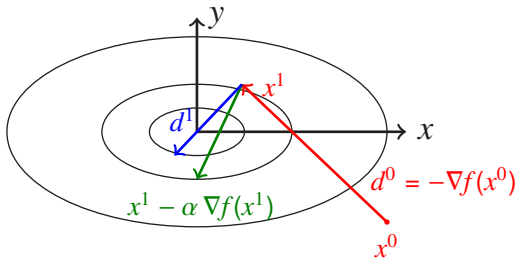
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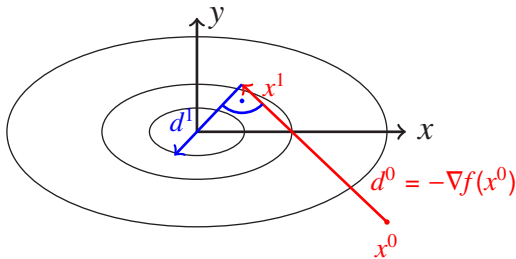
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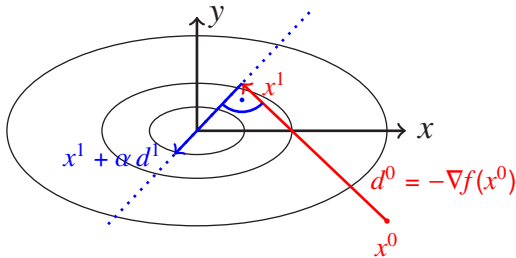
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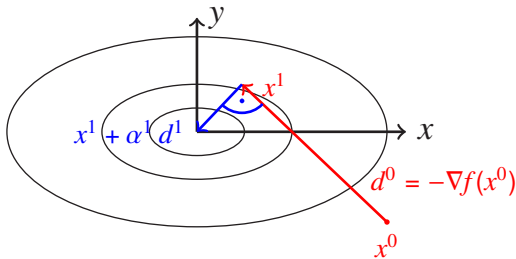
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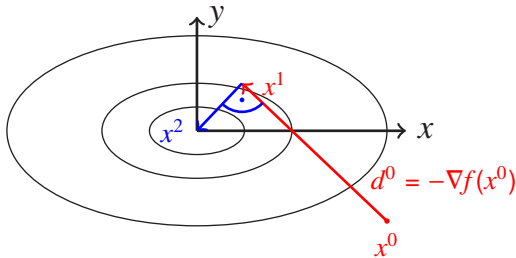
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- **optimal** Krylov method



- goal:
 $\langle (\bar{\varepsilon} + \nabla^s u) : \mathbb{C} : (\bar{\varepsilon} + \nabla^s u) \rangle_Q \rightarrow \min$
- introduced by Brisard-Dormieux (2010) and Zeman et al. (2010)
- $\text{res} = \|\Gamma : \mathbb{C} : \varepsilon\| / \|\bar{\sigma}\|$
- requires four fields, vs. two fields for basic/heavy ball

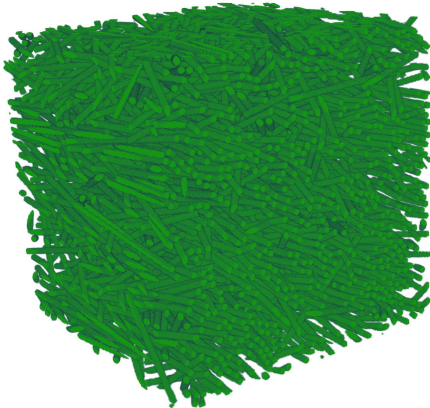
Algorithm 4 Linear CG ($\mathbb{C}, \bar{\varepsilon}, \text{maxit}, \text{tol}$)

```
1:  $G \leftarrow \Gamma : \mathbb{C} : \bar{\varepsilon}$  ▷ Compute  $\bar{\sigma} = \langle \mathbb{C} : \bar{\varepsilon} \rangle_Q$ 
2:  $D \leftarrow -G$ 
3:  $[\mathbf{r}, \text{res}] \leftarrow [ \|G\|, \|G\| / \|\bar{\sigma}\| ]$ 
4:  $k \leftarrow 0$ 
5: while  $k < \text{maxit}$  and  $\text{res} > \text{tol}$  do
6:    $k \leftarrow k + 1$ 
7:    $\mathbf{r}_{\text{old}} \leftarrow \mathbf{r}$ 
8:    $Z \leftarrow \Gamma : \mathbb{C} : D$  ▷  $[\Delta \bar{\sigma}, \hat{Z}(0)] \leftarrow [\hat{Z}(0), 0]$ 
9:    $\alpha \leftarrow \mathbf{r}^2 / (D, Z)_{L^2}$ 
10:   $\varepsilon \leftarrow \varepsilon + \alpha D$ 
11:   $\bar{\sigma} \leftarrow \bar{\sigma} + \alpha \Delta \bar{\sigma}$ 
12:   $\text{res} \leftarrow r / \|\bar{\sigma}\|$ 
13:   $G \leftarrow G + \alpha Z$ 
14:   $\mathbf{r} \leftarrow \|G\|$ 
15:   $\gamma \leftarrow \mathbf{r}^2 / \mathbf{r}_{\text{old}}^2$ 
16:   $D \leftarrow -G + \gamma D$ 
17: end while
18:  $\varepsilon \leftarrow \varepsilon + \bar{\varepsilon}$ 
19: return  $\varepsilon, \bar{\sigma}$ 
```

[S. Brisard and L. Dormieux, Computational Materials Science, 2010]

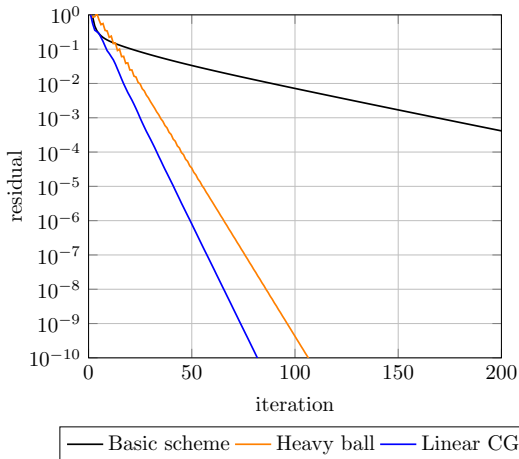
[J. Zeman, J. Vondřejc, J. Novák, and I. Marek, Journal of Computational Physics, 2010]

Practical performance - setup



[MS, International Journal for Numerical Methods in Engineering, 2019]

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



[MS, International Journal for Numerical Methods in Engineering, 2019]

- solve

$$G(x) \stackrel{!}{=} 0 \quad \text{via} \quad G(x+d) \approx G(x) + G'(x) d \stackrel{!}{=} 0$$

via

$$x^{k+1} = x^k + \alpha^k d^k, \quad G'(x^k) d^k = -G(x^k)$$

- locally quadratic convergence ($\alpha^k = 1$) under
 - non-degeneracy of root
 - technical smoothness conditions at root
 - exact computation of d^k
- global convergence via globalization strategy, i.e., via backtracking with $\alpha^k \in (0, 1]$

$$\|G(x^k + \alpha^k d^k)\| \leq (1 - \delta) \|G(x^k)\|, \quad \alpha^k = (1 - \rho)^m, \quad \rho, \delta \in (0, 1)$$

Newton's method in optimization

■ solve

$$\nabla f(x) \stackrel{!}{=} 0 \quad \text{via} \quad \nabla f(x+d) \approx \nabla f(x) + \nabla^2 f(x) d \stackrel{!}{=} 0$$

via

$$x^{k+1} = x^k + \alpha^k d^k, \quad \nabla^2 f(x^k) d^k = -\nabla f(x^k)$$

Newton-CG method

■ solve

$$\nabla f(x) \stackrel{!}{=} 0 \quad \text{via} \quad \nabla f(x+d) \approx \nabla f(x) + \nabla^2 f(x) d \stackrel{!}{=} 0$$

via

$$x^{k+1} = x^k + \alpha^k d^k, \quad \nabla^2 f(x^k) d^k = -\nabla f(x^k) \quad \leftarrow \quad \text{solved with CG}$$

Newton-CG method

■ solve

$$\nabla f(x) \stackrel{!}{=} 0 \quad \text{via} \quad \nabla f(x+d) \approx \nabla f(x) + \nabla^2 f(x) d \stackrel{!}{=} 0$$

via

$$x^{k+1} = x^k + \alpha^k d^k, \quad \nabla^2 f(x^k) d^k = -\nabla f(x^k) \quad \leftarrow \quad \text{solved with CG}$$

- solve

$$\nabla f(x) \stackrel{!}{=} 0 \quad \text{via} \quad \nabla f(x+d) \approx \nabla f(x) + \nabla^2 f(x) d \stackrel{!}{=} 0$$

via

$$x^{k+1} = x^k + \alpha^k d^k, \quad \nabla^2 f(x^k) d^k = -\nabla f(x^k) \quad \leftarrow \quad \text{solved with CG}$$

- under same assumptions as Newton provided, if

$$\|\nabla^2 f(x^k) d^k + \nabla f(x^k)\| \leq \text{const} \|\nabla f(x^k)\|^p,$$

will converge with rate $p \in [1, 2]$

- in practice: $p = 1$, $\text{const} = 0.1$
- global convergence via globalization strategy

- solve

$$\operatorname{div} S(\cdot, \bar{\varepsilon} + \nabla^s(u + v)) \approx \operatorname{div} S(\cdot, \bar{\varepsilon} + \nabla^s u) + \operatorname{div} \frac{\mathbb{S}}{\partial \varepsilon}(\cdot, \bar{\varepsilon} + \nabla^s u) : \nabla^s v \stackrel{!}{=} 0$$

via

$$u^{k+1} = u^k + \alpha^k v^k,$$

$$\operatorname{div} \frac{\mathbb{S}}{\partial \varepsilon}(\cdot, \bar{\varepsilon} + \nabla^s u^k) : \nabla^s v^k = -\operatorname{div} S(\cdot, \bar{\varepsilon} + \nabla^s u^k) \quad \leftarrow \quad \text{solved with CG}$$

■ solve

$$\operatorname{div} S(\cdot, \bar{\varepsilon} + \nabla^s(u + v)) \approx \operatorname{div} S(\cdot, \bar{\varepsilon} + \nabla^s u) + \operatorname{div} \frac{S}{\partial \varepsilon}(\cdot, \bar{\varepsilon} + \nabla^s u) : \nabla^s v \stackrel{!}{=} 0$$

via

$$\varepsilon^{k+1} = \varepsilon^k + \alpha^k \xi^k,$$

$$\xi^k = -\Gamma^0 : \left[\frac{S}{\partial \varepsilon}(\cdot, \varepsilon^k) : \xi^k - \mathbb{C}^0 : \xi^k + S(\cdot, \varepsilon^k) \right] \leftarrow \text{solved with CG}$$

[L. Gélébart and R. Mondon-Cancel, Computational Materials Science, 2013]

■ careful with residuals & forcing

[D. Wicht, MS and T. Böhlke, International Journal for Numerical Methods in Engineering, 2020]

- solve

$$\operatorname{div} S(\cdot, \bar{\varepsilon} + \nabla^s(u + v)) \approx \operatorname{div} S(\cdot, \bar{\varepsilon} + \nabla^s u) + \operatorname{div} \frac{S}{\partial \varepsilon}(\cdot, \bar{\varepsilon} + \nabla^s u) : \nabla^s v \stackrel{!}{=} 0$$

via

$$\varepsilon^{k+1} = \varepsilon^k + \alpha^k \xi^k,$$

$$\xi^k = -\Gamma^0 : \left[\frac{S}{\partial \varepsilon}(\cdot, \varepsilon^k) : \xi^k - \mathbb{C}^0 : \xi^k + S(\cdot, \varepsilon^k) \right] \quad \leftarrow \quad \text{solved with CG}$$

- memory: 1 (ε) + 4 (CG) + 3.5 (tangent) = 8.5 strain fields
- only **linear convergence** in practice

Synopsis first two parts

- trade memory vs speed
- high-memory versions: CG / Newton-CG
- low-memory solvers: basic / fast gradient
- **Why** are CG and Newton-CG faster??

$$\begin{aligned}d^k &= -\nabla f(x^k) + \gamma^{k-1} d^{k-1} \\ \text{CG: } x^{k+1} &= x^k + \alpha^k d^k\end{aligned}$$

$$\text{Heavy ball: } x^{k+1} = x^k - s^k \nabla f(x^k) + \beta^k (x^k - x^{k-1})$$

$$\begin{aligned}d^k &= -\nabla f(x^k) + \gamma^{k-1} d^{k-1} \\ \text{CG: } x^{k+1} &= x^k + \alpha^k d^k \\ d^k &= \frac{1}{\alpha^k} (x^{k+1} - x^k)\end{aligned}$$

$$\text{Heavy ball: } x^{k+1} = x^k - s^k \nabla f(x^k) + \beta^k (x^k - x^{k-1})$$

$$\begin{aligned}d^k &= -\nabla f(x^k) + \gamma^{k-1} d^{k-1} \\ \text{CG: } x^{k+1} &= x^k + \alpha^k d^k \\ d^{k-1} &= \frac{1}{\alpha^{k-1}} (x^k - x^{k-1})\end{aligned}$$

$$\text{Heavy ball: } x^{k+1} = x^k - s^k \nabla f(x^k) + \beta^k (x^k - x^{k-1})$$

$$\begin{aligned} d^k &= -\nabla f(x^k) + \frac{\gamma^{k-1}}{\alpha^{k-1}} (x^k - x^{k-1}) \\ \text{CG: } x^{k+1} &= x^k + \alpha^k d^k \end{aligned}$$

$$\text{Heavy ball: } x^{k+1} = x^k - s^k \nabla f(x^k) + \beta^k (x^k - x^{k-1})$$

$$\begin{aligned}d^k &= -\nabla f(x^k) + \frac{\gamma^{k-1}}{\alpha^{k-1}} (x^k - x^{k-1}) \\ \text{CG: } x^{k+1} &= x^k + \alpha^k \left(-\nabla f(x^k) + \frac{\gamma^{k-1}}{\alpha^{k-1}} (x^k - x^{k-1}) \right)\end{aligned}$$

$$\text{Heavy ball: } x^{k+1} = x^k - s^k \nabla f(x^k) + \beta^k (x^k - x^{k-1})$$

$$\text{CG: } x^{k+1} = x^k - \alpha^k \nabla f(x^k) + \frac{\alpha^k \gamma^{k-1}}{\alpha^{k-1}} (x^k - x^{k-1})$$

$$\text{Heavy ball: } x^{k+1} = x^k - s^k \nabla f(x^k) + \beta^k (x^k - x^{k-1})$$

$$\text{CG: } x^{k+1} = x^k - \alpha^k \nabla f(x^k) + \frac{\alpha^k \gamma^{k-1}}{\alpha^{k-1}} (x^k - x^{k-1})$$

$$\text{Heavy ball: } x^{k+1} = x^k - s^k \nabla f(x^k) + \beta^k (x^k - x^{k-1})$$

$$\Rightarrow \quad \alpha^k = s^k \quad \text{and} \quad \frac{\alpha^k \gamma^{k-1}}{\alpha^{k-1}} = \beta^k$$

$$\text{CG: } x^{k+1} = x^k - \alpha^k \nabla f(x^k) + \frac{\alpha^k \gamma^{k-1}}{\alpha^{k-1}} (x^k - x^{k-1})$$

$$\text{Heavy ball: } x^{k+1} = x^k - s^k \nabla f(x^k) + \beta^k (x^k - x^{k-1})$$

$$\Rightarrow \quad \alpha^k = s^k \quad \text{and} \quad \frac{\alpha^k \gamma^{k-1}}{\alpha^{k-1}} = \beta^k$$

HB \Rightarrow Linear CG

- plane search

$$(s^k, \beta^k) = \operatorname{argmin}_{s, \beta} f(x^k - s \nabla f(x^k) + \beta (x^k - x^{k-1}))$$

- CG = heavy ball with **adaptive parameters**

HB \Rightarrow Linear CG

- plane search

$$(s^k, \beta^k) = \operatorname{argmin}_{s, \beta} f(x^k - s \nabla f(x^k) + \beta (x^k - x^{k-1}))$$

- CG = heavy ball with **adaptive parameters**

Similarly

$$\begin{aligned} \text{Newton: } x^{k+1} &= x^k - \alpha^k \left[\nabla^2 f(x^k) \right]^{-1} \nabla f(x^k) \\ \text{Gradient method: } x^{k+1} &= x^k - s^k \nabla f(x^k) \end{aligned}$$

↗ Newton is gradient descent with **adaptive (anisotropic) step size**

Overview

1. Accelerated gradient methods

2. Newton - CG

3. Adaptive parameter selection

4. Summary and conclusions

- gradient scheme

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

- 1D secant method:

$$s^k = \frac{x^k - x^{k-1}}{f'(x^k) - f'(x^{k-1})} \approx \frac{1}{f''(x^k)}$$

- higher dimension (Barzilai-Borwein, 1988):

$$s^k = \frac{\|x^k - x^{k-1}\|^2}{\langle \nabla f(x^k) - \nabla f(x^{k-1}), x^k - x^{k-1} \rangle}$$

[J. Barzilai and J. M. Borwein, IMA Journal of Numerical Analysis, 1988]

$$x^{k+1} = x^k - s^k \nabla f(x^k) \quad \text{with} \quad s^k = \frac{\|x^k - x^{k-1}\|^2}{\langle \nabla f(x^k) - \nabla f(x^{k-1}), x^k - x^{k-1} \rangle}$$

■ if

$$\alpha_- \leq \lambda \leq \alpha_+ \quad \forall x \forall \lambda \in \text{Eig}(\nabla^2 f(x)),$$

then

$$\frac{1}{\alpha_+} \leq s^k \leq \frac{1}{\alpha_-}$$

$$x^{k+1} = x^k - s^k \nabla f(x^k) \quad \text{with} \quad s^k = \frac{\|x^k - x^{k-1}\|^2}{\langle \nabla f(x^k) - \nabla f(x^{k-1}), x^k - x^{k-1} \rangle}$$

■ practical implementation

$$s^k = \frac{\|\nabla f(x^{k-1})\|^2}{\|\nabla f(x^{k-1})\|^2 - \langle \nabla f(x^k), \nabla f(x^{k-1}) \rangle} s^{k-1}$$

$$\varepsilon^{k+1} = \varepsilon^k - s^k \Gamma : S(\cdot, \varepsilon^k) \quad \text{with} \quad \langle \varepsilon^0 \rangle_Q = \bar{\varepsilon}$$

■ practical implementation

$$s^k = \frac{\|\Gamma : S(\cdot, \varepsilon^{k-1})\|^2}{\|\Gamma : S(\cdot, \varepsilon^{k-1})\|^2 - (S(\cdot, \varepsilon^k), \Gamma : S(\cdot, \varepsilon^{k-1}))_{L^2}} s^{k-1}$$

[MS, International Journal for Numerical Methods in Engineering, 2019]

$$\xi^k = \Gamma : S(\cdot, \varepsilon^k)$$
$$\varepsilon^{k+1} = \varepsilon^k - s^k \xi^k \quad \text{with} \quad \langle \varepsilon^0 \rangle_Q = \bar{\varepsilon}$$

■ practical implementation

$$s^k = \frac{\|\xi^{k-1}\|^2}{\|\xi^{k-1}\|^2 - (S(\cdot, \varepsilon^k), \xi^{k-1}))_{L^2}} s^{k-1}$$

[MS, International Journal for Numerical Methods in Engineering, 2019]

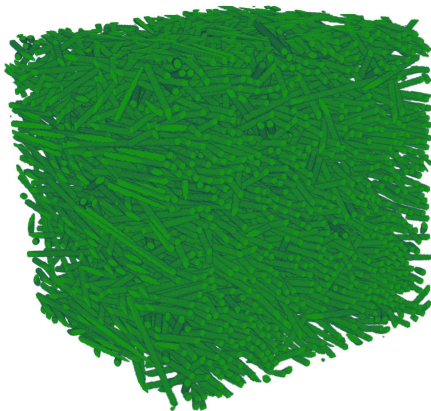
Algorithm 5 Alternative basic scheme ($\bar{\varepsilon}$, maxit, tol, α_0)

- 1: $[\varepsilon, \xi] \leftarrow [\varepsilon^0, 0]$ $\triangleright \langle \varepsilon^0 \rangle_Q \stackrel{!}{=} \bar{\varepsilon}$
 - 2: $[\text{res}, s, k, r] \leftarrow [1, 1/\alpha^0, 0, 1]$
 - 3: **while** $k < \text{maxit}$ **and** $\text{res} > \text{tol}$ **do**
 - 4: $k \leftarrow k + 1$
 - 5: $\xi \leftarrow S(\cdot, \varepsilon)$
 - 6: $\bar{\sigma} \leftarrow \langle \xi \rangle_Q$
 - 7: $\xi \leftarrow \Gamma : \xi$ $\triangleright \hat{\xi}(0) = 0$
 - 8: $\varepsilon \leftarrow \varepsilon - s \xi$ \triangleright use FFT & favorite discretization
 - 9: $r \leftarrow \|\xi\|$
 - 10: $\text{res} \leftarrow r / \|\bar{\sigma}\|$
 - 11: **end while**
 - 12: **return** $\varepsilon, \bar{\sigma}, \text{res}$ \triangleright Requires two strain fields
-

Algorithm 6 Barzilai Borwein basic scheme ($\bar{\varepsilon}, \text{maxit}, \text{tol}, \alpha_0$)

- 1: $[\varepsilon, \xi] \leftarrow [\varepsilon^0, 0]$ $\triangleright \langle \varepsilon^0 \rangle_Q \stackrel{!}{=} \bar{\varepsilon}$
- 2: $[\text{res}, s, k, r] \leftarrow [1, 1/\alpha^0, 0, 1]$
- 3: **while** $k < \text{maxit}$ **and** $\text{res} > \text{tol}$ **do**
- 4: $k \leftarrow k + 1$
- 5: $\begin{bmatrix} \xi \\ \mathbf{p} \end{bmatrix} \leftarrow \begin{bmatrix} S(\cdot, \varepsilon) \\ (S(\cdot, \varepsilon), \xi)_{L^2} \end{bmatrix}$
- 6: $\bar{\sigma} \leftarrow \langle \xi \rangle_Q$
- 7: $\xi \leftarrow \Gamma : \xi$ $\triangleright \hat{\xi}(0) = 0$
- 8: $s \leftarrow s / (1 - \mathbf{p}/r^2)$
- 9: $\varepsilon \leftarrow \varepsilon - s \xi$ \triangleright use FFT & favorite discretization
- 10: $r \leftarrow \|\xi\|$
- 11: $\text{res} \leftarrow r / \|\bar{\sigma}\|$
- 12: **end while**
- 13: **return** $\varepsilon, \bar{\sigma}, \text{res}$ \triangleright Requires two strain fields

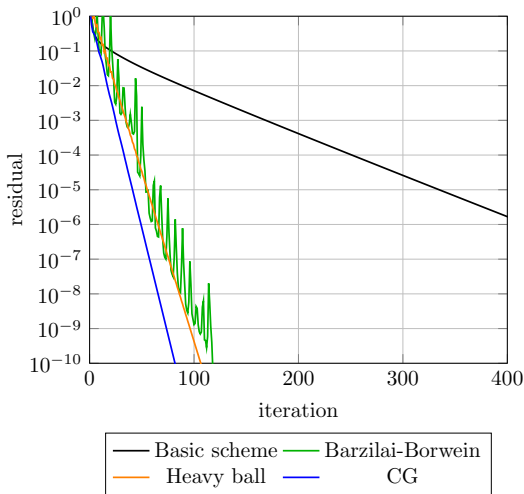
Practical performance - setup



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

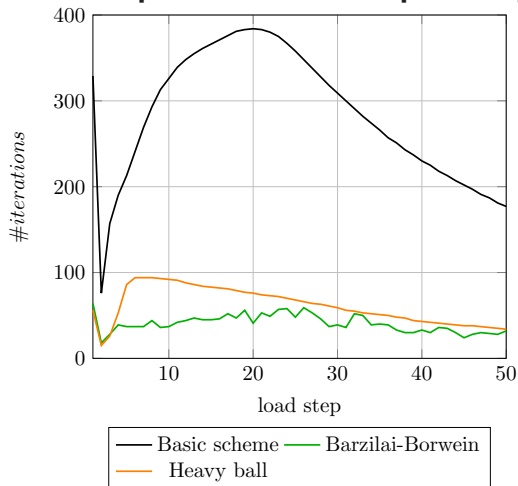
[MS, International Journal for Numerical Methods in Engineering, 2019]

Practical performance - linear elasticity



[MS, International Journal for Numerical Methods in Engineering, 2019]

Practical performance - vM plasticity



- von Mises elastoplastic matrix
- 5% uniaxial extension in x

	average it.		
	Basic	HB	BB
128^3	284.08	64.64	40.58
256^3	382.7	61.58	49.6

[MS, International Journal for Numerical Methods in Engineering, 2019]

Synopsis Barzilai-Borwein

- simple to implement
- two strain fields
- no manual update of α^0
- no eigenvalue decompositions (!)
- but: no monotonicity

$$x^{k+1} = x^k - s^k \nabla f(x^k) + \beta^k (x^k - x^{k-1}), \quad \beta^k = s^k \gamma^{k-1} / s^{k-1}$$

- heavy ball: $s^k = \text{const}$, $\beta^k = \text{const}$, requires **meticulous care**
- CG: line search ↗ **bottleneck**

$$s^k \approx \operatorname{argmin}_s f(x^k + s d^k)$$

and

$$\gamma^k = \|\nabla f(x^{k+1})\|^2 / \|\nabla f(x^k)\|^2 \quad (\text{Fletcher-Reeves, 1964})$$

[R. Fletcher and C. Reeves, The Computer Journal, 1964]

Heavy ball + CG

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

- combine advantages

$$s^k = \text{const}$$

$$\beta^k = \|\nabla f(x^k)\|^2 / \|\nabla f(x^{k-1})\|^2$$

Heavy ball + CG & FFT

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

- combine advantages

$$s^k = \text{const}$$

$$\beta^k = \|\Gamma : S(\cdot, \varepsilon^k)\|^2 / \|\Gamma : S(\cdot, \varepsilon^{k-1})\|^2$$

$$\xi^k = \Gamma : S(\cdot, \varepsilon^k)$$

$$\varepsilon^{k+1} = \varepsilon^k - s^k \xi^k + \beta^k (\varepsilon^k - \zeta^k)$$

$$\zeta^{k+1} = \varepsilon^k$$

- combine advantages

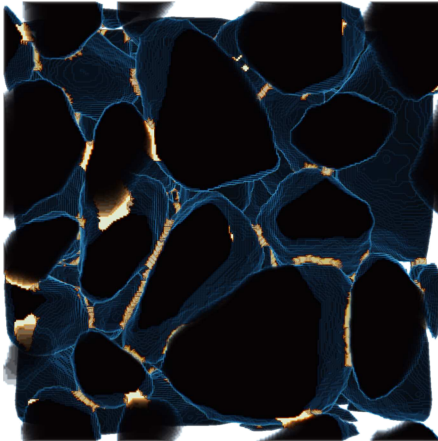
$$s^k = \text{const}$$

$$\beta^k = \|\xi^k\|^2 / \|\xi^{k-1}\|^2$$

Algorithm 7 Fletcher-Reeves Nonlinear CG ($\bar{\varepsilon}$, maxit, tol, α_0)

- 1: $[\varepsilon, \xi, \zeta] \leftarrow [\varepsilon^0, 0, \zeta]$ $\triangleright \langle \varepsilon^0 \rangle_Q \stackrel{!}{=} \bar{\varepsilon}$
- 2: $[\text{res}, s, k, r, \beta] \leftarrow [1, 1/\alpha^0, 0, 1, 0]$
- 3: **while** $k < \text{maxit}$ **and** $\text{res} > \text{tol}$ **do**
- 4: $k \leftarrow k + 1$
- 5: $\xi \leftarrow S(\cdot, \varepsilon)$
- 6: $\bar{\sigma} \leftarrow \langle \xi \rangle_Q$
- 7: $\xi \leftarrow \Gamma : \xi$ $\triangleright \hat{\xi}(0) = 0$
- 8: $r \leftarrow \|\xi\|$
- 9: $\beta \leftarrow r^2 \beta$
- 10: $\begin{bmatrix} \varepsilon \\ \zeta \end{bmatrix} \leftarrow \begin{bmatrix} \varepsilon - s\xi + \beta(\varepsilon - \zeta) \\ \varepsilon \end{bmatrix}$
- 11: $\beta \leftarrow 1/r^2$
- 12: $\text{res} \leftarrow r/\|\bar{\sigma}\|$
- 13: **end while**
- 14: **return** $\varepsilon, \bar{\sigma}, \text{res}$ \triangleright Requires three strain fields

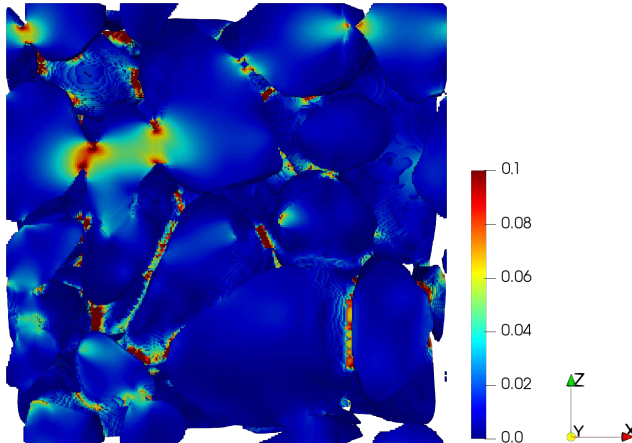
Practical performance - sandcore



Sand (black) and binder (gold)

↗ [MS, Computational Mechanics, 2020]

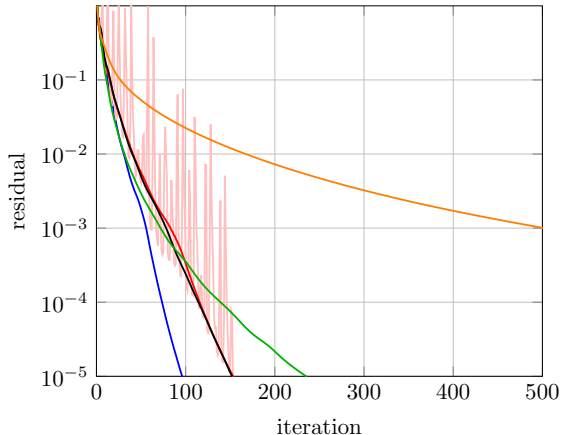
Practical performance - sandcore



Strain magnitude at 5%, on **staggered grid** [MS-Ospald-Kabel, IJNME, 2016]

↗ [MS, Computational Mechanics, 2020]

Practical performance - sandcore



↗ [MS, Computational Mechanics, 2020]

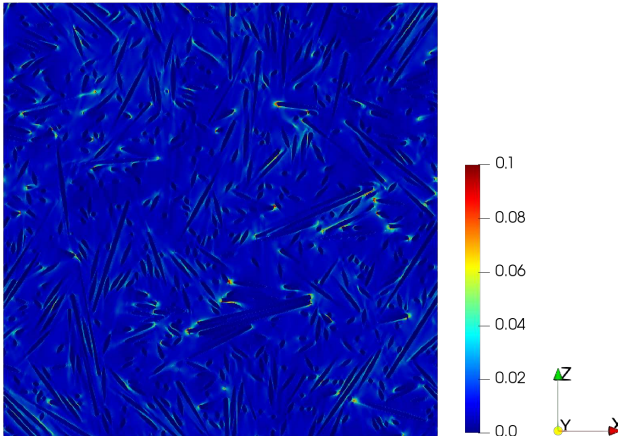
Practical performance - FRP



Planar isotropic SFRP

↗ [MS, Computational Mechanics, 2020]

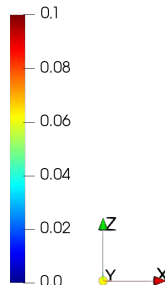
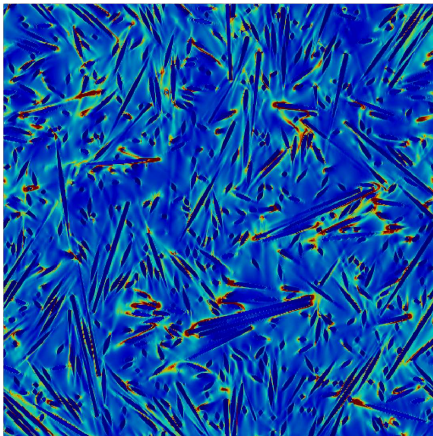
Practical performance - FRP



Planar isotropic SFRP - strain magnitude @ 1% strain

↗ [MS, Computational Mechanics, 2020]

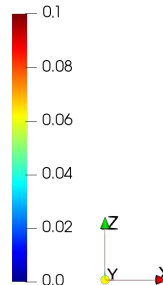
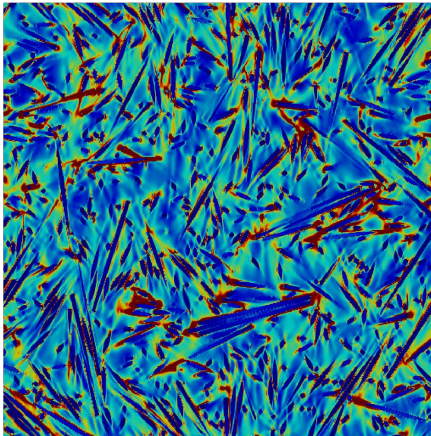
Practical performance - FRP



Planar isotropic SFRP - strain magnitude @ 2% strain

↗ [MS, Computational Mechanics, 2020]

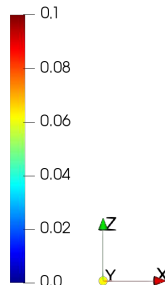
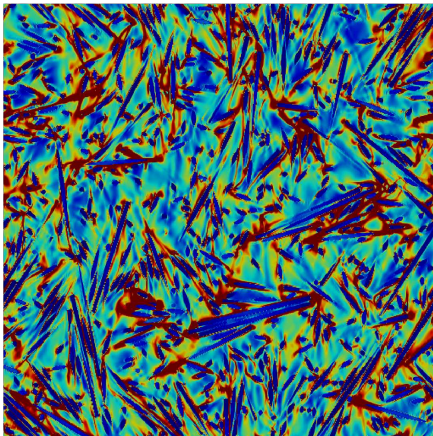
Practical performance - FRP



Planar isotropic SFRP - strain magnitude @ 3% strain

↗ [MS, Computational Mechanics, 2020]

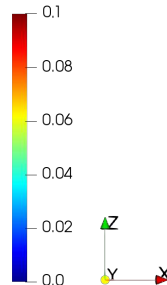
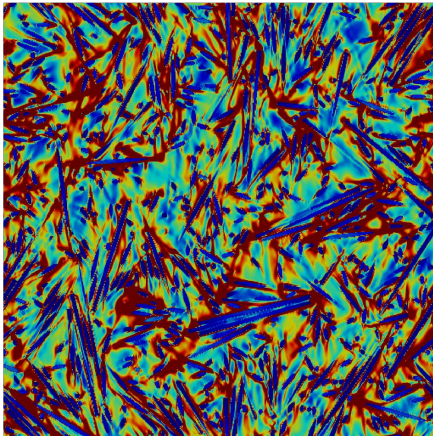
Practical performance - FRP



Planar isotropic SFRP - strain magnitude @ 4% strain

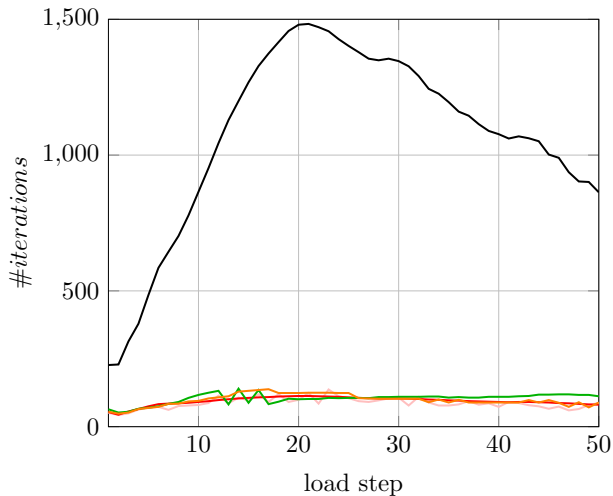
↗ [MS, Computational Mechanics, 2020]

Practical performance - FRP



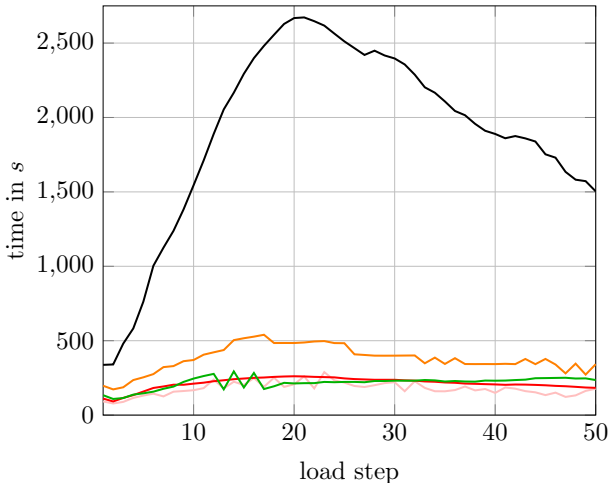
Planar isotropic SFRP - strain magnitude @ 5% strain

↗ [MS, Computational Mechanics, 2020]



— Basic scheme — Barzilai-Borwein — Fletcher-Reeves — Newton-CG — L-BFGS (4)

Practical performance - FRP - run time



— Basic scheme — Barzilai-Borwein — Fletcher-Reeves — Newton-CG — L-BFGS (4)

↗ [MS, Computational Mechanics, 2020]

Overview

1. Accelerated gradient methods

2. Newton - CG

3. Adaptive parameter selection

4. Summary and conclusions

- speed vs. memory
- **adaptive** parameter selection !
- recommendations:

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

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

- not covered: Anderson (↗ L. Gélébart)
- not covered: polarization schemes (next lecture)

Acta Mech 232, 2051–2100 (2021)
<https://doi.org/10.1007/s00707-021-02962-1>



REVIEW AND PERSPECTIVE IN MECHANICS

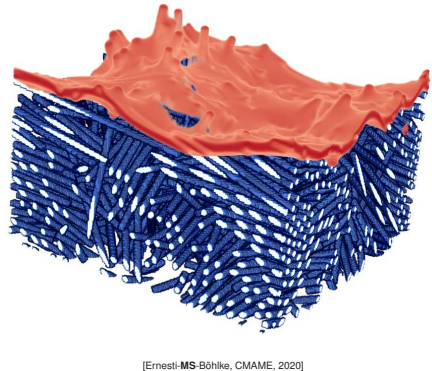
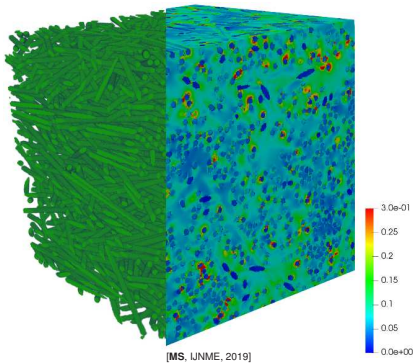
Matti Schneider 

A review of nonlinear FFT-based computational homogenization methods

Received: 9 December 2020 / Revised: 18 January 2021 / Accepted: 16 February 2021 / Published online: 24 March 2021
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Abstract Since their inception, computational homogenization methods based on the fast Fourier transform (FFT) have grown in popularity, establishing themselves as a powerful tool applicable to complex, digitized microstructures. At the same time, the understanding of the underlying principles has grown, in terms of both discretization schemes and solution methods, leading to improvements of the original approach and extending the applications. This article provides a condensed overview of results scattered throughout the literature and guides the reader to the current state of the art in nonlinear computational homogenization methods using the fast Fourier transform.

The end

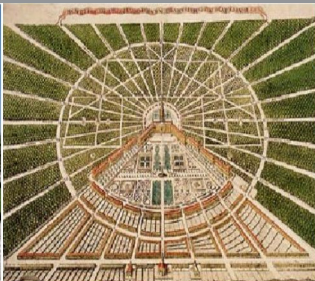


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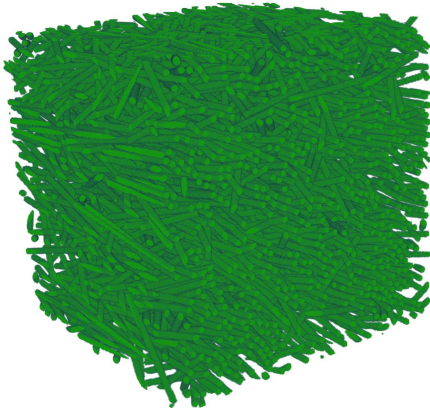
Matti Schneider

Polarization methods

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

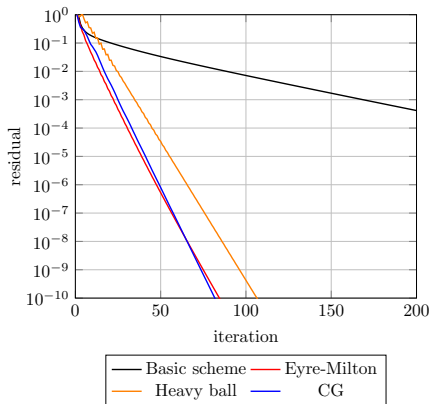


Practical performance - setup



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

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

The Eyre-Milton equation

Lippmann-Schwinger equation

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

The Eyre-Milton equation

Lippmann-Schwinger equation

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

The Eyre-Milton equation

Lippmann-Schwinger equation

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

■ $\sigma = S(\cdot, \varepsilon)$

The Eyre-Milton equation

Lippmann-Schwinger equation

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

■ $\sigma = S(\cdot, \varepsilon)$

The Eyre-Milton equation

Lippmann-Schwinger equation

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

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

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

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

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

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

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

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

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

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

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

The Eyre-Milton equation

Lippmann-Schwinger equation

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

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

The Eyre-Milton equation

Lippmann-Schwinger equation

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

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

The Eyre-Milton equation

Lippmann-Schwinger equation

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

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

The Eyre-Milton equation

Lippmann-Schwinger equation

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

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

The Eyre-Milton equation II

ε solves the Lippmann-Schwinger equation

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

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

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

The Eyre-Milton equation II

ε solves the Lippmann-Schwinger equation

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

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

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

► constant

The Eyre-Milton equation II

ε solves the Lippmann-Schwinger equation

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

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

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

► local in Fourier space

The Eyre-Milton equation II

ε solves the Lippmann-Schwinger equation

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

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

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

with

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

► local in real space

The Eyre-Milton equation II

ε solves the Lippmann-Schwinger equation

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

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

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

► unknown explicit on left-hand side

The Eyre-Milton method

Basic scheme

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

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

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

Basic scheme

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

Polarization scheme

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

- 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?

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

Damping basic scheme?

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

Damping basic scheme?

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

Damping basic scheme?

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

Damping basic scheme?

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

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?

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

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]

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

Convergence criterion

- if $P^k = \sigma^k + \mathbb{C}^0 : \varepsilon^k$,
then $\operatorname{div} \sigma^k \neq 0$ **and** $\varepsilon^k \neq \bar{\varepsilon} + \nabla^s u$
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equilibrium

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]

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

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]

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

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]

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

- use

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

Implementations

- two different implementations
- each with distinct advantages

Algorithm 1 Eyre-Milton scheme ($\bar{\varepsilon}$, maxit, tol, α_0 , γ)

- 1: $P \leftarrow S(\cdot, \varepsilon^0) + \mathbb{C}^0 : \varepsilon^0$ ▷ $\varepsilon^0 \equiv \bar{\varepsilon}$ or via extrapolation
 - 2: res $\leftarrow 1$
 - 3: $k \leftarrow 0$
 - 4: **while** $k < \text{maxit}$ **and** res $> \text{tol}$ **do**
 - 5: $k \leftarrow k + 1$
 - 6: $R \leftarrow P$
 - 7: $P \leftarrow (S - \mathbb{C}^0)(S + \mathbb{C}^0)^{-1}(P)$ ▷ compute $\bar{\sigma}$
 - 8: $P \leftarrow 2\mathbb{C}^0 : \bar{\varepsilon} + (\text{Id} - 2\Gamma) : P$ ▷ use FFT & favorite discretization
 - 9: res $\leftarrow 0.5\|P - R\|/\|\bar{\sigma}\|$
 - 10: $P \leftarrow \gamma R + (1 - \gamma)P$
 - 11: **end while**
 - 12: $\varepsilon \leftarrow (S + \mathbb{C}^0)^{-1}(P)$
 - 13: **return** $\varepsilon, \bar{\sigma}, \text{res}$ ▷ Requires two polarization fields
-

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

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

▷ basic step

▷ implicit solve

↗ [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

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

▷ basic step

▷ implicit solve

↗ [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

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

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

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

1: $e \leftarrow \varepsilon^0$ ▷ $\varepsilon^0 \equiv \bar{\varepsilon}$ or via extrapolation
2: $\sigma \leftarrow S(\cdot, \varepsilon^0)$
3: $\text{res} \leftarrow 1$
4: $k \leftarrow 0$
5: **while** $k < \text{maxit}$ **and** $\text{res} > \text{tol}$ **do**
6: $k \leftarrow k + 1$
7: $\bar{\sigma} \leftarrow \langle \sigma \rangle_Q$
8: $\varepsilon \leftarrow \sigma - \mathbb{C}^0 : e$
9: $\varepsilon \leftarrow \bar{\varepsilon} - 1/\alpha_0 \Gamma : \varepsilon$ ▷ use FFT & favorite discretization
10: $\text{res} \leftarrow \alpha_0 \|\varepsilon - e\|_{L^2} / \|\bar{\sigma}\|$
11: $\varepsilon \leftarrow (1 - 2\gamma)e + 2(1 - \gamma)\varepsilon$
12: $\begin{bmatrix} e \\ \sigma \end{bmatrix} \leftarrow \begin{bmatrix} (S + \mathbb{C}^0)^{-1}(\sigma + \mathbb{C}^0 : \varepsilon) \\ \sigma + \mathbb{C}^0 : (\varepsilon - e) \end{bmatrix}$
13: **end while**
14: **return** $e, \bar{\sigma}, \text{res}$ ▷ 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:

$$P \leftarrow (S - \mathbb{C}^0)(S + \mathbb{C}^0)^{-1}(P) \quad (\text{Implementation \# 1})$$

$$e \leftarrow (S + \mathbb{C}^0)^{-1}(\sigma + \mathbb{C}^0 : \varepsilon) \quad (\text{Implementation \# 2})$$

How to **invert** the stress function?

Overview

1. Polarization methods
2. Evaluating the Cayley operator
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The Cayley operator

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

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

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

- $S(x, \varepsilon) = C(x) : \varepsilon$

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

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

Linear elasticity

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

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

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

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

Beyond linear elasticity

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

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

■ digression:

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

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

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"disassemble" P

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

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

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

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

"disassemble" P :

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

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

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

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

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

■ digression:

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

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

"disassemble" P :

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

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

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

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

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"disassemble" P :

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

Hook-type materials

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

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

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

Hook-type materials & polarization

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

- classically: ε given, σ sought

Hook-type materials & polarization

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

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

Hook-type materials & polarization

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

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

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

Hook-type materials & polarization

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

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

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

Hook-type materials & polarization

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

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

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

Hook-type materials & polarization

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

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

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

Hook-type materials & polarization

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

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

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

Hook-type materials & polarization

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

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

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

Hook-type materials & polarization

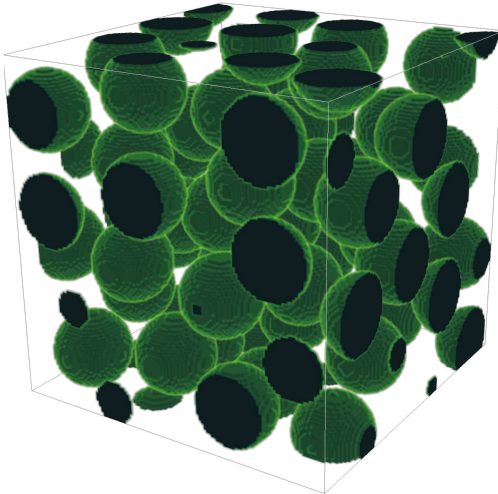
$$\begin{aligned}\sigma &= \mathbf{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\text{in}}) \\ 0 &= g(\sigma, z, \dot{z}) \quad \triangleright z = (\boldsymbol{\varepsilon}^{\text{in}}, \tilde{z})\end{aligned}$$

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

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

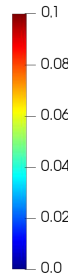
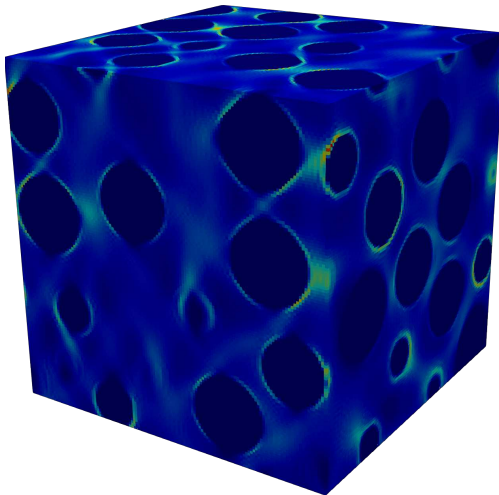
- solving for σ **implicitly** \equiv computing σ **explicitly**

Practical performance - setup



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

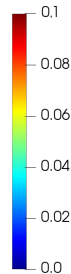
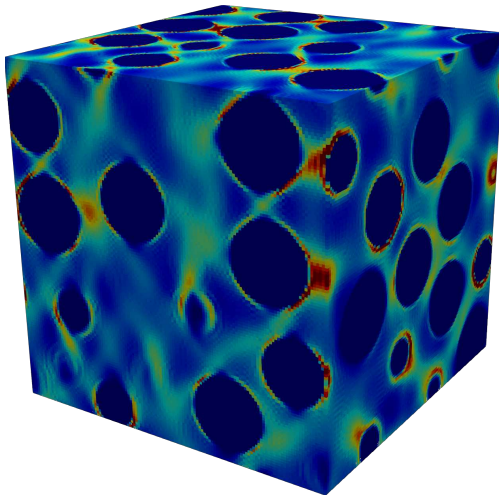
Practical performance - fields



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

plastic strain @ 1% strain

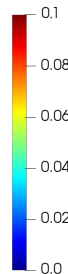
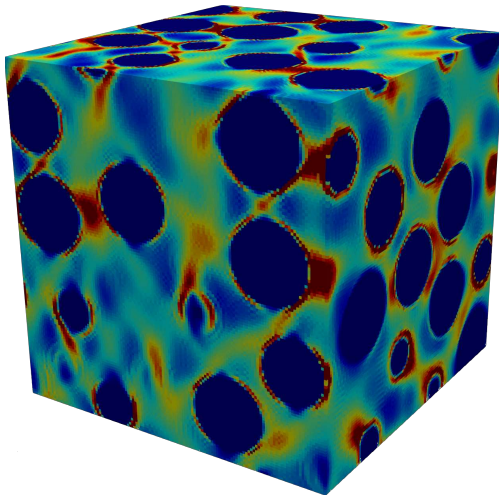
Practical performance - fields



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

plastic strain @ 2% strain

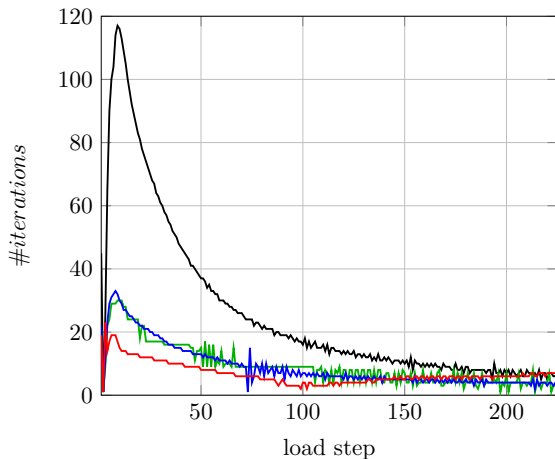
Practical performance - fields



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

plastic strain @ 3% strain

Practical performance - iterations



— Basic scheme — Barzilai-Borwein — Nonlinear CG — Polarization, $\gamma = 1/4$

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

↗ average iterations for 225 load steps

performance of
polarization schemes



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

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

Goal:

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

explicit gradient descent

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

↗ unstable for $s \gg 1$

Goal:

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

implicit gradient descent

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

Goal:

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

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↗ stable for any $s > 0$

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

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

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

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↗ stable for any $s > 0$

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

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

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

■ $\lambda \equiv s/2$

Composite optimization

Goal:

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

semi-implicit gradient descent

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

■ $\lambda \equiv s/2$

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Goal:

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

semi-implicit gradient descent

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

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

■ $\lambda \equiv s/2$

Composite optimization

Goal:

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

semi-implicit gradient descent

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

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

■ $\lambda \equiv s/2$

Composite optimization

Goal:

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

semi-implicit gradient descent

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

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

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

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

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

■ $\lambda \equiv s/2$

Composite optimization



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semi-implicit gradient descent

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

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Composite optimization

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semi-implicit gradient descent

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

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

Composite optimization

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semi-implicit gradient descent

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

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Composite optimization



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Composite optimization

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semi-implicit gradient descent

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

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

Composite optimization

Goal:

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

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

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

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

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

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

Application to hyperelasticity

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

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

- 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

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

- import knowledge from optimization
- Eyre-Milton \iff Douglas-Rachford splitting
- Michel-Moulinec-Suquet \iff 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:

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

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makes **no sense** for $\alpha_- = 0$

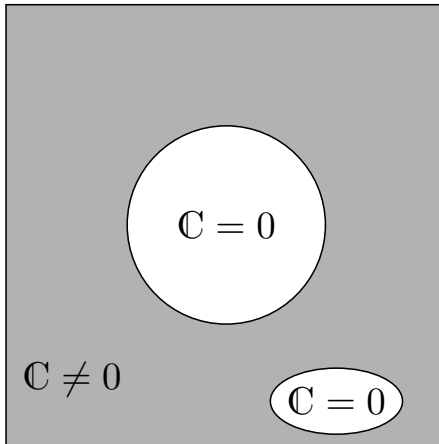
Why?

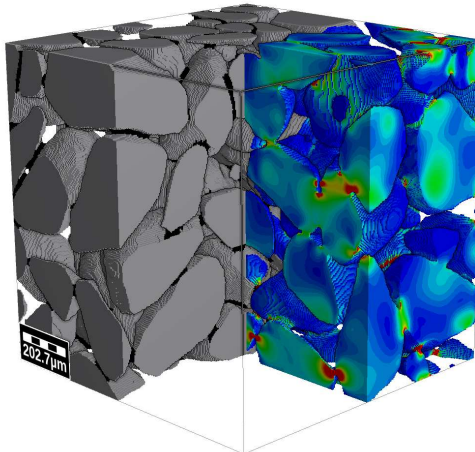
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makes **no sense** for $\alpha_- = 0$ ↗ porous materials

Porous materials - schematic





bound sand grains

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



- 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]

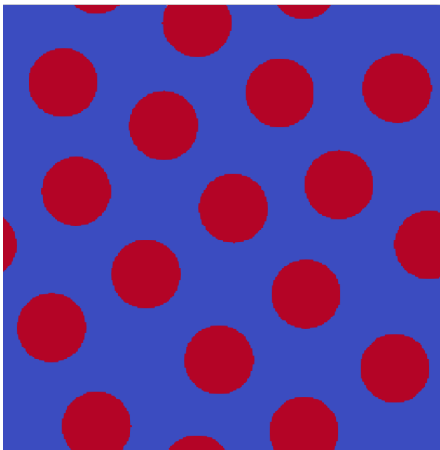
[MS, F. Ospald, and M. Kabel, International Journal for Numerical Methods in Engineering, 2016]

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

Minimal example - geometry

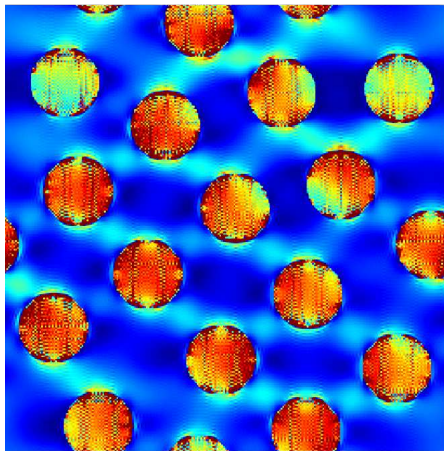


Universität
franco-allemande
Deutsch-Französische
Hochschule



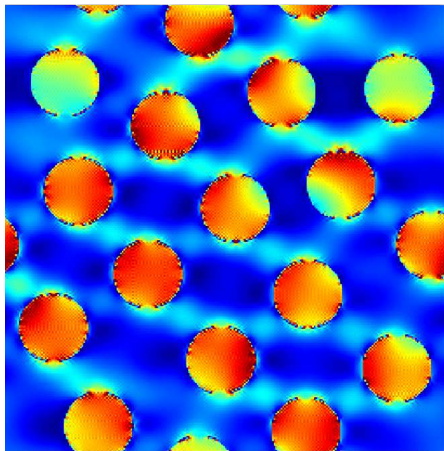
30% pores, 256^2 , quartz sand, $E = 66.9$ GPa and $\nu = 0.25$
5% strain in x

Minimal example - Moulinec-Suquet



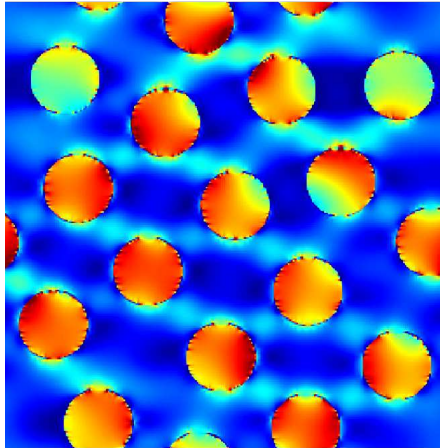
$$\|\varepsilon\|$$

Minimal example - rotated staggered



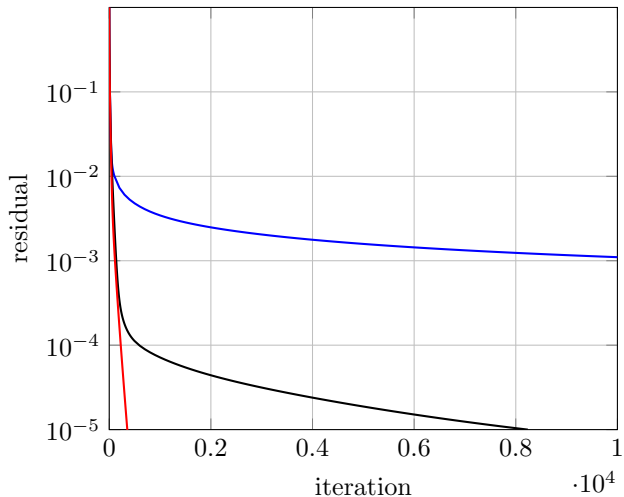
$$\|\varepsilon\|$$

Minimal example - staggered grid



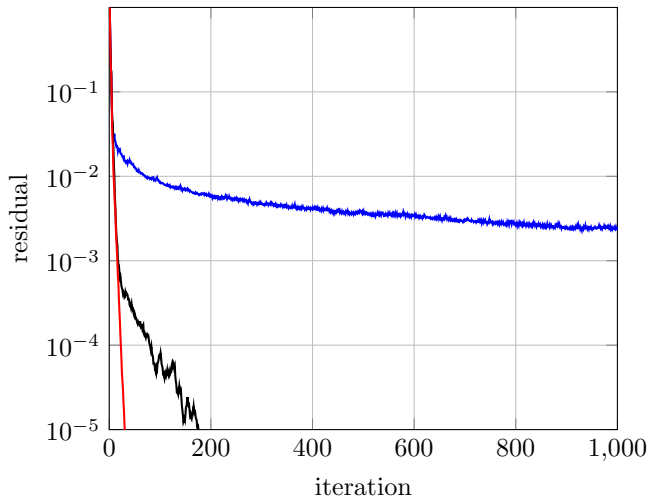
$$\|\varepsilon\|$$

Minimal example - basic



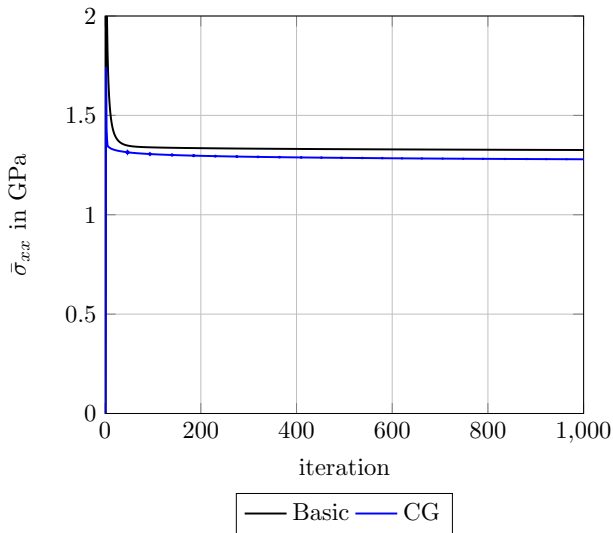
— Moulinec-Suquet — Rotated staggered — Staggered grid

Minimal example - CG

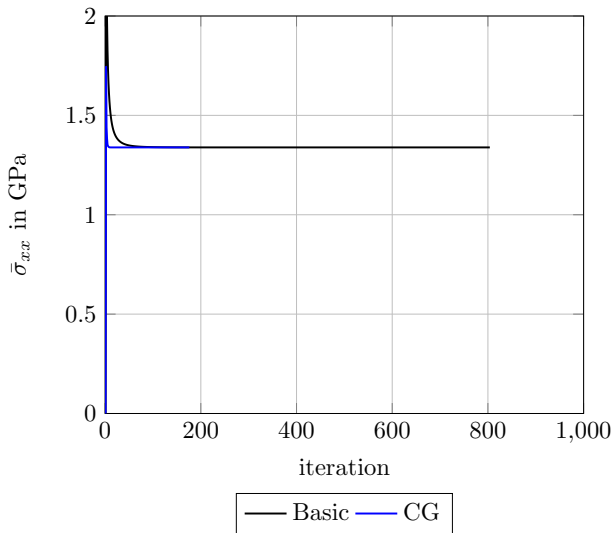


— Moulinec-Suquet — Rotated staggered — Staggered grid

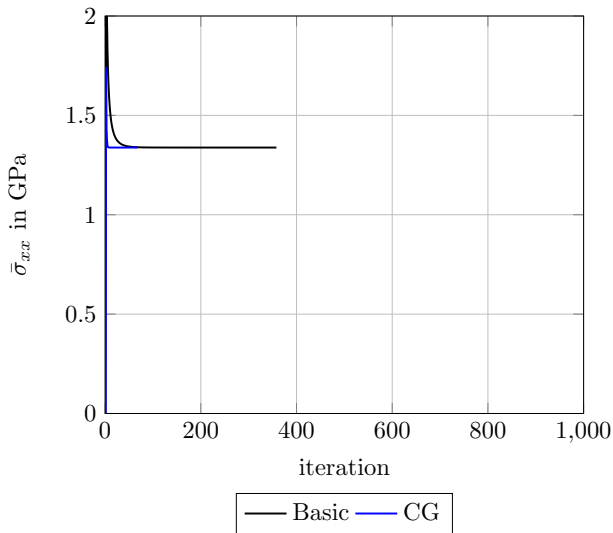
Minimal example - Moulinec-Suquet



Minimal example - Rotated staggered



Minimal example - Staggered grid



Upshot for porous microstructures

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

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

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

two flavors:

- Eyre-Milton ↗ less suitable for adaptivity

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

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■ Michel-Moulinec-Suquet

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■ 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]

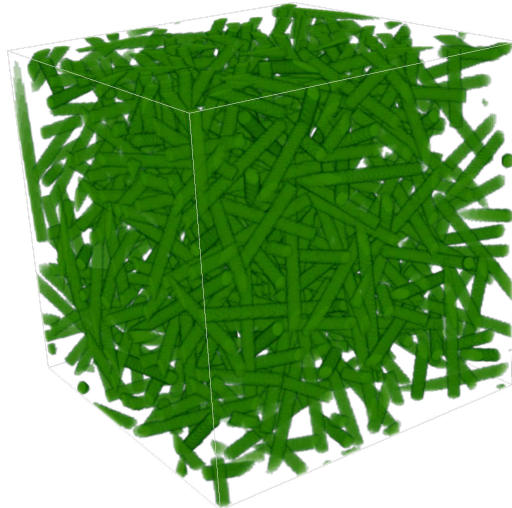
Algorithm 3 ADMM ($\bar{\varepsilon}, \text{maxit}, \text{tol}, \alpha_0 = \alpha_0^{\text{init}}, \gamma$)

1: $e \leftarrow \varepsilon^0$ ▷ $\varepsilon^0 \equiv \bar{\varepsilon}$ or via extrapolation
2: $\sigma \leftarrow S(\cdot, \varepsilon^0)$
3: $\text{res} \leftarrow 1$
4: $k \leftarrow 0$
5: **while** $k < \text{maxit}$ **and** $\text{res} > \text{tol}$ **do**
6: $k \leftarrow k + 1$
7: $\bar{\sigma} \leftarrow \langle \sigma \rangle_Q$
8: $\alpha_0 \leftarrow \|\sigma\|_{L^2} / \|e\|_{L^2}$
9: $\varepsilon \leftarrow \sigma - \mathbb{C}^0 : e$
10: $\varepsilon \leftarrow \bar{\varepsilon} - 1/\alpha_0 \Gamma : \varepsilon$ ▷ use FFT & favorite discretization
11: $\text{res} \leftarrow \alpha_0 \|\varepsilon - e\|_{L^2} / \|\bar{\sigma}\|$
12: $\varepsilon \leftarrow (1 - 2\gamma)e + 2(1 - \gamma)\varepsilon$
13: $\begin{bmatrix} e \\ \sigma \end{bmatrix} \leftarrow \begin{bmatrix} (S + \mathbb{C}^0)^{-1}(\sigma + \mathbb{C}^0 : \varepsilon) \\ \sigma + \mathbb{C}^0 : (\varepsilon - e) \end{bmatrix}$
14: **end while**
15: **return** $e, \bar{\sigma}, \text{res}$ ▷ Requires three fields

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

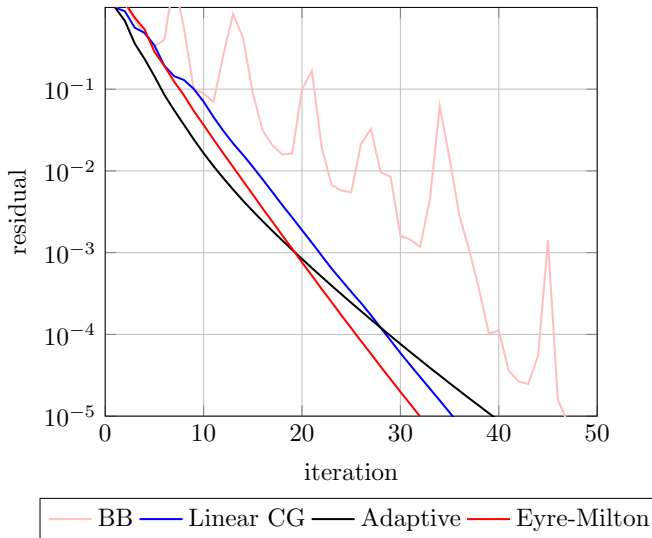
[MS, International Journal for Numerical Methods in Engineering, 2021]

Performance - setup

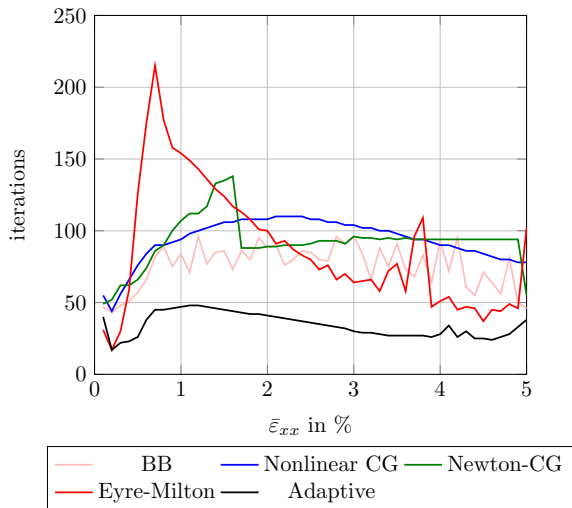


PA6, 15% short glass fibers

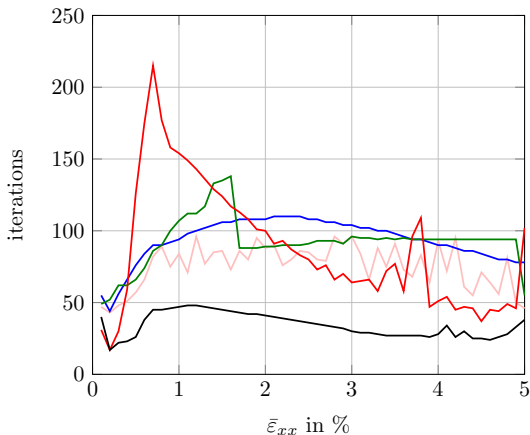
Performance - linear



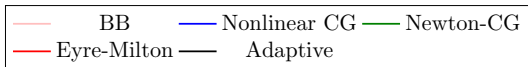
Performance - vM plastic

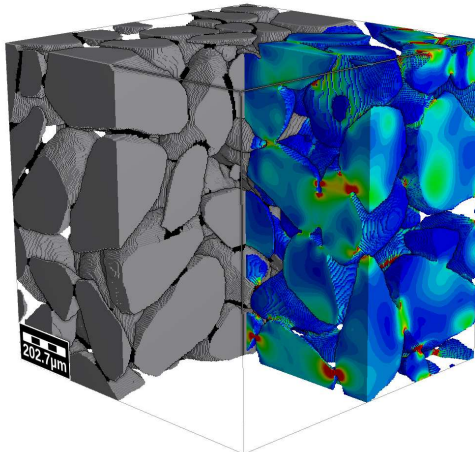


Performance - vM plastic



	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)

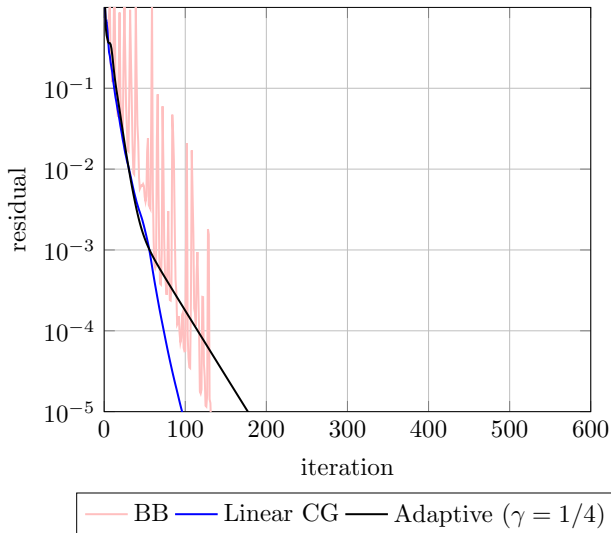




bound sand grains

[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

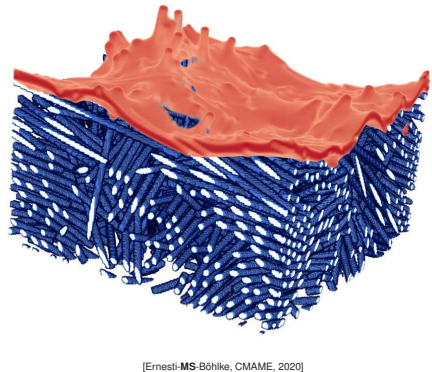
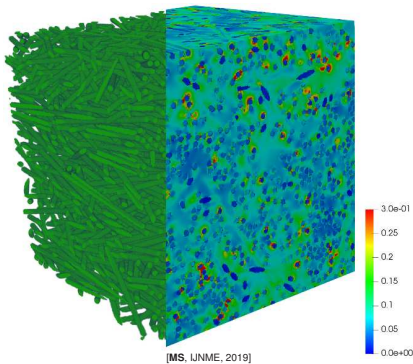
1. Polarization methods
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- polarization schemes specific to FFT-based methods
- extremely powerful
- not for beginners
- recommendations:

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



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Matti Schneider

Polarization methods: Implementation # 1 → # 2

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



Bonus - EM \rightarrow MMS

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

Bonus - EM \rightarrow MMS

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

■ $P^k = \sigma^k + \mathbb{C}^0 : e^k$

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Bonus - EM \rightarrow MMS

$$P^{k+1} = \gamma \sigma^k + \gamma \mathbb{C}^0 : e^k + (1 - \gamma) \sigma^k - (1 - \gamma) \mathbb{C}^0 : e^k + 2(1 - \gamma) \mathbb{C}^0 : \varepsilon^{k+1/2}$$

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Bonus - EM \rightarrow MMS

$$P^{k+1} = \sigma^k - (1 - 2\gamma) \mathbb{C}^0 : e^k + 2(1 - \gamma) \mathbb{C}^0 : \varepsilon^{k+1/2}$$

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Bonus - EM \rightarrow MMS

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

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Bonus - EM → MMS

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Bonus - EM \rightarrow MMS

$$P^{k+1} = \sigma^k + \mathbb{C}^0 : \varepsilon^k$$

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Bonus - EM \rightarrow MMS

$$\sigma^{k+1} + \mathbb{C}^0 : e^{k+1} = \sigma^k + \mathbb{C}^0 : \varepsilon^k$$

- $P^k = \sigma^k + \mathbb{C}^0 : e^k$
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Bonus - EM \rightarrow MMS

$$\sigma^{k+1} + \mathbb{C}^0 : e^{k+1} = \sigma^k + \mathbb{C}^0 : \varepsilon^k \quad \text{and} \quad \sigma^{k+1} + \mathbb{C}^0 : e^{k+1} = \sigma^k + \mathbb{C}^0 : \varepsilon^k$$

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Bonus - EM \rightarrow MMS

$$\sigma^{k+1} + \mathbb{C}^0 : e^{k+1} = \sigma^k + \mathbb{C}^0 : \varepsilon^k \quad \text{and} \quad \sigma^{k+1} + \mathbb{C}^0 : e^{k+1} = \sigma^k + \mathbb{C}^0 : \varepsilon^k$$

- $P^k = \sigma^k + \mathbb{C}^0 : e^k$ with $\sigma^k = S(\cdot, e^k)$
- $\tau^k = \sigma^k - \mathbb{C}^0 : e^k \equiv Z^0(P^k)$
- $Y^0 = \text{Id} - 2\mathbb{C}^0 : \Gamma^0$
- $\varepsilon^{k+1/2} = \bar{\varepsilon} - \Gamma^0 : \tau^k$
- $\varepsilon^k = (1 - 2\gamma) e^k + 2(1 - \gamma) \varepsilon^{k+1/2}$

$$S(\cdot, e^{k+1}) + \mathbb{C}^0 : e^{k+1} = \sigma^k + \mathbb{C}^0 : \varepsilon^k \quad \text{and} \quad \sigma^{k+1} + \mathbb{C}^0 : e^{k+1} = \sigma^k + \mathbb{C}^0 : \varepsilon^k$$

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Bonus - EM \rightarrow MMS

$$S(\cdot, e^{k+1}) + \mathbb{C}^0 : e^{k+1} = \sigma^k + \mathbb{C}^0 : \varepsilon^k \quad \text{and} \quad \sigma^{k+1} = \sigma^k + \mathbb{C}^0 : (\varepsilon^k - e^{k+1})$$

- $P^k = \sigma^k + \mathbb{C}^0 : e^k$ with $\sigma^k = S(\cdot, e^k)$
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$$S(\cdot, e^{k+1}) + \mathbb{C}^0 : e^{k+1} = \sigma^k + \mathbb{C}^0 : \varepsilon^k \quad \text{and} \quad \sigma^{k+1} = \sigma^k + \mathbb{C}^0 : (\varepsilon^k - e^{k+1})$$



$$\varepsilon^{k+1/2} = \bar{\varepsilon} - \Gamma^0 : (\sigma^k - \mathbb{C}^0 : e^k)$$

$$\varepsilon^k = (1 - 2\gamma) e^k + 2(1 - \gamma) \varepsilon^{k+1/2}$$

The RVE method for random sets and homogenization problems

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Introduction to FFT methods – Mines Paris, March 16, 2022

Outline

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Preliminary on random set theory

Covariance, integral range and RVE

The RVE method in homogenization

Conclusion

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Introduction

Context and motivation

- ▶ The mechanical properties of materials are strongly influenced by their microstructure. A key issue in materials science consists in studying and describing material microstructures by quantitative rigorous means.
- ▶ Experimental imaging is a straightforward method to probe material microstructure.
- ▶ Yet, a mathematically-rigorous approach must also be considered : that of probabilistic models of structures , a.k.a. as stochastic materials.
- ▶ In this lecture, our aim is to introduce basic notions on random set theory and methods, applications that allow one to characterize experimental materials and structures, and tools for studying the representativity of material images with respect to their apparent properties.

Example : inclusions in a matrix

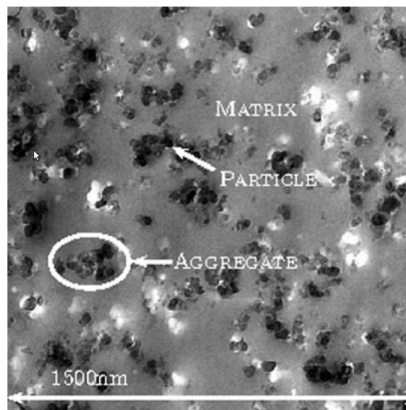


FIGURE – Inclusion of black carbon particles in a rubber matrix (Jean et al., Journal of microscopy, 2011).

Example : Coldspray film

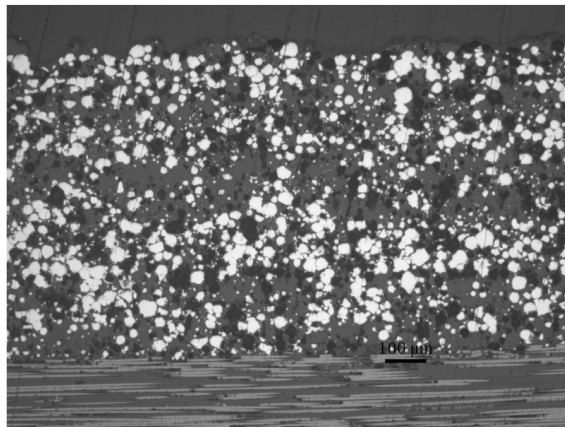
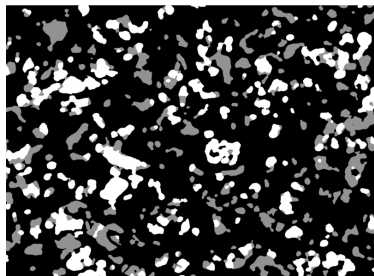
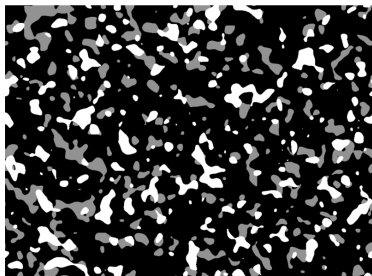


FIGURE – Coating made from a coldsprayed thin film (Bortolussi et al., 2018).

Example : fuel cell



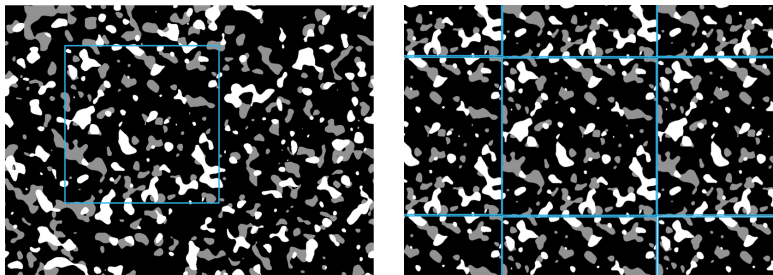
SEM image (segmented)



Model

FIGURE – Multi-phasic anode material from cold-spray (Abdallah et al., 2016).

Example : fuel cell



Compute the physical response on many subvolumes assuming periodic boundary conditions (as in FFT). Does the mean apparent property tends to the effective property as the number of subvolumes $\rightarrow \infty$?

Models of random structures

- ▶ Microstructure models must be able to account for a wide range of geometries
- ▶ They must enable the study of various physical and mechanical properties
- ▶ These models are interesting in that they rely on strong mathematical foundations

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Models of random structures

- ▶ Random set theory : modern developments originate in the works of Choquet (1954), Matheron (1965) and Kendall (1974). It aims to quantify and simulate the morphology of heterogeneous media by probabilistic means.
- ▶ A random set is usually a stochastic model whose realizations are closed subsets of \mathbb{R}^d ($d = 2$ or 3 is the dimension). More generally, scalar or tensorial functions on \mathbb{R}^d (or on a manifold).
- ▶ Random sets based on a *rigorous* definition theorized by G. Matheron, defined as random variables in an appropriate metric space. The probability distribution function of a random set is completely specified by a probability measure defined on a σ -algebra, that is, a space containing \mathbb{R}^d , the empty set, and which is stable by a countless number of unions and intersections and by complement. This algebra is used to define measures on sets of \mathbb{R}^d .

Models of random structures

Early attempts on specific models (Rice, S.O., 1944 ; Miles, R.E., 1964). The general theory and modern understanding was initiated by Matheron and Kendall.

References :

- ▶ Matheron, G. (1975). Random Sets and Integral Geometry, Wiley, New York.
- ▶ Kendall, D. (1974). Foundations of a theory of random sets.
- ▶ Serra, J. (1983). Image Analysis and Mathematical Morphology. Academic Press, Cambridge.
- ▶ Lantuéjoul (2002). Geostatistical Simulation : Models and Algorithms. Springer, Berlin, Chapter 2.
- ▶ Schneider, R., Weil, W. (2008). Stochastic and Integral Geometry. Springer-Verlag, Berlin, Heidelberg.

Models of random structures

The theory of random sets originate in image analysis (or mathematical morphology), i.e. the interest in finding criteria for characterizing random sets.

Usually, this is achieved in two steps : (i) a transformation of the set ; (ii) a measure on the transformed set. Mathematical morphology considers transformations that involve comparing two sets, one of them called the “structuring element”.

Models of random structures

The fundamental theoretical tool for characterizing random sets is the Choquet capacity (Choquet, 1954) :

$$T(K) = P\{X \cap K \neq \emptyset\}, \quad (1)$$

The Choquet capacity satisfies :

- i) $0 \leq T(K) \leq 1$ for any compact subset K , and $T(\emptyset) = 0$,
 $T(\mathbb{R}^d) = 1$,
- ii) $T(K) \leq T(K \cup K')$ all compact subsets K and K' ,
- iii) If K_n is a sequence of decreasing compact subsets (for inclusion) in \mathbb{R}^d , with limit \mathcal{K} , then

$$\lim_{n \rightarrow \infty} T(K_n) = T(\mathcal{K}).$$

Models of random structures

The “hitting functional” T “Choquet capacity” plays the same role for random sets with inclusion as that of the cumulative distribution function for random scalar variables with order relation $<$ (Matheron, 1975). This interpretation is justified by the following theorem (Choquet 1954; Kendall 1974; Matheron 1975) :

Theorem Let T be a functional defined on the set of compact subsets \mathbb{K} of \mathbb{R}^d . Then a single probability measure P defined on the σ -algebra \mathbb{F}_K exists such that :

$$P(\mathbb{F}_K) = T(K),$$

if, and only if, T is a Choquet capacity verifying (i), (ii) and (iii) in the previous slide.

Models of random structures

The σ -algebra \mathbb{F}_K is then the smallest σ -algebra containing the closed sets that meet the compact subsets of \mathbb{R}^d :

$$\mathbb{F}_K = \{F \in \mathbb{F} : F \cap K \neq \emptyset\}, \quad K \in \mathbb{K},$$

where \mathbb{F} is the set of the closed subsets of \mathbb{R}^d and \mathbb{K} the set of compact subsets.

This property allows one to define random structures, but also to characterize them.

Models of random structures

Stationarity : a random set is stationary iff its Choquet capacity is translation-invariant : $T(K) = T(K_x)$ for all x .

Isotropy : the Choquet capacity is rotation-invariant.

Ergodicity : all realizations of the random set model have the same Choquet capacity. There are other definitions of ergodicity, see Heinrich, 1992.

Models of random structures

Example : the Boolean random set with homogeneous Poisson point process \mathcal{P} of intensity θ and primary grain G .

$$T(K) = 1 - e^{-\theta \bar{\mu}_d(G \oplus \check{K})}$$

where $\check{K} = \{-\mathbf{x} | \mathbf{x} \in K\}$, \oplus is the Minkowski addition :

$$G \oplus \check{K} = \{\mathbf{x} | K_{\mathbf{x}} \cap G \neq \emptyset\} \quad (K_{\mathbf{x}} = \{\mathbf{x} + \mathbf{y} | \mathbf{y} \in K\}).$$

This capacity is that of realizations of the Boolean model (Serra, 1981) :

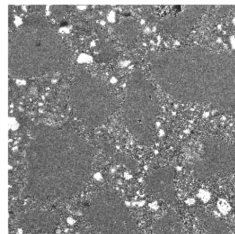
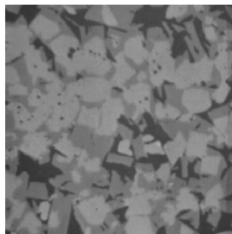
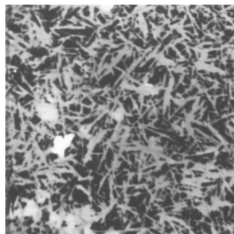
$$X = \bigcup_{x \sim \mathcal{P}} G_x$$

The set X is stationary and ergodic.

Boolean models can be considered to play the same role as the normal distribution for random sets with addition replaced by union. There exists the equivalent of a central limit theorem for random sets, where unions of i.i.d. random sets asymptotically tend to Boolean sets (Serra, 1981).

Models of random structures

Random media (microstructures) that fit with Boolean model



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Covariance

Probe the microstructure with compact sets. Spatial law : set of points $K = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$ ($n \geq 1$).

Examples :

- ▶ $K = \{\mathbf{x}\}$. Then : $T(K) = P\{\mathbf{x} \in X\}$.
- ▶ Linear erosion : $K = \{\mathbf{x} + s(\mathbf{y} - \mathbf{x}) \mid 0 \leq s \leq 1\}$.
- ▶ Covariance : $K = \{\mathbf{x}, \mathbf{y}\}$. Then :
 $T(K) = P\{\mathbf{x} \in X \text{ and } \mathbf{y} \in X\} = C(\mathbf{x}, \mathbf{y})$.

Covariance

Useful properties of the covariance function :

- ▶ For stationary media, the covariance depends only on $\mathbf{h} = \mathbf{x} - \mathbf{y}$:
 $C(\mathbf{h}) = C(\mathbf{x}, \mathbf{y})$.
- ▶ For isotropic random sets, $C(h) = C(\mathbf{x}, \mathbf{y})$ where $h = |\mathbf{x} - \mathbf{y}|$ is a one-dimensional function.
- ▶ $C(0) = V(X)$ the mean d -dimensional volume fraction of X .
- ▶ $\lim_{h \rightarrow \infty} C(h) = C(0)^2$
- ▶ $C(X; h) = 1 - 2C(X^c; 0) + C(X^c; h)$ where X^c is X 's complementary set
- ▶ $C(h)$ is periodic if the set X is periodic
- ▶ If $C(h)$ admits the Taylor expansion $C(h) = C(0) - c_0 h + O(h^2)$, c_0 is the specific surface area in dimension 3, or specific perimeter, in dimension 2, of the set X .
- ▶ $C(h) - C(0) \sim h^\nu$ ($0 < \nu < 1$) for a fractal set X of Hausdorff dimension $d_h = 3 - \nu$ (Matheron, 1989).
- ▶ Anti-correlation phenomena, mean length of cords, angular points, cusp are some of the geometrical properties that can be related to covariances (e.g. Emery and Lantuéjoul, 2011)

Covariance examples

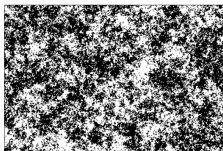
Any function does not define a covariance. Covariances are definite positive :

$$\sum_{\alpha, \beta=1}^n \lambda_{\alpha} \lambda_{\beta} C(h_{\alpha} - h_{\beta}) \geq 0, \quad \lambda_{\alpha}, h_{\alpha} \in \mathbb{R}.$$

Some exact covariances.

Stable

$$C(h) = e^{-\sqrt{|h|/a}}$$



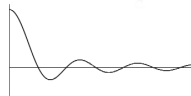
Gaussian

$$C(h) = e^{-|h|^2/a^2}$$



Cardinal sine

$$C(h) = \frac{\sin(|h|/a)}{|h|/a}$$



Covariance examples

For a Boolean model of primary grains G ,

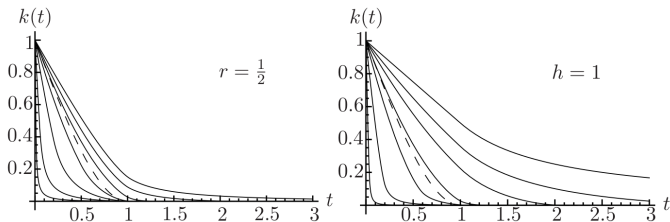
$$C(h) = 2p - 1 + (1 - p)^{2 - k(h)/k(0)}$$

with k the covariogram :

$$k(h) = \langle |G \cap G_h| \rangle_{|h|=h}$$

where the mean is taken over all directions.

Ex : covariogram of cylinders with varying aspect ratio (first obtained by



Gille, 1987)

Integral range

The integral range, homogeneous to a d -dimensional volume, is by definition :

$$A_d = \int_{h \in \mathbb{R}^d} d^d \mathbf{h} \frac{C(\mathbf{h}) - C(0)^2}{C(0)[1 - C(0)]}$$

where $p = C(0)$ is the density of X .

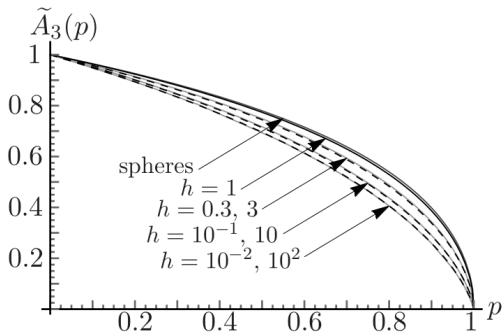
For isotropic models :

$$A_d = \frac{1}{p(1-p)} \int_{h=0}^{\infty} S_d dh [C(h) - p^2]$$

where S_d is the surface of the d -dimensional sphere.

Integral range

Example : integral range of Boolean models of cylinders vs. density p (in units of primagry grain volume).



Varying aspect ratios (Willot, 2017)

Representative volume element

Variance $D_X^2(V)$ of the apparent density of a stationary random set X , computed on d -dimensional domain Ω of volume V :

$$D_X^2(V) = \left\langle \left(\bar{\rho} - \frac{1}{V} \int_{\Omega} d^d \mathbf{x} \chi_X(\mathbf{x}) \right)^2 \right\rangle$$

computed over random realizations of X , where $\bar{\rho}$ is the observed mean density, computed over all realizations and χ_X the characteristic function of X . For ergodic media, the mean can be computed over subvolumes “sufficiently” far from each other.

Representative volume element

For $N \gg 1$ we have $\bar{p} \rightarrow p$ and :

$$D_X^2(V) = \frac{1}{NV^2} \sum_{i=1}^N \int_{\mathbf{x}, \mathbf{y} \in \Omega} d^d \mathbf{x} d^d \mathbf{y} [\chi_X(\mathbf{x}) \chi_X(\mathbf{y}) - p^2].$$

Property : when $V \gg A_d$:

$$D_X^2(V) = p(1-p) \frac{A_d}{V} + o(1/V).$$

Representative volume element

Proof :

$$D_X^2(V) = \frac{1}{NV^2} \sum_{i=1}^N \int_{\mathbf{x}, \mathbf{y} \in \Omega} d^d \mathbf{x} d^d \mathbf{y} [\chi_X(\mathbf{x}) \chi_X(\mathbf{y}) - \rho^2].$$

Use the variable change $\mathbf{t} = \mathbf{x} - \mathbf{y}$.

Representative volume element

Interpretation of the relation :

$$D_X^2(V) = p(1-p)\frac{A_d}{V} + o(1/V).$$

When $V \gg A_d$,

$$D_X^2(V) \sim \frac{\text{var}(\chi(0))}{V/A_d}$$

where $\text{var}(\chi(0))$ is the point variance and $n = V/A_d$ is the volume size, expressed in units of integral range.

The $D_X^2(V) = \text{var}(\chi(0))/n$ represents the variance of a mean of n independent observations. This is as if the domain V had been divided into n independent domains of the same size A_d . A_d must then be interpreted as the scale of the phenomenon (see Lantuéjoul, 1991).

Representative volume element

Special case : when $A_d = 0$ (possible when anti-correlations are present), the variance displays “super-convergence”, i.e. goes to 0 faster than $1/V$.



Fig. 7. Realization of an SERF with a zero integral range (dilution random function).

From Lantuéjoul (1991). Dilution function : $\sum_{\mathbf{y} \in \mathcal{P}} f(\mathbf{x} - \mathbf{y})$ with $\langle f \rangle = 0$.

Representative volume element

Extensions and properties.

Miles-Lantuéjoul correction for subvolumes V of a larger volume V_0 (Lantuéjoul, 1991) :

$$D_X^2(V) = p(1-p) \frac{A_d}{V} \left(1 - \frac{V}{V_0}\right) + o(1/V).$$

Interpretation : the mean of the values computed on subvolumes is biased (equal to that in V_0), hence there are two sources for the variance, that of “regular” domains of volume V and that for V_0 .

Representative volume element

The absolute and relative errors for n samples of volume V are defined as :

$$\varepsilon_{\text{abs}} = \frac{2D_X(V)}{\sqrt{n}}, \quad \varepsilon_{\text{rela}} = \frac{\varepsilon_{\text{abs}}}{p} = \frac{2D_X(V)}{p\sqrt{n}}$$

The RVE size for a given relative precision $\varepsilon_{\text{rela}}$ is then :

$$V_{\text{RVE}} = \frac{4\text{var}(\chi(0))A_d}{n\varepsilon_{\text{rela}}^2 p^2}$$

Note the $\varepsilon_{\text{rela}}^2$ term. This is because ε is proportional to the standard deviation. Hence, one additional digit of precision requires in general $100\times$ -larger volume size.

Representative volume element

The precision of a given prediction can conversely be computed as :

$$\varepsilon_{\text{rela}} = \frac{2\text{std}(\chi(0))\sqrt{A_d}}{\rho\sqrt{nV_{\text{RVE}}}}$$

In terms of absolute error :

$$V_{\text{RVE}} = \frac{4\text{var}(\chi(0))A_d}{n\varepsilon_{\text{abs}}^2}$$

$$\varepsilon_{\text{abs}} = \frac{2\text{std}(\chi(0))\sqrt{A_d}}{\sqrt{nV_{\text{RVE}}}}$$

Representative volume element

Example : Voronoi tessellation of space (Kanit et al, 2003) Every cell colored at random.

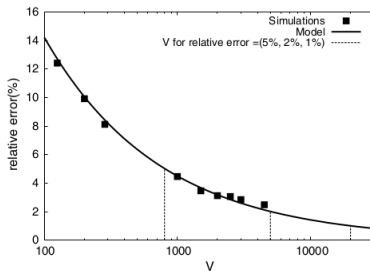


Fig. 14. Relative precision ϵ_{rel} for volume fraction $P = 70\%$ and $n = 1$ realization: It decreases when the size of the domain increases.

RVE for random fields

Straightforward extension of the theory to random functions, i.e. *scalar fields*. Spatial distribution of an ergodic, stationary random function $Z(\mathbf{x})$:

$$F_{x_1, \dots, x_n}(z_1, \dots, z_n) = P\{Z(\mathbf{x}_i) < z_i\}$$

The spatial distribution can be extended to a unique probability measure on a σ -algebra (Kolmogorov, 1933; Neveu, 1965).

Covariogram :

$$K(\mathbf{h}) = \int_{\mathbb{R}^d} d\mathbf{x} Z(\mathbf{x}) Z(\mathbf{x} + \mathbf{h})$$

Covariance : $C(\mathbf{h}) = \text{Cov}(Z(\mathbf{x}), Z(\mathbf{x} + \mathbf{h})) = K(\mathbf{h}) - \rho^2$ where
 $\rho = \int_{\mathbb{R}^d} d\mathbf{x} Z(\mathbf{x})$

Integral range :

$$A_d = \int_{\mathbb{R}^d} d\mathbf{h} [C(\mathbf{h}) - C(0)^2] = \lim_{V \rightarrow \infty} \frac{VD_Z^2(V)}{\text{var}(Z(\mathbf{x}))}$$

Extensions to vectorial (Jeulin, 1990) and tensorial fields are delicate.

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The RVE method in homogenization

To apply Matheron's formula to random fields from stochastic homogenization one need to solve two problems :

- ▶ (i) The random fields are NOT stationary when boundary conditions are applied on a volume element ;
- ▶ (ii) Unknown correlations length.

Solution for these two issues :

- ▶ Problem (i) can be solved by considering the solutions of auxiliary problems with stationary fields that approximate (in a way that can be controlled) the fields of interest.
- ▶ Problem (ii) can be tracted for certain problems by applying Matheron's techniques on the auxiliary fields. Correlation length are provided by the Green operator.

The RVE method in homogenization

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Solution for these two issues for elliptic problems :

- ▶ Problem (i) can be solved by considering the solutions of auxiliary problems with stationary fields that approximate (in a way that can be controlled) the fields of interest.
- ▶ Problem (ii) can be treated for certain problems by applying Matheron's techniques on the auxiliary fields. Correlation lengths are provided by the Green operator.

Main results obtained by Yurinskii (Sibirsk Mat. Zh. ; 1986), Naddaf and Spencer (1998) and the theory subsequently developed by Gloria and Otto (2011). More general results by Kozlov (1979), Papanicolaou and Varadhan (1981) and Künnemann (1983) in the continuum and discrete case, with ergodic hypothesis.

The RVE method in homogenization

Consider the simple case of a d -dimensional lattice \mathbb{Z}^d with random conductivity $a(\mathbf{x}, \mathbf{x})$ along each bond connecting \mathbf{x} and $\mathbf{y} = \mathbf{x} + \mathbf{e}_j$.

“Conductivity” problem with macroscopic loading ξ for the gradient field :

$$-\nabla^* \cdot [A(\xi + \nabla\Phi)](\mathbf{x}) = \sum_{|\mathbf{x}-\mathbf{y}|=1} = a(\mathbf{x}, b\mathbf{m}\mathbf{y})[\phi(\mathbf{x}) - \phi(\mathbf{y})] = 0.$$

Hypothesis :

- ▶ Uniform ellipticity :

$$0 < \alpha \leq a(\mathbf{x}, b\mathbf{m}\mathbf{y}) \leq \beta$$

for some $\alpha, \beta < \infty$.

- ▶ The $a(\mathbf{x}, b\mathbf{m}\mathbf{y})$ are independently and identically distributed ;

The RVE method in homogenization

Homogenized conductivity defined by :

$$\xi \cdot A_{\text{hom}} \xi = \langle (\xi + \nabla \phi) \cdot A(\xi + \nabla \phi) \rangle$$

where the mean is evaluated over random configurations (at any given point, since the model is stationary).

Since the corrector field ϕ is ergodic :

$$\sum (\xi + \nabla \phi) \cdot A(\xi + \nabla \phi) \eta_L \rightarrow \xi \cdot A_{\text{hom}} \xi$$

as $L \rightarrow \infty$ where η_L is an averaging function so that $\text{supp}(\eta_L) \subset \{|x| \leq L\}$, $|\eta_L| \lesssim L^{-d}$, $\sum \eta_L = 1$.

Convergence rate w.r.t. L ?

The RVE method in homogenization

Main problem : the field ϕ has to be solved on the whole space \mathbb{Z}^d (for a single realization).

It is natural to replace the field ϕ by the field ϕ_R solution of :

$$\begin{aligned} -\nabla^* \cdot [A(\xi + \nabla \Phi_R)] &= 0 && \text{in } \mathbb{Z}^d \cap \{|\mathbf{x}| < R\}, \\ \Phi_R &= 0 && \text{in } \mathbb{Z}^d \cap \{|\mathbf{x}| \geq R\}, \end{aligned}$$

where $R \gg L$.

However ϕ_R is not stationary anymore.

The RVE method in homogenization

The main idea in a nutshell : replace the elliptic PDE for the conductivity problem by :

$$\frac{1}{T} \phi_T - \nabla^* \cdot [A(\xi + \nabla \phi_T)] = 0$$

the field solution (ϕ_T) is

The zero-order term introduces a characteristic length $\sim \sqrt{T}$ in ϕ_T .

In a second step, one replaces the above PDE with :

$$\begin{aligned} \frac{1}{T} \phi_T - \nabla^* \cdot [A(\xi + \nabla \phi_{T,R})] &= 0 && \text{in } \mathbb{Z}^d \cap \{|\mathbf{x}| < R\}, \\ \phi_{T,R} &= 0 && \text{in } \mathbb{Z}^d \cap \{|\mathbf{x}| \geq R\}, \end{aligned}$$

with unknown $\phi_{T,R}$.

With suitable choice of R and L , $\phi_{T,R}$ (which can be computed) is a very good approximation of ϕ_T which is a very good approximation of ϕ as $T \rightarrow \infty$.

The RVE method in homogenization

Error we make when replacing :

$$\xi \cdot A_{\text{hom}} \xi \rightarrow \sum (\xi + \nabla \phi_T) \cdot A (\xi + \nabla \phi_T) \eta_L$$

Two sources of error : finite-size effects ($L \neq \infty$) and that related to the cut-off length-scale T :

$$\begin{aligned} \langle |\sum (\xi + \nabla \phi_T) \cdot A (\xi + \nabla \phi_T) \eta_L - \xi \cdot A_{\text{hom}} \xi|^2 \rangle &= \langle |\sum (\xi + \nabla \phi_T) \cdot A (\xi + \nabla \phi_T) \eta_L - \langle (\xi + \nabla \phi) \cdot A (\xi + \nabla \phi) \rangle|^2 \rangle \\ &= \underbrace{\text{var}[\sum (\xi + \nabla \phi_T) \cdot A (\xi + \nabla \phi_T) \eta_L]}_{\sim L^{-d} \text{ in the low-limit contrast}} + \underbrace{|\langle \sum (\xi + \nabla \phi_T) \cdot A (\xi + \nabla \phi_T) \eta_L \rangle - \langle (\xi + \nabla \phi) \cdot A (\xi + \nabla \phi) \rangle|^2}_{\langle (\nabla \phi_T - \nabla \phi) \cdot A (\nabla \phi_T - \nabla \phi) \rangle \text{ stationarity of } \phi, \phi_T} \\ &\quad \sim T^{-d} \text{ in the low-contrast limit} \end{aligned}$$

The RVE method in homogenization

The choice $L \sim \sqrt{T} \sim R$ is “optimal” in the sense that errors due to the cut-off can then be neglected and finite-size effects are the leading order term, which scales as :

$$\text{var} \left[\sum (\xi + \nabla \phi_T) \cdot A(\xi + \nabla \phi_T) \eta_L \right] \lesssim L^{-d}$$

In the above, an additional assumption on the smoothness of η_L is made : $|\nabla \eta_L| \lesssim L^{-d-1}$.

Proof in Gloria and Otto (2011), Annex A. Consider the low-contrast regime. In that setting, the Lippman-Schwinger equation gives an exact solution to first-order in the contrast, and depends only on the statistics of $A - \langle A \rangle$. Variations are given by derivatives w.r.t. $a(\mathbf{x})$, and the Green identity results in terms $\eta_L^2 \sim L^{-d}$.

The RVE method in homogenization

This leads to the scaling-law (Kozlov, Math. Sb, 1979) :

$$|\langle A_L \rangle - A_{\text{hom}}| \sim \begin{cases} C(\alpha, \beta)L^{-1} & \text{if } d = 2, \\ C(\alpha, \beta)L^{-3/2} & \text{if } d = 3, \\ C(\alpha, \beta)L^{-2} \log L & \text{if } d = 4, \\ C(d, \alpha, \beta)L^{-2} & \text{if } d \geq 5. \end{cases}$$

with $d = 4$ the critical dimension. Different from the result of random fields with finite correlation length.

The same scaling laws hold for periodic boundary conditions (Gloria, ESAIM, 2012). Results have been extended to the continuum (Gloria and Otto, 2018).

The RVE method in homogenization

Furthermore, fluctuations are asymptotically Gaussian :

Central limit theorem for the conductivity problem on a d -dimensional lattice (Gloria & Nolen, 2016) :

$$d_K \left(L^{d/2} \frac{A_{L,\#} - A_{\text{hom}}}{\sigma}, \mathcal{G} \right) \lesssim L^{-d/2} \log^d L, \quad L \rightarrow \infty$$

with d_K the Kolmogorov distance, $\sigma > 0$, \mathcal{G} a standard normal variable.
Conductivity i.i.d. bounded from below and above.

The RVE method in homogenization

For Dirichlet and Neuman boundary conditions :

$$|\langle A_{L,\#} \rangle - A_{\text{hom}}| \sim \begin{cases} C(\alpha, \beta) L^{-1/2} & \text{if } d = 2, \\ C(\alpha, \beta) L^{-1} & \text{if } d = 3. \end{cases}$$

In general, the fields are disturbed in a region along the surface with a width of the same order as the characteristic length in the microstructure. See Gloria and Mourrat (2012).

Representative volume element

Example : stress field in multi-scale rigidly-reinforced Boolean models in elasticity (Willot and Jeulin, 2010)

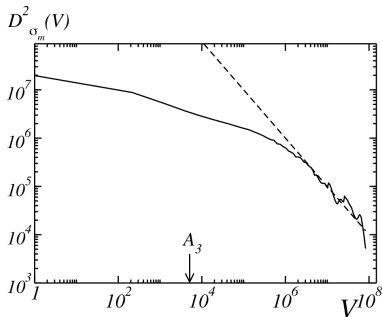
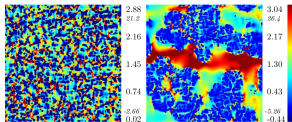


FIG. 10.7. Variance of the mean average stress field (σ_m), proportional to the material apparent bulk-modulus, as computed on volumes of size V , as a function of the volume size, for two-scales iterated Boolean model (IB) with quasi rigid inclusions, at $f = 0.7$ (solid line). The dotted line represents a fit of the variance $D_m^2(V)$ with Eq. 9.2, which holds for volumes much larger than the integral range, i.e. $V \gg A_3$.



Representative volume element

Comparison between finite element and FFT computations (Jean et al, 2009). Elasticity.

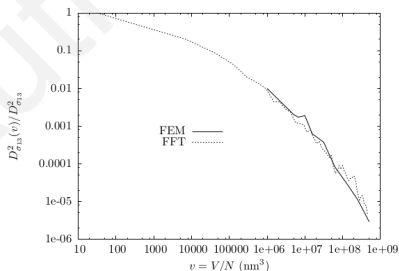
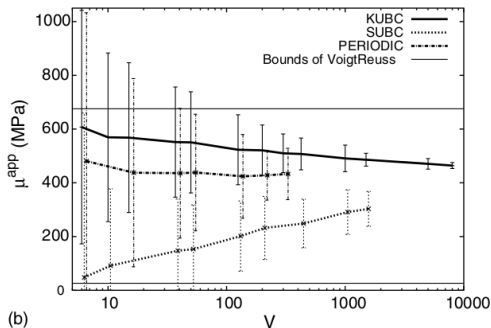


FIG. 17: Variance of apparent mechanical properties on punctual variance as a function of volume of subdomains.

Representative volume element

Example : effect of boundary conditions (Kanit et al, 2003), uniform (static, kinematic) and periodic.



(b)

As expected, $C_{app}^{subc} \leq C^{hom} \leq C_{app}^{kubc}$. Yet, huge size effects are observed for uniform boundary conditions, particularly SUBC (porous media).

The RVE method in homogenization

Some references related to RVEs for physical properties :

- ▶ Elasticity in concrete (Escoda et al, 2011).
- ▶ Elasticity and thermal conductivity in fibrous media (Altendorf et al, 2011). Role of the shape of the RVE.
- ▶ Multiscale RVEs (Willot and Jeulin, 2011).
- ▶ Optics in electrostatics for deposit models (Azzimonti et al, 2013). Singular scaling laws due to surface effects (in 3D) induced by deposit models.
- ▶ Acoustics (Peyrega et al, 2009)
- ▶ Plasticity (Dirrenberger et al, 2016)
- ▶ Mesoporous alumina (Wang et al, 2014)
- ▶ Permeability (Abdallah et al, 2016)
- ▶ Schneider et al, 2021.

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Preliminary on random set theory

Covariance, integral range and RVE

The RVE method in homogenization

Conclusion

Conclusion

- ▶ The size of the representative volume element depends in general on the property sought for and on the required precision.
- ▶ For the density of random sets, its scaling law can be derived in the limit of a large RVE as a Taylor expansion. In the absence of large-scale correlation, this results in a Taylor expansion.
- ▶ The scaling law obeys that of random independent, identically-distributed scalar variables where the number of i.i.d. variables is the volume size, expressed in integral-range unit-size
- ▶ The integral range is the integral of the correlation function. Accordingly, singular behavior occur when the integral range is infinite (correlation at infinite length) or zero.

Conclusion (II)

- ▶ Elliptic PDEs (for the simple conductivity problems, with finite contrast) follow the same trend, up to logarithmic corrections, provided one uses periodic boundary conditions.
- ▶ The theory may be applied to any self-averaging quantity, e.g. the field fluctuations, or local fields in one given phase of a composite.
- ▶ Do consider several samples when doing numerical mechanics! In most cases, the standard deviation decreases as $1/\sqrt{n}$ so you gain a lot at the beginning.
- ▶ Mechanics.

FFT solvers for transport problems in heterogeneous media

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Introduction to FFT methods – Champs-sur-Marne, Gustave Eiffel
University, March 18, 2022

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Scope of FFT methods

- ▶ By principle, FFT methods rely on a Green operator associated to a homogeneous material
- ▶ In mechanics, this operator serves as a projector onto the space of curl-free strain fields (small strain assumption) parallel to the space of divergence-free stress fields (quasi-static balance of linearmomentum)
- ▶ Conservation laws and field admissibility are treated in the Fourier domain whereas constitutive laws are enforced in the real space
- ▶ As such, many problems of physics involving the equivalent of the “Lippmann-Schwinger” equation can be tackled with FFT. Deriving FFT schemes is (almost) straightforward in many problems of quasi-static physics involving heterogeneous materials.

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Conductivity

Linear conductivity in the continuum :

$$\partial_i J_i(\mathbf{x}) = 0, \quad E_i(\mathbf{x}) = -\partial_i \Phi(\mathbf{x}), \quad J_i(\mathbf{x}) = \sigma_{ij}(\mathbf{x}) E_j(\mathbf{x}),$$

where $\Phi(\mathbf{x})$ is the electric potential and $\sigma(\mathbf{x})$ is the local conductivity tensor of the material phase at point \mathbf{x} .

Periodic boundary conditions are employed, in the form

$$\mathbf{J}(\mathbf{x}) \cdot \mathbf{n} = \#, \quad \Phi(\mathbf{x} + L\mathbf{e}_j) \equiv \Phi(\mathbf{x}) - \bar{E}_j L, \quad \mathbf{x}, \mathbf{x} + L\mathbf{e}_j \in \partial\Omega,$$

All FFT schemes presented in the previous talks can be deduced from the following “Lippmann-Schwinger” equation :

$$E_i = \bar{E}_i - G_{ij}^0 * P_j, \quad P_j = J_j - \sigma^0 E_j,$$

Conductivity

Linear conductivity in the continuum :

$$\partial_i J_i(\mathbf{x}) = 0, \quad E_i(\mathbf{x}) = -\partial_i \Phi(\mathbf{x}), \quad J_i(\mathbf{x}) = \sigma_{ij}(\mathbf{x}) E_j(\mathbf{x}),$$

where $\Phi(\mathbf{x})$ is the electric potential and $\sigma(\mathbf{x})$ is the local conductivity tensor of the material phase at point \mathbf{x} .

Periodic boundary conditions are employed, in the form

$$\mathbf{J}(\mathbf{x}) \cdot \mathbf{n} = \#, \quad \Phi(\mathbf{x} + L\mathbf{e}_i) \equiv \Phi(\mathbf{x}) - \bar{E}_i L, \quad \mathbf{x}, \mathbf{x} + L\mathbf{e}_i \in \partial\Omega,$$

Equivalent of the “Lippmann-Schwinger” equation in conductivity :

$$E_i = \bar{E}_i - G_{ij}^0 * P_j, \quad P_j = J_j - \sigma^0 E_j,$$

Conductivity

This gives the equivalent of Moulinec & Suquet's "basic scheme" (Eyre and Milton, 1998)

$$\mathbf{E}^{(k+1)} = \bar{\mathbf{E}} - \mathbf{G}^0 * \mathbf{P}, \quad \mathbf{P} = \mathbf{J} - \sigma^0 \mathbf{E}^{(k)},$$

with e.g. $\mathbf{E}^{(k=0)} \equiv \bar{\mathbf{E}}$.

An equivalent 'dual' formulation stems from writing the problem in terms of the electric current as

$$J_i = \bar{J}_i - H_{ij}^0 * T_j, \quad T_j = E_j - \rho^0 J_j,$$

where $\rho^0 = 1/\sigma^0$ is the reference resistivity, and $\bar{\mathbf{J}}$ is the prescribed macroscopic current. The Green operator associated to the governing equation for the current reads

$$H_{ij}^0(\mathbf{x}) = \sigma^0 \{ [\delta(\mathbf{x}) - 1] \delta_{ij} - \sigma^0 G_{ij}^0(\mathbf{x}) \},$$

where $\delta(\mathbf{x})$ is Dirac's distribution and δ_{ij} is the Kronecker symbol. Thus, for all \mathbf{T} ,

$$H_{ij}^0 * T_j = \sigma^0 (T_i - \langle T_i \rangle_{\Omega} - \sigma^0 G_{ij}^0 * T_j).$$

Conductivity

Remarks :

- ▶ Straightforward extension of all (or nearly all) previously-described schemes in mechanics to conductivity
- ▶ Not just algorithms, but also *all* discretization schemes can be extended to conductivity. Discretization is enforced when applying the Green operator. Symbolically :

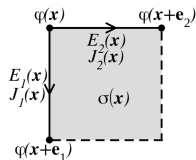
$$\sigma_0 G^{(0)} = \frac{\text{grad}(\text{div}\cdot)}{\Delta} = \frac{\nabla^* \nabla \cdot}{\nabla^* \cdot \nabla}$$

To do so, use the representation in Fourier space for the operators ∇ and adjoint ∇^* .

Conductivity

$$\sigma_0 G^{(0)} = \frac{\text{grad}(\text{div}\cdot)}{\Delta} = \frac{\nabla^* \nabla \cdot}{\nabla^* \cdot \nabla}$$

Remark (i) : in linear and nonlinear conductivity, we are dealing with lower-order tensors. It is often sufficient to consider the forward-and-backward finite-difference scheme which is centered.



This finite-difference scheme is centered.

The “classical” discretization (all fields are trigonometric polynomials) is also possible and works fine if $\partial J(\mathbf{x})/\partial E(\mathbf{x}) > 0$.

Conductivity

$$\sigma_0 G^{(0)} = \frac{\text{grad}(\text{div}\cdot)}{\Delta} = \frac{\nabla^* \nabla \cdot}{\nabla^* \cdot \nabla}$$

Remark (ii) : when utilizing finite differences, the operators ∇ and ∇^* can be computed easily in the real space.

Fourier transforms are required, only when applying $(\nabla^* \cdot \nabla)^{-1} = \Delta^{-1}$.

$$\phi^{k+1} = \frac{1}{\sigma^0 \Delta} \mathbf{div} [(\sigma - \sigma^0)(\bar{\mathbf{E}} - \mathbf{grad}\phi^k)]$$

Provides a rewriting of the basic scheme in terms of potential (not the electric field) which is the scalar. Only one FFT (and one FFT^{-1}) is required at each step (could be more depending on the convergence criterion).

This is optimal in terms of memory (1 potential + 1 microstructure). On a 16 Gb laptop : 1560^3 voxels.

Conductivity

Remark (iii) : remark (ii) extends to mechanics, for finite-difference schemes in which strain fields are admissible at each step. For instance : staggered discretization schemes with basic gradient descent scheme.

Drawback : harder to parallelize because the computations in the real space are not local (need to provide for overlap zones).

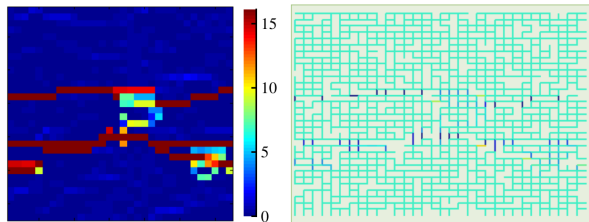
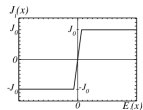
Conductivity

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Conductivity

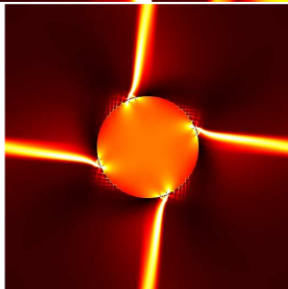
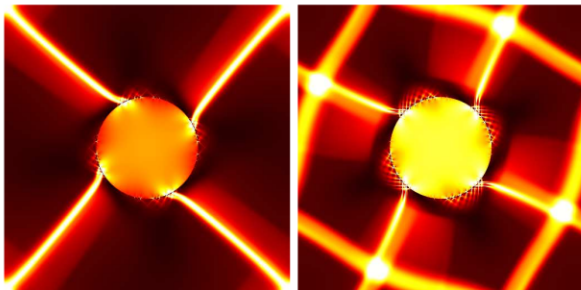
Illustration : nonlinear conductivity on a square lattice with strongly-nonlinear law.



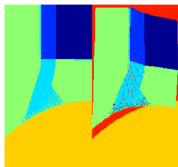
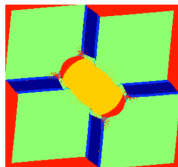
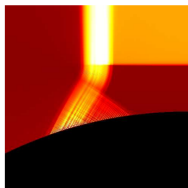
Electric field localization along minimal path. FFT computation with forward-and-backward discretization + polarization scheme (Eyre and Milton, 1998).

Perfect-plasticity

Disgression : Polarization schemes with finite-difference discretization are good at handling perfect-plasticity in mechanics in porous materials.

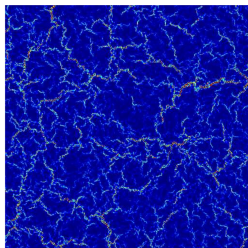
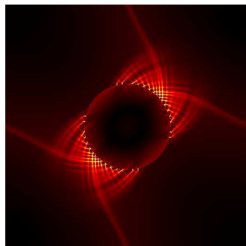
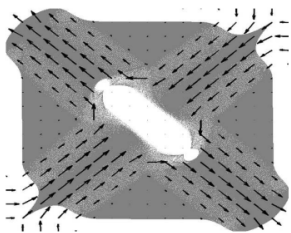


Perfect-plasticity



The periodic part of the displacement is computed from the strain field as (Gasnier et al, 2018) :

$$|\mathbf{k}|^4 u_1 = (2|\mathbf{k}|^2 - |k_1|^2) k_1^* \varepsilon_{11} - k_1 \left[(k_2^*)^2 \varepsilon_{22} + (k_3^*)^2 \varepsilon_{33} \right] + 2 (|\mathbf{k}|^2 - |k_1|^2) \left[k_2^* \varepsilon_{12} + k_3^* \varepsilon_{13} \right] - 2k_1 k_2^* k_3^* \varepsilon_{23}$$



Conductivity

Remark (iv) this scheme solves all “diffusion” problems with many mathematically – albeit not physically – identical equations, equivalent to the first and second Fick law in static.

Heat conduction (Fourier's law) : $\mathbf{J}(\mathbf{x}) = k \text{grad} T(\mathbf{x})$

- ▶ $T(\mathbf{x})$ [T] : temperature at point \mathbf{x}
- ▶ $\mathbf{J}(\mathbf{x})$ [W/m²] : local heat flux
- ▶ k [W/m/K] : thermal conductivity
- ▶ Steady-state (constant temperature gradient) : $\text{div} \mathbf{J}(\mathbf{x}) = 0$

Magnetic permeability : $\mathbf{B}(\mathbf{x}) = \mu(\mathbf{x}) \mathbf{H}(\mathbf{x})$

First Maxwell equation : $\text{rot} \mathbf{H} = 0$ or $\mathbf{H} = -\text{grad} U$

- ▶ $\mathbf{B}(\mathbf{x})$ [T] : magnetic field at point \mathbf{x}
- ▶ $\mathbf{H}(\mathbf{x})$ [TA²/N] : auxiliary magnetic field
- ▶ μ [N/A²] : magnetic permeability
- ▶ U : magnetic potential
- ▶ Gauss's law : $\text{div} \mathbf{B}(\mathbf{x}) = 0$

Conductivity

Darcy's law : $\mathbf{q}(\mathbf{x}) = \frac{-k}{\mu} \text{grad}P(\mathbf{x})$

- ▶ $P(\mathbf{x})$ [N/m²] : pressure at point \mathbf{x}
- ▶ $\mathbf{q}(\mathbf{x})$ [(m³/(m²s))] : fluid flow
- ▶ k [m²] : permeability
- ▶ μ [Pa s] fluid viscosity

Hydrogeology, gaz diffusion.

Dielectric permittivity : $\mathbf{D}(\mathbf{x}) = \varepsilon\mathbf{E}(\mathbf{x})$

- ▶ ε [F/m] : absolute permittivity
- ▶ $\mathbf{D}(\mathbf{x})$ [C/m²] : electric displacement field at point \mathbf{x}
- ▶ $\mathbf{E}(\mathbf{x})$ [N/C] : electric field

Conductivity

Coupling. Piezoelectricity (Brenner et al, Phys Rev. B 2009).

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}} - \boldsymbol{\Gamma}^0 * \boldsymbol{\tau}(\mathbf{x}) - {}^T\boldsymbol{\Upsilon}^0 * \mathbf{P}(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega,$$

$$\mathbf{E}(\mathbf{x}) = \bar{\mathbf{E}} + \boldsymbol{\Upsilon}^0 * \boldsymbol{\tau}(\mathbf{x}) + \boldsymbol{\Delta}^0 * \mathbf{P}(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega,$$

NB : imperfect interfaces are much more difficult to handle. Schemes developed by Monchiet for Kapitza interfaces (2018).

Wicht et al (2020) : thermechanical coupling.

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Extension to quasi-optics with time-harmonic solicitations. All fields are proportional to $\mathbf{e}^{i\omega t}$ where ω is the frequency of the solicitation.

Maxwell equations : $\text{rot}[\text{rot}\mathbf{E}(\mathbf{x})] = \omega^2\mathbf{D}(\mathbf{x})$

Quasi-static assumption $\omega \ll \delta$: $\text{rot}\mathbf{E} = 0$ or $\mathbf{E} = -\text{grad}U$

$\text{div}\mathbf{D}(\mathbf{x}) \equiv 0$ also in electrodynamics.

Optical properties at wavelengths small compared to the typical size of the material.

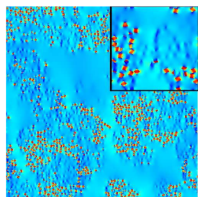
Green operator :

$$G_{ij}^{(0)} = \frac{1}{\sigma_0} \frac{k_i k_j^*}{k_i k_i^*}.$$

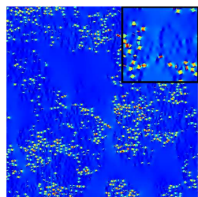
In a way, the implementation becomes even easier as complex-to-complex Fourier transforms are required.

Electrostatics

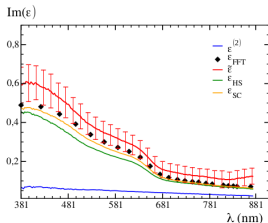
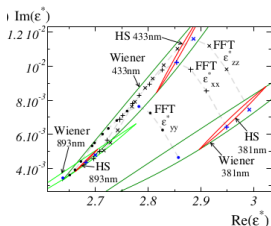
Prediction of optical properties of a hematite coating, with nanoparticles.



(a) $\text{Re}(D_1)$, $\lambda = 401\text{nm}$



(b) $\text{Im}(D_1)$, $\lambda = 401\text{nm}$



(Couka et al, Adv. Sc. Med. and Engng, 2014 ; Azzimonti et al, J. of Modern Optics, 2014)

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Viscoelasticity with Prony series

Time-harmonic regime in mechanics ?

- ▶ *Fourier decomposition in time* : strain and stress history specified as a series of harmonics. *Complex elastic moduli*
- ▶ *Fourier decomposition in space* : use of a Green operator associated to the solution for a homogeneous elastic stiffness tensor
- ▶ Discretization of complex microstructures on a regular grid of voxels ; periodic boundary conditions
- ▶ Full-fields reconstruction in space and time

Problem setup

Time-harmonic sollicitation

$$\tilde{\boldsymbol{\varepsilon}}(\mathbf{x}; t) = \boldsymbol{\varepsilon}(\mathbf{x})\mathbf{e}^{i\omega t}, \quad \tilde{\boldsymbol{\sigma}}(\mathbf{x}; t) = \boldsymbol{\sigma}(\mathbf{x})\mathbf{e}^{i\omega t}, \quad \tilde{\mathbf{u}}(\mathbf{x}; t) = \mathbf{u}(\mathbf{x})\mathbf{e}^{i\omega t} \quad (1)$$

N.B. physical fields

$$\hat{\boldsymbol{\varepsilon}}(\mathbf{x}; t) = \mathbf{Re} [\tilde{\boldsymbol{\varepsilon}}(\mathbf{x}; t)], \quad \hat{\boldsymbol{\sigma}}(\mathbf{x}; t) = \mathbf{Re} [\tilde{\boldsymbol{\sigma}}(\mathbf{x}; t)], \quad \hat{\mathbf{u}}(\mathbf{x}; t) = \mathbf{Re} [\tilde{\mathbf{u}}(\mathbf{x}; t)]$$

Small deformation, steady-state regime

$$\tilde{\varepsilon}_{ij}(\mathbf{x}; t) = \frac{1}{2} [\partial_j \tilde{u}_i(\mathbf{x}; t) + \partial_i \tilde{u}_j(\mathbf{x}; t)], \quad \partial_i \tilde{\sigma}_{ij}(\mathbf{x}; t) = 0.$$

$$\varepsilon_{ij}(\mathbf{x}; t) = \frac{1}{2} [\partial_j u_i(\mathbf{x}; t) + \partial_i u_j(\mathbf{x}; t)], \quad \partial_i \sigma_{ij}(\mathbf{x}; t) = 0.$$

Local response

Linear-elastic inclusions :

$$\tilde{\sigma}(\mathbf{x}; t) = \mathbb{C}_2 : \tilde{\varepsilon}(\mathbf{x}; t), \quad \sigma(\mathbf{x}) = \mathbb{C}_2 : \varepsilon(\mathbf{x}),$$

Visco-elastic matrix :

$$\tilde{\sigma}(\mathbf{x}; t) = \int_{-\infty}^t d\tau \mathbb{C}_1(t - \tau) : \frac{d\tilde{\varepsilon}(\mathbf{x}; \tau)}{d\tau}.$$

For an isotropic tensor \mathbb{C}_1 :

$$\sigma(\mathbf{x}) = \mathbb{C}_1^*(\kappa_1^*, \mu_1^*) : \varepsilon(\mathbf{x})$$

with :

$$\kappa_1^*(\mathbf{i}\omega) = \overline{\kappa_1} + \mathbf{i}\omega \int_0^{\infty} d\eta [\kappa_1(\eta) - \overline{\kappa_1}] \mathbf{e}^{-\mathbf{i}\omega\eta},$$

$$\mu_1^*(\mathbf{i}\omega) = \overline{\mu_1} + \mathbf{i}\omega \int_0^{\infty} d\eta [\mu_1(\eta) - \overline{\mu_1}] \mathbf{e}^{-\mathbf{i}\omega\eta},$$

$$\overline{\kappa_1} = \lim_{t \rightarrow \infty} \kappa_1(t) \geq 0, \quad \overline{\mu_1} = \lim_{t \rightarrow \infty} \mu_1(t) \geq 0.$$

Local response

Example (Maxwell model) :

$$\frac{\tilde{\sigma}'(t)dt}{t_1} + d\tilde{\sigma}'(t) = 2\mu_0 d\tilde{\varepsilon}'(t), \quad \frac{\tilde{\sigma}_{kk}(t)dt}{t_1} + d\tilde{\sigma}_{kk}(t) = 3\kappa_0 d\tilde{\varepsilon}_{kk}(t)$$

This is equivalent to (Christensen, 2012) :

$$\tilde{\sigma}'(t) = \int_{-\infty}^t d\tau 2\mu_1(t-\tau) \frac{d\tilde{\varepsilon}'(\tau)}{d\tau}, \quad \tilde{\sigma}_{kk}(t) = \int_{-\infty}^t d\tau 3\kappa_1(t-\tau) \frac{d\tilde{\varepsilon}_{kk}(\tau)}{d\tau},$$

with

$$\mu_1(t) = \mu_0 e^{-t/t_1} \mathcal{H}(t), \quad \kappa_1(t) = \kappa_0 e^{-t/t_1} \mathcal{H}(t), \quad \mathcal{H}(t) = \begin{cases} 0 & \text{if } t < 0, \\ 1 & \text{if } t > 0. \end{cases}$$

Time-FFT provides the complex moduli :

$$\mu_1^*(i\omega) = \frac{\mu_0}{1 + 1/(i\omega t_1)}, \quad \kappa_1^*(i\omega) = \frac{\kappa_0}{1 + 1/(i\omega t_1)}.$$

Boundary conditions

Periodic boundary conditions with time-harmonic macroscopic strain loading

$$\langle \boldsymbol{\varepsilon}(\mathbf{x}) \rangle = \bar{\boldsymbol{\varepsilon}}, \quad \boldsymbol{\varepsilon}(\mathbf{x}) \# , \quad \boldsymbol{\sigma}(\mathbf{x}) \# .$$

Effective properties

$$\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma}(\mathbf{x}) \rangle = \mathbb{C}^{\text{eff}} : \bar{\boldsymbol{\varepsilon}} .$$

N.B. for non-harmonic strain loading $\alpha(t) = \langle \tilde{\boldsymbol{\varepsilon}}(\mathbf{x}; t) \rangle$

$$\alpha(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \alpha(\omega) \mathbf{e}^{i\omega t} .$$

Strain field recovered as a superposition of harmonic responses

$$\tilde{\boldsymbol{\varepsilon}}(\mathbf{x}; t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \boldsymbol{\varepsilon}_{\omega}(\mathbf{x}) \mathbf{e}^{i\omega t} .$$

FFT scheme for the viscoelastic response

Extension of FFT scheme to complex elastic moduli straightforward but differ in one instance. Symmetry with complex-valued fields :

$$\hat{\varepsilon}_{kl}(\mathbf{x}; t) = \hat{\varepsilon}_{lk}(\mathbf{x}; t), \quad \hat{\sigma}_{kl}(\mathbf{x}; t) = \hat{\sigma}_{lk}(\mathbf{x}; t),$$

$$\varepsilon_{kl}(\mathbf{x}) = \varepsilon_{lk}(\mathbf{x}), \quad \sigma_{kl}(\mathbf{x}) = \sigma_{lk}(\mathbf{x}).$$

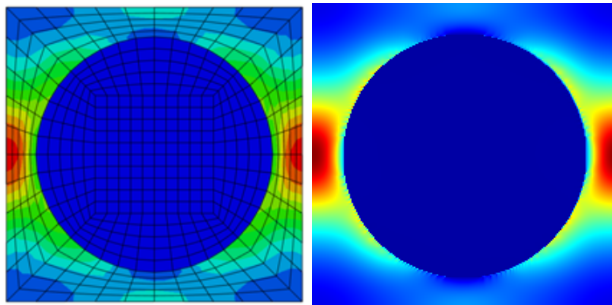
$$G_{ij,kl}^0(\mathbf{q}) = G_{ji,kl}^0(\mathbf{q}) = G_{ij,lk}^0(\mathbf{q}) = [G_{kl,ij}^0(\mathbf{q})]^*.$$

$$C_{ij,kl}^0 = C_{ji,kl}^0 = C_{ij,lk}^0 = (C_{kl,ij}^0)^* = C_{kl,ij}^0,$$

The reference must be real. Scheme applied with basic scheme (Figliuzzi et al, 2016) or polarization-based method (Gallican et al, 2019; André et al, 2021). They use : $\kappa_0 = \sqrt{\kappa_1 \kappa_2}$, $\mu_0 = \sqrt{\mu_1 \mu_2}$.

Validation : FE-FFT comparison

Stiff inclusion with periodic boundary conditions embedded in a viscoelastic matrix defined by a Prony series. Local stress $\sigma_m(\mathbf{x})$ (2D section). FEM (Abaqus) vs. FFT.



From Figliuzzi et al, 2016.

Validation : comparison with analytical estimates

Loss angle $\delta = \mathcal{I}(\mu^{\text{eff}}) / \mathcal{R}(\mu^{\text{eff}})$, periodic array of spheres of radius R
Viscoelastic matrix defined by a Prony series.

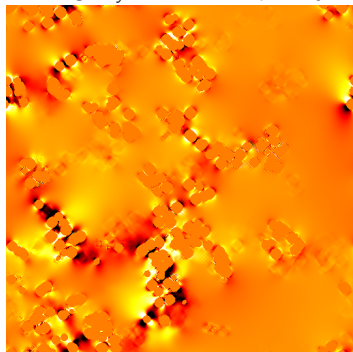
f (Hz)	$R = 0$		$R = 5$	
	Cohen (2004)	FFT	Cohen (2004)	FFT
1	0.033504	0.033504	0.033504	0.033502
5	0.038662	0.038662	0.038661	0.038659
10	0.040469	0.040469	0.040468	0.040466
50	0.04646	0.04646	0.04646	0.046456
100	0.050326	0.050326	0.050325	0.050322

	$R = 20$		$R = 40$	
1	0.033479	0.033451	0.033054	0.032757
5	0.038631	0.038598	0.038123	0.037769
10	0.040436	0.040401	0.039895	0.039519
50	0.046421	0.04638	0.045773	0.045326
100	0.050282	0.050237	0.049567	0.049074

FFT maps

Silica and carbon black materials used as nanoscopic fillers to improve the stiffness of rubbers (from Figliuzzi et al.).

Mean stress field $\mathbf{Im}(\sigma_{xy})$ (2D section). Material subjected to strain loading $\varepsilon_{xy} = 1\%$. Frequency : $\omega = 1117$ Hz.

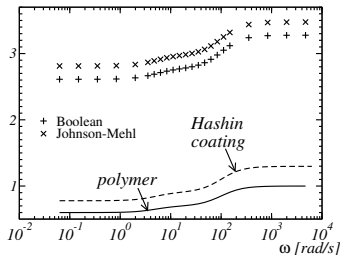


512^3 voxel grids (Figliuzzi et al, 2016)

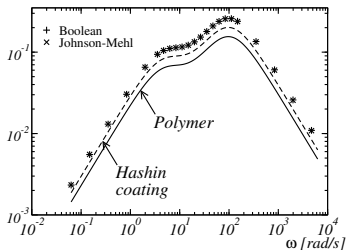
Effective response

Effective shear modulus μ^{eff} vs. frequency ω

$Re(\mu)$ [MPa]



$Imag(\mu)$ [MPa]



Rigorous bounds on the complex shear and bulk moduli of two-phase media given by Milton & Berryman (1997)

Viscoelasticity

Comparison with a time-explicit scheme :

$$\frac{\tilde{\sigma}'(t)dt}{t_1} + d\tilde{\sigma}'(t) = 2\mu_0 d\tilde{\varepsilon}'(t), \quad \frac{\tilde{\sigma}_{kk}(t)dt}{t_1} + d\tilde{\sigma}_{kk}(t) = 3\kappa_0 d\tilde{\varepsilon}_{kk}(t)$$

$$\hat{\varepsilon}(\mathbf{x}; t) = 0, \quad \hat{\sigma}(\mathbf{x}; t) = 0$$

for $t < t_0$. For $t \geq t_0$, the material is subject to harmonic strain loading :

$$\langle \hat{\varepsilon}(\mathbf{x}; t) \rangle = \cos(\omega t) \bar{\varepsilon}$$

Take $t_0 = \pi/(2\omega)$. The stress field σ at time $t + dt$ is then computed by explicit time-discretization. For instance, for the deviatoric parts :

$$\Delta \hat{\sigma}'(\mathbf{x}, t) = 2\mu^0 \Delta \hat{\varepsilon}'(\mathbf{x}, t) - \frac{\hat{\sigma}'(\mathbf{x}, t) \Delta t}{t_1},$$

$$\Delta \hat{\sigma}'(\mathbf{x}, t) = \hat{\sigma}'(\mathbf{x}, t + \Delta t) - \hat{\sigma}'(\mathbf{x}, t), \quad \Delta \hat{\varepsilon}'(\mathbf{x}, t) = \hat{\varepsilon}'(\mathbf{x}, t + \Delta t) - \hat{\varepsilon}'(\mathbf{x}, t).$$

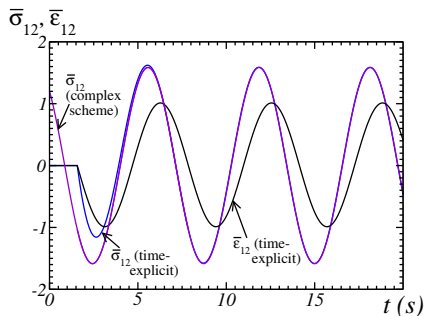
Equivalent to a thermoelastic stress-strain relation with unknown $\Delta \hat{\varepsilon}$ and $\Delta \hat{\sigma}$ and with applied strain loading :

$$\langle \Delta \hat{\varepsilon}'(\mathbf{x}, t) \rangle = -\omega \sin(\omega t) \Delta t \bar{\varepsilon}$$

See e.g. Badulescu et al (2015).

Viscoelasticity

Example (stiff inclusion in Maxwell matrix, periodic array of spheres, from Figliuzzi et al.)



Pros and cons : the Prony series FFT scheme is useful for complex viscoelastic laws that require a large number of fields at previous time steps. In the harmonic case, the memory required is only two times that of the classical “real” schemes. Cons : harmonic regimes only ; must be linear viscoelasticity.

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Damage in heterogeneous media

Polycrystal subjected to thermal cycles (cooling, re-heating)



Describe damage evolution : initiation, propagation. Strongly nonlinear problem. Irreversibility.

Variational principle

Total energy of a domain Ω containing cracks along surfaces Γ , submitted to a deformation field $\varepsilon(\mathbf{x})$.

$$E(\varepsilon, \Gamma) = E(\varepsilon) + E(\Gamma) = \int_{\Omega \setminus \Gamma} W(\varepsilon(\mathbf{x})) d\mathbf{x} + \gamma_c \int_{\Gamma} dS$$

$E(\varepsilon)$: stored elastic energy ; $E(\Gamma)$ fracture surface energy, according to Griffith criterion of fracture ; γ_c toughness (specific surface energy).

Variational principle of Francfort and Marigo (JMPS, 1998). The total energy (over all admissible fields ε) is minimized during the fracture process :

$$(\varepsilon, \Gamma) = \operatorname{arginf}_{(\varepsilon, \Gamma)} \left\{ \int_{\Omega \setminus \Gamma} \frac{1}{2} \varepsilon(\mathbf{x}) : \mathbb{C}(\mathbf{x}) : \varepsilon(\mathbf{x}) + \gamma_c \int_{\Gamma} dS \right\}$$

in elasticity.

Variational principle

Solve :

$$(\boldsymbol{\varepsilon}, \Gamma) = \operatorname{arginf}_{(\boldsymbol{\varepsilon}, \Gamma)} \left\{ \int_{\Omega \setminus \Gamma} \frac{1}{2} \boldsymbol{\varepsilon}(\mathbf{x}) : \mathbb{C}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}) + \gamma_c \int_{\Gamma} dS \right\}$$

in the space of physically-admissible strain fields :

$$\boldsymbol{\varepsilon} \in \mathcal{K}(\bar{\boldsymbol{\varepsilon}}) = \{ \boldsymbol{\varepsilon}; \exists \mathbf{u} : \boldsymbol{\varepsilon} = (\nabla \mathbf{u})_{\text{sym}}, \langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}} \}$$

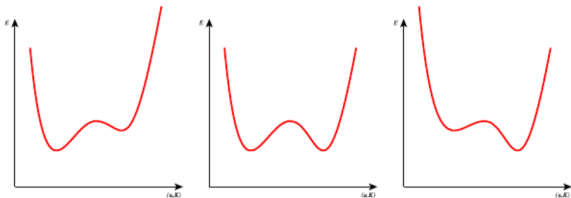
(assuming small deformations). At fixed Γ (no damage evolution) : the stress tensor $\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}$ is divergence-free ($\operatorname{div} \boldsymbol{\sigma} = 0$, $\boldsymbol{\sigma} \cdot \mathbf{n}$ is the force per unit surface)

NB : Mumford-Shah functional :

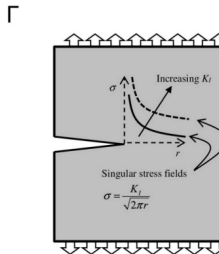
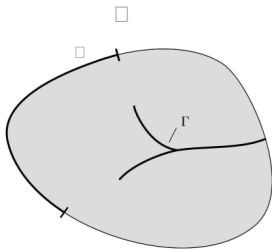
$$\min_{(u, \Gamma)} \left\{ \int_{\Omega \setminus \Gamma} |u - g|^2 + \gamma_c \int_{\Gamma} dS + \int_{\Omega \setminus \Gamma} |\nabla u|^2 \right\}$$

Variational principle

One-dimensional problem : beam under traction (Bourdin, 2007)



Before fracture, at the onset of fracture, after failure



Phase field models for fracture of homogeneous isotropic media

The variational principle can not in general be solved numerically.

Regularization : introduction of a phase field $\Phi(\mathbf{x})$ ($0 \leq \Phi(\mathbf{x}) \leq 1$) with $\Phi(\mathbf{x}) \equiv 1$ along the crack and $\Phi(\mathbf{x}) = 0$ away from the crack. This setting requires an additional length scale parameter ℓ .

The volume integral $E(\varepsilon)$ is replaced by $\int_{\Omega} (1 - \Phi)^2 W(\varepsilon(\mathbf{x})) dx$.

The surface integral $E(\Gamma)$ is replaced by $\gamma_c \int_{\Omega} (\frac{1}{2\ell} \Phi^2 + \frac{\ell}{2} \nabla \Phi \cdot \nabla \Phi) dx$ (Bourdin, 2007 ; Bourdin, Francfort and Marigo, 2008).

Resulting variational principle : minimization over admissible stress field and $\Phi(\mathbf{x})$ of the volume integrals

$$\operatorname{arginf}_{(\varepsilon, \Phi)} \left\{ \int_{\Omega} (1 - \Phi)^2 W(\varepsilon(\mathbf{x})) dx + \gamma_c \int_{\Omega} dx \left(\frac{1}{2\ell} \Phi^2 + \frac{\ell}{2} \nabla \Phi \cdot \nabla \Phi \right) \right\}$$

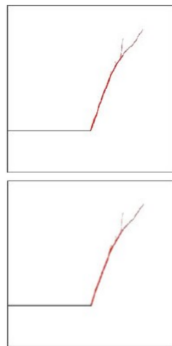
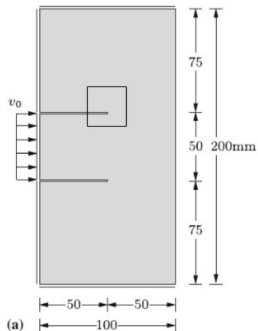
$$\varepsilon \in \mathcal{K}(\bar{\varepsilon}) = \{ \varepsilon; \exists \mathbf{u} : \varepsilon = (\nabla \mathbf{u})_{\text{sym}}, \langle \varepsilon \rangle = \bar{\varepsilon} \}$$

Enough to do initiation and propagation.

Phase field models for fracture of homogeneous isotropic media

Usually solved by Finite Element Methods.

From Kalthoff and Winkler (1987) (left) and Hokacker (2012) (right).



PDE for the phase field model

Functional minimization provides :

$$\begin{aligned}\boldsymbol{\varepsilon}(\mathbf{x}) &= (\nabla \mathbf{u}(\mathbf{x}))_{\text{sym}}, & \langle \boldsymbol{\varepsilon}(\mathbf{x}) \rangle &= \bar{\boldsymbol{\varepsilon}}, \\ \boldsymbol{\sigma} &= (1 - \phi(\mathbf{x}))^2 \mathbb{C}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}), & \text{div}(\boldsymbol{\sigma}) &= 0.\end{aligned}$$

for the linear elastic problem.

For the phase-field problem (Miehe, IJNME 2010) :

$$2(1 - \Phi)\mathcal{H} - \gamma_c/\ell(\Phi - \ell^2\Delta\Phi) = 0$$

with elastic energy $\mathcal{H}(\mathbf{x}, t) = W(\boldsymbol{\varepsilon}) = \frac{1}{2}\boldsymbol{\varepsilon} : \mathbb{C} : \boldsymbol{\varepsilon}$ acting as “source term”.

Irreversibility : $\mathcal{H}(\mathbf{x}, t) = \sup_{\boldsymbol{\varepsilon} < t} W(\boldsymbol{\varepsilon}, \tau)$

Fourier-based method

Unilateral law. Essential in compression. E.g. model of Miehe :

$$\sigma = (1 - \phi)^2 \mathbb{C} : \varepsilon^+ \mathbb{C} : \varepsilon^-, \quad \varepsilon^\pm = \varepsilon_k^\pm n_k \oplus n_k.$$

Irreversibility. ϕ can not decrease. Change the source term :

$\mathcal{H}(\mathbf{x}, t) = \max_{0 \leq s \leq t} \{ \Psi^+(x, s) \}$ with $\Psi^+(\varepsilon) = \Psi^+(\varepsilon^+)$ (depends on the tensile parts of the strain due to unilateral effect).

Anisotropic tenacity (second-order tensor).

Non-zero elastic moduli in regions where $\phi = 1$ using :

$(1 - \phi(\mathbf{x}))^2 \mathbb{C}(\mathbf{x}) \rightarrow (1 - \phi(\mathbf{x}) + k)^2 \mathbb{C}(\mathbf{x})$ with $k \ll 1$

Damping parameter :

$$2(1 - \Phi)\mathcal{H} - \gamma_c/\ell(\Phi - \ell^2 \Delta \Phi) = \eta \dot{\phi}$$

Fourier-based method

Chen and Gelebart (2021) proposed to solve the equation in ϕ with a “basic scheme”

$$\phi^{(k+1)}(\mathbf{q}) = \frac{\chi^k(\mathbf{q})}{A_0 + \mathbf{q} \cdot \mathbf{q}}, \quad \chi^k(\mathbf{x}) = B(\mathbf{x}) - (A(\mathbf{x}) - A_0)\phi(\mathbf{x}),$$

(terms A_0 and B detailed in Chen and Gélébart, 2021). χ is the polarization field for phase-field problem and we use the Green operator associated to the Helmholtz equation (no pole).

Several strategies are possible (not detailed here) :

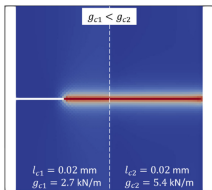
“sequential” : solve each problem for ε and ϕ separately (small time steps required). Each problem in ε and ϕ is convex.

“implicit” : solve the full problem at each time step.

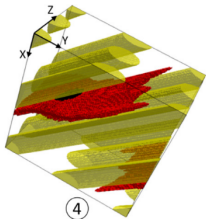
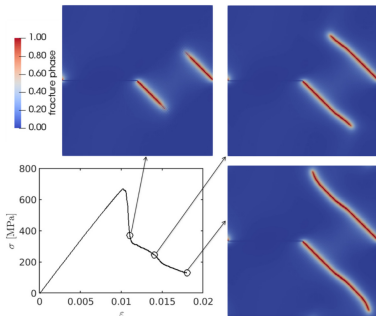
Other authors proposed FFT methods for phase field problem, e.g. Jeulin (IJSS, 2021) or Ernesti et al (2021) who used an implicit solver.

Phase field models for fracture of homogeneous isotropic media

Phase-field predicted by Chen and Gélébart (2021)

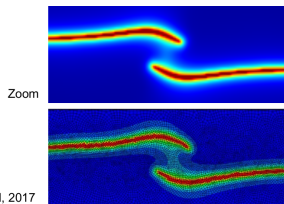
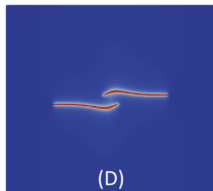
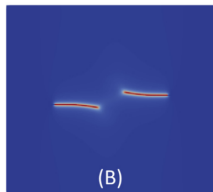


(f)



Phase field models for fracture of homogeneous isotropic media

Comparison with finite element method



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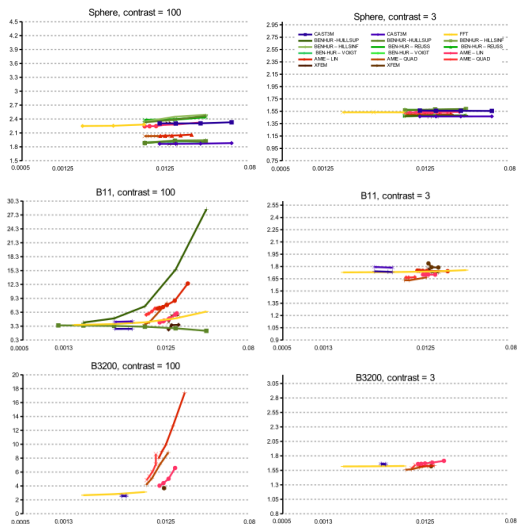
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Performances

From Bary et al, 2011 (linear elasticity)



Performances and accuracy

Numerical optimization of microstructures properties with viscoelastic behavior (Koishi et al, 2017).

4,000 configurations of 1024^3 each on TSUBAME supercomputer at Global Scientific Information and Computing Center in Tokyo Institute of Technology through the HPCI System Research Project

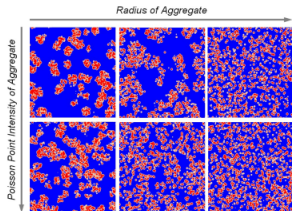
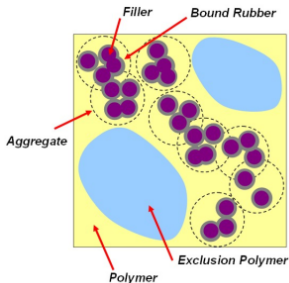


Figure 4. Cross section of six 3D simulation models generated with different Poisson point intensity and radius of aggregate, domain size: $1,000\text{nm} \times 1,000\text{nm} \times 1,000\text{nm}$, the volume fraction of filler: 15%, the radius of filler: 10nm, the thickness of bound rubber: 5nm.

Performances and accuracy

From Koishi et al, 2017. Use of the rotated scheme with polarization method.

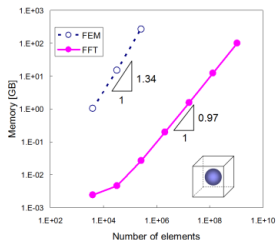


Figure 6. Required memory size of the FFT-based scheme and FEM against the number of elements.

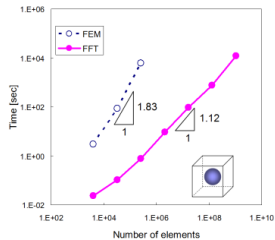
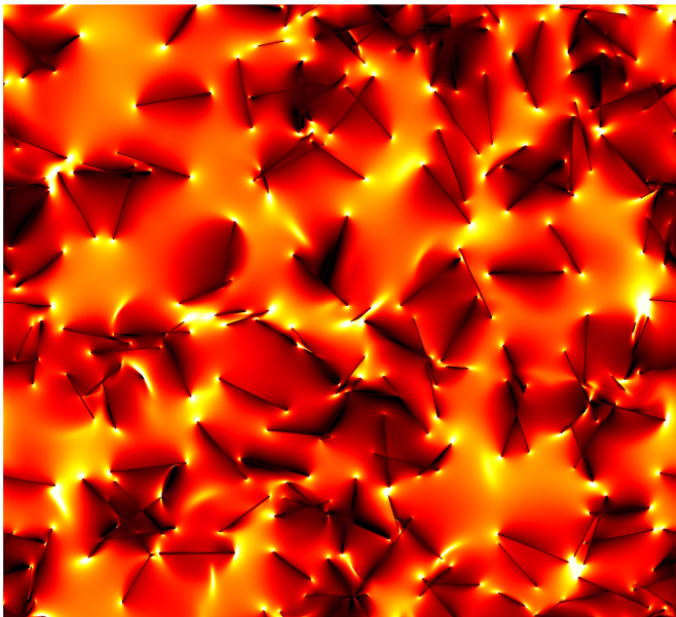


Figure 5. Computation time of the FFT-based scheme and FEM against the number of elements.

Performances and accuracy

Dealing with cracks.



Performances and accuracy

From Gasnier et al (2018).

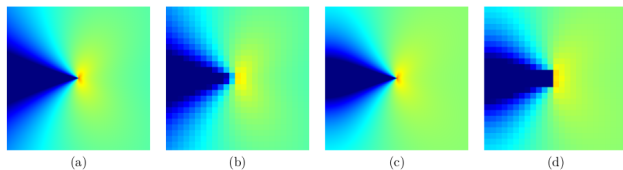


Figure 2: Stress component σ_{yy} in a region centered around an isolated crack tip, in a 2D medium. (a): Asymptotic expansion (5); (c-d): FFT predictions for the backward-and-forward scheme (FFT-BF) on grids of 4096^2 (c) and 128^2 voxels (d); (b): local averages of the asymptotic expansion (a) on the same coarse voxel-grid as used in (d). The same color map, ranging from blue (lowest value) to red (highest value) is used in maps (a-d).

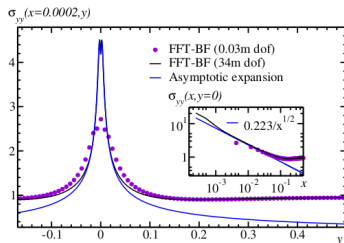


Figure 1: Periodic array of cracks in plane strain: profile of the stress component σ_{yy} along the segment $x = 2 \cdot 10^{-4}$, $-0.15 < y < 0.5$, close to the crack tip at $x = y = 0$. Solid black line and purple dots: Fourier backward-and-forward scheme with 34 millions and 32 thousands degrees of freedom. Solid blue line: asymptotic expansion near the crack tip (5) fitted with the value $K_I = 0.556$. Embedded graph (right): plot of σ_{yy} along the segment $y = 0$, $x > 0$, in log-log scale.

Performances and accuracy

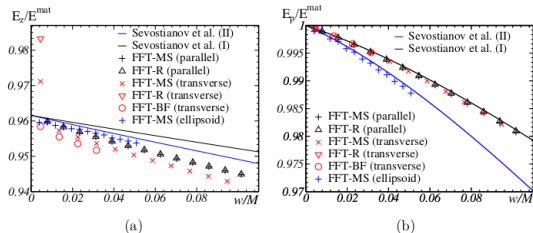


Figure 10: Influence of the crack's width w on the effective elastic moduli of a periodic array of cracks: Young moduli E_z and E_p . Symbols: FFT data points for cracks with cylindrical shape oriented parallel (black) and transverse (red) to the voxel grid and for ellipsoidal cracks with axis parallel to the voxel grid (blue). Solid lines: exact result for non-interacting parallel ellipsoidal voids. Black: with the same volume as the cylinders (method I). Blue: with lowest semi-axis $w/2$ (method II).

Cracks

From Gasnier et al (2018). Displacement field. Use of different discretizations.

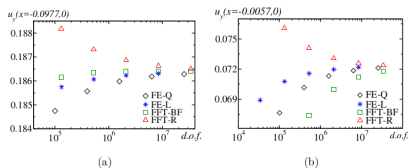


Figure 9: Continuation of Figs. 7 and 8: one value of the displacement component u_y in the middle of the crack ($y = 0$, $x = -0.977$) (a) and near the crack-tip ($y = 0$, $x = -0.0057$) (b), as a function of the number of degrees of freedom: finite element with linear elements (stars), quadratic elements (diamonds), Fourier methods with backward-forward (squares) and rotated (triangles) schemes.

Liu et al, (2020) report a 5 to 10% difference.

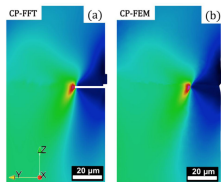


Fig. 6. The σ_{yy} fields for (a) CP-FFT vs. (b) CP-FEM comparison for a zoomed view near the crack tip (displaying the dashed-box region shown in Fig. 5).

- ▶ Lucarini and Segurado (Computational Mechanics, 2019). Crystal plasticity with fatigue. Difference of the order of 7%. FFT is 6-7 times faster *and allows to compute models with sizes not accessible using FEM.*
- ▶ Vondrejč and de Geus (Journal of Computational and Applied Mathematics, 2020) : FEM more accurate than FFT when the material properties display jumps, mixed results obtained when the material properties vary smoothly.

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Stokes flow

Incompressible Newtonian fluid with viscosity μ :

$$\mu \Delta \mathbf{u} = \nabla \cdot P \quad (\text{Stokes equation})$$

$$\mathbf{u} = 0 \quad (\text{no-slip boundary condition at fluid-solid interface})$$

$$\text{div} \mathbf{u} = 0 \quad (\text{fluid incompressibility})$$

Periodic boundary conditions :

$$P(\mathbf{x}) = \boldsymbol{\alpha} \cdot \mathbf{x} + \phi(\mathbf{x}), \quad \phi\#, \quad \mathbf{u}\#$$

Loading : pressure drop $\boldsymbol{\alpha} = \langle \nabla \cdot P \rangle$

Permeability κ :

$$\mu \langle \mathbf{u} \rangle = \kappa \langle \nabla \cdot P \rangle = \kappa \cdot \boldsymbol{\alpha}$$

FFT methods for Stokes flow

Stokes equation equivalent to :

$$\mathbf{d}(\mathbf{x}) = (\text{grad}\mathbf{u}(\mathbf{x}))_{\text{sym}}, \quad \mathbf{d}_m = 0,$$

$$\boldsymbol{\sigma}(\mathbf{x}) = 2\mu\mathbf{d}(\mathbf{x}) - P(\mathbf{x})\mathbf{I}, \quad P(\mathbf{x}) = \boldsymbol{\alpha} \cdot \mathbf{x} + \phi(\mathbf{x})$$

$$\text{div}\boldsymbol{\sigma} = 0$$

Idea (Bignonnet and Dormieux, 2014) : extend the equations over the solid phase, treated as an incompressible viscous fluid with infinite viscosity ($\mu = \infty$). No-slip boundary conditions automatically met, however rigid body motion of the solid domain must be prevented. If there is one connected component spanning the medium, it is sufficient to enforce $u = 0$ at one point in the solid phase or on average.

There must be body forces in the solid phase that counterbalance the macroscopic fluid pressure gradient.

$$\mu(\mathbf{x}) = \begin{cases} \infty & \text{solid} \\ \mu_f & \text{otherwise.} \end{cases} \quad \text{div}\boldsymbol{\sigma} = \begin{cases} -\boldsymbol{\alpha}/f_s & \text{solid} \\ 0 & \text{otherwise.} \end{cases}$$

FFT methods for Stokes flow

Introduce a reference viscosity μ^0 and recast the problem as :

$$\boldsymbol{\sigma}(\mathbf{q}) = -\mathbf{Y}^0(\mathbf{q}) \cdot \bar{\mathbf{f}}(\mathbf{q}) - \Delta^0(\mathbf{q}) : [\mathbf{d}(\mathbf{q}) - \frac{1}{2\mu^0} : \boldsymbol{\sigma}(\mathbf{x})]$$

$$\mathbf{d}(\boldsymbol{\sigma}) = A(\mathbf{x})[\boldsymbol{\sigma}(\mathbf{x}) - P(\mathbf{x})\mathbf{I}], \quad A(\mathbf{x}) = \frac{1}{2\mu} \chi_f(\mathbf{x}) + \frac{1}{2\mu_s} \chi_s(\mathbf{x})$$

$$\mathbf{Y}^0(\mathbf{q}) = \frac{i}{|\mathbf{q}|^4} [(\delta_{ij}q_k + \delta_{ik}q_j + \delta_{jk}q_i)|\mathbf{q}|^2 - 2q_iq_jq_k], \quad f = \text{div}(\alpha_k x_k)$$

Iterative scheme (Monchiet and Bonnet, 2009) :

$$\boldsymbol{\sigma}^{k+1}(\mathbf{q}) = \boldsymbol{\sigma}^k(\mathbf{q}) - \Delta^0(\mathbf{q}) : \mathbf{d}^k(\mathbf{q}), \quad \boldsymbol{\sigma}^1(\mathbf{q}) \equiv -\mathbf{Y}^0(\mathbf{q}) \cdot \bar{\mathbf{f}}(\mathbf{q})$$

Common choices : $\mu^0 = \mu_f$ or $\mu^0 = 2\mu_f, 4\mu_f$ (in-between μ_f and ∞).

FFT methods for Stokes flow

Bignonnet and Dormieux : polarization scheme with variational framework. Introduce a reference viscosity μ^0 :

$$\boldsymbol{\tau}(\mathbf{x}) = \boldsymbol{\sigma}(\mathbf{x}) - 2\mu^0 \mathbf{d}(\mathbf{x})$$

Green function G^0 , third-order Green operator \mathcal{G}^0 , fourth-order Green operator Γ^0 :

$$\begin{aligned}\mathbf{u} &= \bar{\mathbf{u}} + G^0 * f_S^{-1} \chi^S \boldsymbol{\alpha} + \mathcal{G}^0 * \boldsymbol{\tau}, \\ \mathbf{d} &= -\Gamma^0 * \boldsymbol{\tau} + {}^t \mathcal{G}^0 * f_S^{-1} \chi^S \boldsymbol{\alpha},\end{aligned}$$

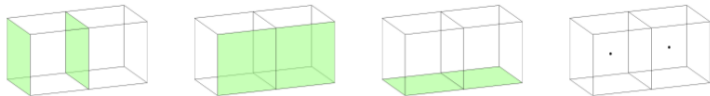
with $\bar{\mathbf{u}} = -f_S^{-2} \overline{\chi^S G^0 * \chi^S} \cdot \boldsymbol{\alpha} = -G_0^{SS} \cdot \boldsymbol{\alpha}$

Tensors G^0 , \mathcal{G}^0 and Γ^0 have simple forms in Fourier space (for the problem in the continuum).

In these methods, the solid phase must form one continuous phase. Different discretizations (e.g. finite-differences) are possible. See Bignonnet (2020).

FFT methods for Stokes flow

Method developed by A. Wiegmann (2007). Velocity field evaluated at the center of the voxel faces, pressure field at the center of the voxels.



With local centered differences, $\Delta \mathbf{u}$ and $\nabla \cdot P$ evaluated at the center of voxel faces, and $\text{div} \mathbf{u}$ at the voxel centers.

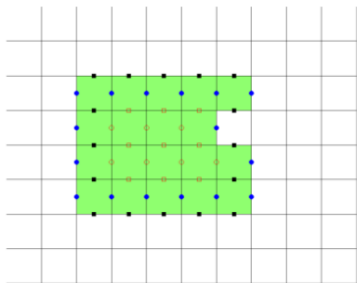
$$\Delta \mathbf{u}(\mathbf{x}) \approx \Delta_h \mathbf{u}(\mathbf{x}) = \frac{\sum_i [\mathbf{u}(\mathbf{x} + \mathbf{e}_i) + \mathbf{u}(\mathbf{x} - \mathbf{e}_i) - 2\mathbf{u}(\mathbf{x})]}{h^2},$$

$$(\partial_i P)(\mathbf{x} + \mathbf{e}_i/2) \approx (\nabla_h P) \cdot \mathbf{e}_i = \frac{P(\mathbf{x} + \mathbf{e}_i) - P(\mathbf{x})}{h},$$

$$(\text{div} \mathbf{u})(\mathbf{x}) \approx (\text{div}_h \mathbf{u})(\mathbf{x}) = \sum_i \frac{u_i(\mathbf{x} + \mathbf{e}_i/2) - u_i(\mathbf{x} - \mathbf{e}_i/2)}{h}$$

FFT methods for Stokes flow

No slip boundary conditions ?



Method “FFF” : $\mathbf{u} = 0$ along blue and black points. Enforces normal and tangential no-slip boundary conditions.

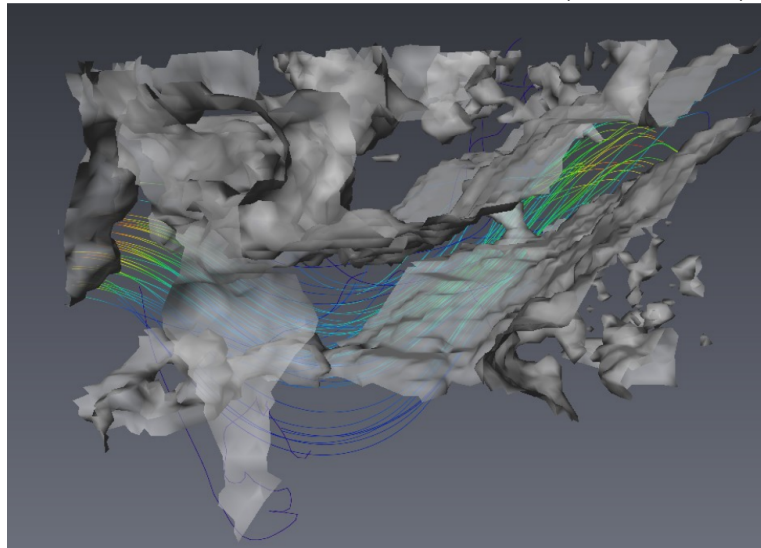
Discretized system rewritten as

$$\mu \Delta_h \mathbf{u} = \nabla_h P + \mathbf{f}$$

The force \mathbf{f} takes non-zero values along the fluid-solid interface. Fields P and \mathbf{u} can be computed from \mathbf{f} . System solved by conjugate gradient method. Poisson equation solved by FFTs (Wiegmann, 2007).

Results : 2D cylindrical obstacle

Fluid flow inside anode material used in fuel cells (Abdallah, 2016).



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Topics not addressed here :

- ▶ Dislocations.
- ▶ Strain gradients.
- ▶ Periodic boundary conditions.
- ▶ Finite strain. Requires a different Green operator to take into account rotations.