

Séminaire du Centre de Recherche de l'École de l'Air (CRÉA)

# An overview of “FFT-based techniques” for numerical homogenization

**S. Brisard**

Laboratoire Navier (UMR 8205),  
École des Ponts ParisTech, Université Gustave Eiffel, CNRS, Marne-la-Vallée, France

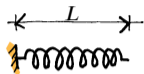
30 sept. 2020



# Outline of this talk

- Mechanics in a (tiny) nutshell
- Homogenization in a nutshell
- The case of continuum mechanics: the homogenization problem and full-field simulations
- Intermezzo # 1: on linear systems
- Intermezzo # 2: on eigenstrains
- The Lippmann–Schwinger equation and its discretization

# From position to displacement to strain



$$F = kx \quad \longrightarrow \quad F = k(\ell - L) \quad \longrightarrow \quad \varepsilon = \frac{\ell - L}{L}$$

# From forces to stresses



$$P = Mg$$

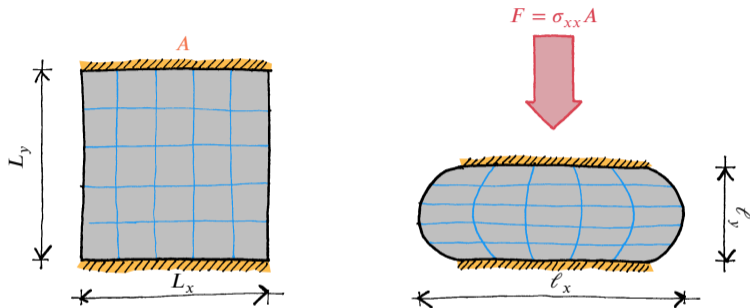
Giacometti exhibition in Washington  
(SIPANY/SIPA)  
(reproduced from [francetvinfo.fr](http://francetvinfo.fr))



Footprint of a prehistoric child, Pech Merle cave  
(reproduced from  
<http://www.pechmerle.com>)

$$\sigma = \frac{\Delta F}{\Delta A}$$

# Strains and stresses are tensors

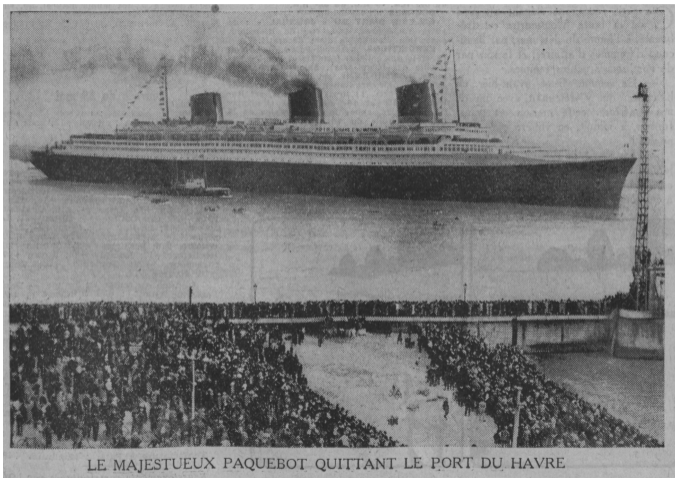


$$\epsilon_{xx} = \frac{l_x - L_x}{L_x}$$

$$\epsilon_{yy} = \frac{l_y - L_y}{L_y}$$

$$\epsilon_{xy} = ???$$

# What is homogenization?



The launch of the *Normandie* ocean liner (1935)  
*Le Journal*, num. 15565. Downloaded from [Gallica](#)

# What is homogenization?



# What is homogenization?

## Three length-scales

- $L_\mu$ : microscopic length-scale (size of dots, dot spacing)
- $L_m$ : mesoscopic length-scale (size of patches)
- $L_M$ : macroscopic length-scale (screen-to-eye distance)

## Separation of scales

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



# What is homogenization?

## In the present context

Homogenization is the process of replacing the complex distribution of dots with an equivalent, homogeneous patch of gray.

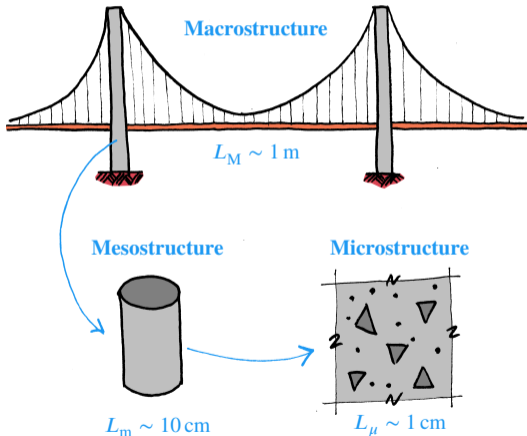
The goal is to establish the (quantitative) rule that relates the dot pattern (size and spacing of dots) to the gray level.

## More generally

Homogenization is the process of replacing the complex *microstructure* with an equivalent, homogeneous *mesostructure*.

The goal is to establish the (quantitative) rule that relates the physical properties of the microstructure to the macroscopic property.

# Homogenization of mechanical properties



# Homogenization of linear elastic properties

## The goal

At the scale of the structure (the towers of the suspension bridge), material heterogeneities (aggregates, ...) are **ignored**. The response of the structure is computed as if it was **homogeneous**.

## Effective (macroscopic) linear elastic properties

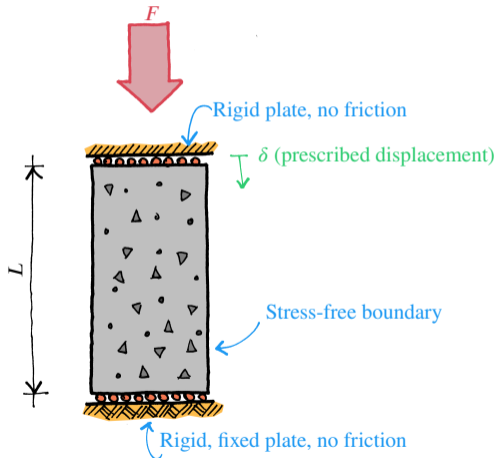
$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{C}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}) \quad \Rightarrow \quad \langle \boldsymbol{\sigma} \rangle = \mathbf{C}^{\text{eff}} : \langle \boldsymbol{\varepsilon} \rangle$$

## The homogenization problem

Effective properties are found **at the mesoscopic scale**

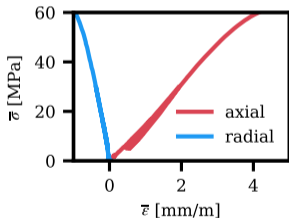
- from experimental characterization (**top-down** approach)
- or from numerical simulation (**bottom-up** approach)

# The top-down approach



## Macroscopic variables

- Macro. stress:  $F/A$
- Macro. strain:  $\delta/L$



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

# Modelling the axial compression test

## Field equations

- Self-weight is negligible  $\Rightarrow$  no body-forces
- Loading comes from boundary conditions only!

## Boundary conditions

- Stress-free lateral surface
- Upper & lower faces: no friction, prescribed vertical displacement

## Macro-homogeneity condition — This is essential!

$$\langle \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \rangle = \langle \boldsymbol{\sigma} \rangle : \langle \boldsymbol{\varepsilon} \rangle = \frac{F}{A} \frac{\delta}{L} = \text{macro. stress} \times \text{macro. strain}$$

**The axial compression test is effectively  
a strain-driven experiment!**

# The bottom-up approach

## The need for a bottom-up approach

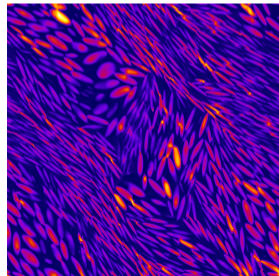
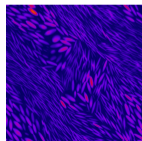
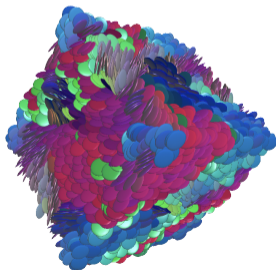
- Experimental approach is not predictive
- How microstructural features affect macroscopic properties cannot be understood

## What is the bottom-up approach?

- Physical exp. replaced with thought exp.
- Essential features of physical exp. are kept
  - “large” sample (a.k.a. **statistical volume element**)
  - no body-forces
  - suitable boundary conditions

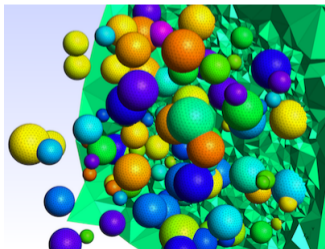
# “Full-field” simulations

- Physical exp.: macro. stress and strain are **measured**
- Thought exp.: they are **computed** a posteriori
- Solve the homogenization problem to find local stresses and strains
- Compute macro. variables as volume averages of local variables



# The homogenization problem is hard

- Standard problem of continuum mechanics
- FE analyses are possible
- There are a lot of interfaces
- Creating the mesh is a tedious procedure
- The FE model is large (many degrees of freedom)



Reproduced from [www.gmsh.info](http://www.gmsh.info)



# Intermezzo #1: on linear systems

- The initial linear system (complex LHS, simple RHS)

$$\begin{cases} 2x - y = 1 \\ -5x + 3y = 1 \end{cases} \quad \text{solution: } x = 4 \quad y = 7$$

- Let's rewrite this linear system ( $\alpha$ : arbitrary number)

$$\begin{cases} \alpha x + (2 - \alpha)x - y = 1 \\ \alpha y - 5x + (3 - \alpha)y = 1 \end{cases}$$

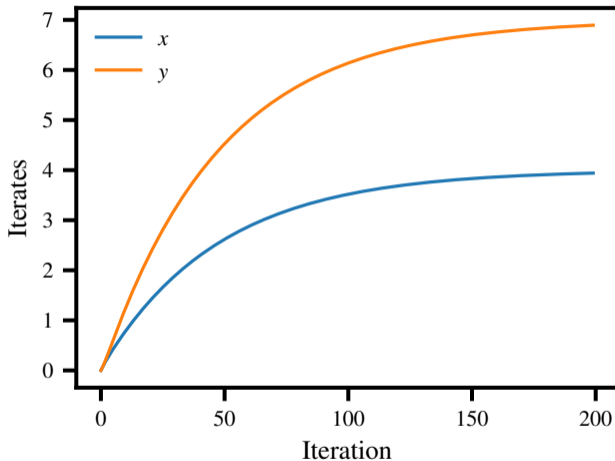
- The equivalent linear system (simple LHS, complex RHS)

$$\begin{cases} \alpha x = 1 - (2 - \alpha)x + y \\ \alpha y = 1 + 5x - (3 - \alpha)y \end{cases}$$

# Iterative solution of transformed system

- Remember transformed system: 
$$\begin{cases} \alpha x = 1 - (2 - \alpha)x + y \\ \alpha y = 1 + 5x - (3 - \alpha)y \end{cases}$$
- Start from e.g.  $x_0 = 0, y_0 = 0$
- Compute  $x_1$  and  $y_1$ : 
$$\begin{cases} \alpha x_1 = 1 - (2 - \alpha)x_0 + y_0 \\ \alpha y_1 = 1 + 5x_0 - (3 - \alpha)y_0 \end{cases}$$
- Compute  $x_2$  and  $y_2$ : 
$$\begin{cases} \alpha x_2 = 1 - (2 - \alpha)x_1 + y_1 \\ \alpha y_2 = 1 + 5x_1 - (3 - \alpha)y_1 \end{cases}$$
- ...iterate until convergence (or the absence of it)

# Iterations with $\alpha = 10$



**Slow convergence!**

## Iterations with $\alpha = 2$

$$x_{10} = 1.67285156$$

$$y_{10} = 7.46191406$$

$$x_{20} = -24.7685709$$

$$y_{20} = 85.29713631$$

$$x_{30} = -790.49446901$$

$$y_{30} = 2223.99702253$$

$$x_{40} = -22267.97299532$$

$$y_{40} = 62174.26642779$$

$$x_{50} = -624455.17753026$$

$$y_{50} = 1743052.24003351$$

**No convergence at all!**

# Back to homogenization

## Summary

- Start from linear system with complex LHS (+ simple RHS)
- Build transformed system with simple LHS (+ more complex RHS)
- Solve transformed system iteratively (pray for convergence!)

## The homogenization problem

- Is a set of **partial differential equations**
- After suitable discretization, it reduces to a **linear system**
- LHS relates to the **material**; complex for heterogeneous materials
- RHS relates to the **loading**
- Idea: introduce a **homogeneous** reference material ( $\simeq \alpha$ ) to transform linear system

# Intermezzo #2: on eigenstrained materials

## Thermoelasticity

- Most materials tend to expand upon heating
- Notable exception: water
- Order of magnitude (steel, concrete):  $\Delta L/L = 1.2 \cdot 10^{-5} \text{ m/m/K}$

## Example: a bridge deck

span = 30 m      width = 6 m      thickness = 25 cm  
temp. diff. = 50°C    Young mod. = 30 GPa

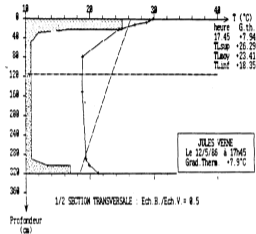
- Unrestrained ends:  $\Delta L = 1.2 \cdot 10^{-5} \times 30 \times 50 = 1.8 \text{ cm}$
- Fixed ends:  $F = 30 \cdot 10^9 \times 1.2 \cdot 10^{-5} \times 50 \times 6 \times 0.25$   
 $= 27 \text{ MN} \equiv 2700 \text{ t}$

# Complex eigenstrain distributions

Temp. elevation across deck of J. Verne bridge, Amiens, Fr.



Credits J. Mossot via Wikimedia

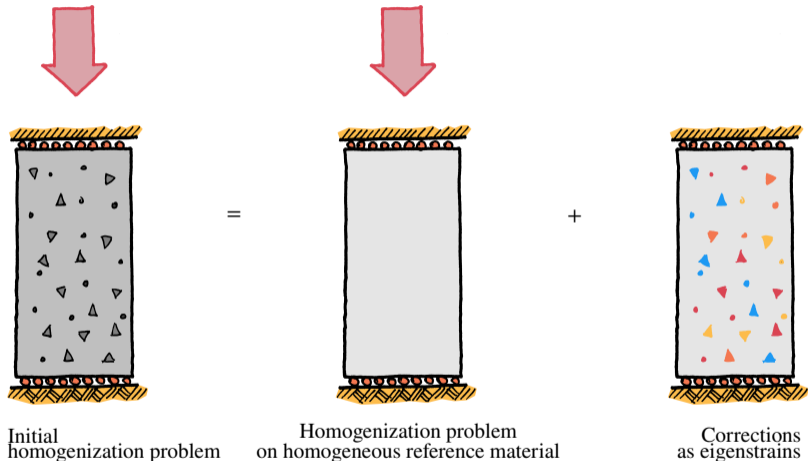


Reproduced from Hadjeb [[Had91](#)]

## Discretization of PDEs

- Eigenstrains affect the RHS of the system!
- Finding the effect of eigenstrains in a homogeneous material is relatively easy! See [[Kor73](#); [ZD73](#); [Krö74](#)]

# The Lippmann–Schwinger equation



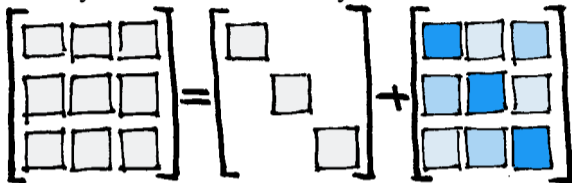
$$\boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} - \boldsymbol{\Gamma}_0 [(\mathbf{C} - \mathbf{C}_0) : \boldsymbol{\varepsilon}]$$

see [Kor73; ZD73; Krö74]



# What did we gain?

- New system has an extremely nice structure



- Block-diagonal: efficient “matvec” product in the real space
- Block-circulant: efficient “matvec” product in the Fourier space
- Globally: efficient, matrix-free “matvec” product
- Need for iterative linear solvers (GC and the likes)
- Straightforward implementation
- Parallelization rather simple

# Introducing “FFT-based” methods

- A very unfortunate name: FFT is just a means to the end
- Better: “Lippmann–Schwinger solvers”
- Even better (credit where credit is due): “Moulinec–Suquet solvers”

## (Sketchy) Historical outline

- Seminal papers: Moulinec, Suquet (and Michel)  
[MS94; MS98; MMS01]
- Early contribution from Eyre and Milton [EM99]
- New contributions started in late 2000: [WP08; Zem+10; BD10]
- Other groups joined soon afterwards: Fraunhofer ITWM (Germany), CEA (France), Eindhoven University (The Netherlands)...
- Small but vibrant community:  
mini-symposium at each Ecomas Congress

# State-of-the art FFT-based methods

- Discretization: [BD10; BD12; SOK15; SMK17; Wil15]
- Fast solvers
  - polarization-based: [EM99; MB12; MS14; SWB19]
  - krylov based: [BD10; Zem+10; BD12; BS18; Sch20; WSB20]
  - fast-gradients: [KBS14; Sch17; Sch19]
- Convergence, stopping criteria: [MMS01; BD12; MS14; SWB19]
- Multiscale simulations (FEM  $\times$  FFT): [GK18]

# State-of-the art FFT-based methods

- Material non-linearities: [MS94; MS98; GM13]...
- Geometric non-linearities: [KBS14; KFS16; dGeu+17]
- Multiphysical couplings
  - piezoelectricity: [BBL12]
  - phase fields for crystal plasticity: [Che+15]...
  - phase fields for cracking: [Che+19; Cao+20]

## Challenges

- Preconditioning
- Adaptative mesh refinement

# Closure

- Introduction to homogenization
- The homogenization problem for continuum mechanics
- The Lippmann–Schwinger equation for full-field simulations

## What we did not cover

- Variational formulation of the Lippmann–Schwinger equation: the principle of Hashin and Shtrikman [[HS62b](#); [Wil77](#)]
- Theoretical results using this principle [[HS62a](#); [Wil77](#)]... and many, many, many more!

# Thank you for your attention

`sebastien.brisard@univ-eiffel.fr`  
`https://cv.archives-ouvertes.fr/sbrisard`  
`https://sbrisard.github.io`



This work is licensed under the Creative Commons Attribution 4.0 International License. To view a copy of this license, visit <http://creativecommons.org/licenses/by/4.0/> or send a letter to Creative Commons, PO Box 1866, Mountain View, CA 94042, USA.

# References

- [BBL12] R. Brenner et al. “Investigation of the Effective Response of 2-1-2 Piezoelectric Composites.” In: *Procedia IUTAM*. IUTAM Symposium on Linking Scales in Computations: From Microstructure to Macro-Scale Properties 3 (2012), pp. 292–300.
- [BD10] S. Brisard and L. Dormieux. “FFT-Based Methods for the Mechanics of Composites: A General Variational Framework.” In: *Computational Materials Science* 49.3 (2010), pp. 663–671.
- [BD12] S. Brisard and L. Dormieux. “Combining Galerkin Approximation Techniques with the Principle of Hashin and Shtrikman to Derive a New FFT-Based Numerical Method for the Homogenization of Composites.” In: *Computer Methods in Applied Mechanics and Engineering* 217–220 (2012), pp. 197–212.
- [BS18] C. Bellis and P. Suquet. “Geometric Variational Principles for Computational Homogenization.” In: *Journal of Elasticity* (2018).
- [Cao+20] Y. J. Cao et al. “A Novel FFT-Based Phase Field Model for Damage and Cracking Behavior of Heterogeneous Materials.” In: *International Journal of Plasticity* 133 (2020), p. 102786.
- [Che+15] L. Chen et al. “An Integrated Fast Fourier Transform-Based Phase-Field and Crystal Plasticity Approach to Model Recrystallization of Three Dimensional Polycrystals.” In: *Computer Methods in Applied Mechanics and Engineering* 285 (2015), pp. 829–848.

- [Che+19] Y. Chen et al. “A FFT Solver for Variational Phase-Field Modeling of Brittle Fracture.” In: *Computer Methods in Applied Mechanics and Engineering* 349 (2019), pp. 167–190.
- [dGeu+17] T. W. J. de Geus et al. “Finite Strain FFT-Based Non-Linear Solvers Made Simple.” In: *Computer Methods in Applied Mechanics and Engineering* 318 (2017), pp. 412–430.
- [EM99] D. J. Eyre and G. W. Milton. “A Fast Numerical Scheme for Computing the Response of Composites Using Grid Refinement.” In: *The European Physical Journal - Applied Physics* 6.01 (1999), pp. 41–47.
- [GK18] F. S. Göküzüm and M.-A. Keip. “An Algorithmically Consistent Macroscopic Tangent Operator for FFT-Based Computational Homogenization.” In: *International Journal for Numerical Methods in Engineering* 113.4 (2018), pp. 581–600.
- [GM13] L. Gélébart and R. Mondon-Cancel. “Non-Linear Extension of FFT-Based Methods Accelerated by Conjugate Gradients to Evaluate the Mechanical Behavior of Composite Materials.” In: *Computational Materials Science* 77 (2013), pp. 430–439.
- [Had91] A. Hadjeb. “Analyse Des Actions Thermiques Sur Les Ouvrages d’art En Béton.” Thèse de doctorat. Université des Sciences et Techniques de Lille-Flandre-Artois, 1991.
- [HS62a] Z. Hashin and S. Shtrikman. “A Variational Approach to the Theory of the Elastic Behaviour of Polycrystals.” In: *Journal of the Mechanics and Physics of Solids* 10.4 (1962), pp. 343–352.



- [HS62b] Z. Hashin and S. Shtrikman. “On Some Variational Principles in Anisotropic and Nonhomogeneous Elasticity.” In: *Journal of the Mechanics and Physics of Solids* 10.4 (1962), pp. 335–342.
- [KBS14] M. Kabel et al. “Efficient Fixed Point and Newton–Krylov Solvers for FFT-Based Homogenization of Elasticity at Large Deformations.” In: *Computational Mechanics* 54.6 (2014), pp. 1497–1514.
- [KFS16] M. Kabel et al. “Mixed Boundary Conditions for FFT-Based Homogenization at Finite Strains.” In: *Computational Mechanics* 57.2 (2016), pp. 193–210.
- [Kor73] J. Korringa. “Theory of Elastic Constants of Heterogeneous Media.” In: *Journal of Mathematical Physics* 14.4 (1973), pp. 509–513.
- [Krö74] E. Kröner. “On the Physics and Mathematics of Self-Stresses.” In: *Topics in Applied Continuum Mechanics*. Ed. by J. L. Zeman and F. Ziegler. Vienna: Springer Verlag Wien, 1974, pp. 22–38.
- [MB12] V. Monchiet and G. Bonnet. “A Polarization-Based FFT Iterative Scheme for Computing the Effective Properties of Elastic Composites with Arbitrary Contrast.” In: *International Journal for Numerical Methods in Engineering* 89.11 (2012), pp. 1419–1436.
- [MMS01] J. C. Michel et al. “A Computational Scheme for Linear and Non-Linear Composites with Arbitrary Phase Contrast.” In: *International Journal for Numerical Methods in Engineering* 52.1-2 (2001), pp. 139–160.

- [MS14] H. Moulinec and F. Silva. “Comparison of Three Accelerated FFT-Based Schemes for Computing the Mechanical Response of Composite Materials.” In: *International Journal for Numerical Methods in Engineering* 97.13 (2014), pp. 960–985.
- [MS94] H. Moulinec and P. Suquet. “A Fast Numerical Method for Computing the Linear and Nonlinear Mechanical Properties of Composites.” In: *Comptes rendus de l’Académie des sciences. Série II, Mécanique, physique, chimie, astronomie* 318.11 (1994), pp. 1417–1423.
- [MS98] H. Moulinec and P. Suquet. “A Numerical Method for Computing the Overall Response of Nonlinear Composites with Complex Microstructure.” In: *Computer Methods in Applied Mechanics and Engineering* 157.1–2 (1998), pp. 69–94.
- [Sch17] M. Schneider. “An FFT-Based Fast Gradient Method for Elastic and Inelastic Unit Cell Homogenization Problems.” In: *Computer Methods in Applied Mechanics and Engineering* 315 (2017), pp. 846–866.
- [Sch19] M. Schneider. “On the Barzilai-Borwein Basic Scheme in FFT-Based Computational Homogenization.” In: *International Journal for Numerical Methods in Engineering* 118.8 (2019), pp. 482–494.
- [Sch20] M. Schneider. “A Dynamical View of Nonlinear Conjugate Gradient Methods with Applications to FFT-Based Computational Micromechanics.” In: *Computational Mechanics* 66.1 (2020), pp. 239–257.
- [SMK17] M. Schneider et al. “FFT-Based Homogenization for Microstructures Discretized by Linear Hexahedral Elements.” In: *International Journal for Numerical Methods in Engineering* 109.10 (2017), pp. 1461–1489.

- [SOK15] M. Schneider et al. “Computational Homogenization of Elasticity on a Staggered Grid.” In: *International Journal for Numerical Methods in Engineering* (2015), n/a–n/a.
- [SWB19] M. Schneider et al. “On Polarization-Based Schemes for the FFT-Based Computational Homogenization of Inelastic Materials.” In: *Computational Mechanics* 64.4 (2019), pp. 1073–1095.
- [Wil15] F. Willot. “Fourier-Based Schemes for Computing the Mechanical Response of Composites with Accurate Local Fields.” In: *Comptes Rendus Mécanique* 343.3 (2015), pp. 232–245.
- [Wil77] J. Willis. “Bounds and Self-Consistent Estimates for the Overall Properties of Anisotropic Composites.” In: *Journal of the Mechanics and Physics of Solids* 25.3 (1977), pp. 185–202.
- [WP08] F. Willot and 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.
- [WSB20] D. Wicht et al. “On Quasi-Newton Methods in Fast Fourier Transform-Based Micromechanics.” In: *International Journal for Numerical Methods in Engineering* 121.8 (2020), pp. 1665–1694.
- [ZD73] R. Zeller and P. H. Dederichs. “Elastic Constants of Polycrystals.” In: *Physica Status Solidi (B)* 55.2 (1973), pp. 831–842.

- [Zem+10] J. Zeman et al. “Accelerating a FFT-Based Solver for Numerical Homogenization of Periodic Media by Conjugate Gradients.” In: *Journal of Computational Physics* 229.21 (2010), pp. 8065–8071.