Overview of FFT-based homogenization techniques from the Galerkin point of view (slides)

Sébastien Brisard

Overview of FFT-based homogenization techniques from the Galerkin point of view

Sébastien Brisard

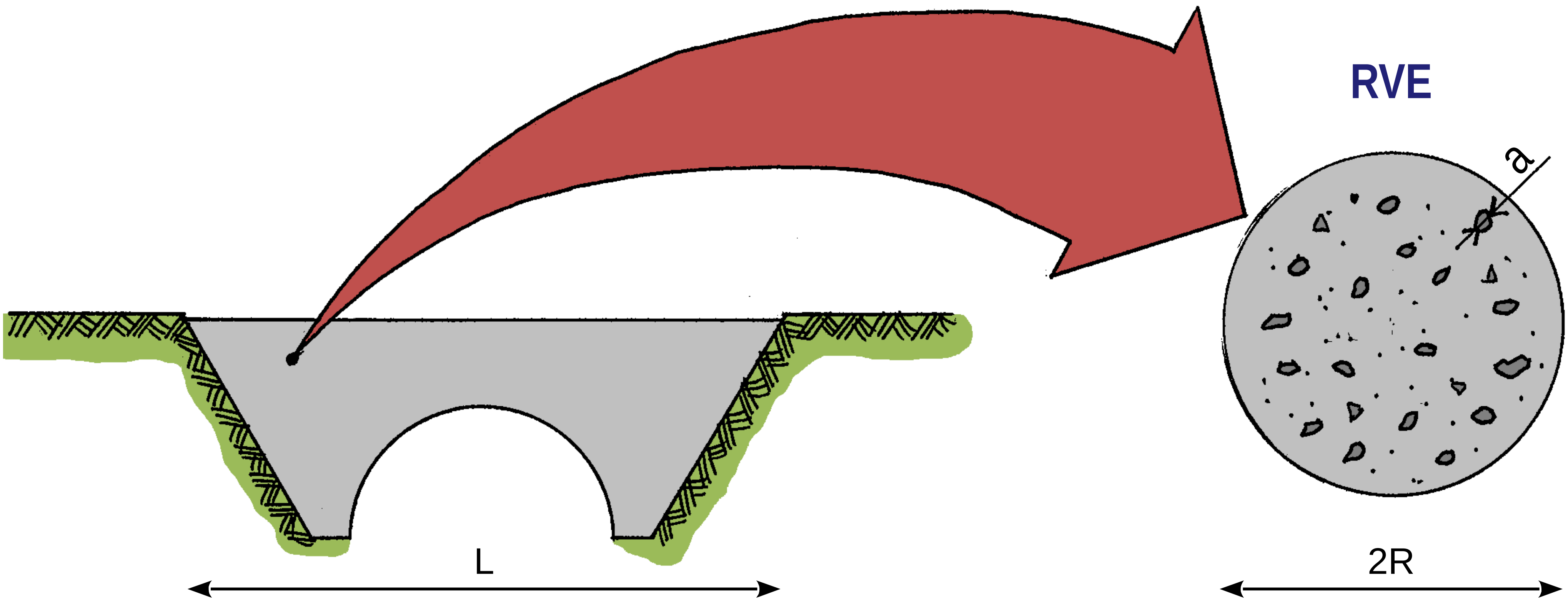
Université Paris-Est, Laboratoire Navier (UMR 8205), CNRS, ENPC, IFSTTAR

Acknowledgements: V.P. Tran, L. Dormieux, F. Legoll, L. Chamoin

Introduction

- Homogenization requires the solution to the so-called “corrector problem”
- Traditional numerical methods (e.g. FEM) can be costly
  - Conforming mesh
  - Large linear system
- Grid-based methods are handy in such situations!
- FFT-based methods first introduced by Moulinec and Suquet (1994)
- Since about 2010, regain of interest for these methods
- Present talk: overview, biased towards a variational point of vew
  - Brief recap on homogenization
  - The Lippmann-Schwinger equation (LS): strong and weak forms
  - Galerkin discretization of LS: consistent and asymptotically consistent discretizations
  - 3D application

Homogenization in a nutshell



Initial problem

$$\operatorname{div}(\mathbf{C}:\boldsymbol{\varepsilon})+\boldsymbol{B}=\mathbf{0}$$
$$\boldsymbol{\varepsilon}=\operatorname{sym}\operatorname{grad}\boldsymbol{u}$$
+ Boundary Conditions

Homogenization

Separation of scales $a \ll R \ll L$

Homogenized problem

$$\operatorname{div}(\mathbf{C}^{\mathrm{eff}}:\boldsymbol{\varepsilon})+\boldsymbol{B}=\mathbf{0}$$
$$\boldsymbol{\varepsilon}=\operatorname{sym}\operatorname{grad}\boldsymbol{u}$$
+ Boundary Conditions

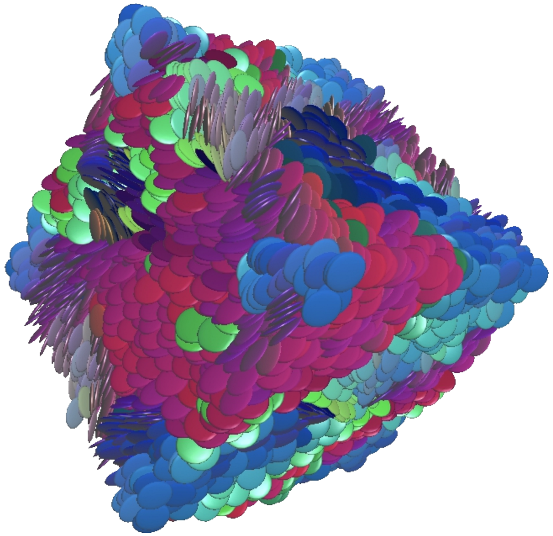
Computation of the homogenized stiffness

Elastic equilibrium of RVE

Heterogeneous

$$\operatorname{div}\left(\boxed{\mathbf{C}} : \boldsymbol{\varepsilon}\right) = \mathbf{0}$$
$$\boldsymbol{\varepsilon} = \operatorname{sym}\operatorname{grad}\boldsymbol{u}$$
$$\mathrm{BC}\left(\boldsymbol{E}\right)$$

Can be complex!



Boundary conditions

- Ensure that average strain is $\boldsymbol{E}$
- Hilll's lemma must hold

Example: periodic BCs

$$\boldsymbol{u}\left(\boldsymbol{x}\right) = \boldsymbol{E}\cdot\boldsymbol{x} + \boxed{\boldsymbol{u}^{\mathrm{per}}}\left(\boldsymbol{x}\right)$$

Periodic

Well-suited to numerical homogenization

Kanit et al. (2003), *Int J Sol Struct* **40**, 3647-3679

Macroscopic stress

$$\boldsymbol{\Sigma} = \overline{\boldsymbol{\sigma}} = \boldsymbol{C}^{\mathrm{eff}} : \overline{\boldsymbol{\varepsilon}} = \boldsymbol{C}^{\mathrm{eff}} : \boldsymbol{E}$$

The Lippmann-Schwinger equation (LS)

Reference material

- Arbitrary, homogeneous stiffness: $\boldsymbol{C}_0$
- Interesting additional properties if reference material stiffer/softer than all phases

Hashin and Shtrikman (1962), *J Mech Phys Sol* **10**, 335-342

Willis (1977), *J Mech Phys Sol* **25**, 185-202

The Green operator for strains

$$\operatorname{div}\left(\boldsymbol{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\varpi}\right) = \mathbf{0}, \quad \boldsymbol{\varepsilon} = \operatorname{sym}\operatorname{grad}\boldsymbol{u}^{\mathrm{per}} \quad \overset{\text{def.}}{\Longleftrightarrow} \quad \boldsymbol{\varepsilon} = -\boldsymbol{\Gamma}_0 * \boldsymbol{\varpi}$$

The Lippmann-Schwinger equation

$$\operatorname{div}\left(\boldsymbol{C} : \boldsymbol{\varepsilon}\right) = \mathbf{0}, \quad \boldsymbol{\varepsilon} = \boldsymbol{E} + \operatorname{sym}\operatorname{grad}\boldsymbol{u}^{\mathrm{per}} \quad \Longleftrightarrow \quad \left(\boldsymbol{C} - \boldsymbol{C}_0\right)^{-1} : \boldsymbol{\tau} + \boldsymbol{\Gamma}_0 * \boldsymbol{\tau} = \boldsymbol{E}, \quad \boldsymbol{\tau} = \left(\boldsymbol{C} - \boldsymbol{C}_0\right) : \boldsymbol{\varepsilon}$$

Korringa (1973), *J Math Phys* **14**, 509-513

Kröner (1974), *Topics in Applied Continuum Mechanics*, 22-38

Nemat-Nasser et al. (1982), *Mech Mat* **15**, 163-181

Zeller and Dederichs (1973), *Physica Status Solidi (B)* **55**, 831-842

LS as a variational problem

Strong form

$$(\mathbf{C}-\mathbf{C}_0)^{-1}:\boldsymbol{\tau}+\boldsymbol{\Gamma}_0*\boldsymbol{\tau}=\mathbf{E}$$

$\Longleftrightarrow$

Weak form: find $\boldsymbol{\tau}\in V$ such that

$$a(\boldsymbol{\tau},\boldsymbol{\varpi})=f(\boldsymbol{\varpi})\text{ for all }\boldsymbol{\varpi}\in V$$

V: space of square integrable, second order, symmetric tensors.

The linear form: $f(\boldsymbol{\varpi})=\mathbf{E}:\int\boldsymbol{\varpi}$

The bilinear form

$$a_{\mathrm{diag}}(\boldsymbol{\tau},\boldsymbol{\varpi})=\int\boldsymbol{\varpi}(\mathbf{x}):[\mathbf{C}(\mathbf{x})-\mathbf{C}_0]^{-1}:\boldsymbol{\tau}(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

$$a(\boldsymbol{\tau},\boldsymbol{\varpi})=\boxed{a_{\mathrm{diag}}(\boldsymbol{\tau},\boldsymbol{\varpi})}+\boxed{a_{\mathrm{circ}}(\boldsymbol{\tau},\boldsymbol{\varpi})}$$

$$a_{\mathrm{circ}}(\boldsymbol{\tau},\boldsymbol{\varpi})=\iint\varpi(\mathbf{x}):\boldsymbol{\Gamma}_0(\mathbf{x}-\mathbf{y}):\boldsymbol{\tau}(\mathbf{y})\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y}$$

Galerkin discretization of the LS equation

Find $\boldsymbol{\tau}\in V$ such that $a_{\text{diag}}(\boldsymbol{\tau},\boldsymbol{\varpi})+a_{\text{circ}}(\boldsymbol{\tau},\boldsymbol{\varpi})=f(\varpi)$ for all $\boldsymbol{\varpi}\in V$

Consistent discretization

Brisard and Dormieux (2010), *Comp Mat Sci* **49**, 663-671

Evaluation over V^h remains difficult!

Find $\boldsymbol{\tau}^h\in \boxed{V^h}$ such that $a_{\text{diag}}(\boldsymbol{\tau}^h,\boldsymbol{\varpi}^h)+\boxed{a_{\text{circ}}(\boldsymbol{\tau}^h,\boldsymbol{\varpi}^h)}=f(\boldsymbol{\varpi}^h)$ for all $\boldsymbol{\varpi}^h\in V^h$

Space of cell-wise constant polarization fields

Asymptotically consistent discretization: exact evaluation is not necessary!

Find $\boldsymbol{\tau}^h\in V^h$ such that $a_{\text{diag}}(\boldsymbol{\tau}^h,\boldsymbol{\varpi}^h)+\boxed{a^h_{\text{circ}}(\boldsymbol{\tau}^h,\boldsymbol{\varpi}^h)}=f(\boldsymbol{\varpi}^h)$ for all $\boldsymbol{\varpi}^h\in V^h$

Asymptotically consistent approximation

Brisard and Dormieux (2012), *Comp Meth Appl Mech Eng* **217-220**, 197-212

Asymptotically consistent approximations

- Periodic Green operator for strains is in fact given by an infinite Fourier series
- Various estimates of this series for cell-wise constant functions
  - **Truncation** of high frequencies: Moulinec and Suquet (1994, 1998)
  - **Exact** (up to round-off errors): Brisard and Dormieux (2010)
  - **Filtering** of high frequencies: Brisard and Dormieux (2012)
  - **Finite elements** approximation: Yvonnet (2012)
  - **Finite differences** approximation: Willot et al. (2014), Willot (2015)
- All these approximations can be fitted in the general framework introduced here!
- If appropriately implemented, they can be switched on-the-fly in a simulation.

Moulinec and Suquet (1994), *CR Acad Sci II* **318**, 1417-1423
Moulinec and Suquet (1998), *Comp Meth Appl Mech Eng* **57**, 69-94
Brisard and Dormieux (2010), *Comp Mat Sci* **49**, 663-671
Brisard and Dormieux (2012), *Comp Meth Appl Mech Eng* **217-220**, 197-212
Yvonnet (2012), *Int J Num Meth Eng* **92**, 178-205
Willot et al. (2014), *Int J Num Meth Eng* **98**, 518-533
Willot (2015), *CR Acad Sci Mec* **343**, 232-245

The underlying linear system

Discrete variational problem results in a linear system

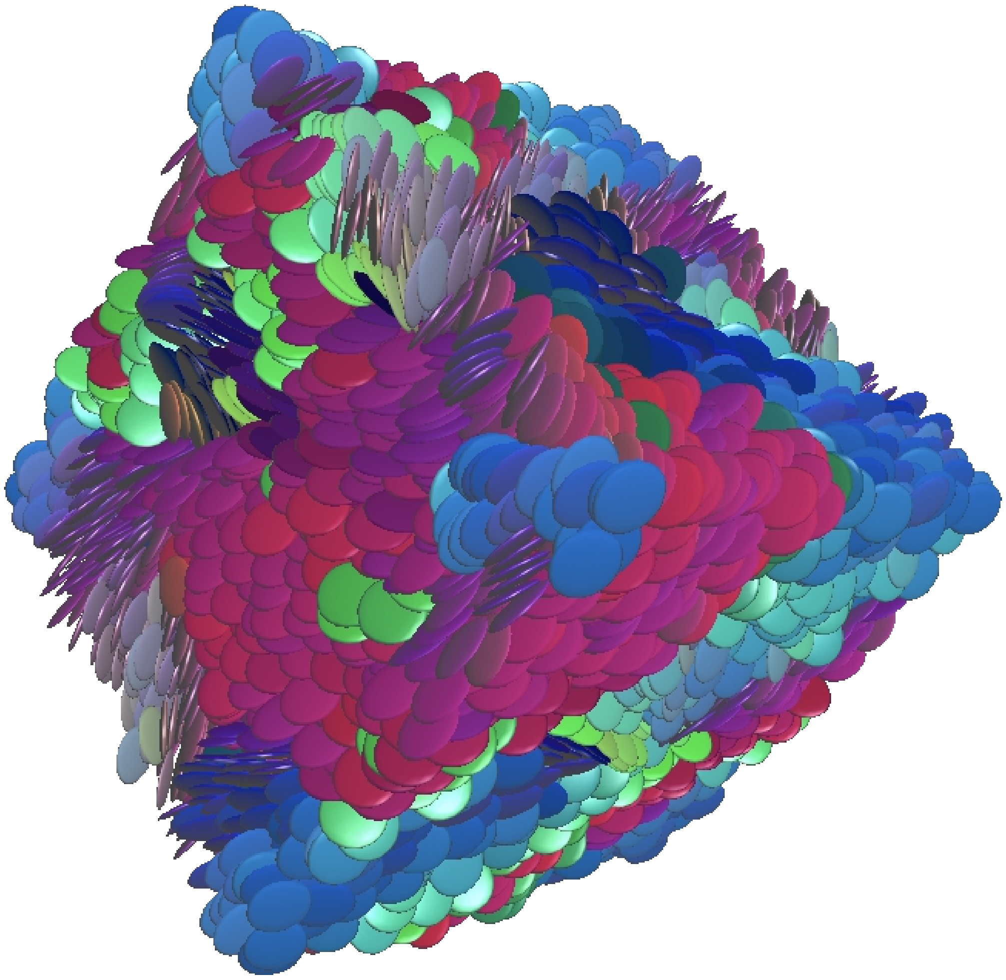
$$\left(\underbrace{\boxed{A_{\mathrm{diag}}}}_{\text{Block-diagonal}} + \underbrace{\boxed{A_{\mathrm{circ}}}}_{\text{Block-circulant}}\right) x = b$$

Solving the linear system

- Matrix is not sparse: matrix-free approach
- Use iterative linear solvers
  - Fixed-point iterations: Moulinec and Suquet (1994, 1998)
  - Augmented-Lagrangian: Michel et al. (2001)
  - Conjugate Gradient: Brisard and Dormieux (2010)
- Use FFT to compute matrix-vector products (Moulinec and Suquet, 1994, 1998)

Moulinec and Suquet (1994), *CR Acad Sci II* **318**, 1417-1423
Moulinec and Suquet (1998), *Comp Meth Appl Mech Eng* ***157***, 69-94
Michel et al. (2001), *Int J Num Meth Eng* **52**, 139-160
Brisard and Dormieux (2010), *Comp Mat Sci* **49**, 663-671

Example: 3D microstructure (1/2)



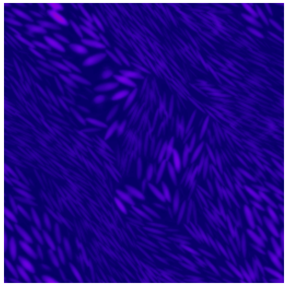
Microstructural parameters

- Flat spheroids (1/8 aspect ratio)
- Dense packing (60%)
- Large model (10000 particles)
- Moderate contrast (inclusions 100 times stiffer than matrix)

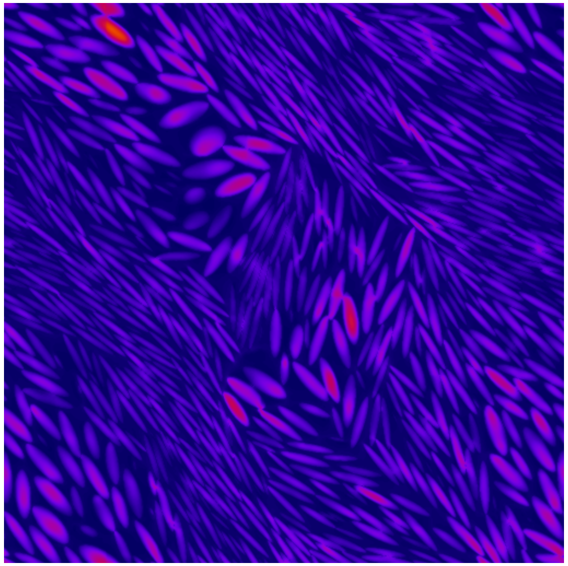
The simulation

- Home-made code
  - Python + Cython + FFTW + MPI
  - Very flexible implementation
  - Soon to be open-sourced (contact me!)
- Simulations run on two servers
  - Intel Xeon X5690, 3.47GHz, 192 Go
  - Intel Xeon E5-2643, 3.30GHz, 762 Go
- Most simulations run on 16 cores

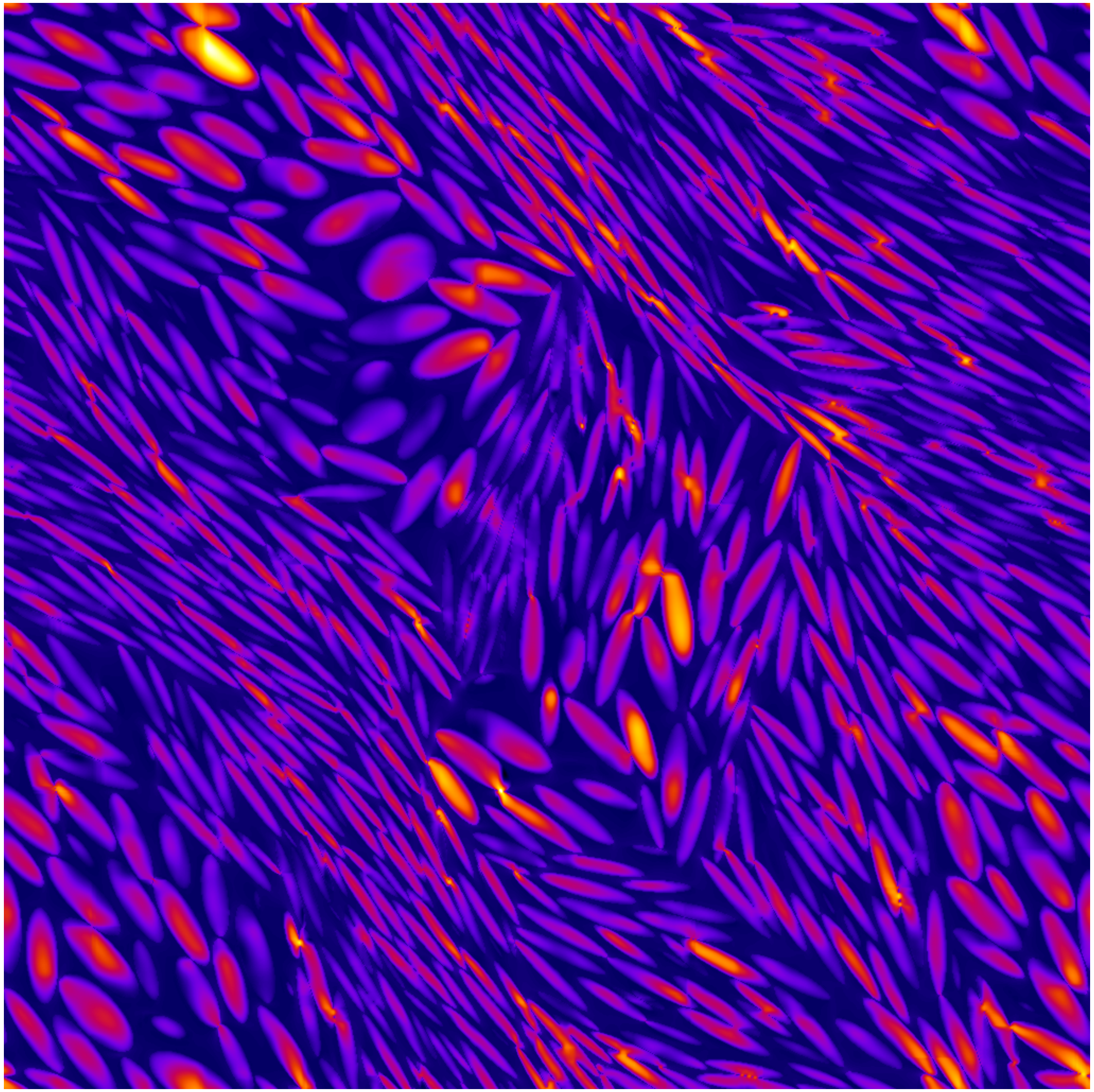
Example: 3D microstructure (2/2)



256^3



512^3



1024^3 (approx. $6 \cdot 10^9$ dofs)

Conclusion and outlook

- Summary
  - **General, unified** framework for FFT-based homogenization techniques
  - All avatars of this method (Moulinec & Suquet; Michel, Moulinec and Suquet; Yvonnet; Willot; Monchiet; …) fit into this unified framework
  - Clear distinction between **discretization** and iterative **solution** of the discretized problem: **any** discrete Green operator can be combined with **any** iterative linear solver
- Work in progress
  - **A priori** error estimates: with F. Legoll (Navier Laboratory, Ecole des Ponts ParisTech)
  - **A posteriori** error estimates: with L. Chamoin (LMT, ENS Cachan)
- Open questions
  - Matrix-free preconditioners
  - What is the “best” discrete Green operator?
  - What is the “best” reference material?

Thank you for your attention!

sebastien.brisard@ifsttar.fr