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

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

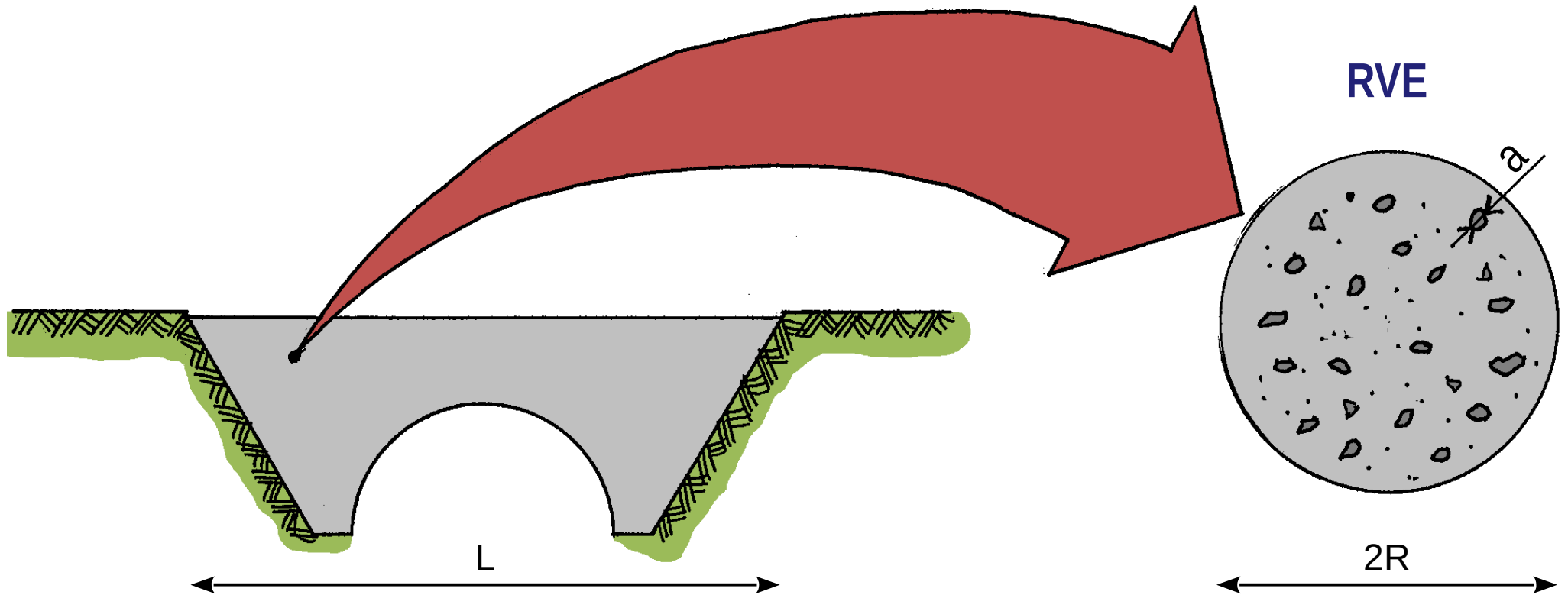
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- Homogenization requires the solution to the so-called “corrector problem”
- Traditional numerical methods (e.g. FEM) can be costly
 - Conforming mesh
 - Large linear system
- Grid-based methods are handy in such situations!
- FFT-based methods first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

Navier Homogenization in a nutshell



Initial problem

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

Homogenization

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

Homogenized problem

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

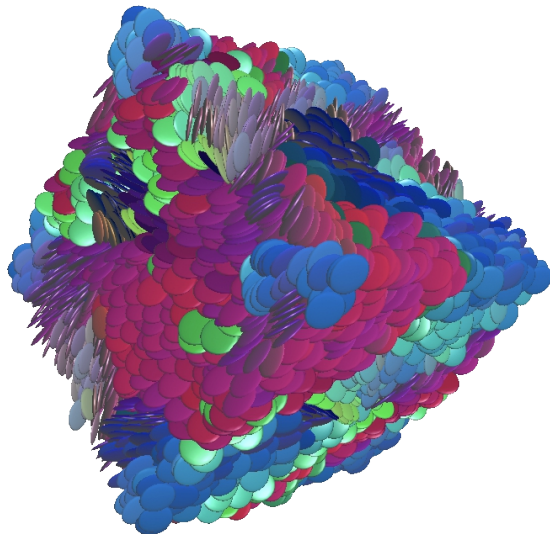
Navier Computation of the homogenized stiffness

Elastic equilibrium of RVE

$$\begin{aligned} \text{div}(\mathbf{C} : \boldsymbol{\varepsilon}) &= \mathbf{0} \\ \boldsymbol{\varepsilon} &= \text{sym grad } \mathbf{u} \\ \text{BC}(\mathbf{E}) \end{aligned}$$

Heterogeneous

Can be complex!



Boundary conditions

- Ensure that average strain is \mathbf{E}
- Hill's lemma must hold

Example: periodic BCs

$$\mathbf{u}(\mathbf{x}) = \mathbf{E} \cdot \mathbf{x} + \mathbf{u}^{\text{per}}(\mathbf{x})$$

Periodic

Well-suited to numerical homogenization

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

Macroscopic stress

$$\boldsymbol{\Sigma} = \bar{\boldsymbol{\sigma}} = \mathbf{C}^{\text{eff}} : \bar{\boldsymbol{\varepsilon}} = \mathbf{C}^{\text{eff}} : \mathbf{E}$$

Reference material

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

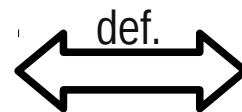
Hashin and Shtrikman (1962), *J Mech Phys Sol* **10**, 335-342

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

The Green operator for strains

$$\text{div}(\mathbf{C}_0 : \boldsymbol{\varepsilon} + \boldsymbol{\varpi}) = \mathbf{0}$$

$$\boldsymbol{\varepsilon} = \text{sym grad } \mathbf{u}^{\text{per}}$$

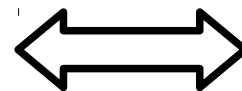


$$\boldsymbol{\varepsilon} = -\boldsymbol{\Gamma}_0 * \boldsymbol{\varpi}$$

The Lippmann-Schwinger equation

$$\text{div}(\mathbf{C} : \boldsymbol{\varepsilon}) = \mathbf{0}$$

$$\boldsymbol{\varepsilon} = \mathbf{E} + \text{sym grad } \mathbf{u}^{\text{per}}$$



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

$$\boldsymbol{\tau} = (\mathbf{C} - \mathbf{C}_0) : \boldsymbol{\varepsilon}$$

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

Navier LS as a variational problem

Strong form

$$(\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} + \Gamma_0 * \boldsymbol{\tau} = \mathbf{E} \quad \longleftrightarrow$$

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

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

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

$$a_{\text{circ}}(\boldsymbol{\tau}, \boldsymbol{\varpi}) = \iint \boldsymbol{\varpi}(\mathbf{x}) : \Gamma_0(\mathbf{x} - \mathbf{y}) : \boldsymbol{\tau}(\mathbf{y}) d\mathbf{x} d\mathbf{y}$$

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

Asymptotically consistent approximation

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

- 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

Discrete variational problem results in a linear system

$$(A_{\text{diag}} + A_{\text{circ}}) x = b$$

Block-diagonal

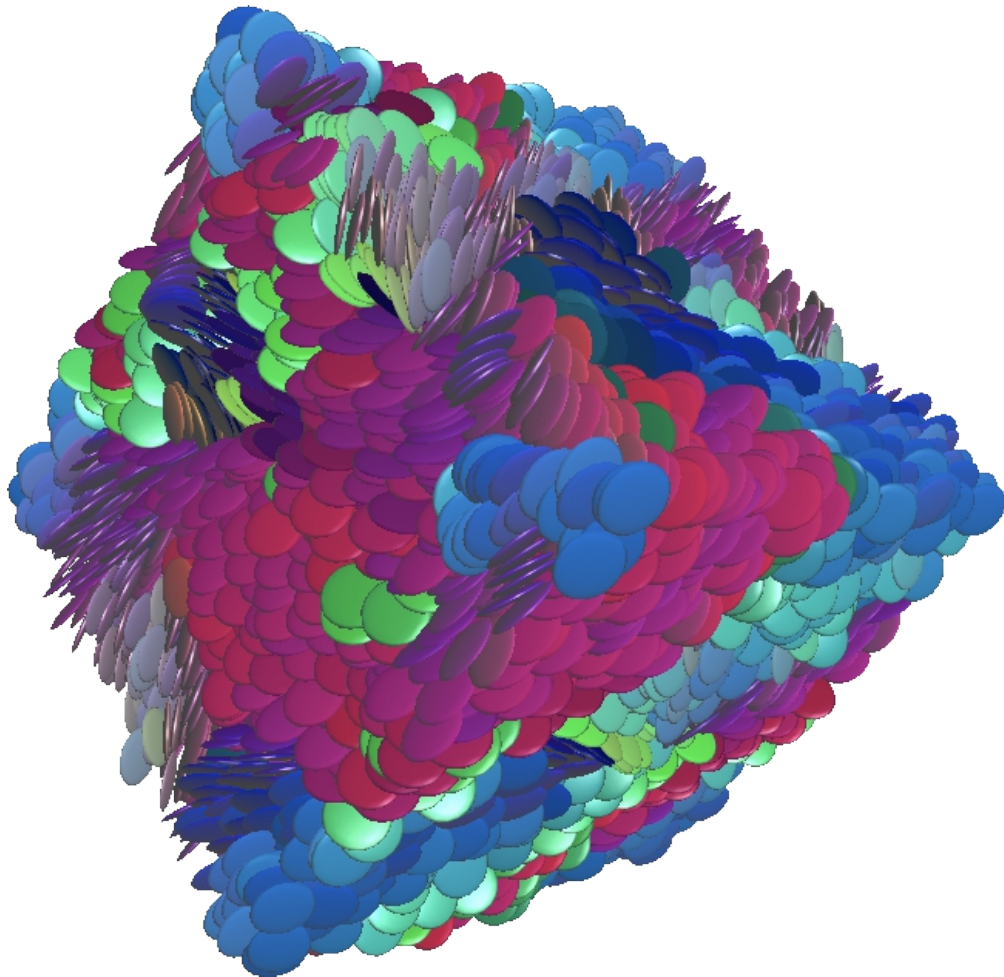
Block-circulant

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

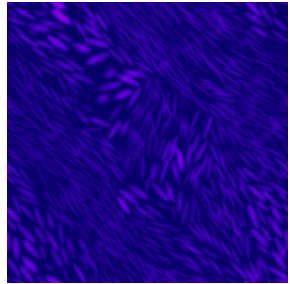
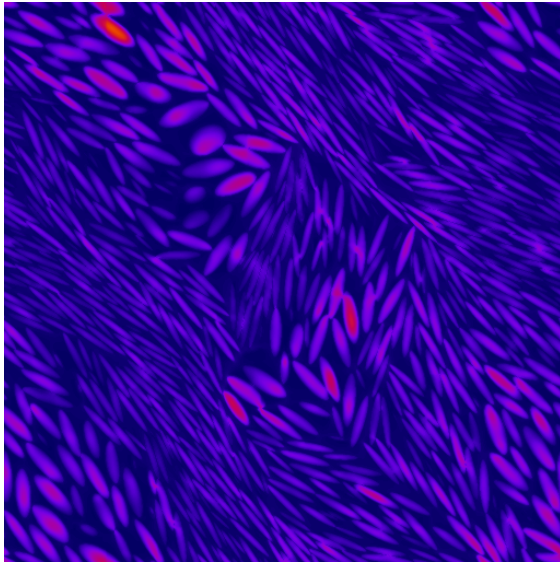
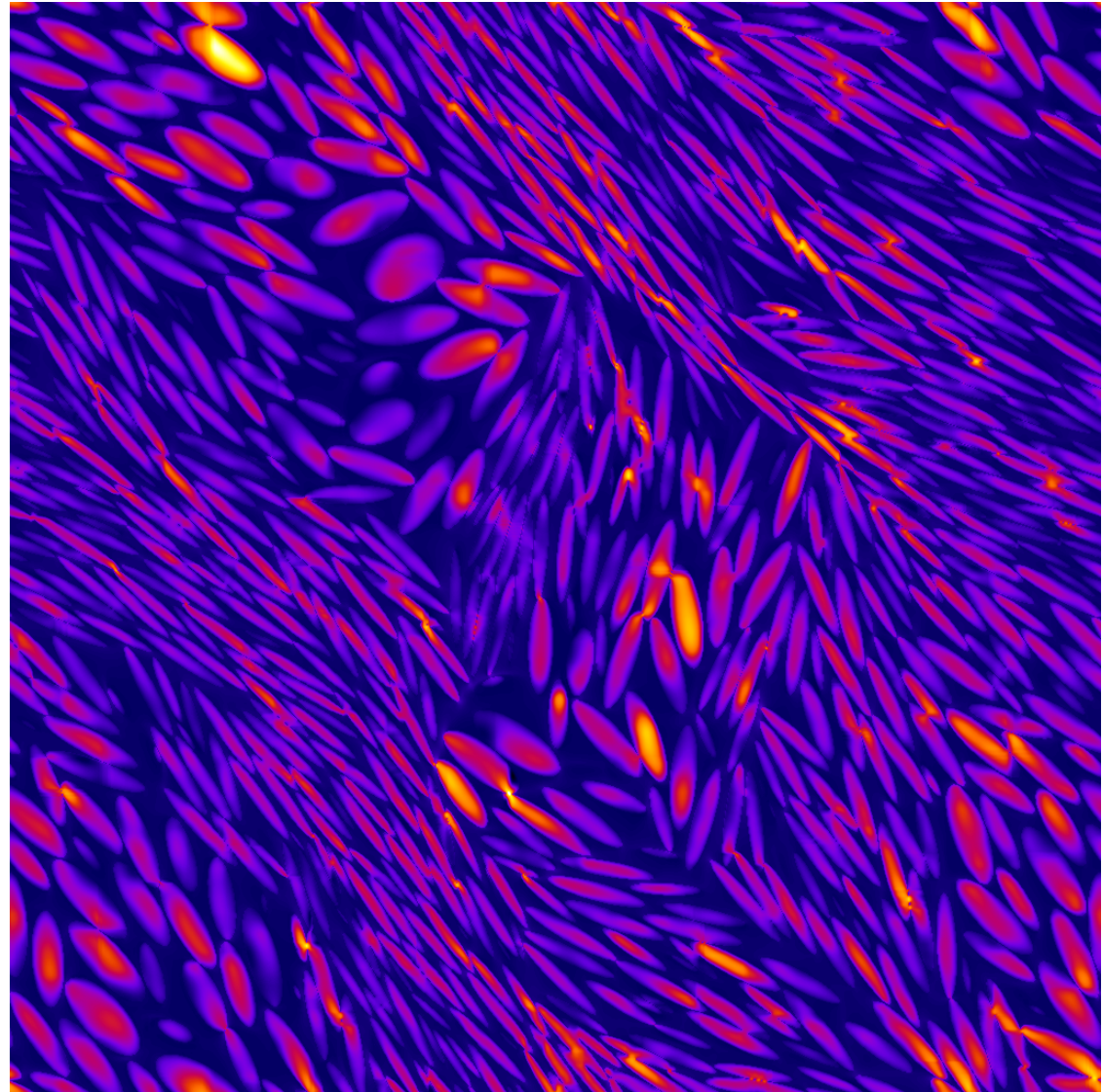


Microstructural parameters

- 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

 256^3  512^3  1024^3 (approx. $6 \cdot 10^9$ dofs)

- 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!

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