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
Homogenization in a nutshell

\[ \text{div} \left( C : \varepsilon \right) + B = 0 \]
\[ \varepsilon = \text{sym grad} \ u \]
+ Boundary Conditions

Homogenization

Separation of scales \( a \ll R \ll L \)

Initial problem

Homogenized problem

\[ \text{div} \left( C^{\text{eff}} : \varepsilon \right) + B = 0 \]
\[ \varepsilon = \text{sym grad} \ u \]
+ Boundary Conditions
**Computation of the homogenized stiffness**

**Elastic equilibrium of RVE**
- \( \text{div} \left( C : \varepsilon \right) = 0 \)
- \( \varepsilon = \text{sym grad} \ u \)

**Boundary conditions**
- Ensure that average strain is \( E \)
- Hilll's lemma must hold

**Example: periodic BCs**
- \( u \left( x \right) = E \cdot x + u_{\text{per}} \left( x \right) \)

**Macroscopic stress**
- \( \Sigma = \overline{\sigma} = C^{\text{eff}} : \varepsilon = C^{\text{eff}} : E \)

**Well-suited to numerical homogenization**


Can be complex!
The Lippmann-Schwinger equation (LS)

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

The Green operator for strains
$$\text{div} \left( \mathbf{C}_0 : \varepsilon + \varpi \right) = 0$$
$$\varepsilon = \text{sym grad} \, \mathbf{u}^{\text{per}}$$

def.

$$\varepsilon = - \Gamma_0 \ast \varpi$$

The Lippmann-Schwinger equation
$$\text{div} \left( \mathbf{C} : \varepsilon \right) = 0$$
$$\varepsilon = \mathbf{E} + \text{sym grad} \, \mathbf{u}^{\text{per}}$$

$$\left( \mathbf{C} - \mathbf{C}_0 \right)^{-1} : \boldsymbol{\tau} + \Gamma_0 \ast \boldsymbol{\tau} = \mathbf{E}$$
$$\boldsymbol{\tau} = \left( \mathbf{C} - \mathbf{C}_0 \right) : \varepsilon$$

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

\[(C - C_0)^{-1} \cdot \tau + \Gamma_0 \ast \tau = E\]

**Weak form:** find \( \tau \in V \) such that

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

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

The linear form:

\[f(\varpi) = E : \int \varpi\]

The bilinear form

\[a(\tau, \varpi) = a_{\text{diag}}(\tau, \varpi) + a_{\text{circ}}(\tau, \varpi)\]

\[a_{\text{diag}}(\tau, \varpi) = \int \varpi(x) : [C(x) - C_0]^{-1} : \tau(x) \, dx\]

\[a_{\text{circ}}(\tau, \varpi) = \iint \varpi(x) : \Gamma_0(x - y) : \tau(y) \, dx \, dy\]
Galerkin discretization of the LS equation

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

**Consistent discretization**

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

Evaluation over \( V^h \) remains difficult!

**Asymptotically consistent discretization:** exact evaluation is not necessary!

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

**Space of cell-wise constant polarization fields**

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


Asymptotically consistent approximation
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
  - Exact (up to round-off errors): Brisard and Dormieux (2010)
  - Filtering of high frequencies: Brisard and Dormieux (2012)
  - Finite elements approximation: Yvonnet (2012)
- 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
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

\[
(A_{\text{diag}} + A_{\text{circ}}) \mathbf{x} = \mathbf{b}
\]

Solving the linear system

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

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Moulinec and Suquet (1994), *CR Acad Sci II* 318, 1417-1423

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!

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