

# Constitutive relation error for FFT-based methods

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# Constitutive relation error for FFT-based methods

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June 9th 2016

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CRE & Uniform Grid, Periodic Lippmann – Schwinger solvers

A local reconstruction of the displacement

The nitty-gritty details

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# CRE: the setting

## Elastic equilibrium of a structure

$\mathrm{div}\,\boldsymbol{\sigma}+\mathbf{b}=\mathbf{0} \quad (\Omega)$

$\boldsymbol{\sigma}\cdot\mathbf{n}=\overline{\mathbf{T}} \quad (\partial\Omega_T)$

$\boldsymbol{\sigma}$ statically admissible with $\mathbf{b}$ and $\overline{\mathbf{T}}$

$\mathbf{u}=\overline{\mathbf{u}} \quad (\partial\Omega_u)$

$\mathbf{u}$ kinematically admissible with $\overline{\mathbf{u}}$

$\boldsymbol{\sigma}=\mathbf{C}:\boldsymbol{\epsilon} \quad (\Omega)$

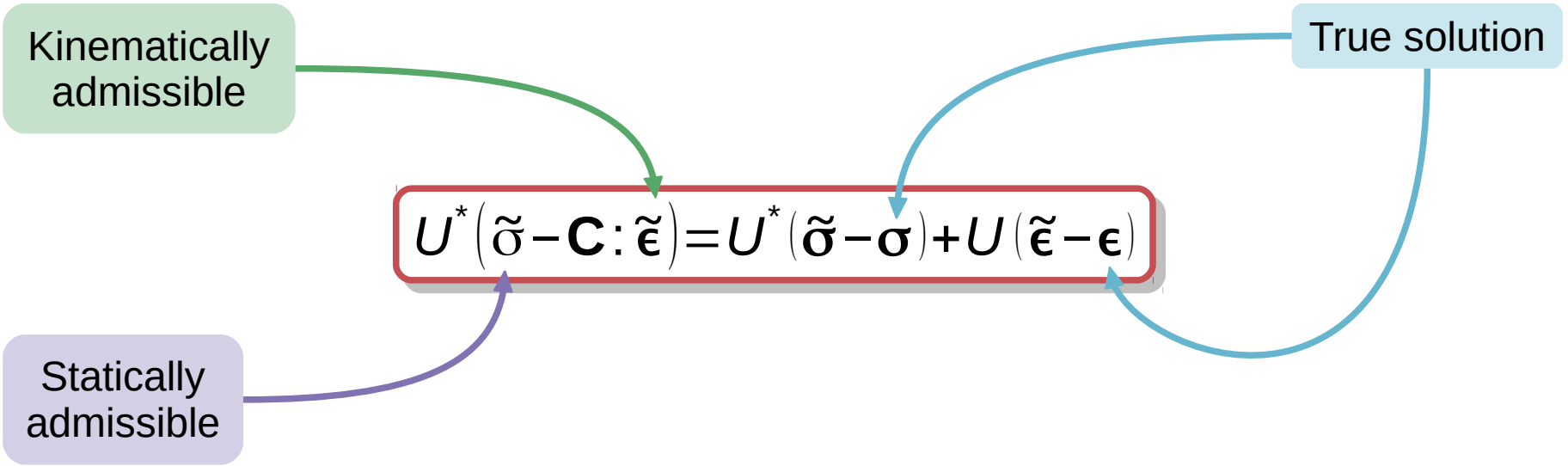
(local) constitutive relation

## Strain energy and complementary strain energy as norms

$$U(\epsilon)=\frac{1}{2}\int_\Omega \boldsymbol{\epsilon}:\mathbf{C}:\boldsymbol{\epsilon}\,\mathrm{d}V$$

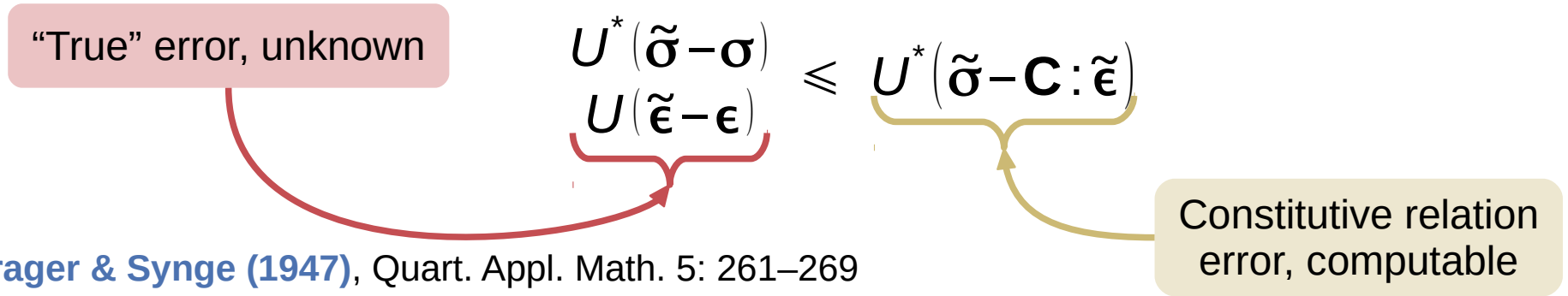
$$U^*(\sigma)=\frac{1}{2}\int_\Omega \boldsymbol{\sigma}:\mathbf{S}:\boldsymbol{\sigma}\,\mathrm{d}V$$

# The Prager – Synge theorem




## Consequence

... even if $\tilde{\sigma} \neq \mathbf{C} : \tilde{\epsilon}$ (of course)




**Prager & Synge (1947)**, Quart. Appl. Math. 5: 261–269

# Application to FEM

**Construction of kinematically admissible displacement**

Trivial with **displacement-based** FEM!

**Construction of statically admissible stress:** the EET method

- Equilibrating Element Tractions
- **Post-processing** of the FEM nodal displacements
- Succession of **local** linear problems
  - **Step 1.** construction of tractions: node-wise
  - **Step 2.** construction of stresses: element-wise

**Ladevèze & Pelle (2005)**, *Mastering Calculations in Linear and Nonlinear Mechanics*, Springer

**Evaluation of constitutive relation error**

Simple integration of standard FE fields, upper bound on “true” error

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# Application to UGPLS solvers

$$\left(\mathbf{C}-\mathbf{C}_0\right)^{-1}:\boldsymbol{\tau}+\boldsymbol{\Gamma}_0[\boldsymbol{\tau}]=\mathbf{E}$$

**The unknown is the stress polarization** (or the strain)

- Strain is **not necessarily** compatible
- Kinematically admissible displacement?
- Statically admissible stress?

**Construction of kinematically admissible displacement**

The main topic of this talk

**Construction of statically admissible stress**

- Arguably the most difficult part
- Don't want to reinvent the wheel: use the EET method!

# Reconstruction of displacements: literature review

## Most UGPLS solvers produce compatible strain fields!

- **But** approximation is **non-local** in space (trig. polynomials)
- Susceptible to Gibbs phenomenon

**Moulinec & Suquet (1998),** *Comp. Meth. Appl. Mech. Eng.* **157(1-2)**, 69–94
**Willot & Pellegrini (2008),** *Continuum Models & Discrete Systems XI*, 443–450
**Zeman et al. (2010),** *J. Comp. Phys*. **229(21)**, 8065–8071
**Monchiet & Bonnet (2012),** *Int. J. Num. Meth. Eng.* **89(11)**, 1419–1436
**Kabel et al. (2014),** *Comp. Mech*. **54(6)**, 1497–1514
**Vondřejc et al. (2014),** *Comp. & Math. Appl*. **68(3),** 156–173
**Willot (2015)**, *Comptes Rendus Mécanique* **343(3)**, 232–245

## Approximation that is local in space is sometimes preferable

- EET method to reconstruct statically admissible stress
- Limit analysis: plastic admissibility checked at the nodes only

**Makrodimopoulos & Martin (2007),** *Int. J. Num. Anal. Meth. Geomechanics* **31(6)**, 835–865

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# From stress-polarization to displacement

## Approximation that is local in space

- Q1 approximation
- Post-processing of estimate of stress-polarization (or strain)

## True displacement from true stress polarization

$$\left(\mathbf{C}-\mathbf{C}_0\right)^{-1}:\boldsymbol{\tau}+\boldsymbol{\Gamma}_0[\boldsymbol{\tau}]=\mathbf{E} \quad \Rightarrow \quad \nabla\cdot\left(\mathbf{C}_0:\nabla^s\mathbf{u}+\boldsymbol{\tau}\right)=\mathbf{0}$$

## Approx. displacement from approx. stress polarization

$$\left(\mathbf{C}^{\mathbf{N}}-\mathbf{C}_0\right)^{-1}:\boldsymbol{\tau}^{\mathbf{N}}+\boldsymbol{\Gamma}_0^{\mathbf{N}}[\boldsymbol{\tau}^{\mathbf{N}}]=\mathbf{E} \quad \Rightarrow \quad \nabla\cdot\left(\mathbf{C}_0:\nabla^s\mathbf{u}^{\mathbf{N}}+\boldsymbol{\tau}^{\mathbf{N}}\right)=\mathbf{0}$$

$\mathbf{N}=(N_1,\ldots,N_d)$: grid-size

# Wait a minute...

## Our two-step approach

1. $\left(\mathbf{C}^{\mathbf{N}}-\mathbf{C}_0\right)^{-1}:\boldsymbol{\tau}^{\mathbf{N}}+\boldsymbol{\Gamma}_0^{\mathbf{N}}[\boldsymbol{\tau}^{\mathbf{N}}]=\mathbf{E}$ (UGPLS solver)

2. $\nabla\cdot\left(\mathbf{C}_0:\nabla^s\mathbf{u}^{\mathbf{N}}+\boldsymbol{\tau}^{\mathbf{N}}\right)=\mathbf{0}$ (FEM solver)

**An alternative one-step approach:** why not use FEM only?

$$\nabla\cdot\left[\mathbf{C}:\left(\mathbf{E}+\nabla^s\mathbf{u}\right)\right]=\mathbf{0}$$

## The two-step approach is more efficient

- Homogeneous reference material
- Periodic boundary conditions

**FFT for both steps!**

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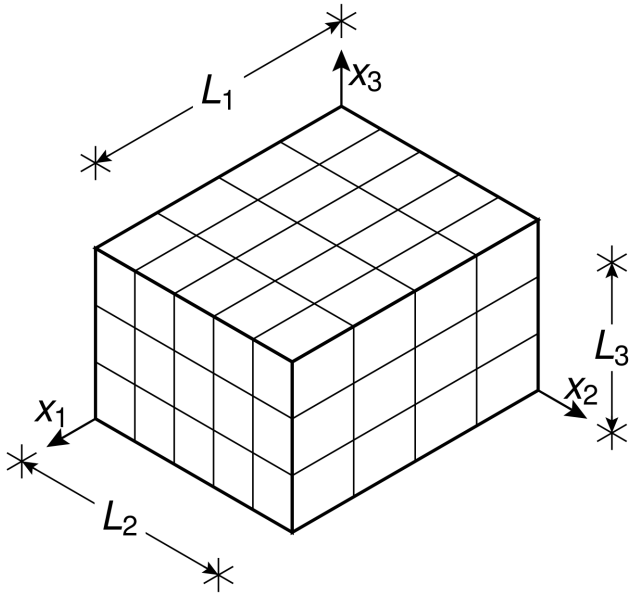
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# Q1 approximation of displacement




$\mathbf{L}=(L_1,\ldots,L_d)$: size of unit-cell

$\mathbf{N}=(N_1,\ldots,N_d)$: grid-size

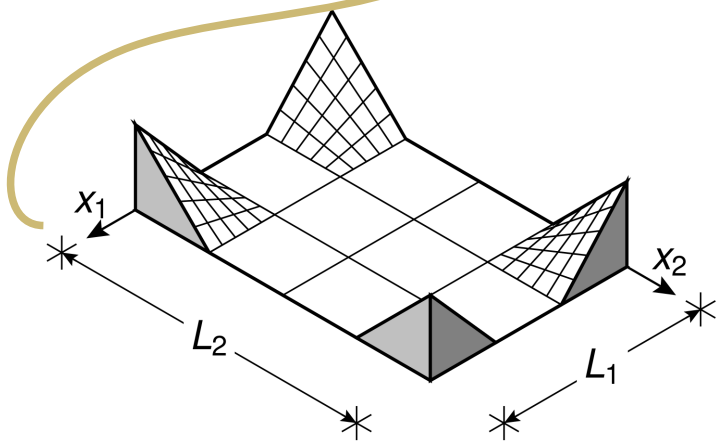
Cell-wise constant

$$\nabla\cdot\left(\mathbf{C}_0:\nabla^s\mathbf{u}^{\mathbf{N}}+\boldsymbol{\tau}^{\mathbf{N}}\right)=\mathbf{0}$$

Nodal displacement

$$\mathbf{u}^{\mathbf{N}}(\mathbf{x})=\sum_{\mathbf{n}}\Phi^{\mathbf{N}}\left(\mathbf{x}-\mathbf{x}_{\mathbf{n}}^{\mathbf{N}}\right)\mathbf{u}_{\mathbf{n}}^{\mathbf{N}}$$

Nodal coordinates




Periodic shape function

# Fourier series, discrete Fourier transform

**Displacement is periodic!** Can be expanded in Fourier series

$$\mathbf{u}(\mathbf{x}) = \frac{1}{N_1 \cdots N_d} \sum_{\mathbf{k} \in \mathbb{Z}^d} \left[ \prod_{j=1}^{d} \operatorname{sinc}^2\left( \frac{\pi k_j}{N_j} \right) \exp\left( \frac{2 i \pi k_j x_j}{L_j} \right) \right] \hat{\mathbf{u}}^{\mathbf{N}}_{\mathbf{k}}$$

**Discrete Fourier transform of nodal displacements**

$$\hat{\mathbf{u}}^{\mathbf{N}}_{\mathbf{k}} = \sum_{n_1=0}^{N_1-1} \cdots \sum_{n_d=0}^{N_d-1} \exp\left[ -2 i \pi \left( \frac{k_1 n_1}{N_1} + \cdots + \frac{k_d n_d}{N_d} \right) \right] \mathbf{u}^{\mathbf{N}}_{\mathbf{n}}$$

**Infinite sum defined by a finite (periodic) series of unknowns (in Fourier space).**

# Total Potential Energy

## Can be computed in Fourier space

$$\Pi = \frac{L_1 \cdots L_d}{N_1^2 \cdots N_d^2} \sum_{k_1=0}^{N_1-1} \sum_{k_d=0}^{N_d-1} \left( \frac{1}{2} \overline{\hat{\mathbf{u}}_{\mathbf{k}}^{\mathbf{N}}} \cdot \hat{\mathbf{K}}_{\mathbf{k}}^{\mathbf{N}} \cdot \hat{\mathbf{u}}_{\mathbf{k}}^{\mathbf{N}} + \overline{\hat{\mathbf{u}}_{\mathbf{k}}^{\mathbf{N}}} \cdot \hat{\boldsymbol{\tau}}_{\mathbf{k}}^{\mathbf{N}} \cdot \overline{\hat{\mathbf{B}}_{\mathbf{k}}^{\mathbf{N}}} \right)$$

$\hat{\mathbf{K}}_{\mathbf{k}}^{\mathbf{N}}$: modal stiffness matrix $(d \times d)$

$\hat{\mathbf{B}}_{\mathbf{k}}^{\mathbf{N}}$: modal strain-displacement vector $(d \times 1)$

**Closed-form expressions!**

## Optimization of total potential energy

$$\hat{\mathbf{K}}_{\mathbf{k}}^{\mathbf{N}} \cdot \hat{\mathbf{u}}_{\mathbf{k}}^{\mathbf{N}} = -\hat{\boldsymbol{\tau}}_{\mathbf{k}}^{\mathbf{N}} \cdot \overline{\hat{\mathbf{B}}_{\mathbf{k}}^{\mathbf{N}}}$$

$N_1 \times \cdots \times N_d$ small $(d \times d)$ linear systems rather than

one single large linear system with $N_1 \times \cdots \times N_d \times d$ unknowns!

# Summary of the method

1. Compute DFT of cell-wise constant stress polarization
2. Compute DFT of nodal displacement: for each discrete freq.
    a. Assemble modal stiffness matrix
    b. Assemble modal strain-displacement vector
    c. Solve resulting $d \times d$ linear system
3. Compute inverse DFT of nodal displacement

**SB (2016),** *Int. J. Num. Meth. Eng.*, early view (10.1002/nme.5263)

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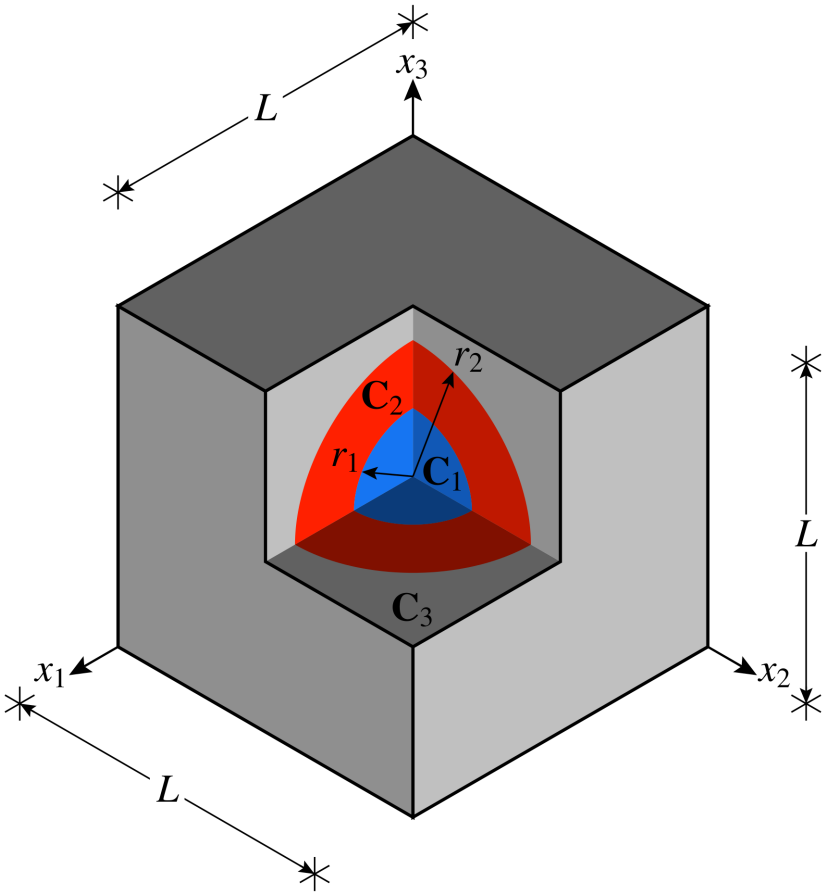
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# Hashin's coated sphere

Example borrowed from Schneider et al. (2015)




$$r_1 = 0.2\,L$$

$$r_2 = 0.4\,L$$

$$\kappa_1 = 100\,\kappa_2$$

$$\kappa_3 = 1.25191\,\kappa_2$$

$$\nu_1 = \nu_2 = \nu_3 = 0.25$$

$$\mathbf{E} = \frac{E_v}{3}\left(\mathbf{e_1}\otimes\mathbf{e_1} + \mathbf{e_2}\otimes\mathbf{e_2} + \mathbf{e_3}\otimes\mathbf{e_3}\right)$$

**Schneider et al. (2015),** *Int. J. Num. Meth. Eng.* **105(9)**, 1419–1436

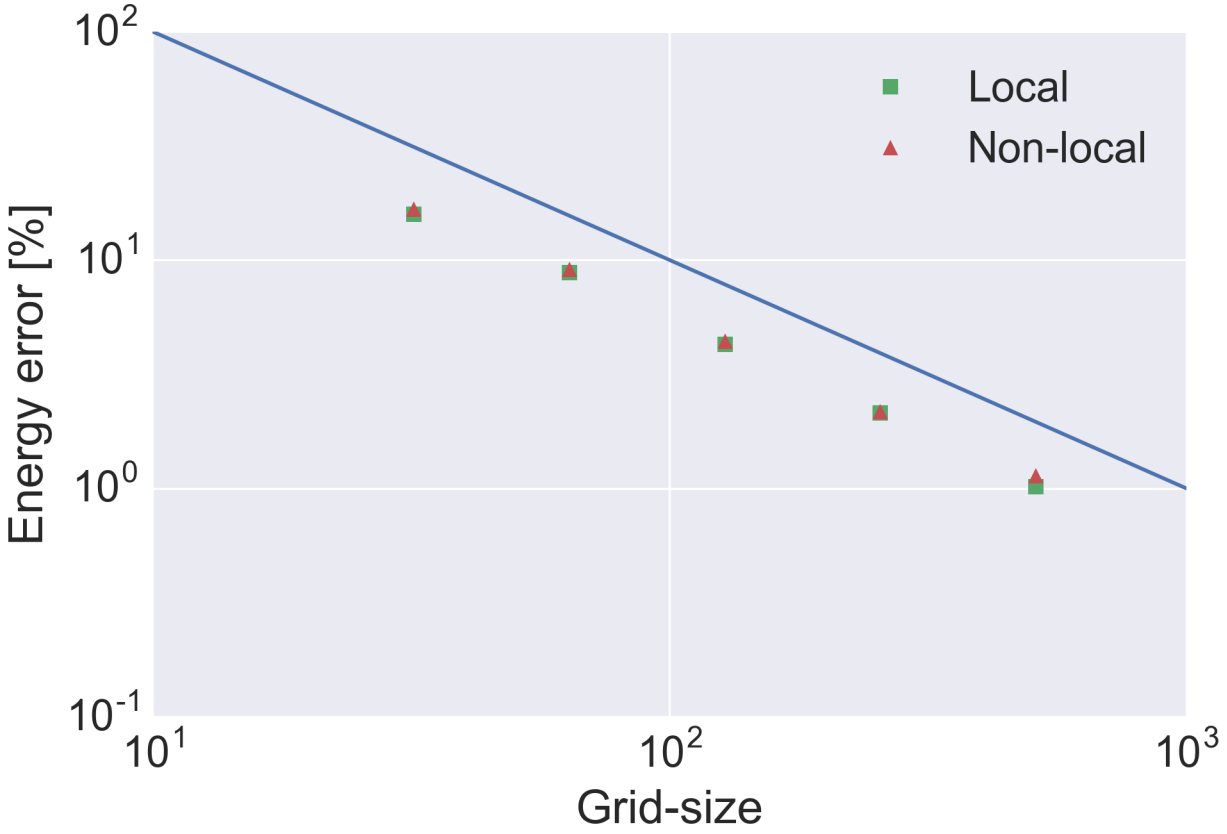
# Error on reconstructed displacement

**Truncated discrete Green operator** (Moulinec & Suquet, 1998)



# Error on reconstructed displacement

## Finite difference discrete Green operator (Willot, 2015)



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# Reconstruction of stress

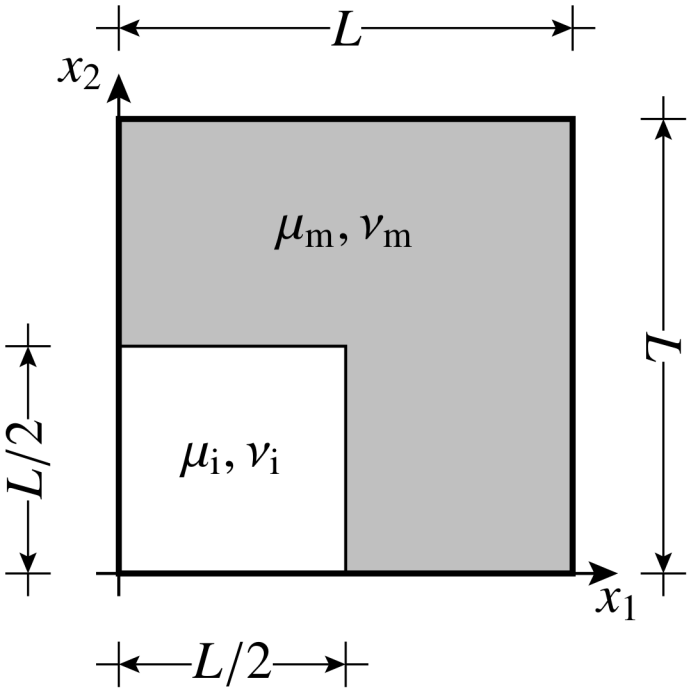
## Reconstructed displacement is a Galerkin solution

$$\int_{\Omega} \left[ \left( \mathbf{C}_0 : \nabla^s \mathbf{u}^{\mathbf{N}} + \boldsymbol{\tau}^{\mathbf{N}} \right) : \nabla^s \mathbf{v} \right] \mathrm{d}V = 0 \quad \text{for all } \mathbf{v} \text{ Q1, periodic}$$

- “Strong extension condition” does not lead to overdetermination
- Equilibrated Element Traction method applies
- Reconstructing statically admissible stress fields becomes standard!
- Constitutive relation error can be evaluated

**Ladevèze & Pelle (2005),** *Mastering Calculations in Linear and Nonlinear Mechanics*, Springer

# A simple, 2D example




$$\mu_i = 100\,\mu_m$$

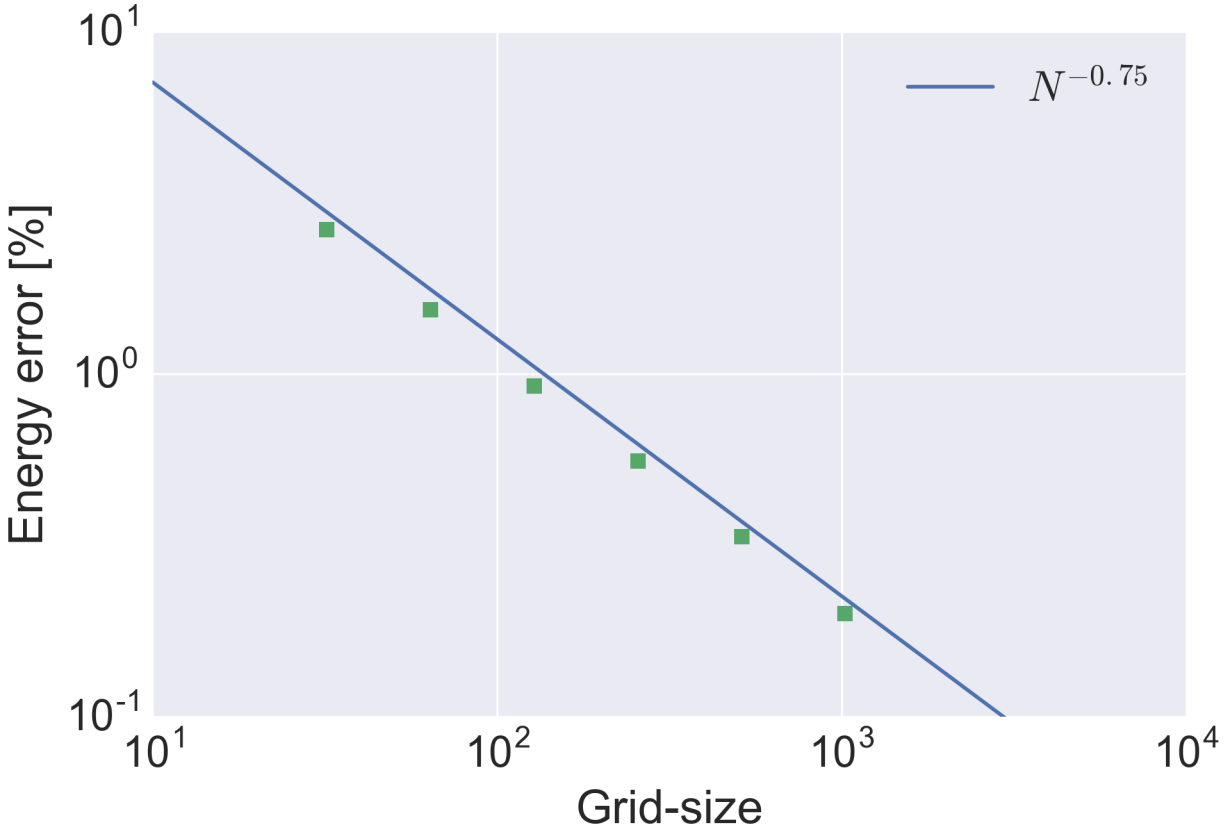
$$\nu_m = 0.3$$

$$\nu_i = 0.2$$

$$\mathbf{E} = E_{12}\left(\mathbf{e_1}\otimes\mathbf{e_2} + \mathbf{e_2}\otimes\mathbf{e_1}\right)$$

# Constitutive relation error

**Work in progress** (with L. Chamoin)



# Conclusion and perspectives

## An “agnostic” method to reconstruct displacements…

- Works with **any** UGPLS solver
- Very low cost (9 FFT in 3D)
- Reconstruction is **local** in space
- Accuracy comparable to other existing approaches

## … Which paves the way to reconstruction of stresses

- Standard post-processing of the reconstructed displacement
- Rigorous bound on energy error

## Perspectives

- Extension to local quantities of interest
- Systematic selection of reference material

# Thank you for your attention !

http://sbrisard.github.io/