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ECCOMAS 2016

# Constitutive relation error for FFT-based methods

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A non-specialist's presentation of constitutive relation error

CRE & **U**niform **G**rid, **P**eriodic **L**ippmann – **S**chwinger solvers

A local reconstruction of the displacement

The nitty-gritty details

Example 1

Example 2

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## Elastic equilibrium of a structure

$$\begin{array}{ll} \operatorname{div} \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0} & (\Omega) \\ \boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{T}} & (\partial \Omega_T) \end{array} \quad \boldsymbol{\sigma} \text{ statically admissible with } \mathbf{b} \text{ and } \bar{\mathbf{T}}$$

$$\mathbf{u} = \bar{\mathbf{u}} \quad (\partial \Omega_u) \quad \mathbf{u} \text{ kinematically admissible with } \bar{\mathbf{u}}$$

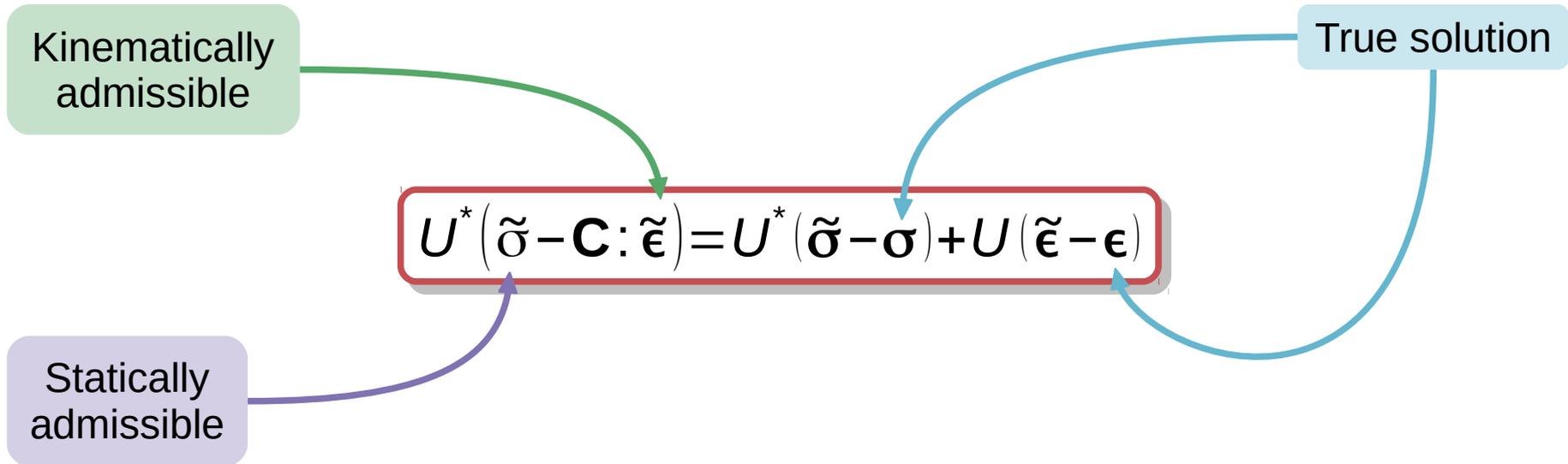
$$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\epsilon} \quad (\Omega) \quad \text{(local) constitutive relation}$$

## Strain energy and complementary strain energy as norms

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

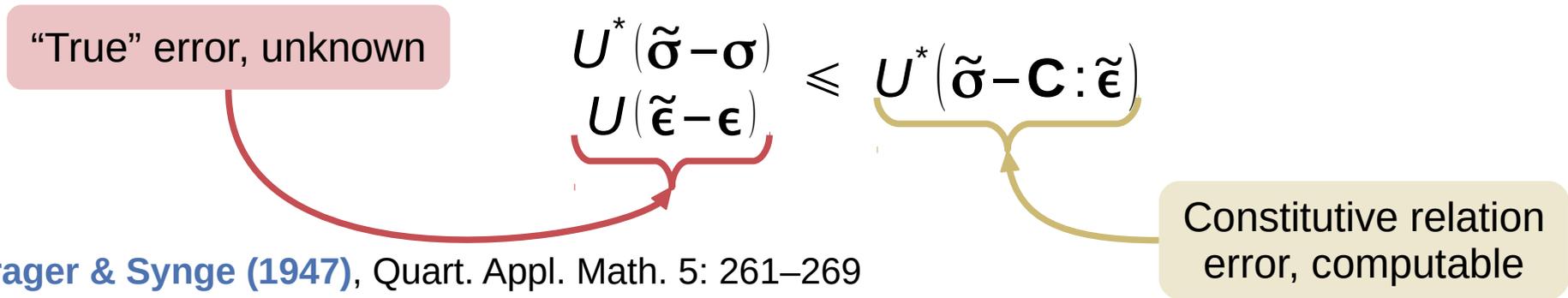
$$U^*(\boldsymbol{\sigma}) = \frac{1}{2} \int_{\Omega} \boldsymbol{\sigma} : \mathbf{S} : \boldsymbol{\sigma} \, dV$$

# 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

## Construction of kinematically admissible displacement

Trivial with **displacement-based** FEM!

## Construction of statically admissible stress: the EET method

- ◆ Equilibrating Element Traction
- ◆ **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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$$(\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} + \boldsymbol{\Gamma}_0[\boldsymbol{\tau}] = \mathbf{E}$$

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

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

## **Approx.** displacement from **approx.** stress polarization

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

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

## Our two-step approach

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

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

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

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

## The two-step approach is more efficient

- ◆ Homogeneous reference material
- ◆ Periodic boundary conditions

**FFT for both steps!**

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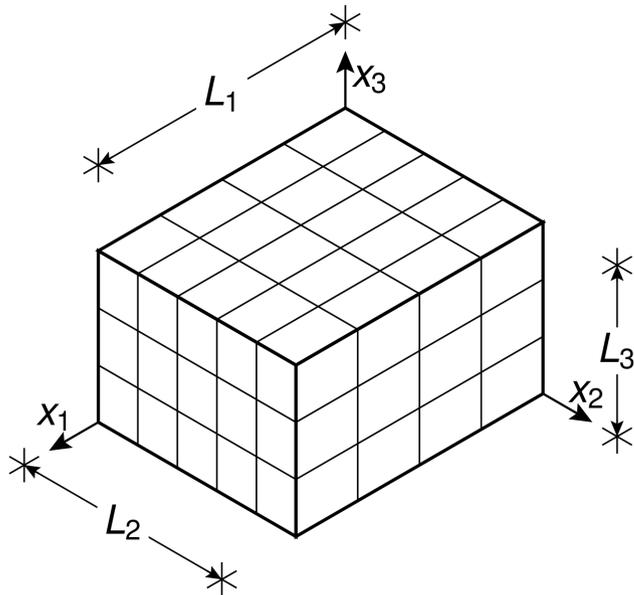
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## Q1 approximation of displacement



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

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

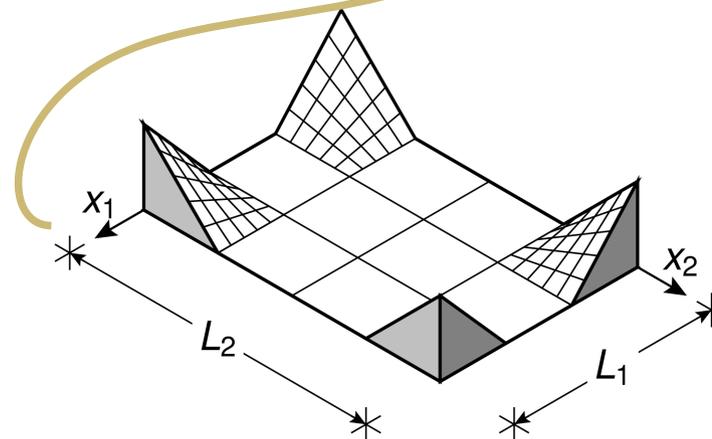
$$\nabla \cdot (\mathbf{C}_0 : \nabla^s \mathbf{u}^N + \boldsymbol{\tau}^N) = \mathbf{0}$$

Cell-wise constant

Nodal displacement

$$\mathbf{u}^N(\mathbf{x}) = \sum_n \Phi^N(\mathbf{x} - \mathbf{x}_n^N) \mathbf{u}_n^N$$

Nodal coordinates



Periodic shape function

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

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

**Discrete Fourier transform of nodal displacements**

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

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

Can be computed in Fourier space

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

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

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

**Closed-form expressions!**

Optimization of total potential energy

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

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

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

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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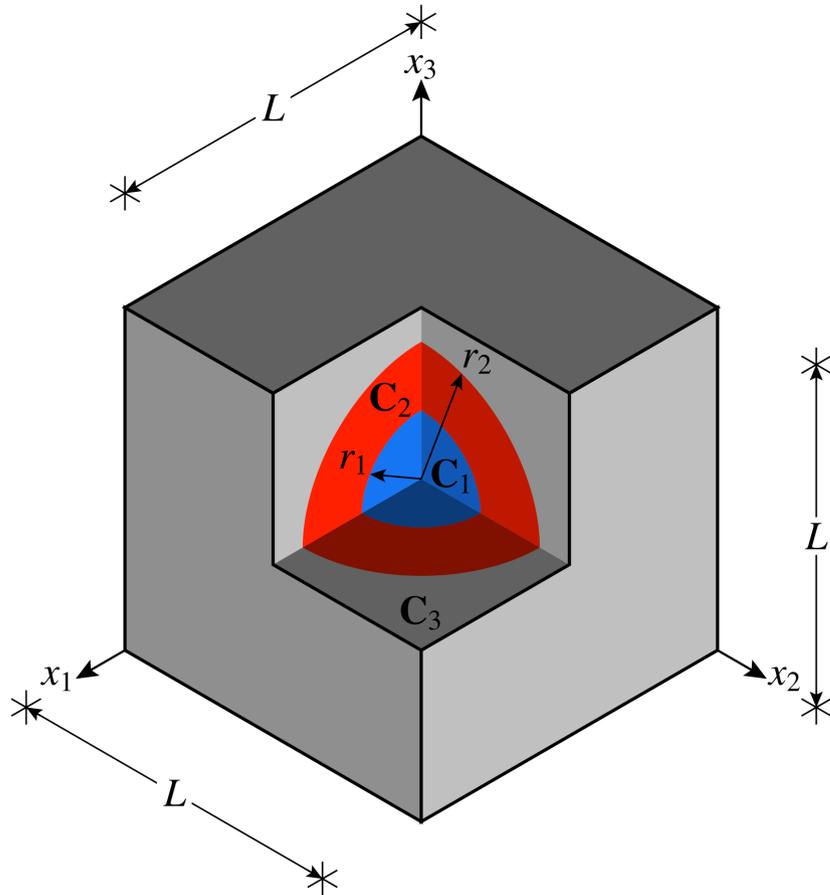
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Example borrowed from Schneider et al. (2015)



$$r_1 = 0.2L$$

$$r_2 = 0.4L$$

$$\kappa_1 = 100 \kappa_2$$

$$\kappa_3 = 1.25191 \kappa_2$$

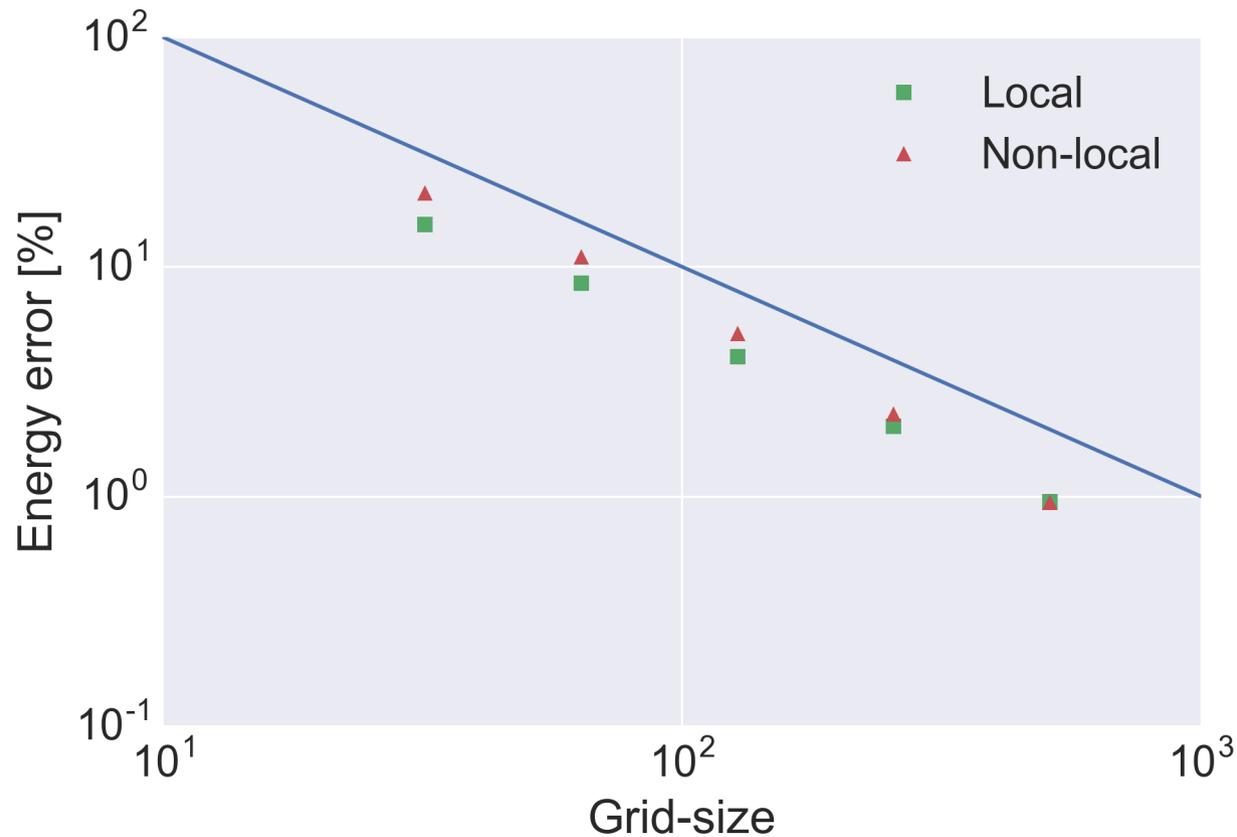
$$\nu_1 = \nu_2 = \nu_3 = 0.25$$

$$\mathbf{E} = \frac{E_v}{3} (\mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_2 \otimes \mathbf{e}_2 + \mathbf{e}_3 \otimes \mathbf{e}_3)$$

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

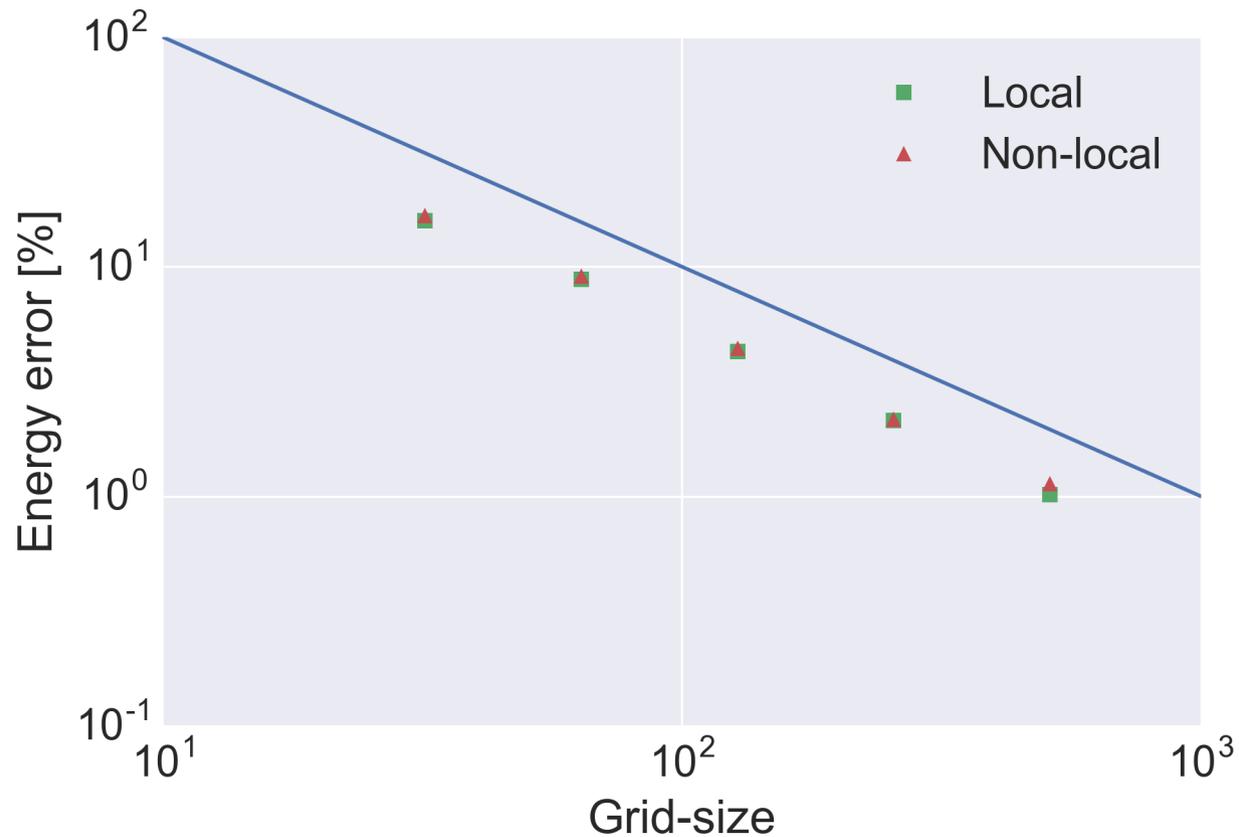
# Error on reconstructed displacement

Truncated discrete Green operator (Moulinec & Suquet, 1998)



# Error on reconstructed displacement

Finite difference discrete Green operator (Willot, 2015)



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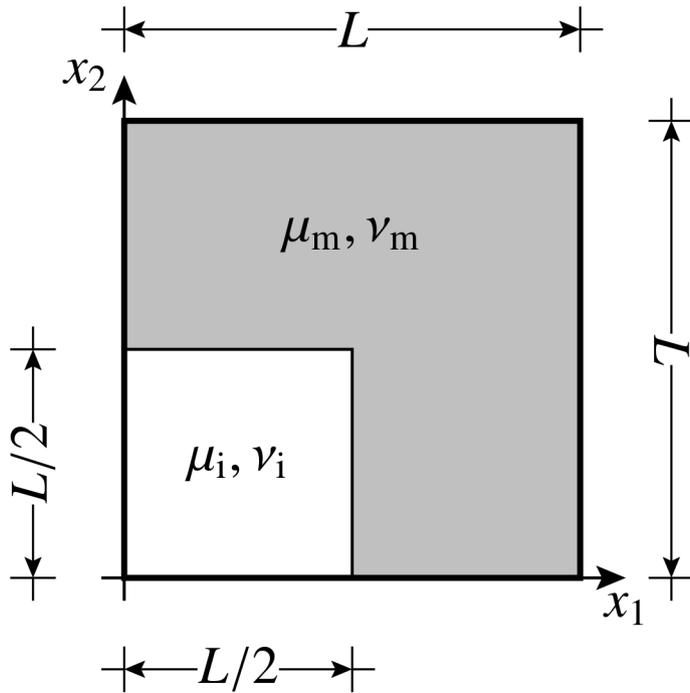
## Reconstructed displacement is a Galerkin solution

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

- ◆ “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



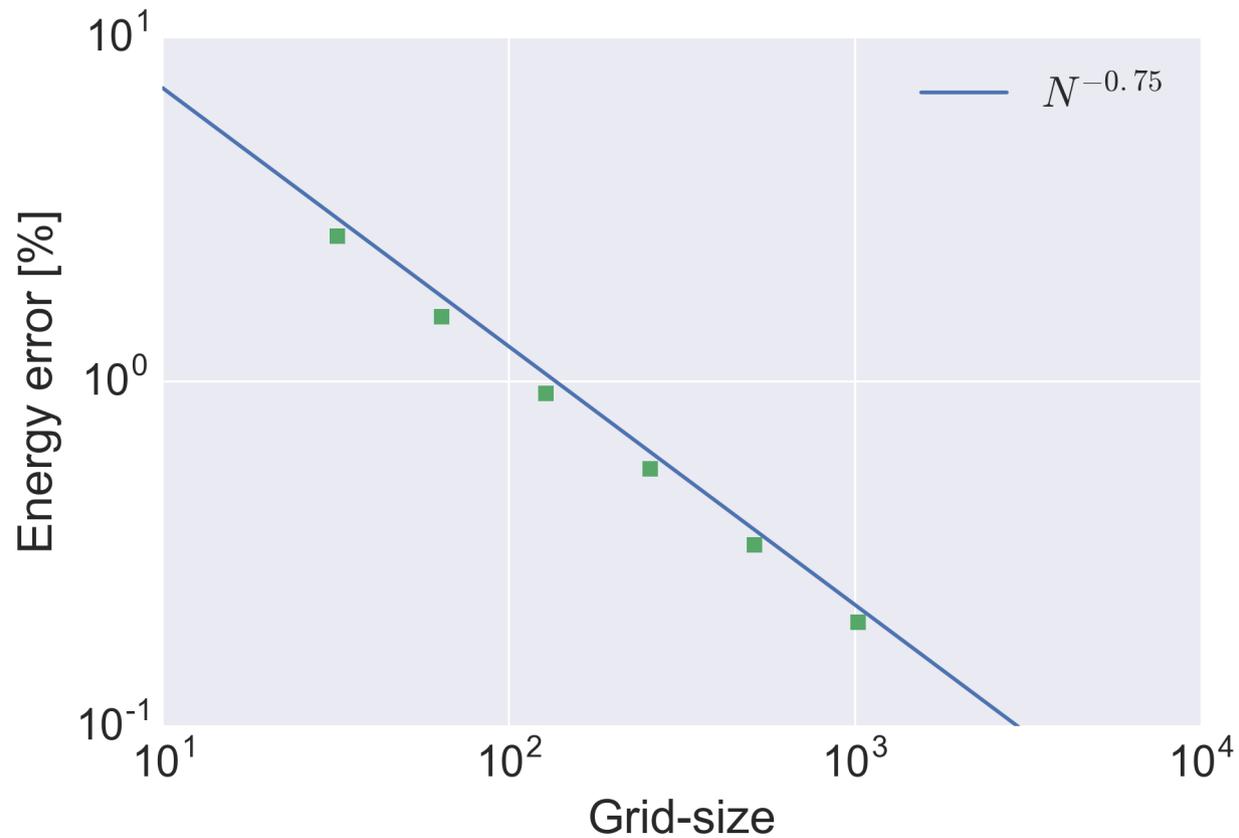
$$\mu_i = 100 \mu_m$$

$$\nu_m = 0.3$$

$$\nu_i = 0.2$$

$$\mathbf{E} = E_{12} (\mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1)$$

Work in progress (with L. Chamoin)



## 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/`