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Constitutive relation error for FFT-based methods

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June 9th 2016



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

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

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

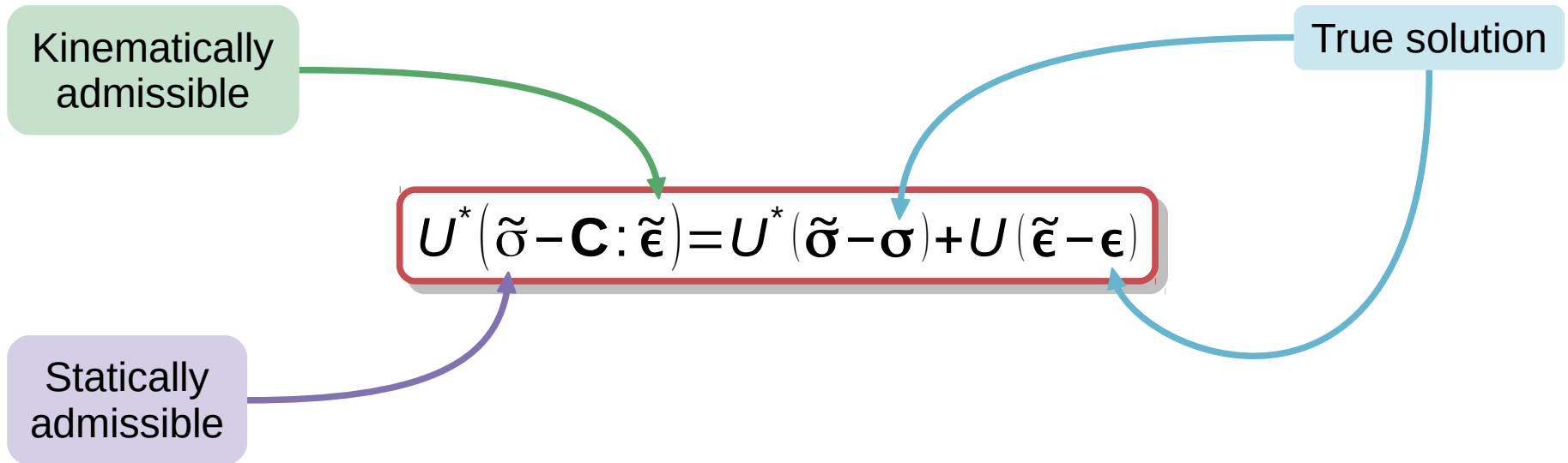
$$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\epsilon} \quad (\Omega) \quad \text{(local) constitutive relation}$$

Strain energy and complementary strain energy as norms

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

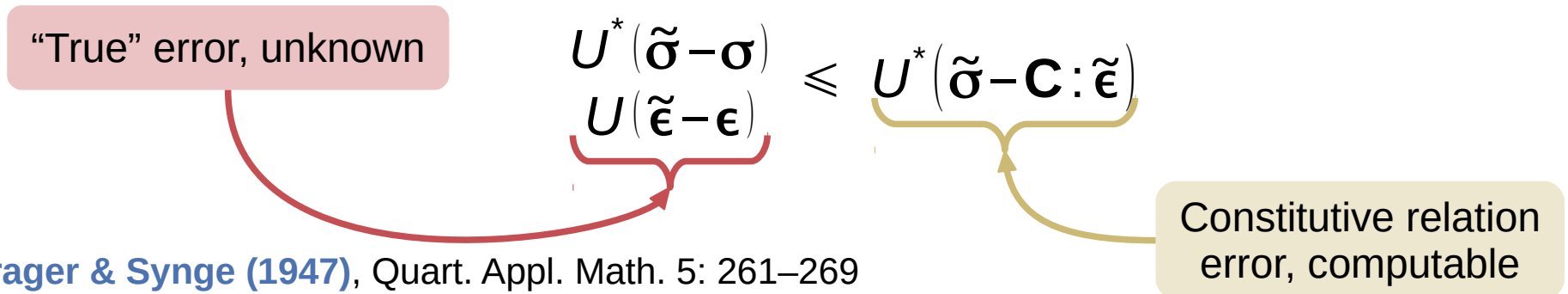
$$U^*(\boldsymbol{\sigma}) = \frac{1}{2} \int_{\Omega} \boldsymbol{\sigma} : \mathbf{S} : \boldsymbol{\sigma} \, dV$$

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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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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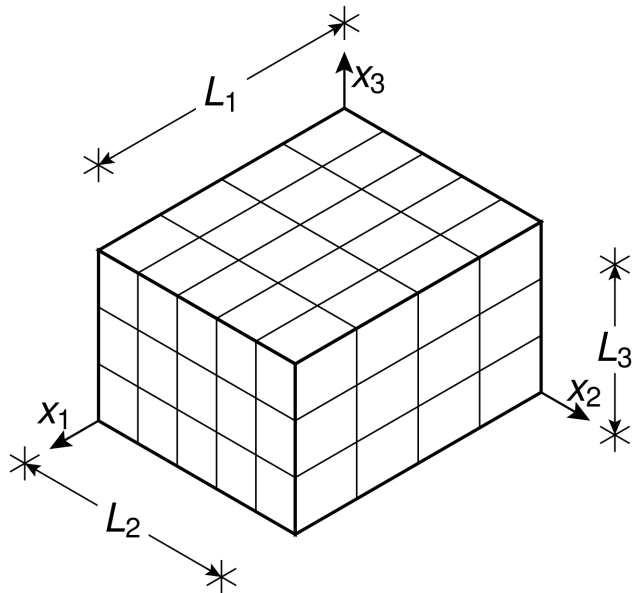
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Q1 approximation of displacement



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

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

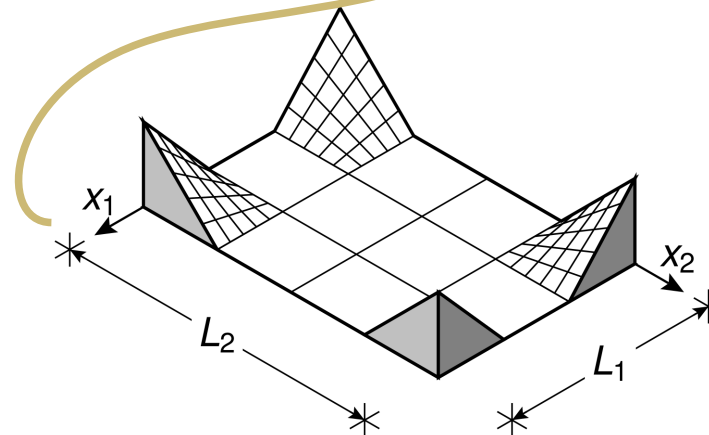
$$\nabla \cdot (\mathbf{C}_0 : \nabla^s \mathbf{u}^N + \boldsymbol{\tau}^N) = 0$$

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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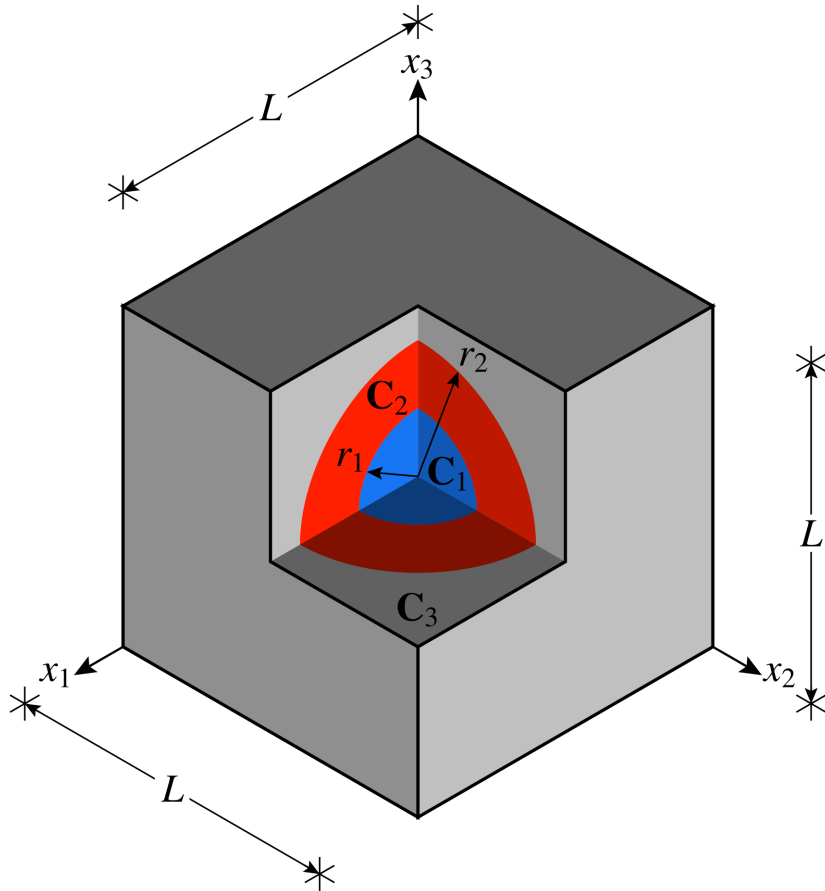
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Example borrowed from Schneider et al. (2015)



$$r_1 = 0.2L$$

$$r_2 = 0.4L$$

$$\kappa_1 = 100 \kappa_2$$

$$\kappa_3 = 1.25191 \kappa_2$$

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

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

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

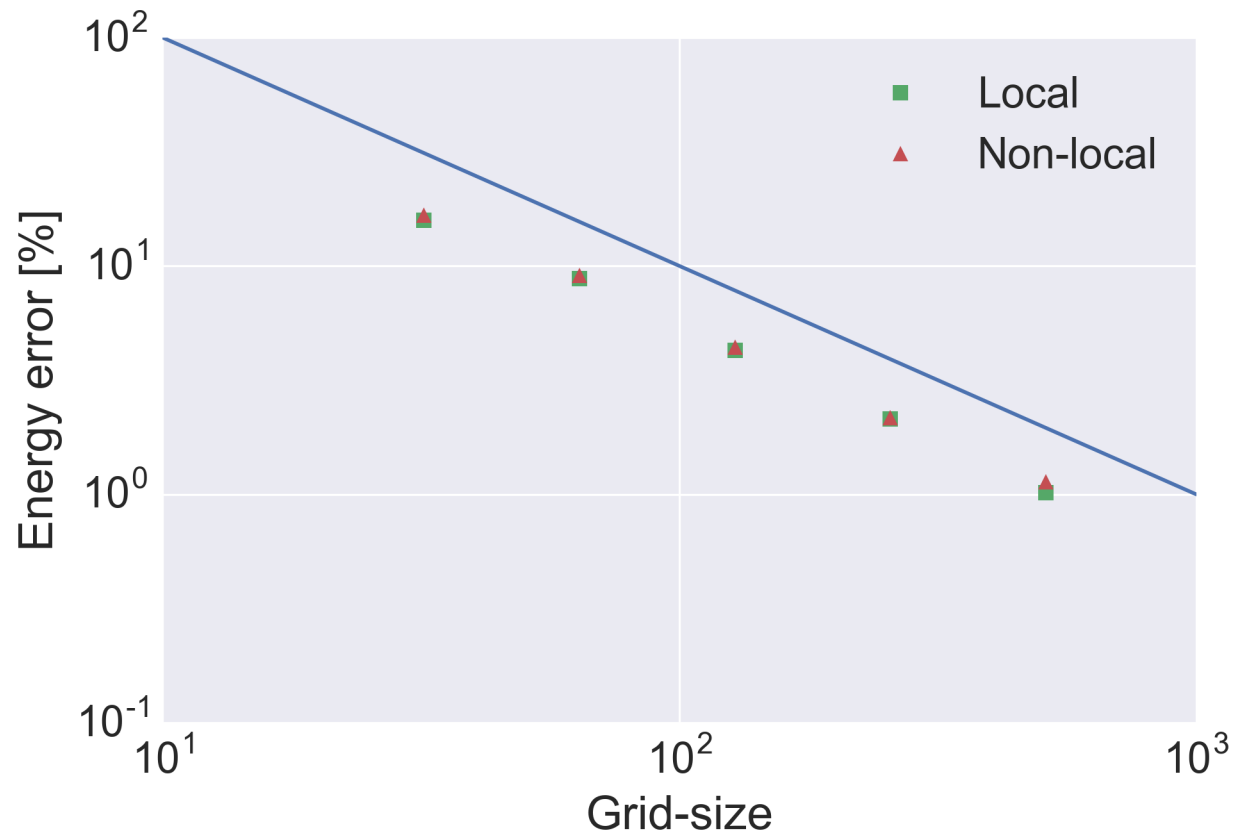
Error on reconstructed displacement

Truncated discrete Green operator (Moulinec & Suquet, 1998)



Error on reconstructed displacement

Finite difference discrete Green operator (Willot, 2015)



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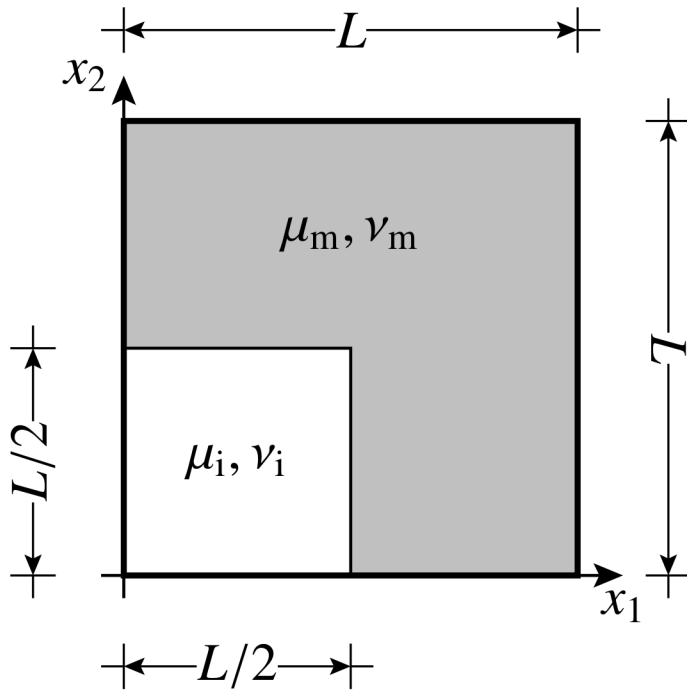
Reconstructed displacement is a Galerkin solution

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

- ◆ “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



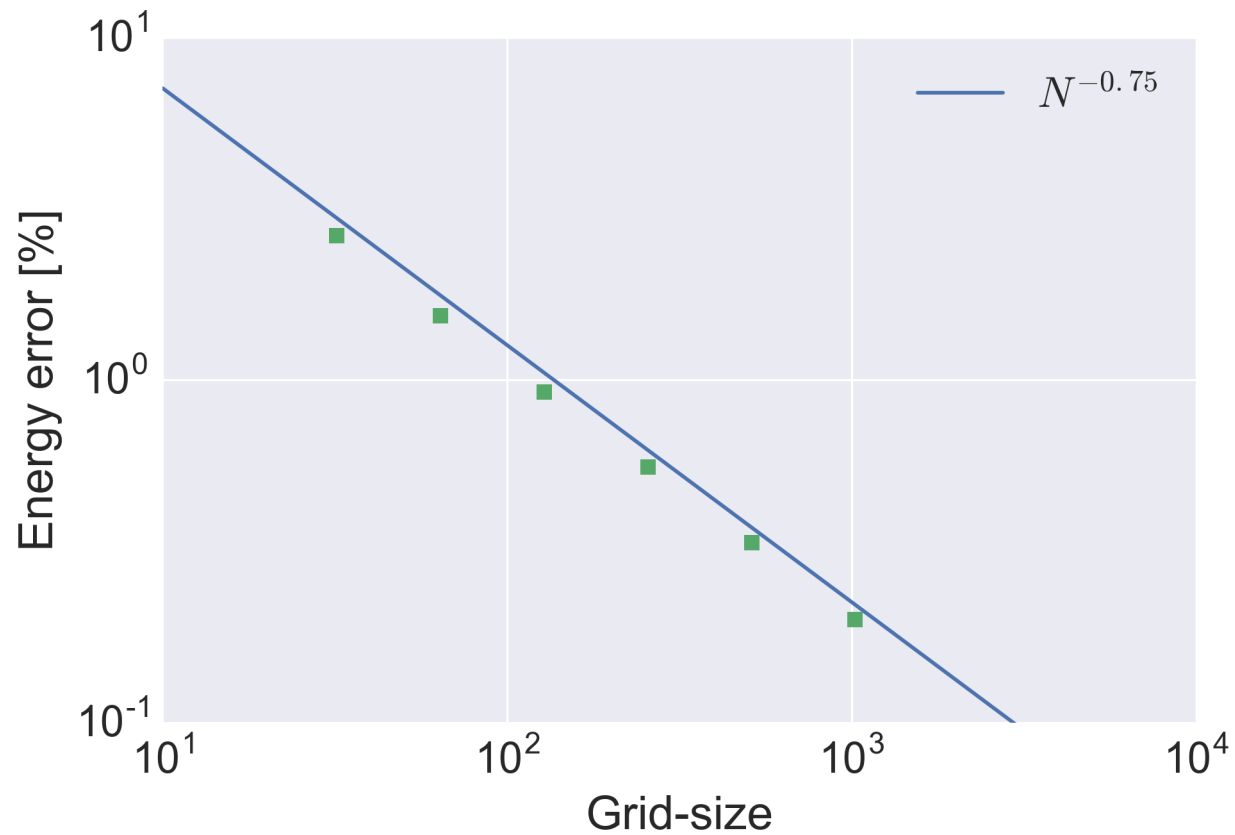
$$\mu_i = 100 \mu_m$$

$$\nu_m = 0.3$$

$$\nu_i = 0.2$$

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

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/>

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