HAL open science

Constitutive relation error for FFT-based methods

Sébastien Brisard, L Chamoin

To cite this version:

Sébastien Brisard, L Chamoin. Constitutive relation error for FFT-based methods. VII European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS Congress 2016), Jun 2016, Crete Island, Greece. hal-01330790v2

HAL Id: hal-01330790
https://enpc.hal.science/hal-01330790v2

Submitted on 6 Jul 2016

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Distributed under a Creative Commons Attribution 4.0 International License

ECCOMAS 2016

Constitutive relation error for FFT-based methods

S. Brisard[1], L. Chamoin[2,3]

[1]Université Paris-Est, Laboratoire Navier, ENPC, IFSTTAR, CNRS, UMR 8205
[2]LMT, ENS Cachan, CNRS, Université Paris-Saclay
[3]INRIA Rocquencourt, MATHERIALS research team

June 9th 2016

Contents

Contents

CRE: the setting

Elastic equilibrium of a structure

$\operatorname{div}\boldsymbol{\sigma}+\mathbf{b}=\mathbf{0}$	(Ω)	σ statically admissible with $\mathbf{b}$ and $\bar{\mathbf{T}}$
$\boldsymbol{\sigma}\cdot\mathbf{n}=\bar{\mathbf{T}}$	$(\partial\Omega_T)$	
$\mathbf{u}=\bar{\mathbf{u}}$	$(\partial\Omega_u)$	$\mathbf{u}$ kinematically admissible with $\bar{\mathbf{u}}$
$\boldsymbol{\sigma}=\mathbf{C}:\boldsymbol{\epsilon}$	(Ω)	(local) constitutive relation

Strain energy and complementary strain energy as norms

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

The Prager – Synge theorem

Kinematically admissible

True solution

$$U^*\left(\tilde{\sigma} - \mathbf{C} : \tilde{\boldsymbol{\epsilon}}\right) = U^*\left(\tilde{\boldsymbol{\sigma}} - \boldsymbol{\sigma}\right) + U\left(\tilde{\boldsymbol{\epsilon}} - \boldsymbol{\epsilon}\right)$$

Statically admissible

Consequence

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

$$\underbrace{\begin{matrix} U^*\left(\tilde{\boldsymbol{\sigma}} - \boldsymbol{\sigma}\right) \\ U\left(\tilde{\boldsymbol{\epsilon}} - \boldsymbol{\epsilon}\right) \end{matrix}}_{\text{“True” error, unknown}} \leqslant \underbrace{U^*\left(\tilde{\boldsymbol{\sigma}} - \mathbf{C} : \tilde{\boldsymbol{\epsilon}}\right)}_{\text{Constitutive relation error, computable}}$$

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

Contents

Application to UGPLS solvers

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

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

Contents

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

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

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

Wait a minute...

Our two-step approach

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

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

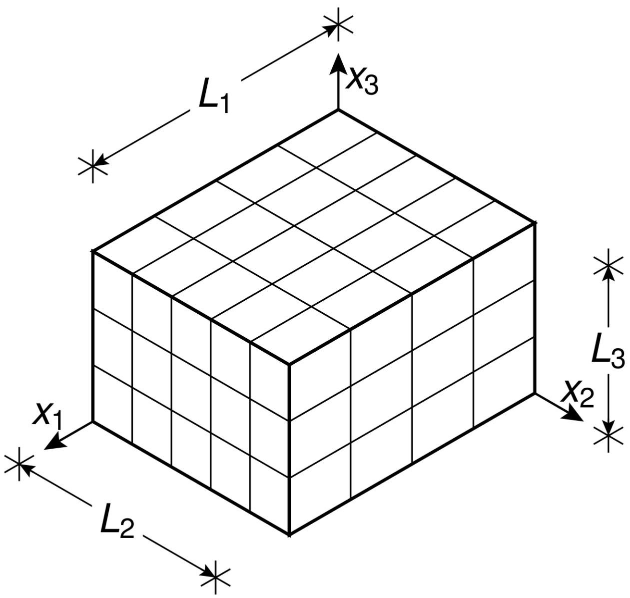
The two-step approach is more efficient

- Homogeneous reference material
- Periodic boundary conditions

FFT for both steps!

Contents

Q1 approximation of displacement



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

Cell-wise constant

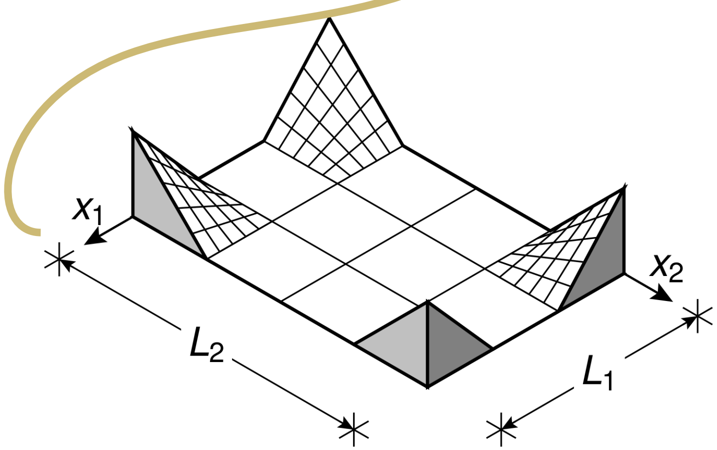
Nodal displacement

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

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

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

Nodal coordinates



Periodic shape function

Fourier series, discrete Fourier transform

Displacement is periodic! Can be expanded in Fourier series

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

Discrete Fourier transform of nodal displacements

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

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)

Contents

A non-specialist's presentation of constitutive relation error

CRE & Uniform Grid, Periodic Lippmann – Schwinger solvers

A local reconstruction of the displacement

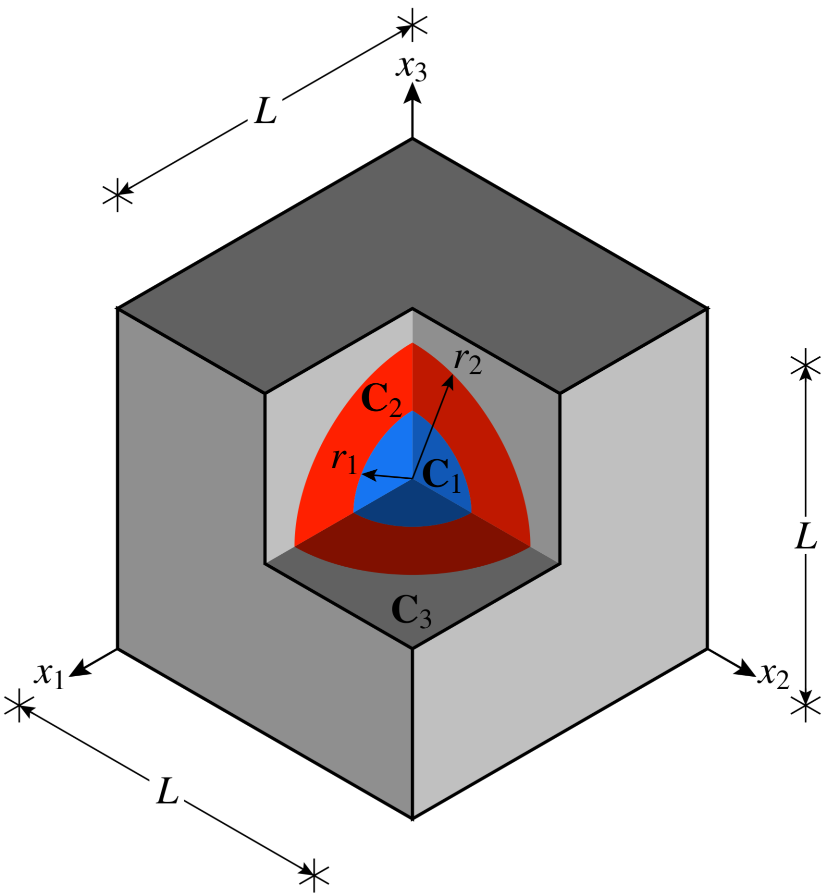
The nitty-gritty details

Example 1

Example 2

Hashin's coated sphere

Example borrowed from Schneider et al. (2015)



$$r_1 = 0.2\,L$$

$$r_2 = 0.4\,L$$

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

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

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

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

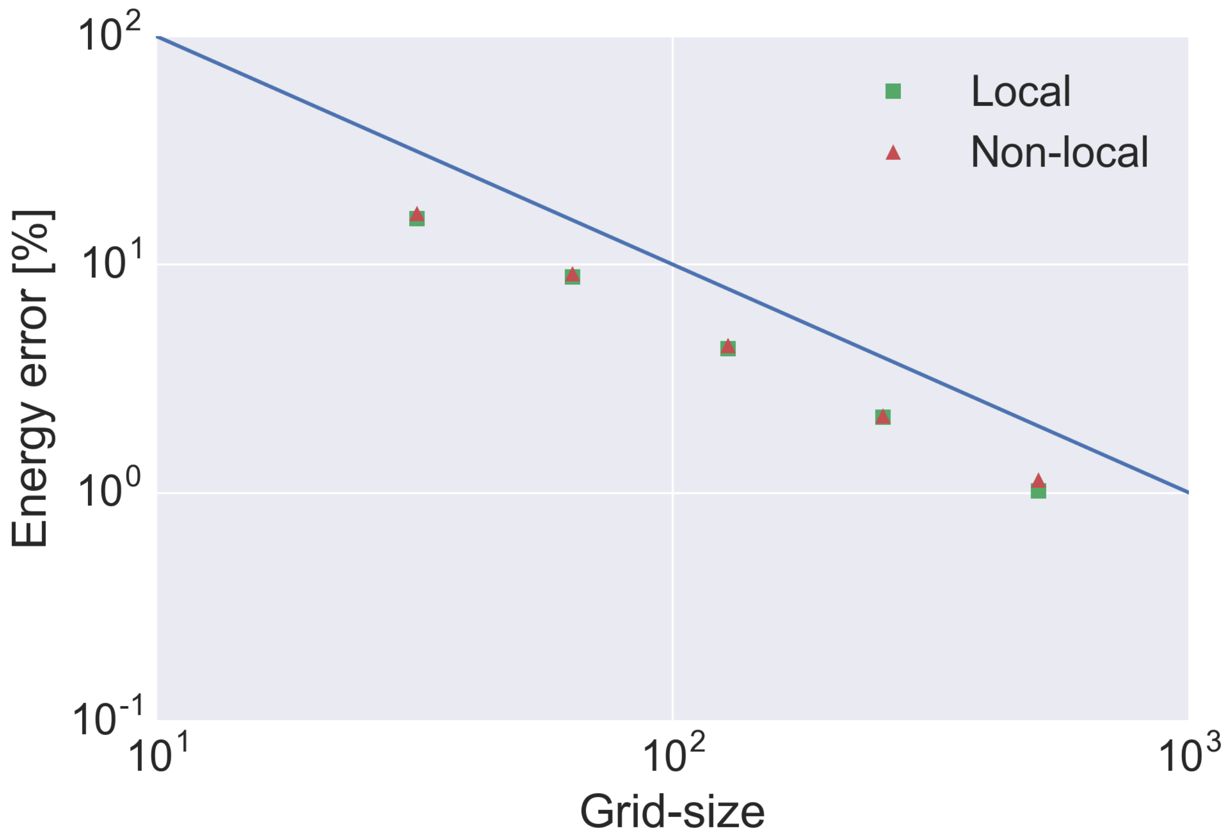
Schneider et al. (2015), *Int. J. Num. Meth. Eng.* **105(9)**, 1419–1436

Error on reconstructed displacement

Truncated discrete Green operator (Moulinec & Suquet, 1998)

Error on reconstructed displacement

Finite difference discrete Green operator (Willot, 2015)



Contents

Reconstruction of stress

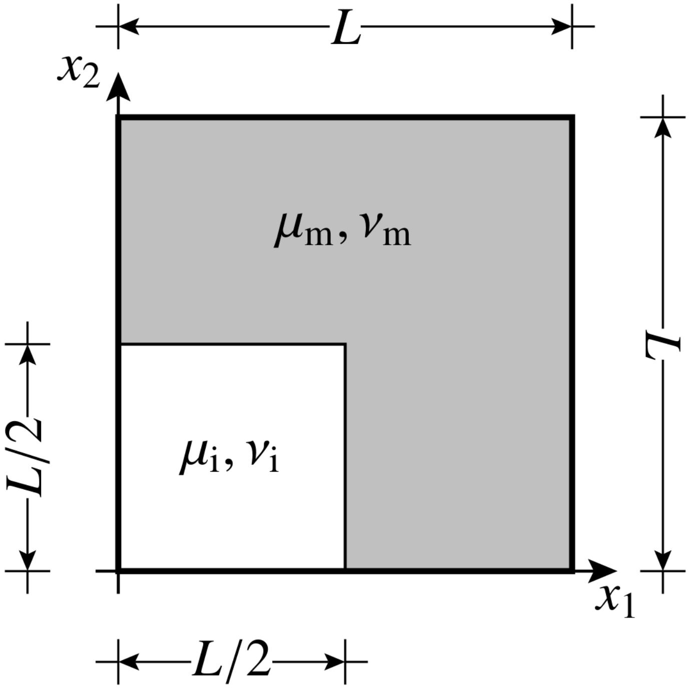
Reconstructed displacement is a Galerkin solution

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

- “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



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

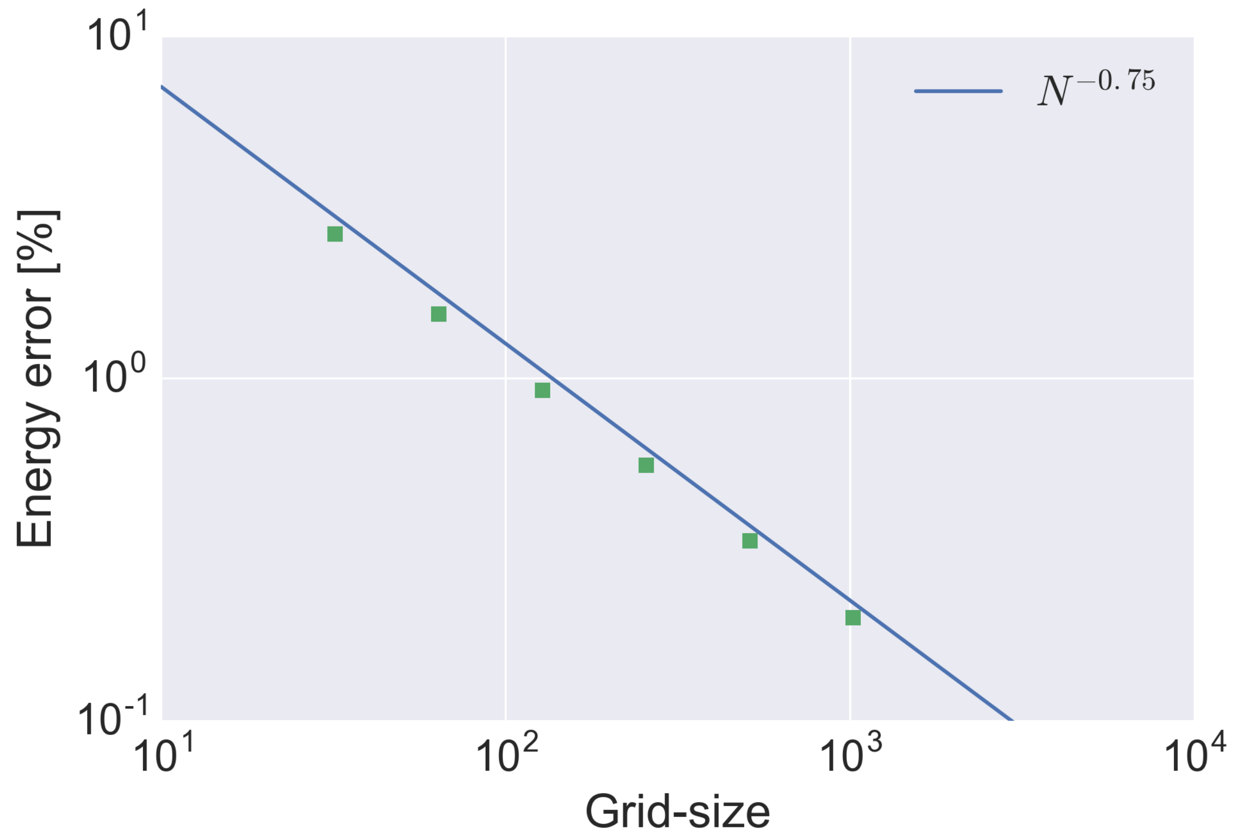
$$\nu_m = 0.3$$

$$\nu_i = 0.2$$

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

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/`

ASSOCIATION FRANÇAISE DE MECANIQUE

Financial support of AFM/CNFM is gratefully acknowledged by SB.