

A posteriori error estimators for FFT-based numerical techniques

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Outline of this talk

Introduction

- constitutive relation error (CRE)
- uniform grid, periodic Lippmann–Schwinger (UGPLS) solvers

Overall strategy

- combining CRE and UGPLS solvers
- reconstructing (kinematically admissible) displacements

Example: a square inclusion

Elastic equilibrium of a structure

$$\Omega : \operatorname{div} \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0} \quad \boldsymbol{\sigma} \text{ statically admissible with } \mathbf{b} \text{ and } \bar{\mathbf{T}}$$

$$\partial\Omega_N : \boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{T}}$$

$$\partial\Omega_D : \mathbf{u} = \bar{\mathbf{u}} \quad \mathbf{u} \text{ kinematically admissible with } \bar{\mathbf{u}}$$

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

Energy norms

$$\langle \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2 \rangle_S = \int_{\Omega} \boldsymbol{\sigma}_1 : \mathbf{S} : \boldsymbol{\sigma}_2 \, dV \quad \|\boldsymbol{\sigma}\|_S^2 = \int_{\Omega} \boldsymbol{\sigma} : \mathbf{S} : \boldsymbol{\sigma} \, dV$$

$$\langle \boldsymbol{\varepsilon}_1, \boldsymbol{\varepsilon}_2 \rangle_C = \int_{\Omega} \boldsymbol{\varepsilon}_1 : \mathbf{C} : \boldsymbol{\varepsilon}_2 \, dV \quad \|\boldsymbol{\varepsilon}\|_C^2 = \int_{\Omega} \boldsymbol{\varepsilon} : \mathbf{C} : \boldsymbol{\varepsilon} \, dV$$

The Prager–Synge theorem

$$\|\hat{\sigma} - C : \hat{\epsilon}\|_S^2 = \|\hat{\sigma} - \sigma\|_S^2 + \|\hat{\epsilon} - \epsilon\|_C^2$$

u, σ : true solution

\hat{u} : kinematically admissible

$\hat{\sigma}$: statically admissible

Consequence

$$\underbrace{\frac{\|\hat{\sigma} - \sigma\|_S^2}{\|\hat{\epsilon} - \epsilon\|_C^2}}_{\text{"True" error, unknown}} \leq \underbrace{\|\hat{\sigma} - C : \hat{\epsilon}\|_S^2}_{\text{Constitutive relation error, computable}}$$

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

Construction of \hat{u}

Trivial with **displacement-based FEM!**

Construction of $\hat{\sigma}$: the EET method (Equilibrating Element Traction)

- Postprocessing 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.
- Provides an upper-bound on the “true” error.

How about Uniform Grid Periodic
Lippmann–Schwinger Solvers
(UGPLS)?

Periodic homogenization: $\Omega = (0, L_1) \times \cdots \times (0, L_d)$ (unit-cell)

The corrector problem

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

The effective stiffness

$$\mathbf{C}^{\text{eff}} : \mathbf{E} \stackrel{\text{def}}{=} \overline{\mathbf{C} : (\mathbf{E} + \nabla^s \mathbf{u})}$$

\mathbf{u} : periodic fluctuation of total displacement

Intermezzo: the Green operator for strains

$$\nabla \cdot (\mathbf{C}_0 : \nabla^s \mathbf{u} + \boldsymbol{\varpi}) = \mathbf{0} \iff \nabla^s \mathbf{u} = -\Gamma_0[\boldsymbol{\varpi}]$$

\mathbf{u} : periodic displacement

\mathbf{C}_0 : homogeneous, reference material

$\boldsymbol{\varpi}$: heterogeneous prestress

$$\begin{aligned} \nabla \cdot (\mathbf{C} : (\mathbf{E} + \nabla^s \mathbf{u})) = \mathbf{0} &\iff \begin{cases} \nabla \cdot (\mathbf{C}_0 : \nabla^s \mathbf{u} + \boldsymbol{\tau}) = \mathbf{0} \\ \boldsymbol{\tau} = (\mathbf{C} - \mathbf{C}_0) : (\mathbf{E} + \nabla^s \mathbf{u}) \end{cases} \\ &\iff \begin{cases} \nabla^s \mathbf{u} = -\boldsymbol{\Gamma}_0[\boldsymbol{\tau}] \\ \boldsymbol{\tau} = (\mathbf{C} - \mathbf{C}_0) : (\mathbf{E} + \nabla^s \mathbf{u}) \end{cases} \\ &\iff \begin{cases} (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} + \boldsymbol{\Gamma}_0[\boldsymbol{\tau}] = \mathbf{E} \\ \boldsymbol{\tau} = (\mathbf{C} - \mathbf{C}_0) : (\mathbf{E} + \nabla^s \mathbf{u}) \end{cases} \end{aligned}$$

Discretization of the Lippmann–Schwinger equation

$$(C - C_0)^{-1} : \boldsymbol{\tau} + \boldsymbol{\Gamma}_0[\boldsymbol{\tau}] = \boldsymbol{E} \quad \rightsquigarrow \quad (C - C_0)^{-1} : \boldsymbol{\tau}^N + \boldsymbol{\Gamma}_0^N[\boldsymbol{\tau}^N] = \boldsymbol{E}$$

Various discretization strategies

- Point collocation (Moulinec & Suquet, 1994, 1998)
- Galerkin, piece-wise constant (Brisard & Dormieux, 2010, 2012)
- Galerkin, trigonometric polynomials (Vondřejc, Zeman & Marek, 2014)

Structure of resulting linear system

Block-diagonal + block-circulant

⇒ Matrix-free implementation, using FFT

$$(C - C_0)^{-1} : \boldsymbol{\tau} + \boldsymbol{\Gamma}_0[\boldsymbol{\tau}] = \boldsymbol{E}$$

Kinematically admissible displacements?

Statically admissible stresses?

Remember: true \mathbf{u} retrieved from true $\boldsymbol{\tau}$

$$\nabla \cdot (C_0 : \nabla^s \mathbf{u} + \boldsymbol{\tau}) = \mathbf{0}$$

The idea: kinematically admissible $\hat{\mathbf{u}}$ derived from approximate $\boldsymbol{\tau}^N$

$$\nabla \cdot (C_0 : \nabla^s \hat{\mathbf{u}} + \boldsymbol{\tau}^N) = \mathbf{0}$$

$\boldsymbol{\tau}^N$: output of the UGPLS solver

Use finite elements on a uniform grid!

1. Compute approximate solution $\boldsymbol{\tau}^N$ to LS (use UGPLS solvers)

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

2. Compute kinematically admissible \mathbf{u}^N as FEM approximation of solution to

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

Question

Why not use FEM to solve the corrector problem

$$\nabla \cdot (\mathbf{C} : (\mathbf{E} + \nabla^s \mathbf{u})) = \mathbf{o} \text{ and be done with it?}$$

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Hint: compare

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

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Why not use FEM to solve the corrector problem

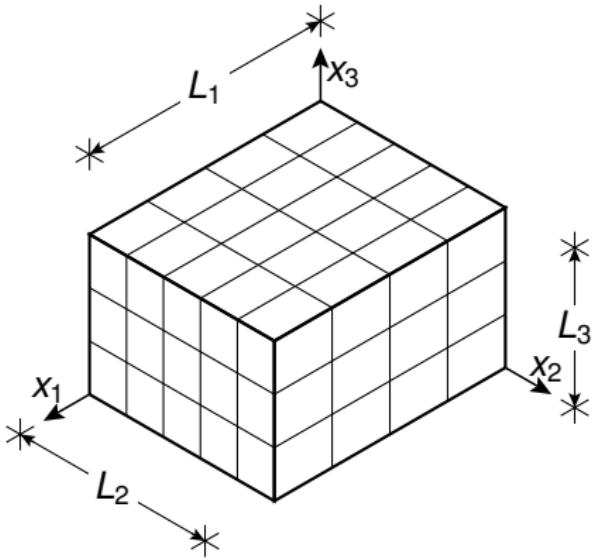
$$\nabla \cdot (\mathbf{C} : (\mathbf{E} + \nabla^s \mathbf{u})) = \mathbf{o} \text{ and be done with it?}$$

Hint: compare

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Answer

The unit-cell is now **homogeneous**,
which makes a **HUGE** difference...



The canonical problem

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

Uniform grid

- $L = (L_1, \dots, L_d)$: size of unit-cell,
- $N = (N_1, \dots, N_d)$: size of grid,
- \mathcal{N} : set of node multi-indices.

$$\mathbf{xy} \stackrel{\text{def}}{=} (x_1 y_1, \dots, x_d y_d)$$

$$\frac{\mathbf{x}}{\mathbf{y}} \stackrel{\text{def}}{=} \left(\frac{x_1}{y_1}, \dots, \frac{x_d}{y_d} \right)$$

$$f(\mathbf{x}) \stackrel{\text{def}}{=} \prod_{j=1}^d f(x_j)$$

f: scalar function

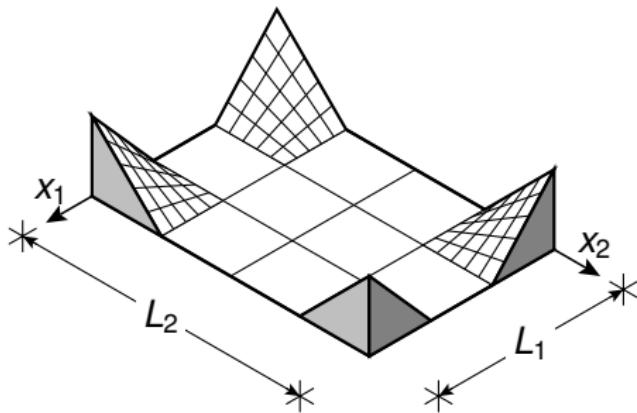
Examples

$$|\mathbf{x}| = |x_1| \cdots |x_d| = |x_1 \cdots x_d|$$

$$\exp\left(2i\pi \frac{\mathbf{kx}}{L}\right) = \exp\left(2i\pi \sum_{j=1}^d \frac{k_j x_j}{L_j}\right)$$

In the following formulas, think of vectors as mere scalars!

Periodic shape function



P1 approx. of displacement

$$u^N(x) = \sum_{n \in \mathcal{N}} \Phi^N(x - x_n^N) u_n^N$$

Φ^N : shape function
 x_n^N : coordinates of nodes

The periodic P1 shape function

$$\Phi^N(x) = \frac{1}{|N|} \sum_{k \in \mathbb{Z}^d} \operatorname{sinc}^2\left(\frac{\pi k}{N}\right) \exp\left(2i\pi \frac{kx}{L}\right)$$

The periodic displacement

$$u^N(x) = \frac{1}{|N|} \sum_{k \in \mathbb{Z}^d} \operatorname{sinc}^2\left(\frac{\pi k}{N}\right) \exp\left(2i\pi \frac{kx}{L}\right) \hat{u}_k^N$$

DFT of nodal displacements

$$\hat{u}_k^N = \sum_{n \in N} \exp\left(-2i\pi \frac{kn}{N}\right) u_n^N$$

The total potential energy

$$\Pi = \frac{|L|}{|N|^2} \sum_{k \in N} \left(\frac{1}{2} \hat{u}_k^N \cdot \hat{K}_k^N \cdot \hat{u}_k^N + \overline{\hat{u}_k^N} \cdot \hat{\boldsymbol{\omega}}_k^N \cdot \overline{\hat{B}_k^N} \right),$$

Notes

1. Finite sum (no approximation)!
2. Closed-form expressions for \hat{K}_k^N and \hat{B}_k^N .

Optimization of potential energy: finite set of $d \times d$ systems

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

Brisard (2015), IJNME, submitted

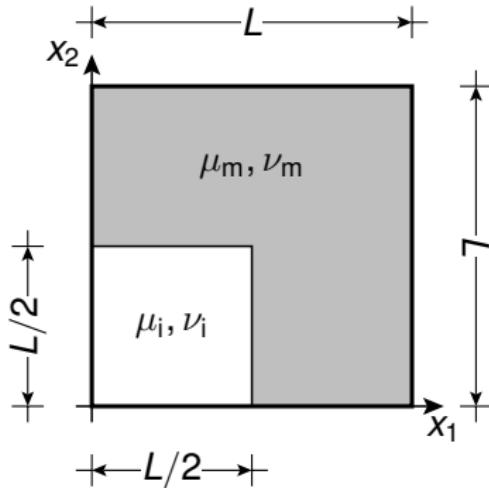
1. Compute DFT of prestress (**use FFT!**).
2. Solve $d \times d$ linear system for each frequency.
3. Compute inverse DFT of displacement (**use FFT!**).

Notes

1. Very simple code, soon available (**meanwhile, contact me!**).
2. Applies to **any** variant of UGPLS!

A very simple example

The problem



Material properties

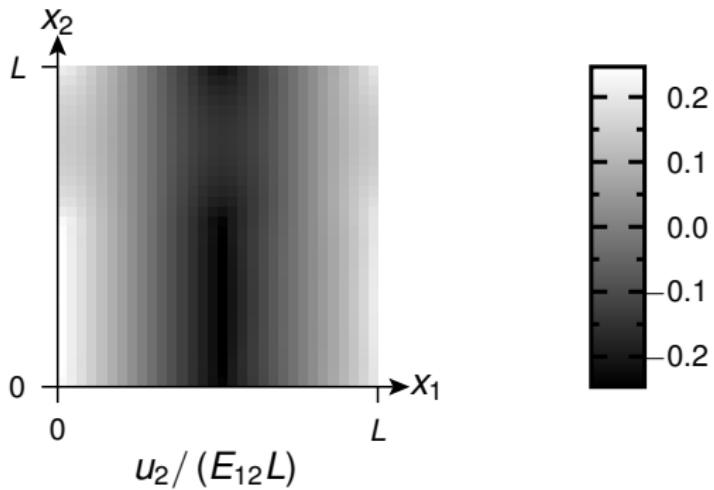
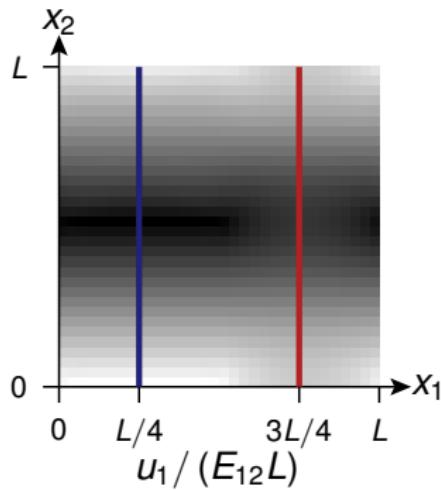
- $\mu_i = 100\mu_m$
- $\nu_m = 0.3$
- $\nu_i = 0.2$

Loading

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

A very simple example

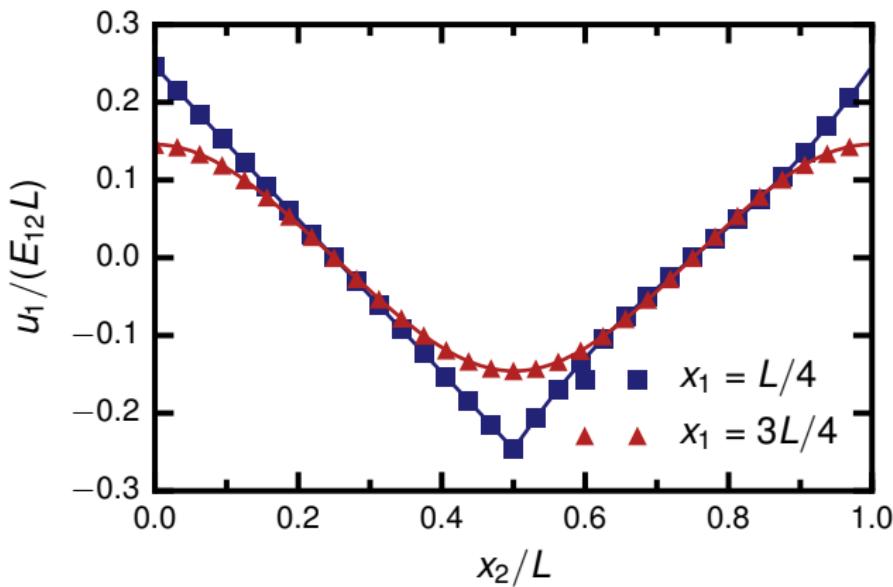
Local displacements



32×32 UGPLS

A very simple example

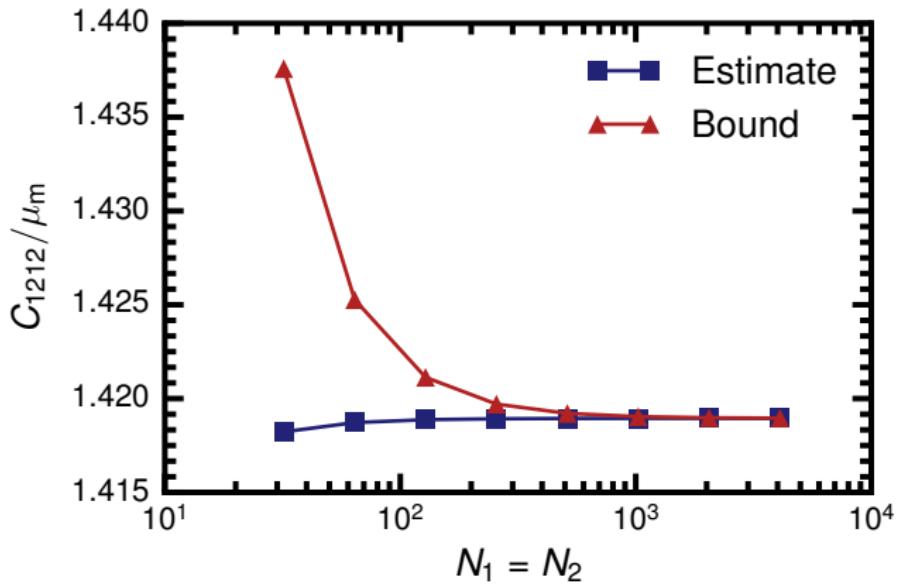
Comparison with direct FEM



32×32 UGPLS, 256×256 FEM

A very simple example

Rigorous upper bound on effective stiffness



Reconstruction of displacements from UGPLS solver output

- **Efficient**: non-iterative, based on FFT.
- Embarrassingly parallel.
- **General**: applies to **any** variant of UGPLS solver.

Application to estimate quality of solution

- Requires statically admissible stresses (cf. FEM).
- Work in progress with L. Chamoin.

Other applications

- Rigorous bounds on macroscopic properties.
- Limit analysis of periodic microstructures.

Thank you for your attention!

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