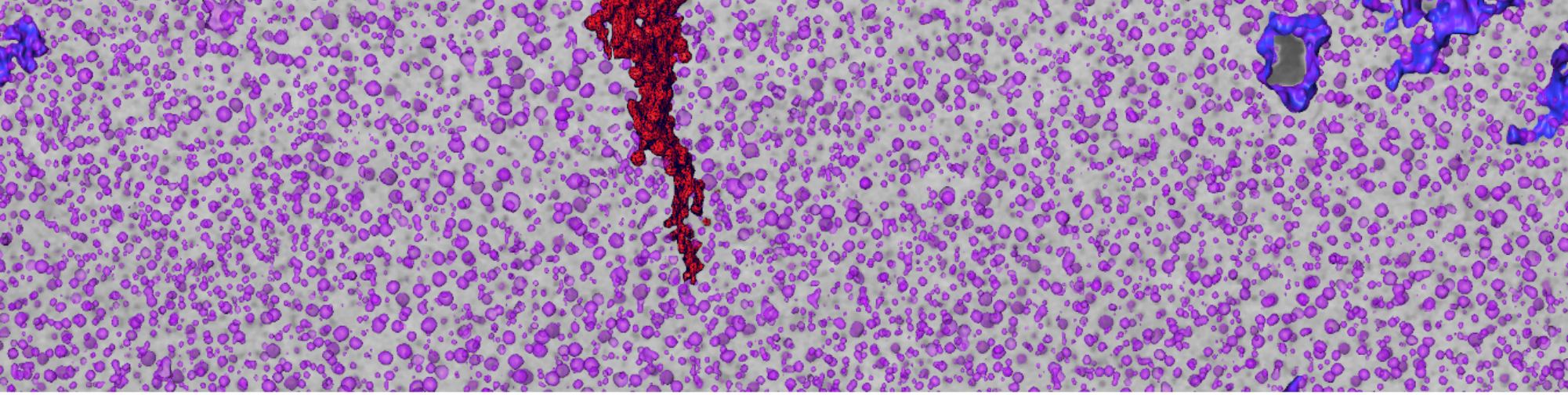

Parallel error estimation for primal and dual domain decomposition methods

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centralelille

cnrs

Context

- Progresses in materials and fabrication lead to complex designs, stressful working regimes for which the adequacy of current sizing methods (aka engineering rules) is not ensured.
- A solution is to run structure-scale computations with mesh size adapted to the meso or micro-scale where critical phenomena are initiated.
- This may result in $\gg$100 Mdof models even for small cases.
- To handle this, we need **distributed data** and **adapted solvers**.
- To ensure quality we need **adapted error estimators**, **parallel remeshers** and **recycling strategies**.

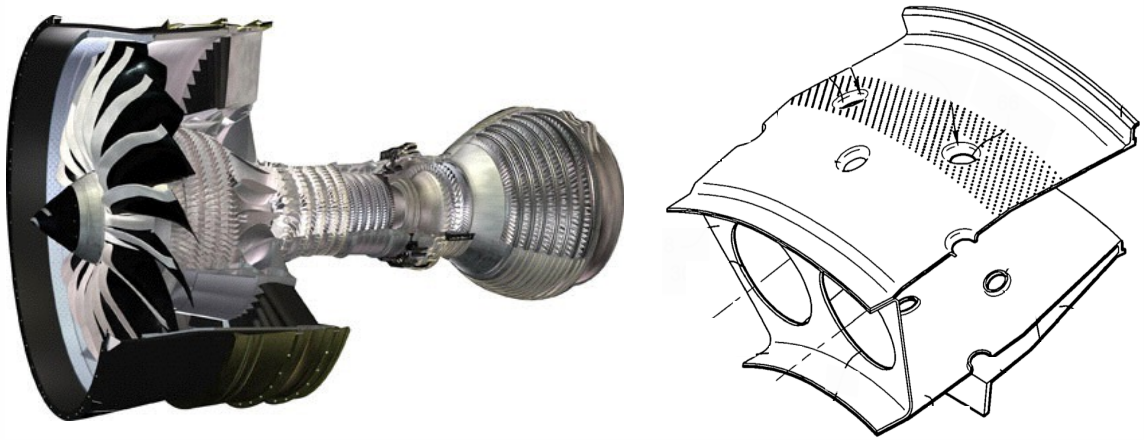

Figure: LEAP engine, combustion chamber (Safran)

This presentation is based on work from before 2015, much progress was done since then, but not by me.

Classical linear elasticity problem

Ω open polyhedral domain of $\mathbb{R}^d$ ($d = 2$ ou 3), $\mathbb{H}$: Hooke's tensor
Load: body force $f \in L^2(\Omega)$,
bcs: Neumann $g \in L^2(\partial_n\Omega)$, Dirichlet $u_d \in H^{1/2}(\partial_d\Omega)$.

Usual variational formulation

Kinematically admissible displacement ($H^1(\Omega)$):
$\mathrm{KA}(\Omega) = \{u \in H^1(\Omega),\ u = u_b \text{ sur } \partial_d\Omega\}$

Find $u \in \mathrm{KA}(\Omega)$ s.t. $\forall v \in \mathrm{KA}_0(\Omega)$,

$$\int_\Omega \varepsilon(u) : \mathbb{H} : \varepsilon(v)\, dx =: a(u,v) = l(v) := \int_\Omega f \cdot v\, dx + \int_{\partial_n\Omega} g \cdot v\, dS$$

with ε the symmetric part of the gradient.

[1] Ladevèze, 1975.

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with ε the symmetric part of the gradient.

Formulation by the **Error in constitutive relation**[1]

Statically admissible stress ($H_{div}(\Omega)$)
$\mathrm{SA}(\Omega) = \{\sigma \in L^2_{sym}(\Omega),\ \forall v \in \mathrm{KA}_0(\Omega), \int_\Omega \sigma : \varepsilon(v)\, dx = \int_\Omega f \cdot v\, dx + \int_{\partial_n\Omega} g \cdot v\, dS\}$

Find $(u,\sigma) \in \mathrm{KA}(\Omega) \times \mathrm{SA}(\Omega)$ s.t. $\mathrm{e_{cr}}(\varepsilon(u),\sigma) := |||\mathbb{H}^{-1} : \sigma - \varepsilon(u)|||_\Omega = 0$

$|||\varepsilon|||_\Omega$ is the energy norm, in particular $|||\varepsilon(u)|||_\Omega = \|u\|_a$.

[1] Ladevèze, 1975.

Classical approximation

continuous Galerkin finite element

Find $u_h \in \mathrm{KA}_h(\Omega)$ subspace of $\mathrm{KA}(\Omega)$ of finite dimension, s.t. $\forall v_h \in \mathrm{KA}_{h0}(\Omega)$

$$r_{u_h}(v_h) := a(u_h, v_h) - l(v_h) = 0$$

and we define $\sigma_h = \mathbb{H} : \varepsilon(u_h)$

Error estimation

Classical approximation

continuous Galerkin finite element

Find $u_h \in \mathrm{KA}_h(\Omega)$ subspace of $\mathrm{KA}(\Omega)$ of finite dimension, s.t. $\forall v_h \in \mathrm{KA}_{h0}(\Omega)$

$$r_{u_h}(v_h) := a(u_h, v_h) - l(v_h) = 0$$

and we define $\sigma_h = \mathbb{H} : \varepsilon(u_h)$

Error estimation

- σ_h is not smooth $\rightarrow$ ZZ2 estimator[2],

Let $\tilde{\sigma}$ be a smoothing of σ_h,

$$\eta_{ZZ2} = |||\sigma_h - \tilde{\sigma}|||$$

Very often $\|u - u_h\|_a \simeq \eta_{ZZ2}$ but no warranty

[2] Zienkiewicz and Zhu, 1987.

Classical approximation

continuous Galerkin finite element

Find $u_h \in \mathrm{KA}_h(\Omega)$ subspace of $\mathrm{KA}(\Omega)$ of finite dimension, s.t. $\forall v_h \in \mathrm{KA}_{h0}(\Omega)$

$$r_{u_h}(v_h) := a(u_h, v_h) - l(v_h) = 0$$

and we define $\sigma_h = \mathbb{H} : \varepsilon(u_h)$

Error estimation

- σ_h is not smooth $\rightarrow$ ZZ2 estimator,
- $\sigma_h \notin \mathrm{SA}(\Omega) \rightarrow$ explicit residuals,[2]

$$\eta^2 = \sum_T h_T^2 \| \operatorname{div} \sigma_h + f \|_{0,T}^2 + \sum_E h_E \| [\sigma_h]_E \cdot n_E \|_{0,E}^2$$

$$\| u - u_h \|_a^2 \leqslant C_1 \eta^2$$

$$C_2 \eta^2 \leqslant \| u - u_h \|_a^2 + \mathrm{osc}^2$$

Oscillation term: $\mathrm{osc}^2 = \sum_T \| h_T (f - \bar{f}_T) \|_{0,T}^2 \ldots$

[2] Verfürth, 1996, review.

Classical approximation

continuous Galerkin finite element

Find $u_h \in \mathrm{KA}_h(\Omega)$ subspace of $\mathrm{KA}(\Omega)$ of finite dimension, s.t. $\forall v_h \in \mathrm{KA}_{h0}(\Omega)$

$$r_{u_h}(v_h) := a(u_h, v_h) - l(v_h) = 0$$

and we define $\sigma_h = \mathbb{H} : \varepsilon(u_h)$

Error estimation

- σ_h is not smooth $\rightarrow$ ZZ2 estimator,
- $\sigma_h \notin \mathrm{SA}(\Omega) \rightarrow$ explicit residuals,
- Stein's formula[2] $\rightarrow$ constant-free explicit residuals,

$$\eta_{new}^2 = \sum_T h_T^2 (\| \operatorname{div} \sigma_h + f \|_{0,T} + C_T \sum_{E \in \partial T} \frac{\sqrt{h_E}}{\sqrt{|T|}} \| [\sigma_h]_E \cdot n_E \|_{0,E})^2$$

$$\| u - u_h \|_a \leqslant C \eta_{new}$$

all constants are computable

[2] Gerasimov, Stein, and Wriggers, 2015.

Classical approximation

continuous Galerkin finite element

Find $u_h \in \mathrm{KA}_h(\Omega)$ subspace of $\mathrm{KA}(\Omega)$ of finite dimension, s.t. $\forall v_h \in \mathrm{KA}_{h0}(\Omega)$

$$r_{u_h}(v_h) := a(u_h, v_h) - l(v_h) = 0$$

and we define $\sigma_h = \mathbb{H} : \varepsilon(u_h)$

Error estimation

- σ_h is not smooth $\rightarrow$ ZZ2 estimator,
- $\sigma_h \notin \mathrm{SA}(\Omega) \rightarrow$ explicit residuals,
- Stein's formula $\rightarrow$ constant-free explicit residuals,
- Error in constitutive relation[2] (implicit residuals),

Prager-Synge theorem: let $\hat{u} \in \mathrm{KA}(\Omega)$, $\hat{\sigma} \in \mathrm{SA}(\Omega)$

$$\|u - \hat{u}\|_a^2 + |||\sigma - \hat{\sigma}|||^2 = \mathrm{e_{cr}}^2(\varepsilon(\hat{u}), \hat{\sigma})$$

Use $\hat{u} = u_h$ and compute $\hat{\sigma}$ from σ_h (aka. equilibration). Better if $\hat{\sigma} \simeq \sigma$:

$$\|u - u_h\|_a \leqslant \mathrm{e_{cr}}(\varepsilon(u_h), \hat{\sigma})$$

[2] Ladevèze and Leguillon, 1983.

Classical approximation

continuous Galerkin finite element

Find $u_h \in \mathrm{KA}_h(\Omega)$ subspace of $\mathrm{KA}(\Omega)$ of finite dimension, s.t. $\forall v_h \in \mathrm{KA}_{h0}(\Omega)$

$$r_{u_h}(v_h) := a(u_h, v_h) - l(v_h) = 0$$

and we define $\sigma_h = \mathbb{H} : \varepsilon(u_h)$

Error estimation

- σ_h is not smooth $\longrightarrow$ ZZ2 estimator,
- $\sigma_h \notin \mathrm{SA}(\Omega) \longrightarrow$ explicit residuals,
- Stein's formula $\longrightarrow$ constant-free explicit residuals,
- Error in constitutive relation (implicit residuals),
- Lower bound by estimation of the residual,

$$\forall \hat{w} \in \mathrm{KA}_0(\Omega), \quad \frac{|r_{u_h}(\hat{w})|}{\|\hat{w}\|_a} \leqslant \|u - u_h\|_a$$

$\hat{w}$ must be of high order. Better if $\hat{w} \simeq (u - u_h)$.

Classical approximation

continuous Galerkin finite element

Find $u_h \in \mathrm{KA}_h(\Omega)$ subspace of $\mathrm{KA}(\Omega)$ of finite dimension, s.t. $\forall v_h \in \mathrm{KA}_{h0}(\Omega)$

$$r_{u_h}(v_h) := a(u_h, v_h) - l(v_h) = 0$$

and we define $\sigma_h = \mathbb{H} : \varepsilon(u_h)$

Error estimation

- σ_h is not smooth $\longrightarrow$ ZZ2 estimator, easy to compute, often efficient but not rigorous (in its early versions)
- $\sigma_h \notin \mathrm{SA}(\Omega) \longrightarrow$ explicit residuals, perfect for adaptation, not for error measurement
- Stein's formula $\longrightarrow$ constant-free explicit residuals, not tested
- Error in constitutive relation (implicit residuals), computationally demanding but constant free $\longleftarrow$
- Lower bound by estimation of the residual, computationally demanding but constant free and by-product of equilibration[2] $\longleftarrow$

[2] Díez, Parés, and Huerta, 2003.

Given an error estimation with local (element) contributions (η_T), there are mainly two strategies:

- The nested discretization method, based on the chain:
  $$SOLVE \longrightarrow ESTIMATE \longrightarrow MARK \longrightarrow REFINE$$
  - MARK: select elements most contributing to the error (most famous: Dörfler's marking[3])
  - REFINE: iterative or recursive bisection of elements (even local errors impact lots of elements)

  $\longrightarrow$ lots of interesting properties (error decrease, quasi-optimality)
- The full remeshing technique based on the definition of map of characteristic lengths computed using a priori estimators with the objective to have all elements contributing identically to the error.

[3] Dörfler, 1996.

Linear quantities of interest

Bounds on the energy norm of the error may not be interesting for an engineer who may prefer the error on specific values (average stress in a region, SIF around a crack, displacement of a node...).

Extractor and adjoint problem

We consider continuous linear quantities of interest of the form $\tilde{l}(u)$.
The adjoint problem writes:

$$\text{Find } \tilde{u} \in \mathrm{KA}_0(\Omega) \text{ s.t. } \forall v \in \mathrm{KA}_0(\Omega),\ a(v, \tilde{u}) = \tilde{l}(v)$$

Let $\tilde{u}_h$ be the finite element approximation of $\tilde{u}$, we have:

$$\tilde{l}(u - u_h) = a(u - u_h, \tilde{u} - \tilde{u}_h)$$

Cauchy-Schwarz bound

$$|\tilde{l}(u - u_h)| \leqslant \|u - u_h\|_a \|\tilde{u} - \tilde{u}_h\|_a \leqslant \mathrm{e_{cr}} \tilde{\mathrm{e}}_{\mathrm{cr}}$$

Parallelogram bound

Let $e_h = u - u_h$ and $\tilde{e}_h = \tilde{u} - \tilde{u_h}$,

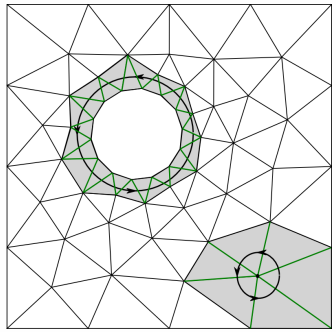
$$\tilde{I}(u - u_h) = \frac{1}{4}\left(\underbrace{\|se_h + \frac{1}{s}\tilde{e}_h\|_a}_{S^+} - \underbrace{\|se_h - \frac{1}{s}\tilde{e}_h\|_a}_{S^-}\right)$$

with $s = \|\tilde{e}_h\|_a / \|e_h\|_a$
Let $\beta^{+/-}_{\text{inf}\,/\,\text{sup}}$ be bounds for $S^{+/-}$, we have:

$$\beta^+_{\text{inf}} - \beta^-_{\text{sup}} \leqslant 4\tilde{I}(u - u_h) \leqslant \beta^+_{\text{sup}} - \beta^-_{\text{inf}}$$

Sequential recovery of admissible fields

$\hat{\sigma} \in \mathrm{SA}(\Omega) \subset H_{div}(\Omega)$
$w \in \mathrm{KA}_0(\Omega)$



- Element equilibration techniques
  - Compute face tractions from σ_h, optimize on closed loops[4] or at least on star-patches[5].
  - Solve Neumann problems on elements with high order elements[6].
- Flux-free technique[7]
  - Using partition of unity, directly solve the error equation $a(e_h, v) = r_h(v)$ with high order on star-patches.
  - Automatically provides both $\hat{\sigma}$ and $\hat{w}$ (for the lower bound).

The recovery involves many localized operations. Evaluating the error roughly doubles the computational cost.

In the following we assume we have a recovery procedure $(\hat{\sigma}, w) = \mathcal{F}(\sigma_h, f, g)$.
It works for pure Neumann problems if rigid body balance is satisfied by (f, g).

---

[4] V. Rey, Gosselet, and C. Rey, 2014.
[5] Pled, Chamoin, and Ladevèze, 2011.
[6] Babuška et al., 1994.
[7] Parés, Díez, and Huerta, 2006.

Parallel processing by domain decomposition methods

Domain decomposition methods

- DDM are a natural tool to distribute the data of a PDE.
- They are an active research domain since 1990's.
- Major breakthrough around 2010–2015 with the propositions of strategies to ensure solvers' robustness (for implicit time integration).
- Now a rather established tool available in software suites (PetSc, HPDDM,...)

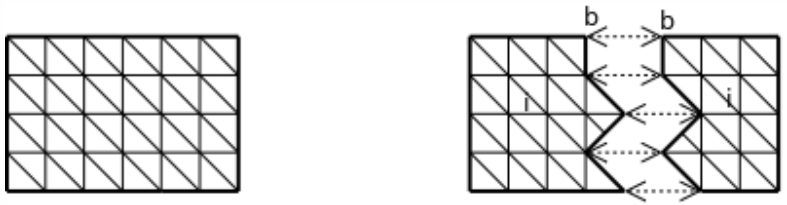
The many flavors of DDMs

- with/wo overlap,
- with Dirichlet/Neumann/Robin bcs,
- with $n \geqslant 2$ levels (a bit like multigrids),
- with ability to run nonlinear iterations inside subdomains,
- with asynchronous capabilities.

Here, we will be working in the frame of **non-overlapping primal or dual DDMs** (aka Dirichlet-Dirichlet and Neumann-Neumann), these methods are known under the acronyms FETI and BDD. The theory is valid for their primal-dual extensions FETI(DP) and BDD(C).

Two subdomains

i = internal, b = boundary = interface



Stiffness matrix and generalized efforts, independent per subdomain

$$\begin{pmatrix} \mathbf{K}^1_{ii} & \mathbf{K}^1_{ib} \\ \mathbf{K}^1_{bi} & \mathbf{K}^1_{bb} \end{pmatrix} \quad , \quad \begin{pmatrix} \mathbf{f}^1_i \\ \mathbf{f}^1_b \end{pmatrix} \qquad \begin{pmatrix} \mathbf{K}^2_{ii} & \mathbf{K}^2_{ib} \\ \mathbf{K}^2_{bi} & \mathbf{K}^2_{bb} \end{pmatrix} \quad , \quad \begin{pmatrix} \mathbf{f}^2_i \\ \mathbf{f}^2_b \end{pmatrix}$$

Virtual assembly $\longrightarrow$ sparse pattern

$$\begin{pmatrix} \mathbf{K}^1_{ii} & 0 & \mathbf{K}^1_{ib} \\ 0 & \mathbf{K}^2_{ii} & \mathbf{K}^2_{ib} \\ \mathbf{K}^1_{bi} & \mathbf{K}^2_{bi} & \mathbf{K}_{bb} \end{pmatrix} \begin{pmatrix} \mathbf{u}^1_i \\ \mathbf{u}^2_i \\ \mathbf{u}_b \end{pmatrix} = \begin{pmatrix} \mathbf{f}^1_i \\ \mathbf{f}^2_i \\ \mathbf{f}_b \end{pmatrix} \qquad \text{with} \begin{cases} \mathbf{K}_{bb} = \mathbf{K}^1_{bb} + \mathbf{K}^2_{bb} \\ \mathbf{f}_b = \mathbf{f}^1_b + \mathbf{f}^2_b \end{cases}$$

Domain decomposition – formulation

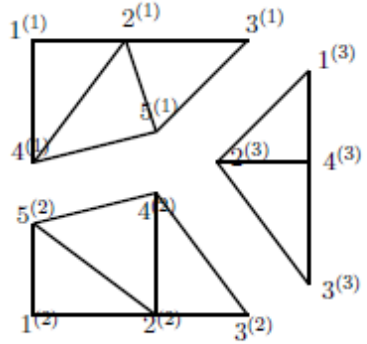
Introduction of neighbor's nodal reaction $\boldsymbol{\lambda}_b^s$
Local balance :

$$\begin{pmatrix} \mathbf{K}_{ii}^1 & \mathbf{K}_{ib}^1 \\ \mathbf{K}_{bi}^1 & \mathbf{K}_{bb}^1 \end{pmatrix} \begin{pmatrix} \mathbf{u}_i^1 \\ \mathbf{u}_b^1 \end{pmatrix} = \begin{pmatrix} \mathbf{f}_i^1 \\ \mathbf{f}_b^1 \end{pmatrix} + \begin{pmatrix} 0 \\ \boldsymbol{\lambda}_b^1 \end{pmatrix} \quad \text{et} \quad \begin{pmatrix} \mathbf{K}_{ii}^2 & \mathbf{K}_{ib}^2 \\ \mathbf{K}_{bi}^2 & \mathbf{K}_{bb}^2 \end{pmatrix} \begin{pmatrix} \mathbf{u}_i^2 \\ \mathbf{u}_b^2 \end{pmatrix} = \begin{pmatrix} \mathbf{f}_i^2 \\ \mathbf{f}_b^2 \end{pmatrix} + \begin{pmatrix} 0 \\ \boldsymbol{\lambda}_b^2 \end{pmatrix}$$

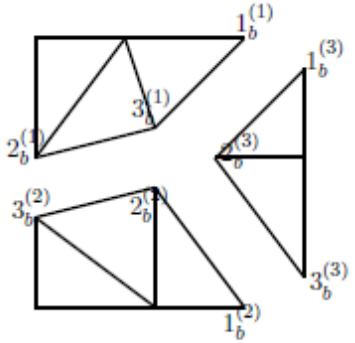
$$\begin{aligned} \mathbf{u}_b^1 - \mathbf{u}_b^2 &= 0 \\ \boldsymbol{\lambda}_b^1 + \boldsymbol{\lambda}_b^2 &= 0 \end{aligned}$$

N-subdomain version: use of assembly and trace operators

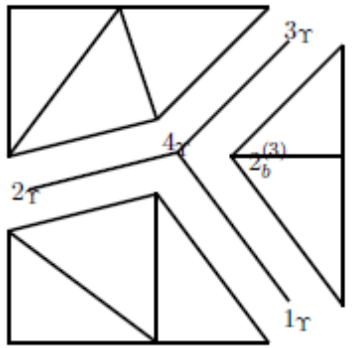
$$\begin{cases} \mathbf{K}^s \mathbf{u}^s = \mathbf{f}^s + \mathbf{T}^{s\,T} \boldsymbol{\lambda}_b^s \\ \sum_s \mathbf{B}^s \mathbf{u}_b^s = \sum_s \mathbf{B}^s \mathbf{T}^s \mathbf{u}^s = 0 \\ \sum_s \mathbf{A}^s \boldsymbol{\lambda}_b^s = 0 \end{cases}$$



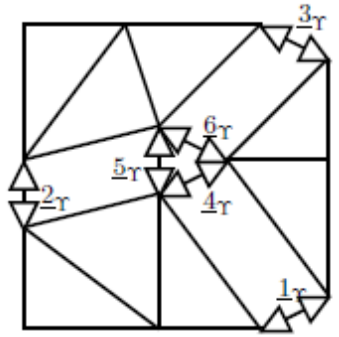
(a) Subdomains



(b) Local interface



(c) Primal interface



(d) Dual interface

$$t^{(1)} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad t^{(2)} = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad t^{(3)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$A^{(1)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad A^{(2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad A^{(3)} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\underline{A}^{(1)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix} \quad \underline{A}^{(2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \underline{A}^{(3)} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$$

Figure 6. Local numberings, interface numberings, trace and assembly operators

Bloc notations

$$\text{Vector } \mathbf{x} = \begin{pmatrix} \vdots \\ \mathbf{x}^s \\ \vdots \end{pmatrix}, \quad \text{Assembly } \begin{matrix} \mathbf{A} = (\ldots \quad \mathbf{A}^s \quad \ldots) \\ \mathbf{B} = (\ldots \quad \mathbf{B}^s \quad \ldots) \end{matrix}, \quad \text{Matrix } \mathbf{X} = \begin{pmatrix} \ddots & & \\ & \mathbf{X}^s & \\ & & \ddots \end{pmatrix}$$

We have:

$$\begin{cases} \mathbf{K}\mathbf{u} = \mathbf{f} + \mathbf{T}^T \boldsymbol{\lambda}_b \\ \mathbf{B}\mathbf{u}_b = \mathbf{B}\mathbf{T}\mathbf{u} = 0 \\ \mathbf{A}\boldsymbol{\lambda}_b = 0 \end{cases}$$

FETI

[Farhat et Roux 91, 94]

Global system on domain Ω

$$\mathbf{K}\mathbf{u} = \mathbf{f}$$

$\mathbf{K}$ is SPD

Substructured formulation

N non-overlapping subdomains, conforming mesh)

$$\mathbf{K}^s\mathbf{u}^s = \mathbf{f}^s + {\mathbf{T}^s}^T{\mathbf{B}^s}^T\boldsymbol{\lambda}$$

$$\sum_s \mathbf{B}^s\mathbf{T}^s\mathbf{u}^s = 0$$

$\boldsymbol{\lambda}$ = Lagrange multipliers that connect subdomains

Classical FETI system

$$\begin{pmatrix} \mathbf{F} & \mathbf{G} \\ \mathbf{G}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda} \\ \alpha \end{pmatrix} = \begin{pmatrix} \mathbf{d} \\ \mathbf{e} \end{pmatrix}$$

Topology

$\mathbf{T}^s$ = trace operators
$\mathbf{B}^s$ = signed Boolean assembly operators

Local operators

$\mathbf{S}^s = \mathbf{K}^s_{bb} - \mathbf{K}^s_{bi}{\mathbf{K}^s_{ii}}^{-1}\mathbf{K}^s_{ib}$ Schur complement
$\mathbf{F}^s = (\mathbf{S}^s)^+ = \mathbf{T}^s{\mathbf{K}^s}^+{\mathbf{T}^s}^T$ Dual Schur (NtD)
$\mathbf{R}^s = \ker(\mathbf{K}^s)$ basis of rigid body modes

Global operators

$$\mathbf{e} = -\left(\ldots, {\mathbf{f}^s}^T\mathbf{R}^s, \ldots\right)^T$$

$$\mathbf{G} = \left(\ldots, \mathbf{B}^s\mathbf{T}^s\mathbf{R}^s, \ldots\right)$$

$$\mathbf{F} = \sum_s \mathbf{B}^s\mathbf{F}^s{\mathbf{B}^s}^T = \mathbf{B}\mathbf{F}\mathbf{B}^T$$

$$\mathbf{d} = -\sum_s \mathbf{B}^s\mathbf{T}^s{\mathbf{K}^s}^+\mathbf{f}^s$$

Rigid body constraint

$$\boldsymbol{\lambda}_0 = \mathbf{Q}\mathbf{G}(\mathbf{G}^T\mathbf{Q}\mathbf{G})^{-1}\mathbf{e}$$
$$\mathbf{P} = \mathbf{I} - \mathbf{Q}\mathbf{G}(\mathbf{G}^T\mathbf{Q}\mathbf{G})^{-1}\mathbf{G}^T$$

Matrix $\mathbf{Q}$ is a SPD matrix, $\mathbf{Q} \simeq \tilde{\mathbf{S}}$ approximates the preconditioner.

$\boldsymbol{\lambda}$ is sought as $\boldsymbol{\lambda} = \boldsymbol{\lambda}_0 + \mathbf{P}\tilde{\boldsymbol{\lambda}}$ where $\tilde{\boldsymbol{\lambda}}$ is a solution of:

$$\mathbf{P}^T\mathbf{F}\mathbf{P}\tilde{\boldsymbol{\lambda}} = \mathbf{P}^T(\mathbf{d} - \mathbf{F}\boldsymbol{\lambda}_0) = \mathbf{P}^T\left(\sum_s \mathbf{B}^s\mathbf{K}^{s^+}(\mathbf{f}^s - \mathbf{B}^{s^T}\boldsymbol{\lambda}_0)\right)$$

Dirichlet preconditioner

This system is solved by an iterative solver, the preconditioner $\tilde{\mathbf{S}}$ being

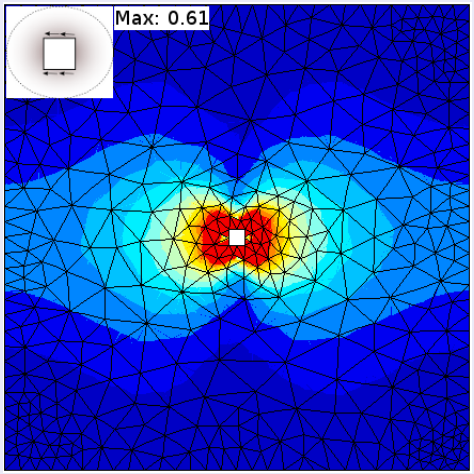
$$\tilde{\mathbf{S}} = \sum_s \tilde{\mathbf{B}}^s\mathbf{S}^s\tilde{\mathbf{B}}^{s^T} = \tilde{\mathbf{B}}\mathbf{S}\tilde{\mathbf{B}}^T$$

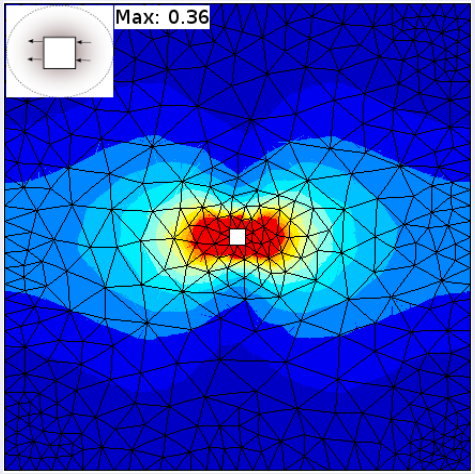
$\tilde{\mathbf{B}}^s$ are scaled[8] assembling operators / $\tilde{\mathbf{B}}^T = \mathbf{B}^+$
$\mathbf{S}^s$ are the Schur complements (Dirichlet-to-Neumann)

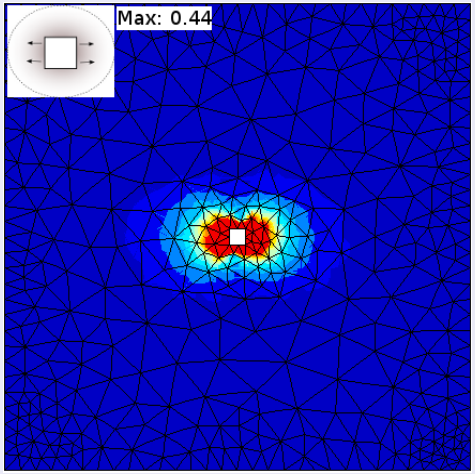
[8] Klawonn and Widlund, 2001; Rixen and Charbel Farhat, 1999.

Coarse problem and Saint-Venant's principle

Effect of a boundary traction distribution







Resultant $R_1 = R_2$ Resultant $R_3 = 0$

- Equal resultant $\longrightarrow$ same long range effects.
- Null resultant $\longrightarrow$ only local effects
- Null torsor $\Leftrightarrow$ tractions orthogonal to RBM

The coarse grid makes long range effects spread instantaneously.[9].
What remains only depend on neighbors.

[9] [Mandel 1993, Farhat 1994 2001, Ladevèze 1999, Dohrmann 2003]

Illustration of local equilibrium

Dirichlet and Neumann bcs

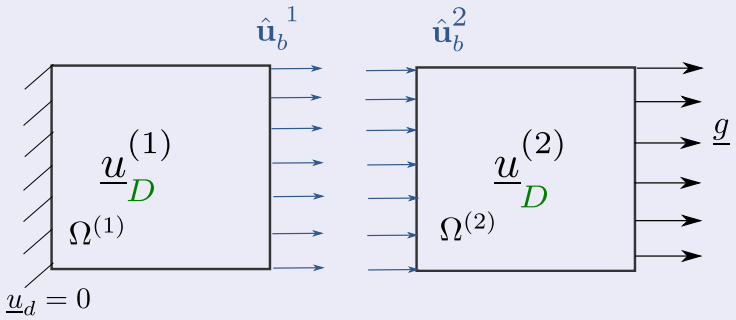
Continuous displacement at the interface

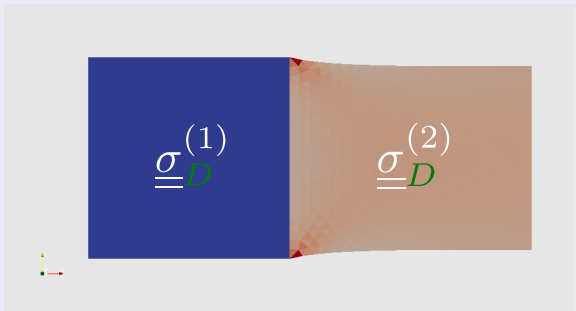
$$\hat{\mathbf{u}}_b^2 - \hat{\mathbf{u}}_b^1 = 0 \Rightarrow \hat{\mathbf{u}}_b^2 = \hat{\mathbf{u}}_b^1$$

Balanced reactions at the interface

$$\hat{\boldsymbol{\lambda}}_N^2 + \hat{\boldsymbol{\lambda}}_N^1 = 0 \Rightarrow \hat{\boldsymbol{\lambda}}_N^2 = -\hat{\boldsymbol{\lambda}}_N^1$$

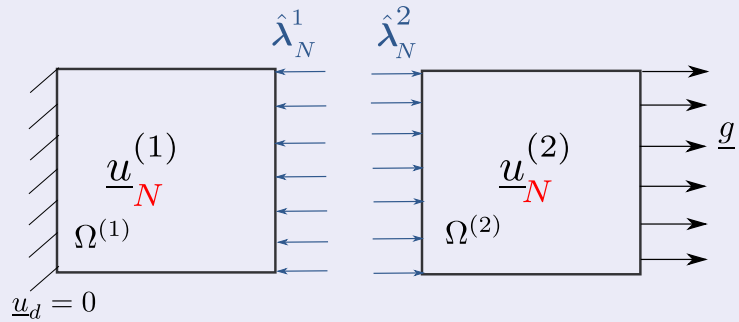
Dirichlet problem on Ω^s

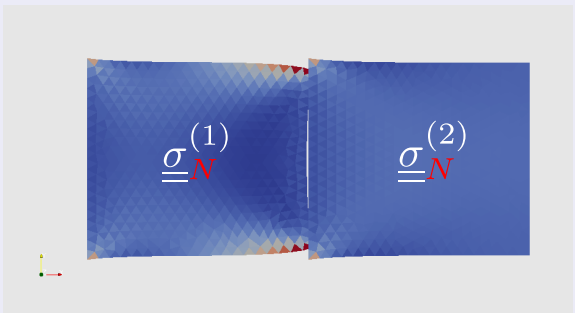




out of balance reactions

Neumann problem on Ω^s

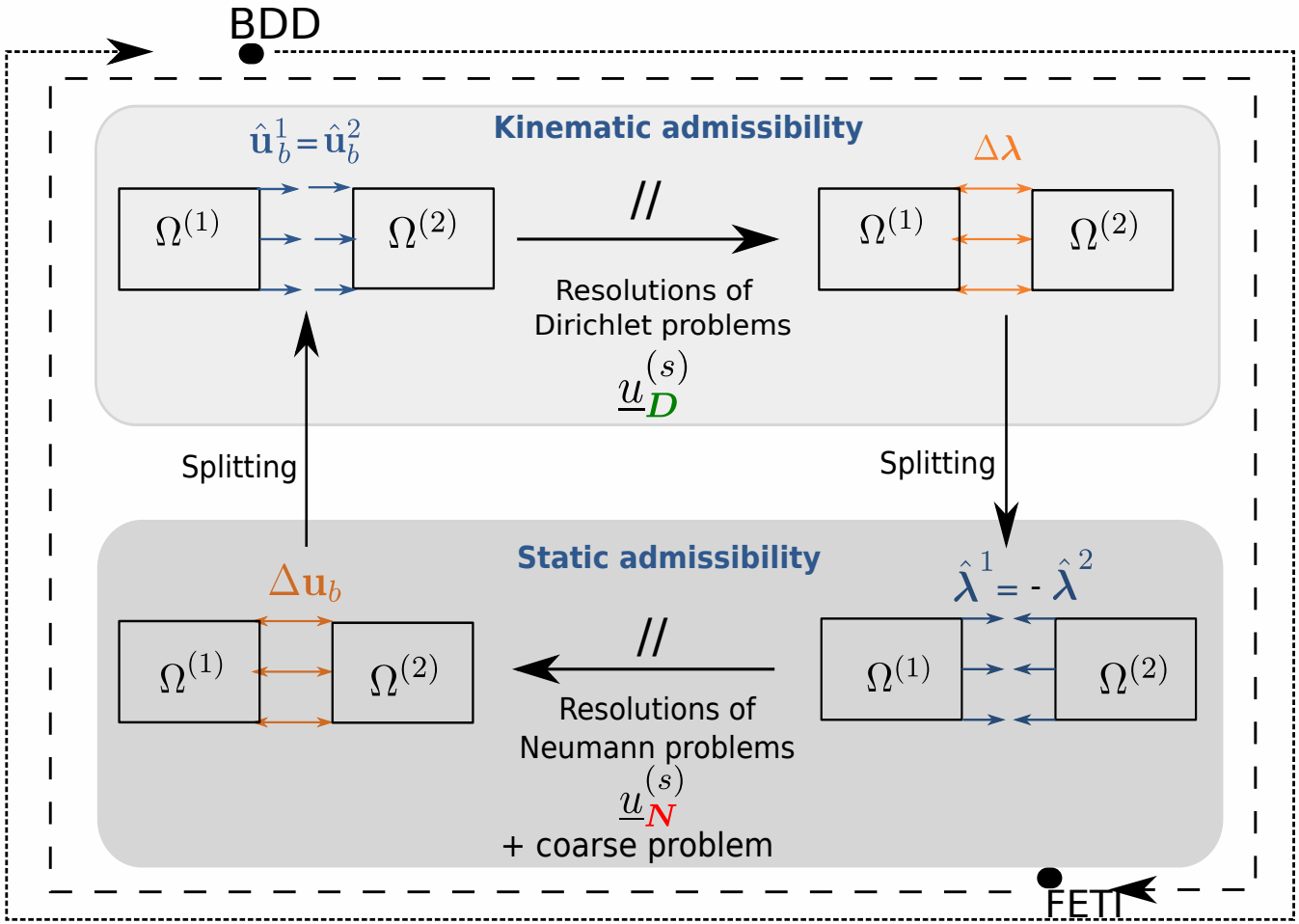




discontinuous displacements

Interface iterations

Dual (FETI)[10] and primal (BDD)[11] approaches



+ **no stationarity, Krylov solver is mandatory**

[10] C. Farhat and Roux, 1994.

[11] Mandel, 1993.

Algorithm 1: FETI: main unknown $\boldsymbol{\Lambda}$

$\boldsymbol{\Lambda} = \texttt{Initialize}(\mathbf{f}^s)$

Local reactions $\boldsymbol{\lambda}_N^s = \mathbf{B}^{s\,T}\boldsymbol{\Lambda}$

$(\mathbf{u}_N^s) = \texttt{Solve}_N(\boldsymbol{\lambda}_N^s, \mathbf{f}^s)$

Compute residual $\mathbf{r} = \mathbf{P}^T(\sum_s \mathbf{B}^s\mathbf{T}^s\mathbf{u}_N^s)$

Define local displacement $\tilde{\mathbf{u}}_b^s = \widetilde{\mathbf{B}}^{s\,T}\mathbf{r}$;

$(\tilde{\boldsymbol{\lambda}}^s, \tilde{\mathbf{u}}^s) = \texttt{Solve}_D(\tilde{\mathbf{u}}_b^s, 0)$

// $\mathbf{u}_D^s = \mathbf{u}_N^s - \tilde{\mathbf{u}}^s$

// $\boldsymbol{\lambda}_D^s = \boldsymbol{\lambda}_N^s - \tilde{\boldsymbol{\lambda}}^s$

Preconditioned residual $\mathbf{z} = \mathbf{P}(\sum_s \widetilde{\mathbf{B}}^s\tilde{\boldsymbol{\lambda}}^s)$

Search direction $\mathbf{w} = \mathbf{z}$

while $\sqrt{(\mathbf{r},\mathbf{z})} > \epsilon\sqrt{(\mathbf{r}_0,\mathbf{z}_0)}$ **do**

$(\delta\mathbf{u}_N^s) = \texttt{Solve}_N(\mathbf{B}^{s\,T}\mathbf{w}, 0)$

$\mathbf{p} = \mathbf{P}^T(\sum_s \mathbf{B}^s\mathbf{T}^s\delta\mathbf{u}_N^s)$

$\alpha = (\mathbf{r},\mathbf{z})/(\mathbf{p},\mathbf{w})$

$\boldsymbol{\Lambda} \leftarrow \boldsymbol{\Lambda} + \alpha\mathbf{w}$

// $\mathbf{u}_N^s \leftarrow \mathbf{u}_N^s + \alpha\delta\mathbf{u}_N^s$

// $\boldsymbol{\lambda}_N^s = \mathbf{B}^{s\,T}\boldsymbol{\Lambda}$

$\mathbf{r} \leftarrow \mathbf{r} - \alpha\mathbf{p}$

$\tilde{\mathbf{u}}_b^s = \widetilde{\mathbf{B}}^{s\,T}\mathbf{r}$

$(\tilde{\boldsymbol{\lambda}}^s, \tilde{\mathbf{u}}^s) = \texttt{Solve}_D(\tilde{\mathbf{u}}_b^s, 0)$

// $\mathbf{u}_D^s = \mathbf{u}_N^s - \tilde{\mathbf{u}}^s$

// $\boldsymbol{\lambda}_D^s = \boldsymbol{\lambda}_N^s - \tilde{\boldsymbol{\lambda}}^s$

$\mathbf{z} = \mathbf{P}(\sum_s \widetilde{\mathbf{B}}^s\tilde{\boldsymbol{\lambda}}^s)$

$\mathbf{w} \leftarrow \mathbf{z} - (\mathbf{p},\mathbf{z})/(\mathbf{p},\mathbf{w})\mathbf{w}$

end

Distributed admissible fields

Let $\omega \subset \Omega$

- Subspace of kinematically admissible fields (KA)

$$\mathrm{KA}(\omega) = \left\{ \mathbf{u} \in \left(\mathrm{H}^1(\omega)\right)^d,\ \mathbf{u} = \mathbf{u}_d \text{ on } \partial\omega \bigcap \partial_u\Omega \right\}$$

- Subspace of statically admissible fields(SA)

$$\mathrm{SA}(\omega) = \left\{ \tau \in \left(\mathrm{L}^2(\omega)\right)^{d\times d}_{\mathrm{sym}};\ \forall v \in \mathrm{KA}_{00}(\omega), \int_\omega \tau : \varepsilon(v)\, dx = \int_\omega f \cdot v\, dx + \int_{\partial_g\Omega \bigcap \partial\omega} g \cdot v\, dS \right\}$$

Global admissibility

$$u \in \mathrm{KA}(\Omega) \Leftrightarrow \begin{vmatrix} u^s \in \mathrm{KA}(\Omega^s),\ \forall s \\ \mathrm{tr}(u^s) = \mathrm{tr}(u^{s'}) \text{ on } \Gamma^{(s,s')} \end{vmatrix}$$

$$\sigma \in \mathrm{SA}(\Omega) \Leftrightarrow \begin{vmatrix} \sigma^s \in \mathrm{SA}(\Omega^s),\ \forall s \\ \sigma^s \cdot n^s + \sigma^{(s')} \cdot n^{(s')} = 0 \text{ on } \Gamma^{(s,s')} \end{vmatrix}$$

Construction of global admissible fields

At each iteration of FETI(DP)/BDD(C)[12]

- $u_D \in H^1(\Omega)$ continuous everywhere and in equilibrium inside subdomains,
- $u_N \in H^1(\cup\Omega^s)$ in equilibrium inside subdomains, with associated interface nodal reactions $\boldsymbol{\lambda}_N^s$ in balance between subdomains $\boldsymbol{\lambda}_N^{s^T} = \mathbf{B}^{s^T}\boldsymbol{\Lambda}$ and in balance wrt rigid body motions and external load. Let σ_N be the associated FE stress field.

[12] A. Parret-Fréaud et al., 2010.

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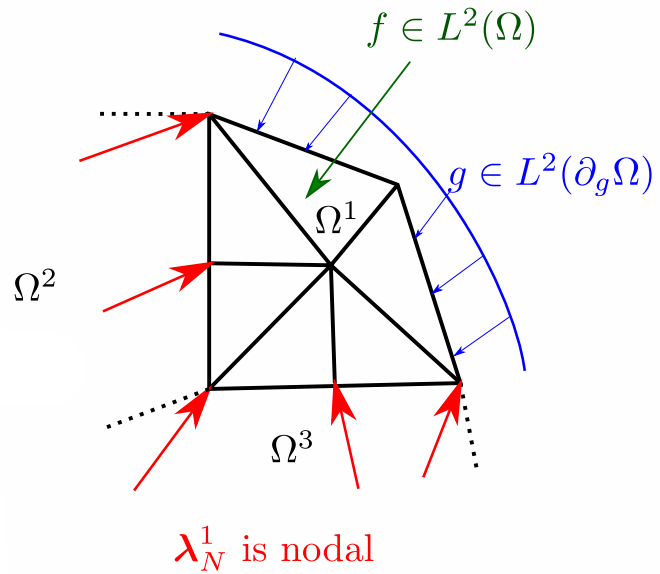

Figure: Subdomain and its surrounding

[12] A. Parret-Fréaud et al., 2010.

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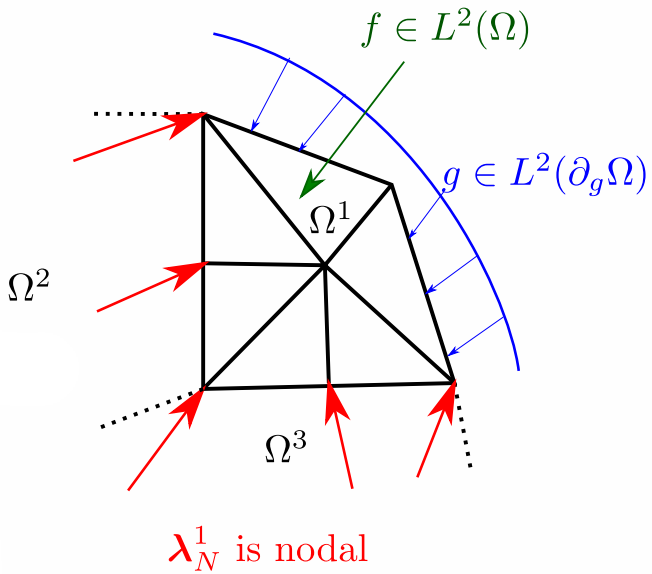

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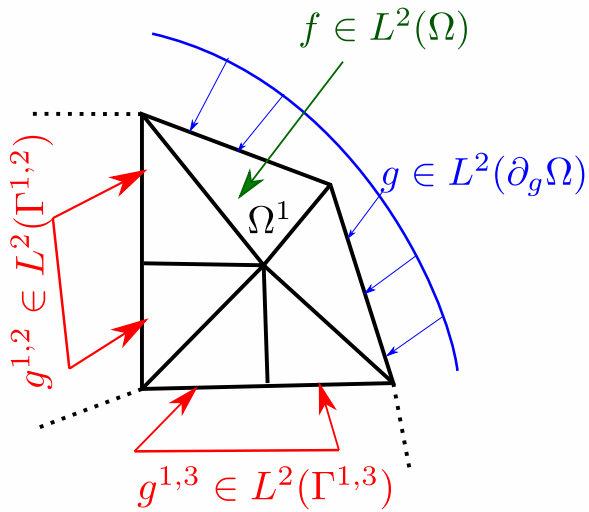

Figure: Preprocessing before recovery

Once we have a L^2 representation of interface traction, we can compute in parallel:

$$\hat{\sigma}_N^s = \mathcal{F}(\sigma_N, f, g, (g^{s,i})_i) \text{ with } \hat{\sigma}_N = (\hat{\sigma}_N^s)_s \in \mathrm{SA}(\Omega)$$

[12] A. Parret-Fréaud et al., 2010.

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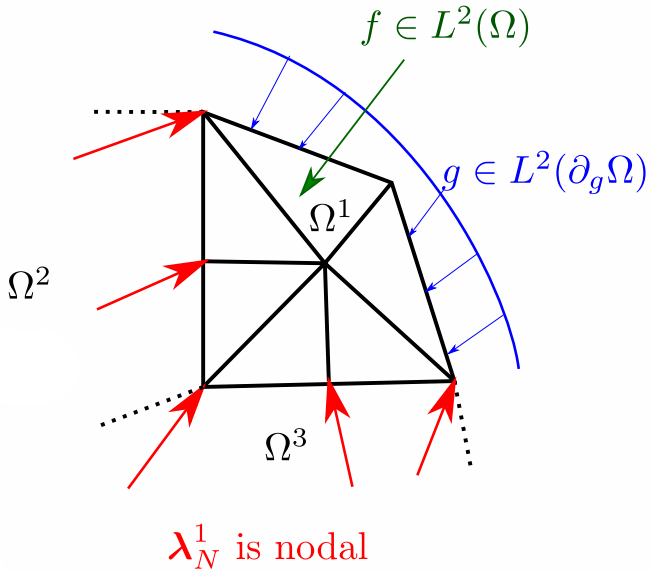

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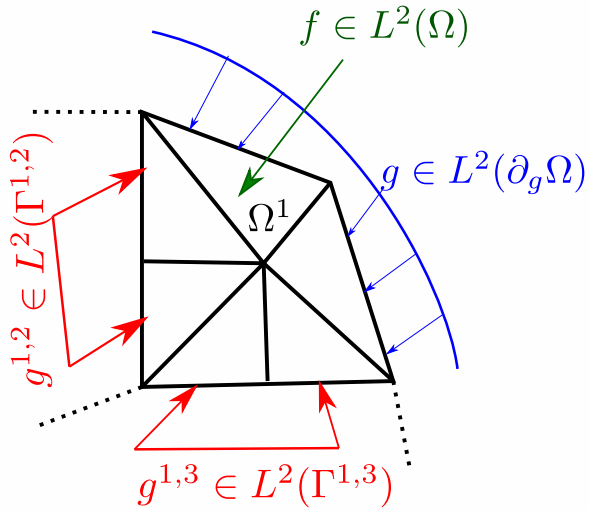

Figure: Preprocessing before recovery

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$$\hat{\sigma}_N^s = \mathcal{F}(\sigma_N, f, g, (g^{s,i})_i) \text{ with } \hat{\sigma}_N = (\hat{\sigma}_N^s)_s \in \mathrm{SA}(\Omega)$$

For the construction of $w \in \mathrm{KA}_0(\Omega)$ we use 0-Dirichlet bc on the interface.

[12] A. Parret-Fréaud et al., 2010.

The little difficulty of multiple points[13]

For Ω^s, $g^{s,i}$ is typically developed on the FE basis.
Its nodal components are adjusted in order to develop the same work as $\boldsymbol{\lambda}_N^{s,i}$.

At multiple points, we first need to define $(\boldsymbol{\lambda}_N^{s,i})_i$ from $\boldsymbol{\lambda}_N^s$.
$(\boldsymbol{\lambda}_N^{s,i})_i$ is defined up to an effect-less "cyclic" stress in $\ker({B^s}^T)$.
Optimization is necessary, it must take heterogeneity into account.
One neighbor communication is required.
This is equivalent to what is encountered in the Element Equilibration Technique.

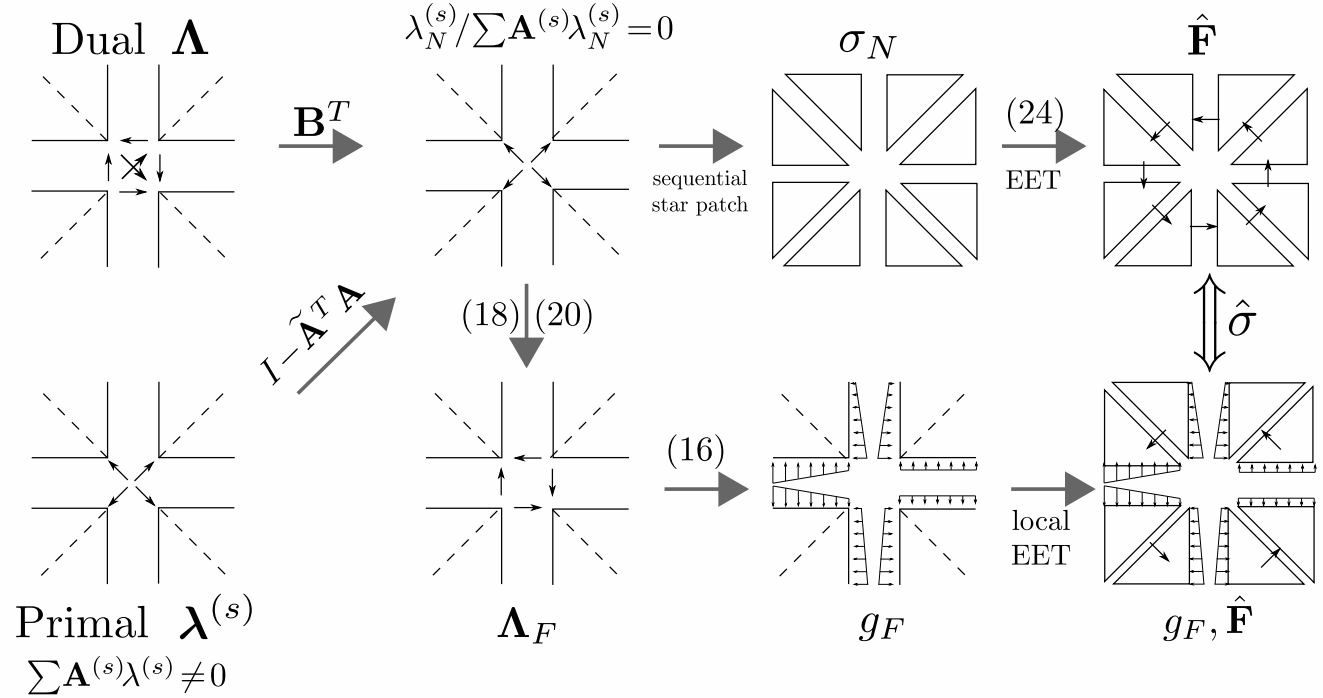


Figure: Methodology for parallel stress recovery / equivalent sequential star-patch

[13] Augustin Parret-Fréaud et al., 2016.

First bounds

Direct transcription of the chosen bounds

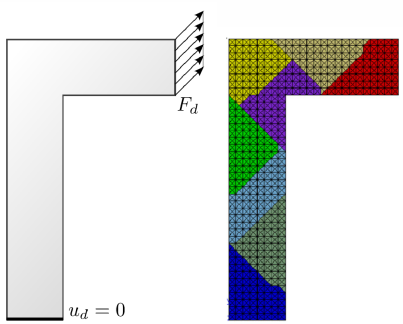
$$\frac{\sum_s R_D^s(\hat{w}^s)}{\sqrt{\sum_s \|\hat{w}^s\|_a^2}} \leqslant \|u - u_D\|_a \leqslant \sqrt{\sum_s \mathrm{e}_{\mathrm{cr}}^2(u_D^s, \hat{\sigma}_N^s)}$$

with

$$R_D^s(\hat{w}^s) := \left(\int_{\Omega^s} f \cdot \hat{w}^s d\Omega + \int_{\partial_g \Omega^s} g \cdot \hat{w}^s dS - \int_{\Omega^s} \varepsilon(u_D^s) : \mathbb{H} : \varepsilon(\hat{w}^s) d\Omega^s \right)$$

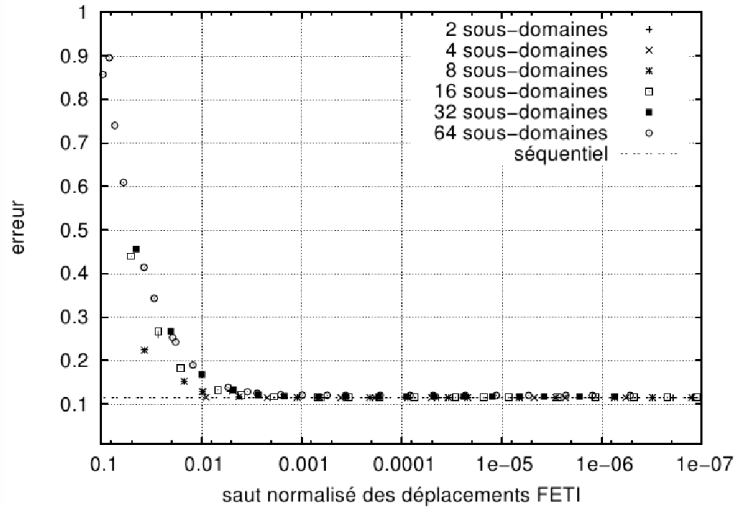
we recall that $\hat{w}^s$ is 0 on the interface.

Γ-shaped structure — first upper bound[14]

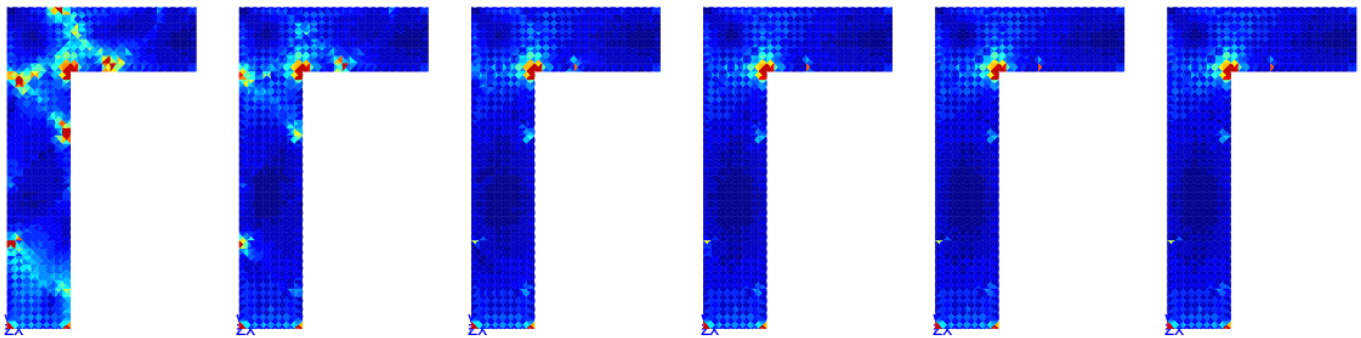


Parallel error estimator:

$$\|u - u_D\|_a \leqslant \sqrt{\sum_s e_{\mathrm{CR}}(\mathbf{u}_D^s, \hat{\sigma}_N^s)_{\Omega^s}}$$



Fast convergence of the estimator



Fast convergence of error maps

The solver converges but the error stagnates

[14] A. Parret-Fréaud et al., 2010.

Bounds with separated contributions

Lemma[15]

For FETI(DP) and BDD(C), we have:

$$\|u_D - u_N\|_a = \|\mathbf{r}\|_{\tilde{\mathbf{S}}} =: |r|$$

The energy norm of the gap between u_N and u_D equals the preconditioner-norm of the residual which is naturally computed at each iteration. It can be chosen to control the iterative solver.
Usually iterations stop when $\|\mathbf{r}_i\|_{\tilde{\mathbf{S}}} \leqslant \epsilon \|\mathbf{r}_0\|_{\tilde{\mathbf{S}}}$ and typically $\epsilon = 10^{-6}$.

Bounds

$$\|u - u_N\|_a \leqslant \sqrt{\sum_s \mathrm{e}_{\mathrm{cr}}^2(u_N^s, \hat{\sigma}_N^s)} + |r|$$

$$\frac{\sum_s R_N^s(\hat{w}^s)}{\sqrt{\sum_s \|\hat{w}^s\|_a}} - |r| \leqslant \|u - u_D\|_a \leqslant \sqrt{\sum_s \mathrm{e}_{\mathrm{cr}}^2(u_N^s, \hat{\sigma}_N^s)} + |r|$$

The first bound is adapted from Vohralik. The second bounds simply uses triangular inequality.

$|r|$ only depends on iterations, other quantities depend on the discretization and (very) weakly on the iterations.

[15] Augustin Parret-Fréaud et al., 2016; V. Rey, C. Rey, and Gosselet, 2014.

Unbiased stopping criterion

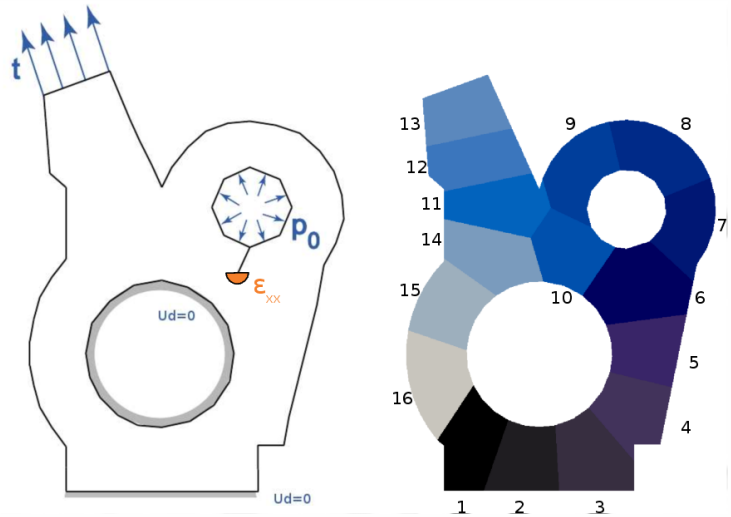


Figure: Pre-cracked structure: forward and adjoint load, decomposition into 16 sd

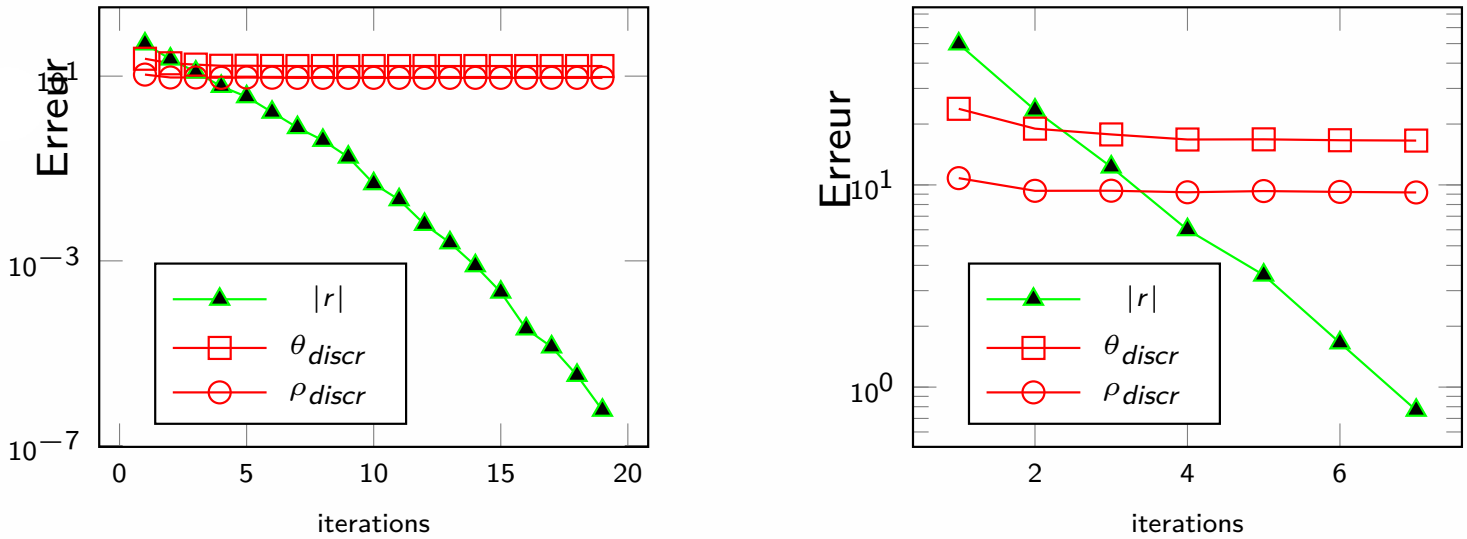


Figure: Envelop of the error due to the discretization and evolution of the residual

Practical considerations

When to compute bounds

- Evaluate discretization bounds at iteration 1 (avoid 0).
- Iterate until residual is smaller than the inf bound.
- Reevaluate the discretization bounds if they changed to much go on with iterations.
- If needed prepare for adaptation (compute remeshing map)

Quantities of interest

Assuming same mesh is used for forward and adjoint problems

- Solve forward and adjoint problem at the same time using a **block** solver.
- Also use block computations for the recovery of admissible fields.
- Stop when both residuals are less than their inf bounds.

First bounding (based on [Ladeveze 2008] et [Rey V., Rey C. Gosselet 14])

$$|\widetilde{L}(\mathbf{u}_{ex}) - \widetilde{L}(\mathbf{u}_{\boldsymbol{D}}) - A_1| \leqslant [\sqrt{\mathbf{r}^{\boldsymbol{T}}\mathbf{z}} + \sqrt{\sum_s e^2_{CR_{(s)}}(\mathbf{u}^s_{\boldsymbol{N}}, \hat{\boldsymbol{\sigma}}^s_N)}][\sqrt{\tilde{\mathbf{r}}^{\boldsymbol{T}}\tilde{\mathbf{z}}} + \sqrt{\sum_s e^2_{CR_{(s)}}(\tilde{u}^{(s)}_{\boldsymbol{N}}, \hat{\tilde{\sigma}}^s_N)}]$$

$$\leqslant (\sqrt{\mathbf{r}^{\boldsymbol{T}}\mathbf{z}} + \theta_{discr})(\sqrt{\tilde{\mathbf{r}}^{\boldsymbol{T}}\tilde{\mathbf{z}}} + \tilde{\theta}_{discr})$$

$$A_1 = \int_\Omega (\hat{\boldsymbol{\sigma}}_N - \mathbb{H}\varepsilon(\mathbf{u}_{\boldsymbol{D}})) : \varepsilon(\tilde{u}_{\boldsymbol{D}})d\Omega = \sum_s {\boldsymbol{\lambda}^s_{\boldsymbol{D}}}^T \mathbf{T}^s \tilde{\mathbf{u}}^{(s)}_{\boldsymbol{D}} \rightarrow \text{interface quantities}$$

Second bounding (based on [Ladeveze 2008] et [Rey V., Rey C. Gosselet 14])

$$|\widetilde{L}(\mathbf{u}_{ex}) - \widetilde{L}(\mathbf{u}_{\boldsymbol{D}}) - A_2| \leqslant \frac{1}{2}[\sqrt{\mathbf{r}^{\boldsymbol{T}}\mathbf{z}} + \sqrt{\sum_s e^2_{CR_{(s)}}(\mathbf{u}^s_{\boldsymbol{N}}, \hat{\boldsymbol{\sigma}}^s_N)}][\sqrt{\tilde{\mathbf{r}}^{\boldsymbol{T}}\tilde{\mathbf{z}}} + \sqrt{\sum_s e^2_{CR_{(s)}}(\tilde{u}^{(s)}_{\boldsymbol{N}}, \hat{\tilde{\sigma}}^s_N)}]$$

$$\leqslant \frac{1}{2}(\sqrt{\mathbf{r}^{\boldsymbol{T}}\mathbf{z}} + \theta_{discr})(\sqrt{\tilde{\mathbf{r}}^{\boldsymbol{T}}\tilde{\mathbf{z}}} + \tilde{\theta}_{discr})$$

$$A_2 = \int_\Omega (\hat{\boldsymbol{\sigma}}_N - \mathbb{H}\varepsilon(\mathbf{u}_{\boldsymbol{D}})) : \mathbb{H}^{-1} : \frac{1}{2}(\hat{\tilde{\sigma}}_N + \mathbb{H}\varepsilon(\tilde{u}_{\boldsymbol{D}}))d\Omega$$

Application on the pre-cracked structure 2

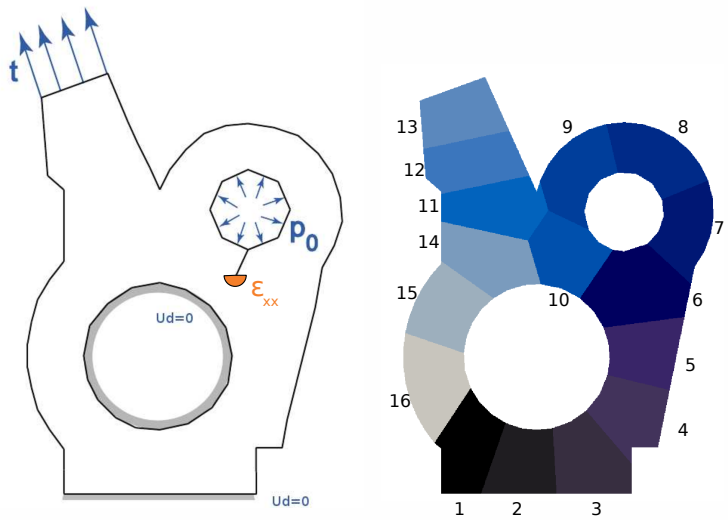


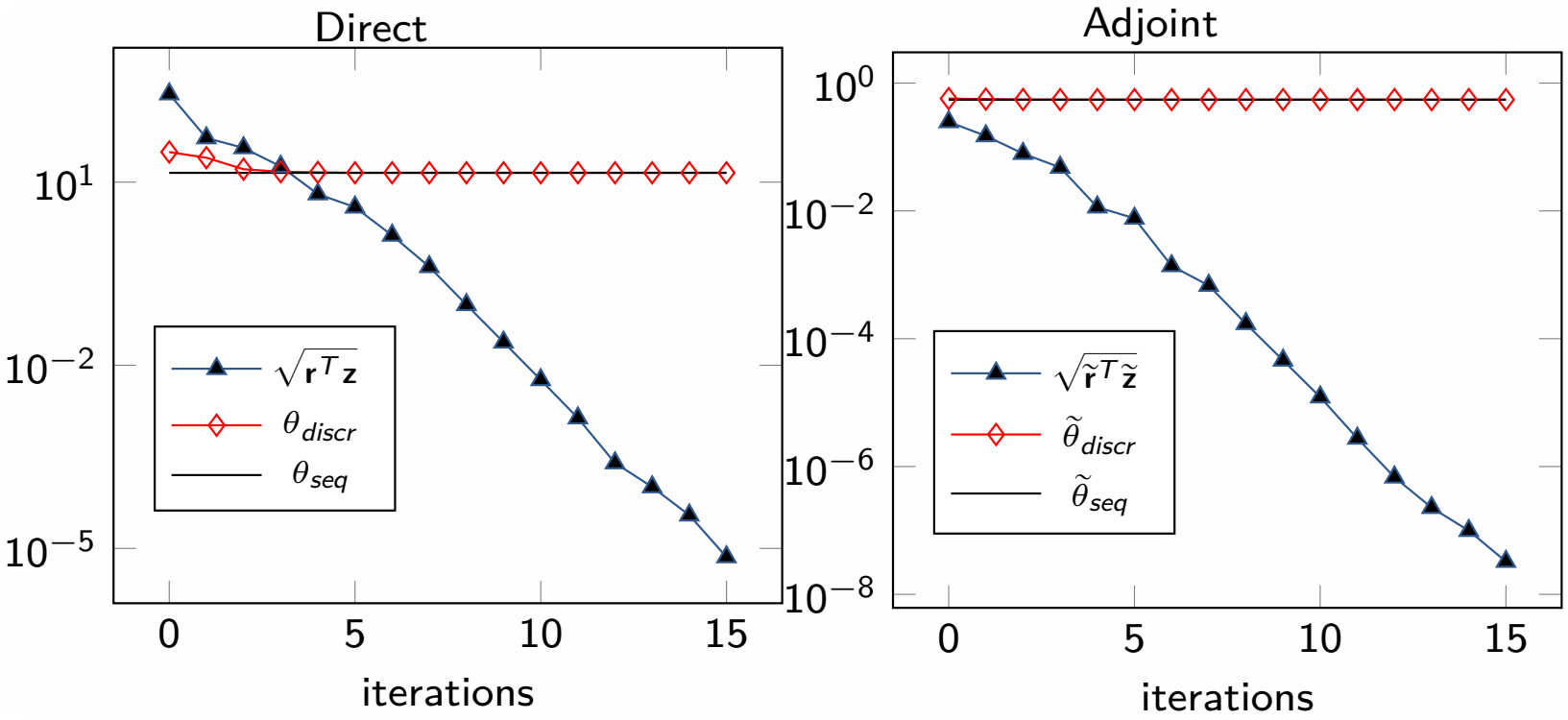
Figure: Loading of direct problem (blue) and adjoint problem (orange)

dof	7180
Approach	dual
Algorithm	FETI
Preconditioner	Dirichlet
Projector	Identity
SA technique	SPET [Pares 06, Cottereau 07]
Local problems	p+2

The interesting quantity of interest would have been the stress intensity factor [Pannetier Ladeveze Louf 2009].

For sake of simplicity, we choose the mean of the xx component of the stress field over a region near the crack.

Application on pre-cracked structure 2



Quantity of interest

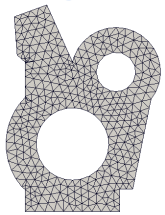
$$I_H = 3,0019$$

$$I_H + \frac{1}{4}(\beta^+_{inf} - \beta^-_{sup}) \leqslant I_{ex} \leqslant I_H + \frac{1}{4}(\beta^+_{sup} - \beta^-_{inf})$$

β^-_{inf}	β^+_{inf}	$\frac{1}{4}\beta^-_{sup}$	$\frac{1}{4}\beta^+_{sup}$	$I_H + \frac{1}{4}(\beta^+_{sup} - \beta^-_{inf})$	$I_H + \frac{1}{4}(\beta^+_{inf} - \beta^-_{sup})$
0	0	12,969	4,2554	4,1332	-0,24041
1,1025	1,5765	12,969	4,2554	3,8576	0,15372

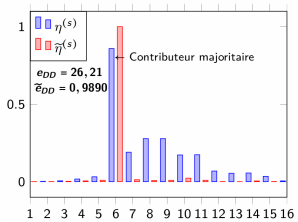
Strategy for adaptation with recycling

Maillage initial



Résolution $\mathrm{S}\underline{x} = \underline{b}$

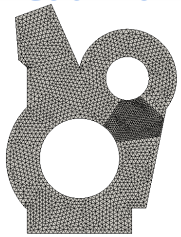
Contributions à l'erreur



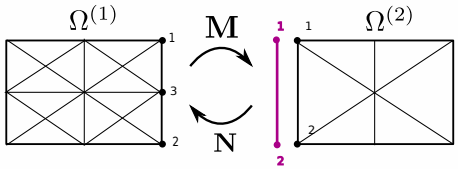
Raffinement local parallèle

discrétisation
de l'interface inchangée

Nouveau maillage



Gestion des incompatibilités aux interfaces



Directions de recherche

V_p base de $K_p(\mathbf{S}, \underline{r}_0)$

Utilisation directe des directions de recherche

$\mathbf{C}$

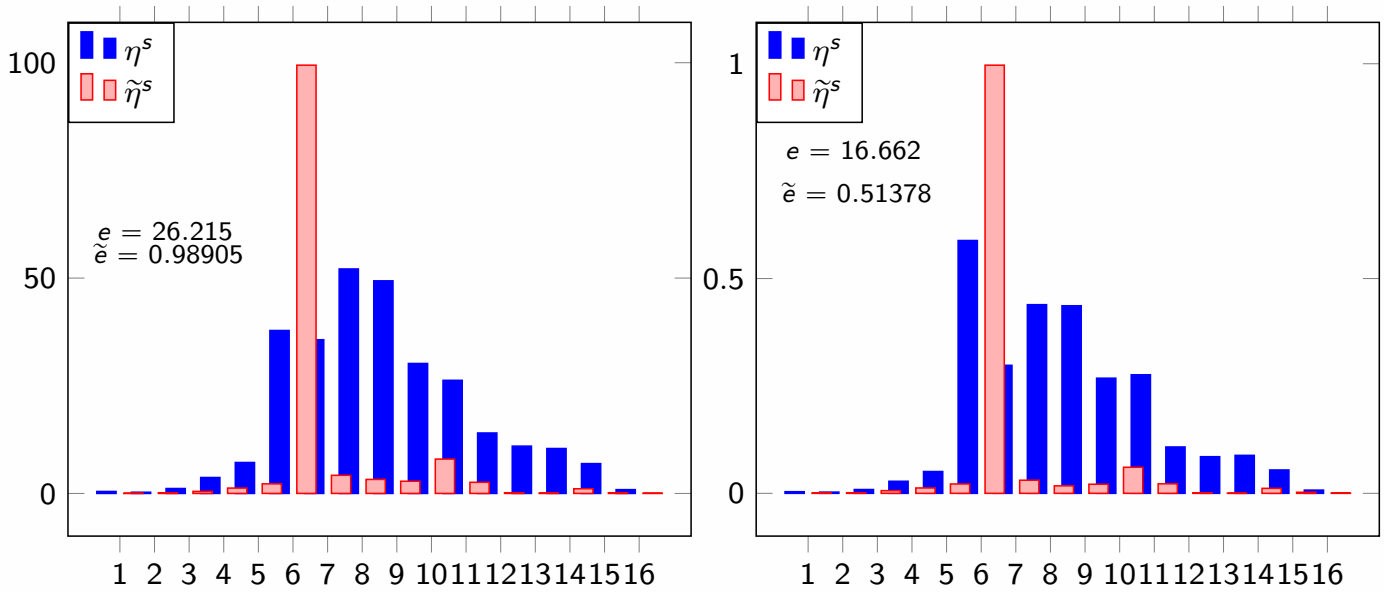
Espace de recherche réduit

$$\widetilde{K}_m(\mathbf{S}\underline{r}_0, \mathbf{C}) = \mathrm{Ker}(\mathbf{C^T S}) \oplus \mathrm{Im}(\mathbf{C})$$

LaM CU3E
Laboratoire de mécanique, multiphysique, multiéchelle

Strategy for adaptation with recycling

We select subdomains most contributing to the errors.
We use hierarchical refinement (at least on the interface)so that the building of admissible fields remains easy.



(a) Initial mesh (b) Locally refined mesh

Figure: Distribution of error within subdomains

Mesh	e	$\widetilde{e}$	I_H	$I_{HH,2}$	$\frac{1}{2}e\widetilde{e}$
Uniform	26.215	0.98905	2.4915	3.1935	12.964
Locally refined	16.662	0.51378	3.2165	0.086055	4.2803

Table: Performance of local refined for the cracked structure

Adaptation and recycling

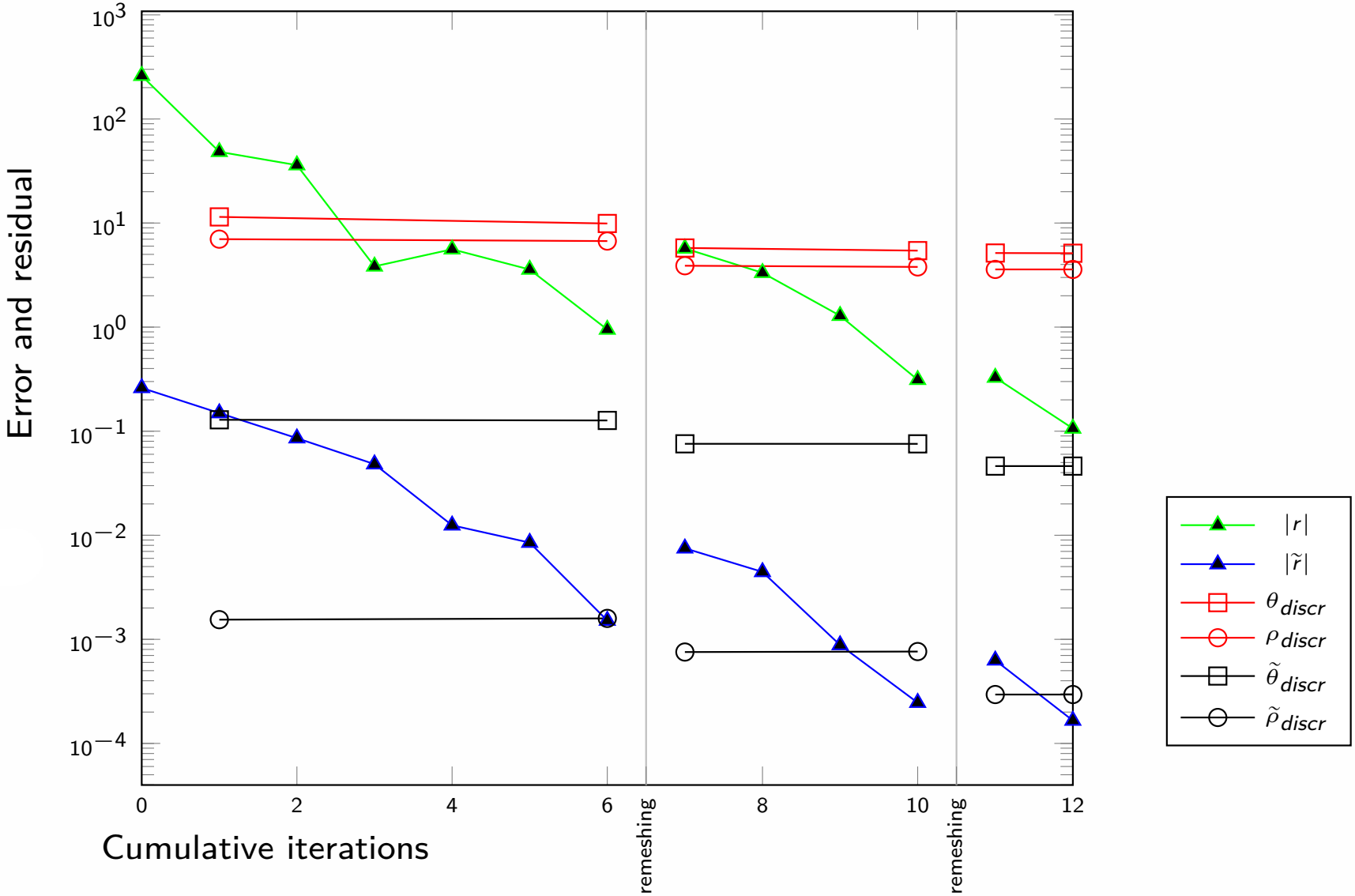


Figure: Erreurs de discrétisation et résidus au cours des itérations

Conclusion

- The recovery of admissible fields can be fully parallel (after just one neighbor communication).
- There are inf and sup bounds of the error which separates the contribution of the solver and of the discretization.
- We can stop the iterative solver based on an unbiased criterion. In practice the discretization error quickly dominates.
- If quantity of interest are wanted, block solvers can be used.
- For the adaptation, hierarchical refinement of interfaces allows to reuse the numerical information.

Ongoing and future work:

- Real implementation for HPC, with improved sequential recovery techniques.
- Error estimation for nonlinear problems[16] with separation of sources[17] with nonlinear DD solvers[18].
- More evolved marking and refinement techniques with good load balancing $\rightarrow$ adaptation of the mesh and of the decomposition.

[16] Ladevèze, 2008.

[17] El Alaoui, Ern, and Vohralik, 2010; Moës, 1996.

[18] Dolean et al., 2015; Klawonn, Lanser, and Rheinbach, 2014; Negrello et al., 2016.