Summer School CEA-EDF-INRIA
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Goal-oriented error control with various applications (FEM, model reduction & adaptivity, ...)

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Outline

- **Motivation**
- **Theoretical aspects of goal-oriented error estimation in FEM**
- **Some applications**
- **Extensions to modeling error (multiscale analysis, model coupling)**

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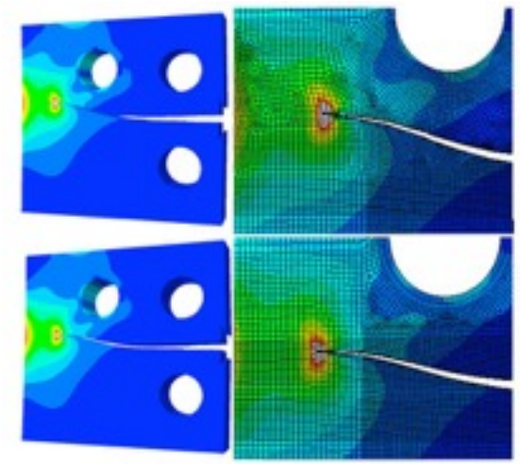
Motivation

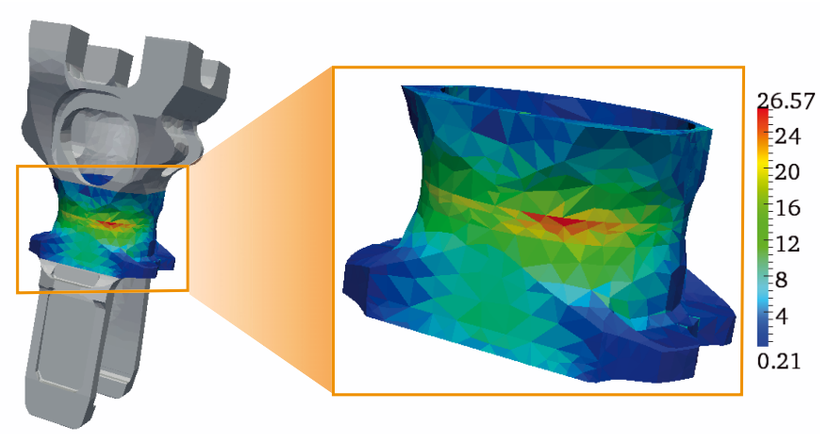
Can we trust numerical simulations?

→ construction of smart numerical procedures

→ adaptive approaches with error estimation tools

- **Usually, the objective of numerical simulation is only to assess values of outputs of interest (local displacement, SIF, max of Mises stress,...)**





- **It is thus sufficient and simpler to control models with respect to these quantities only**

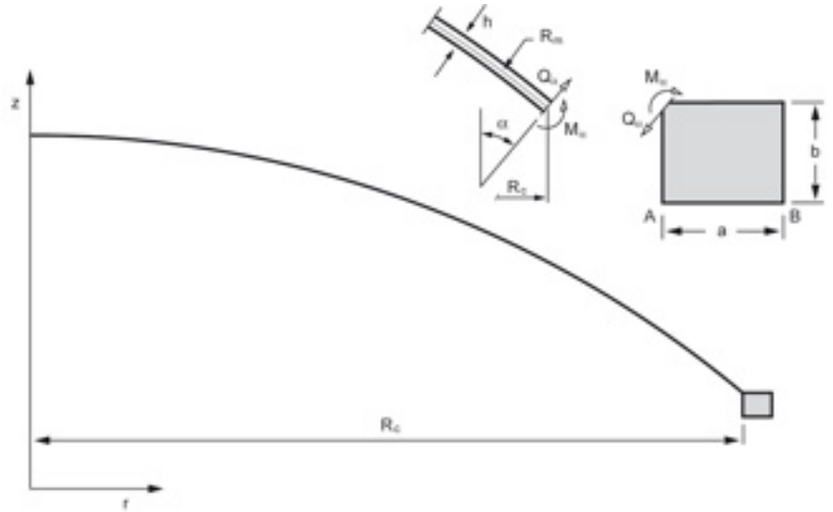
GOAL: compute right at the right engineering cost!!!

Motivation

Girkman's problem (Timoshenko *et al.* 1959)

→ *benchmark* proposed by J. Pitkäranta / I. Babuska / B. Szabo (IACM expression 2008)

Objective : «*assess how analysts, working with commercially available FE software tools, would meet the requirement of verification*»



- spherical shell connected to a stiffening ring
- gravity loading
- all model parameters are known (geometry, material,...)
- exact 3D solution unknown → FE approximation

Particular requirements :
- value of the bending moment at the junction (exact value = -37 Nm/m +/- 2%)
- proof of 5% accuracy

15 answers :
- very few verification procedures (except converging meshes)
- large dispersion (between 205 Nm/m and + 17977 Nm/m...)
- 9 answers out of 5% tolerance

Motivation

Conclusions

«analysts who cannot solve the Girkmann problem are not in a position to claim that they can solve much more complicated problems reliably»

«the requirements of verification pose challenges that users and vendors of commercial finite element analysis software products should urgently address»

- Editorial Policy Statement for AIAA journals :

«we will not accept for publication any manuscript reporting numerical solutions of an engineering problem that fails to adequately address the accuracy of the computed results…»

- Guidelines for the numerical treatment of mathematical models in the field of Solid Mechanics were published by the American Society of Mechanical Engineers (ASME):

V&V 10-2006: Guide for Verification and Validation in Computational Solid Mechanics, ISBN 0-7918-3042-X, 2006.

Objectives

REAL

Q_{real}

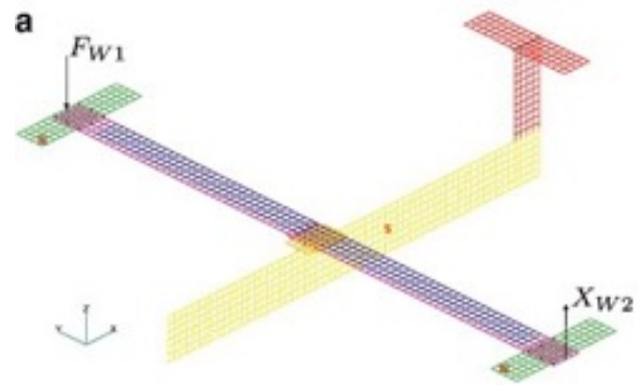
measure error

choice of observations

experimental data

VIRTUAL

$Q_{0,h}$

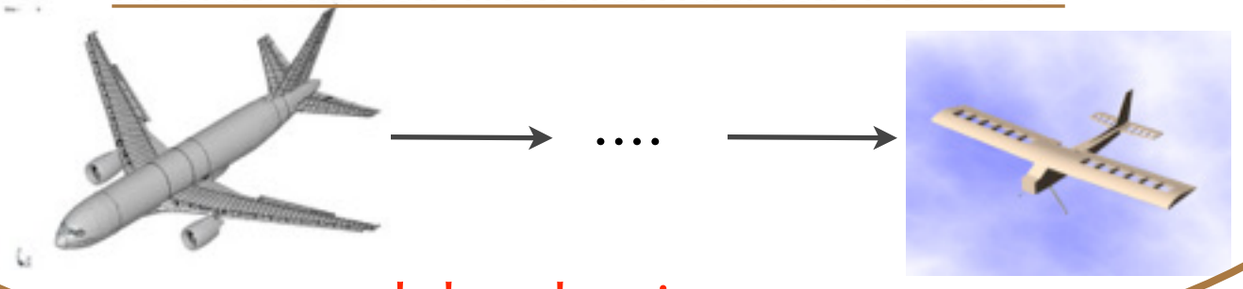


numerical model

Goal: predict a QoI

Ensure the relevance of $Q_{0,h}$ with respect to Q_{real}

hierarchical mathematical models



modeling error

Q

model reduction error

Q_0

discretization error

For FEM: [Paraschivoiu *et al.* 97, Prudhomme & Oden 99, Becker & Rannacher 01,…]

Objectives

GOAL: accurate and efficient computation of the value of a functional $Q(u)$(target quantity), with accuracy TOL , from the solution of a continuous model by using a discrete model of dimension N

$$\mathcal{A}(u) = 0 \qquad\qquad \mathcal{A}_h(u_h) = 0$$

→ the evaluation of the solution by functional $Q(.)$ represents what exactly we want to know of the solution

→ the goal of adaptivity is then the optimal use of computing resources according to one of the following principles:

- Minimal work N for prescribed accuracy TOL
- Maximal accuracy TOL for prescribed work N

→ the traditional approach estimates the error with respect to the generic energy norm of the problem. However, this is generally not what applications need

Typical Example

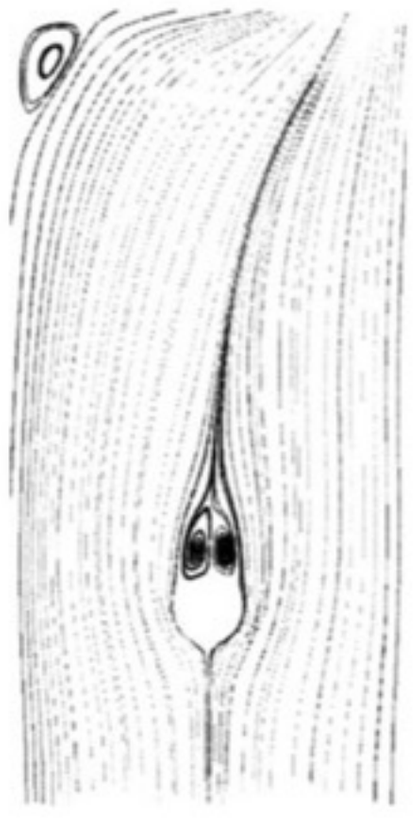
[Bangerth & Rannacher 2003]

Computation of drag coefficient

- viscous incompressible flow around a cylinder in a channel with a narrowed outlet
- 2D configuration, with Poiseuille inflow, and Re=50

  → the flow is laminar and stationary

  → the narrowing of the outlet causes a corner singularity of the pressure

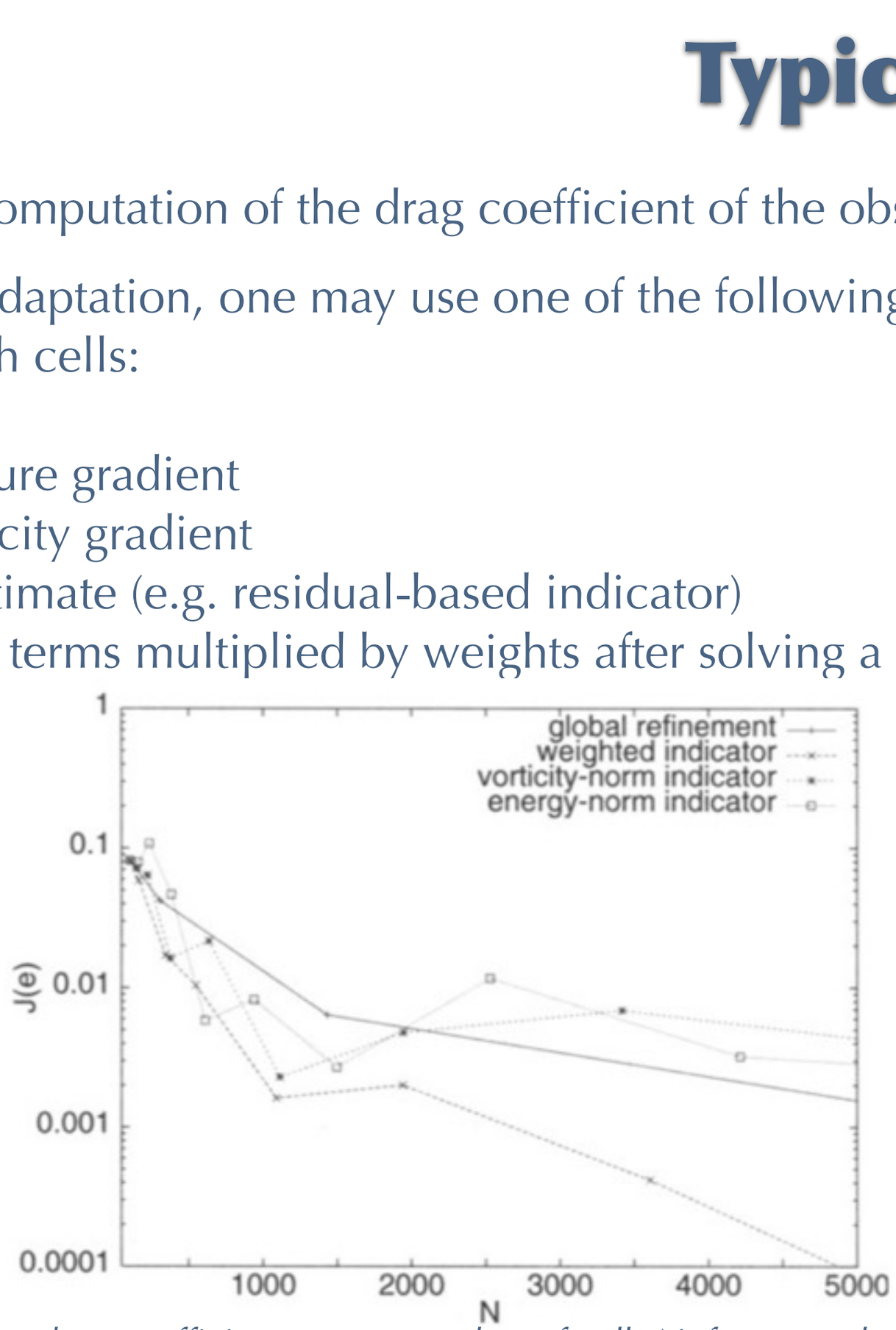


Typical Example

GOAL: accurate computation of the drag coefficient of the obstacle

To control mesh adaptation, one may use one of the following heuristic refinement indicators on mesh cells:

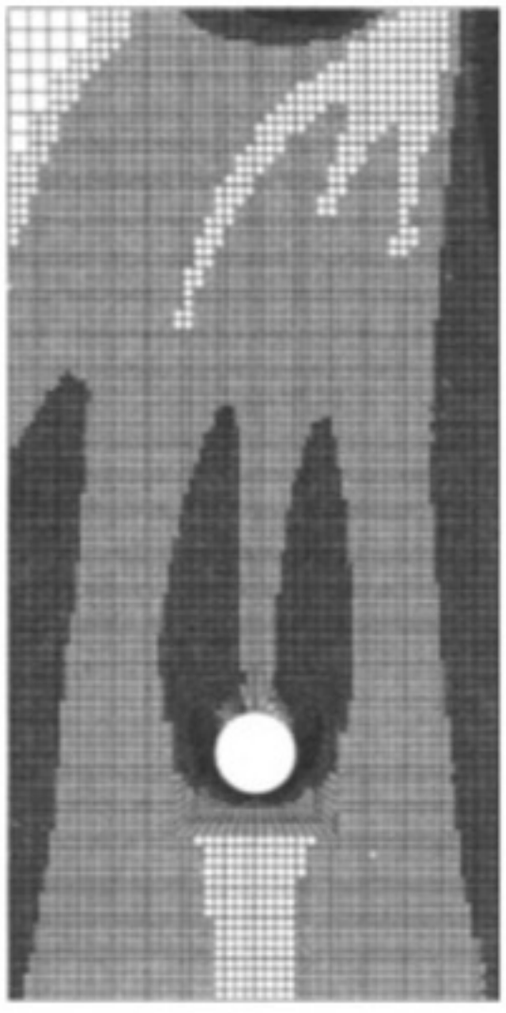
- vorticity
- 1st order pressure gradient
- 2nd order velocity gradient
- global error estimate (e.g. residual-based indicator)
- DWR (residual terms multiplied by weights after solving a global dual problem)



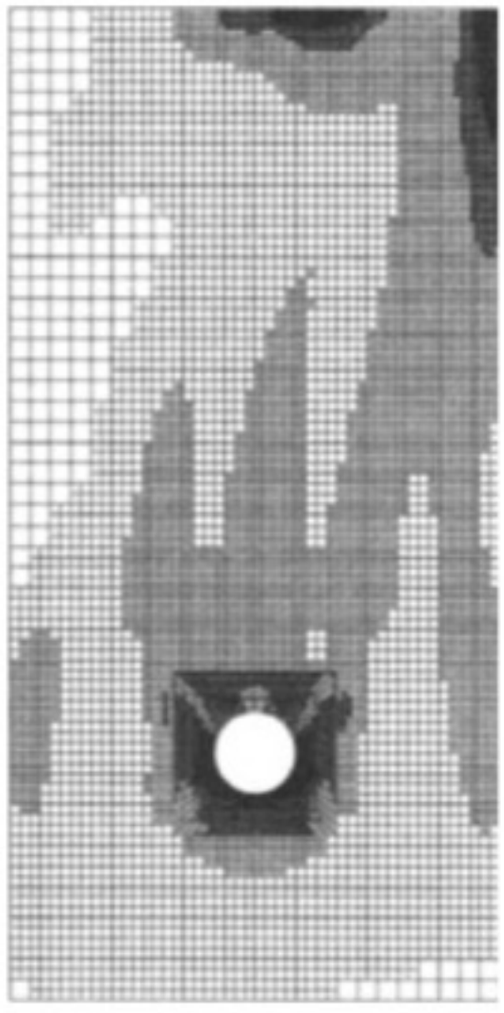
Error in the drag coefficient versus number of cells N, for several adaptive strategies

Typical Example

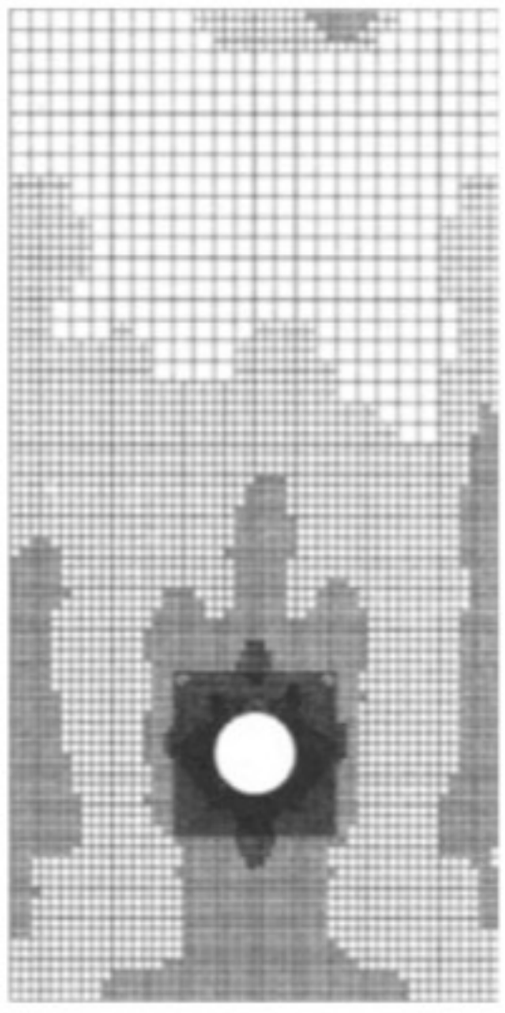
Meshes with 5,000 cells



with vorticity indicator



with residual-based indicator



with DWR indicator

Concepts for goal-oriented approach

Framework of linear algebra (to introduce important aspects)

For regular matrices $A, A_h \in \mathbb{R}^{n\times n}$ and vectors $b, b_h \in \mathbb{R}^n$, consider the problem of finding $x, x_h \in \mathbb{R}^n$ from

$$Ax = b \qquad\qquad A_h x_h = b_h$$

approximation error $e := x - x_h$

truncation error $\tau := A_h x - b_h$

residual $\rho := b - Ax_h$

A priori error analysis is based on the truncation error: $A_h e = A_h x - b_h = \tau$

→ a priori error bound derived involving a stability constant c

$$\|e\| \le c\|\tau\| \qquad\qquad c = \|A_h^{-1}\|$$

In contrast, **a posteriori error analysis** uses the relation $Ae = b - Ax_h = \rho$

→ a posteriori error bound derived involving another stability constant

$$\|e\| \le c\|\rho\| \qquad\qquad c = \|A^{-1}\|$$

Concepts for goal-oriented approach

To estimate error with respect to arbitrary moments of x, we employ a duality argument

For some $j \in \mathbb{R}^n$ assume we want to estimate the value of the linear error functional

$$J(e) = J(x) - J(x_h) = (e, j)$$

Consider the solution $z \in \mathbb{R}^n$ of the associated dual (or adjoint) problem

$$A^* z = j$$

This leads to the identity

$$J(e) = (e, j) = (e, A^* z) = (Ae, z) = (\rho, z)$$

→ weighted estimate $|J(e)| = |\sum_i \rho_i z_i| \leq \sum_i |\rho_i||z_i|$

→ the gain in using weights z_i is that they tell us about the influence of local residuals ρ_i on the error in the target quantity

Concepts for goal-oriented approach

We now switch to PDEs [Rannacher & Suttmeier 1997, Becker & Rannacher 2001]

$$Lu = f \qquad \text{(with BC, and } L \in \mathcal{L}(\mathcal{U}, \mathcal{F})\text{)}$$

We consider a scalar quantity of interest $Q(u) = \langle u, Q \rangle$

$\longrightarrow$ Q in the dual space $\mathcal{U}^*$ equipped with norm $||Q||_* = \sup_{w \in \mathcal{U}, w \neq 0} \frac{|Q(w)|}{\|w\|}$

$\longrightarrow |Q(u)| \leq ||u||.||Q||_*$ (crude estimate)

We introduce the adjoint operator $L^* \in \mathcal{L}(\mathcal{F}^*, \mathcal{U}^*)$ of L, satisfying:

$$\langle Lu, v \rangle = \langle u, L^* v \rangle \quad \forall u \in \mathcal{U}, \forall v \in \mathcal{F}^*$$

Rem: a 1st order time problem thus has final conditions (integration by parts)

Concepts for goal-oriented approach

Direct problem: find $u \in \mathcal{U}$ such that

$$A(u,v) = \langle Lu - f, v \rangle = 0 \quad \forall v \in \mathcal{F}^*$$

Adjoint/dual problem: find $\tilde{u} \in \mathcal{F}^*$ such that [Giles & Süli 2002]

$$\langle v, L^*\tilde{u} - Q \rangle = 0 \quad \forall v \in \mathcal{U}$$

We thus get the following representation:

$$Q(u) = \langle u, Q \rangle = \langle u, L^*\tilde{u} \rangle = \langle Lu, \tilde{u} \rangle = \langle f, \tilde{u} \rangle$$

⟶ generalized Green function (sensitivity of Q with respect to f

A posteriori error estimation: $Q(u) - Q(u_h) = \langle e, L^*\tilde{u} \rangle = \langle f - Lu_h, \tilde{u} \rangle$

Weighting of the residual: $|Q(u) - Q(u_h)| \leq \sum_K |\langle R(u_h), \tilde{u} \rangle_K|$

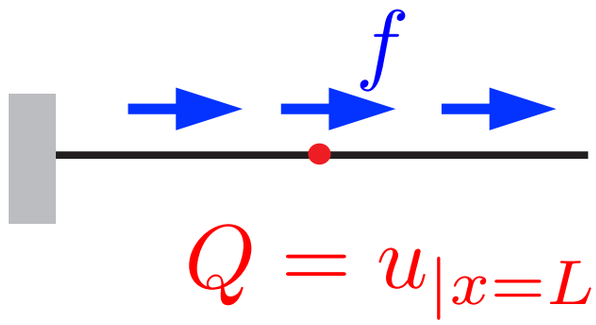
Adjoint Solution

- Linear elasticity (beam in tension)

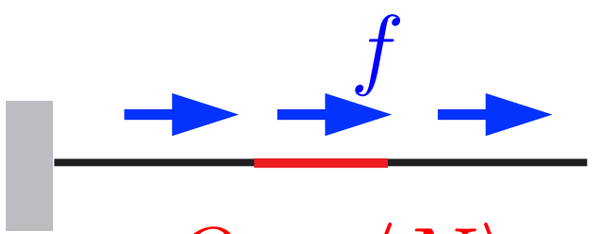
$$-\frac{d}{dx}(ES\frac{du}{dx}) = 0$$
+ BC

$$\longrightarrow \quad Q(u) - Q(u_h) = \int_0^L \frac{d(u-u_h)}{dx}.ES\frac{d\tilde{u}}{dx}$$

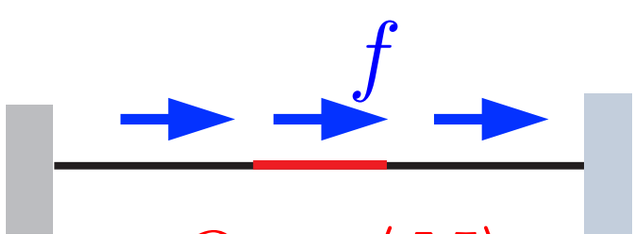
$\tilde{N}$



$$Q = u_{|x=L/2}$$



$$Q = \langle N \rangle_\omega$$



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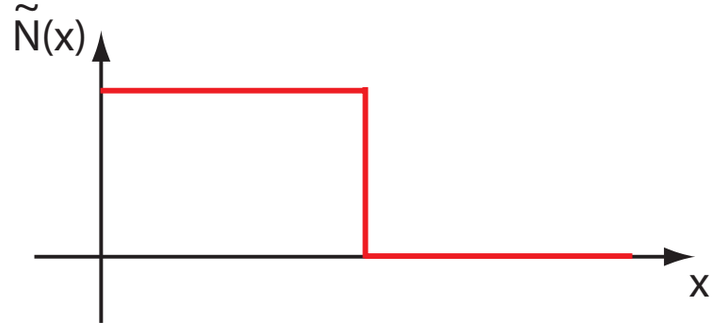
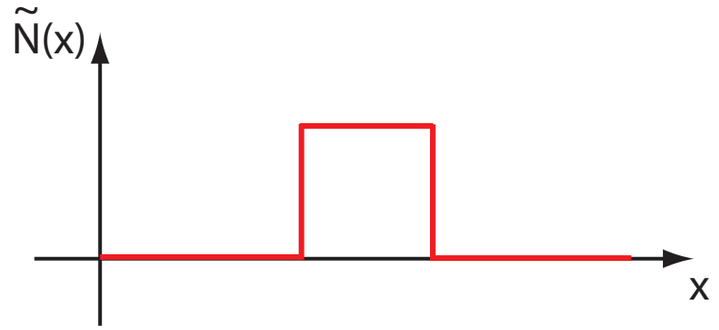
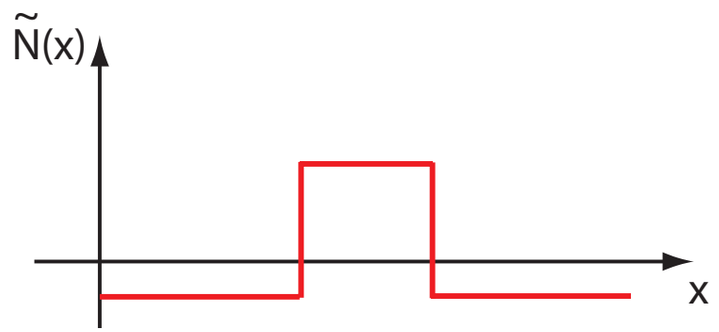


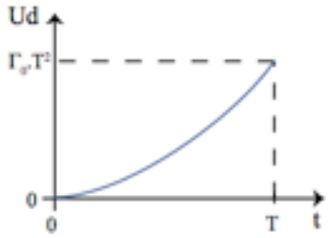


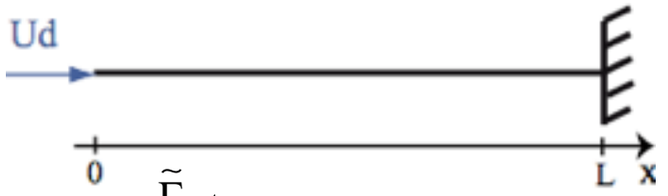


Adjoint Solution

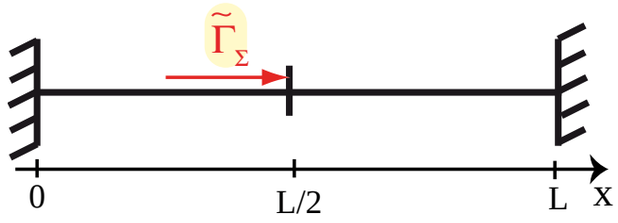
- Linear elastodynamics (beam in tension) over $]0, L[\times[0, T]$

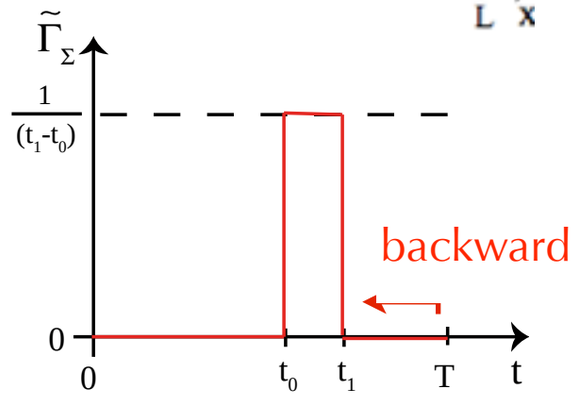
$$\begin{aligned} &-ku'' + \ddot{u} = f \quad \forall (x,t) \in]0, L[\times[0, T] \\ &u(0,t) = U_d(t), u(L,t) = 0 \\ &u(x,0) = \dot{u}(x,0) = 0 \end{aligned}$$





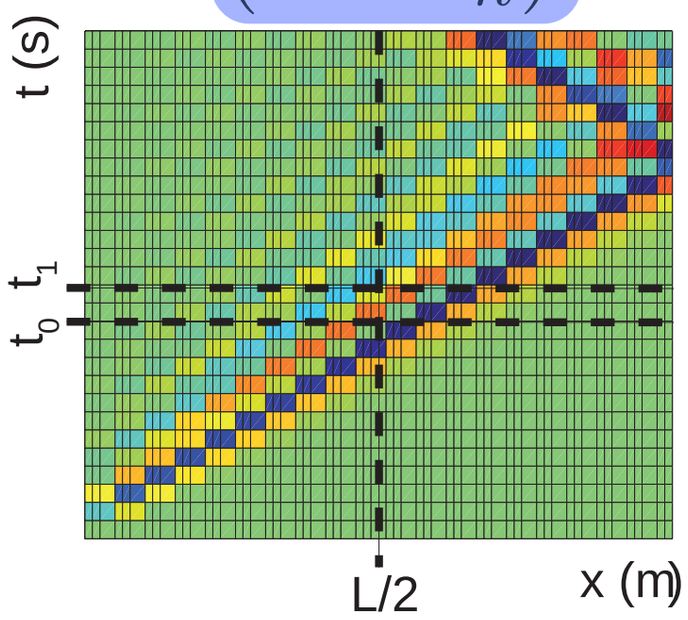
$$Q(u) = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} \dot{u}(x = L/2)$$



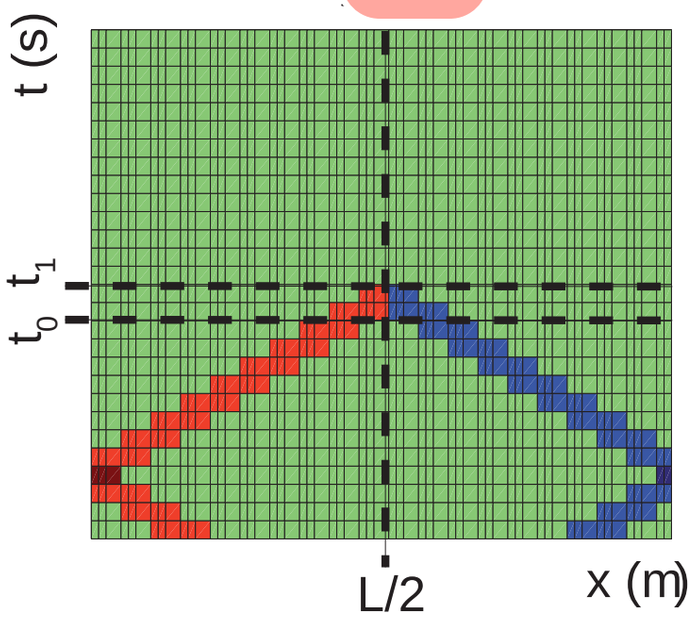


$$Q(u) - Q(u_h) = \int_0^T \int_0^L k\tilde{u}'.(\dot{u} - \dot{u}_h)' dx dt$$

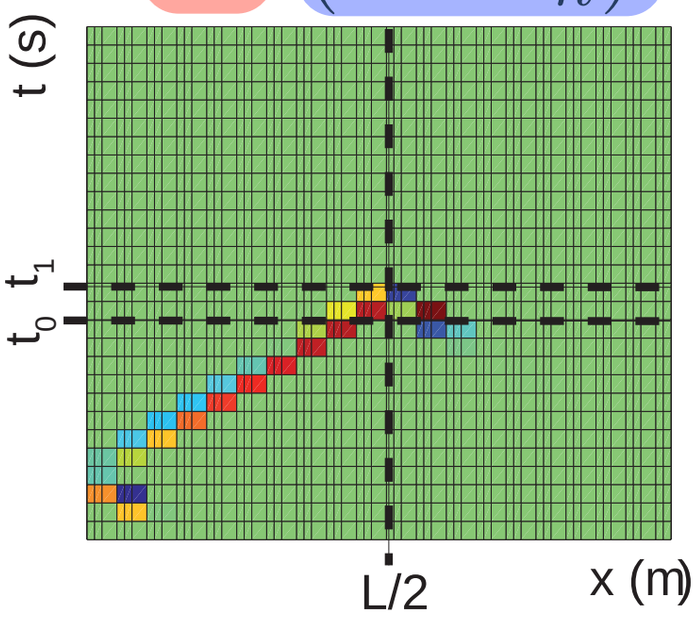
$(\dot{u} - \dot{u}_h)'$



$k\tilde{u}'$



$k\tilde{u}'.(\dot{u} - \dot{u}_h)'$



Optimal control point-of-view

[Becker & Rannacher 2001]

Link with adjoint state method:

$$Q(u) = \min_{u^* \in \mathcal{U}_{sol}} Q(u^*) \qquad \mathcal{U}_{sol} = \{w \in \mathcal{U}, A(w,v) = 0 \; \forall v \in \mathcal{F}^*\}$$

We introduce the associated Lagrangian

$$\mathcal{L}(u,\lambda) = Q(u) - A(u,\lambda)$$

→ the search for the saddle point leads to:

$$\langle \delta u, Q \rangle = \langle L\delta u, \lambda \rangle = \langle \delta u, L^*\lambda \rangle \quad \forall \delta u \in \mathcal{U}$$

which corresponds to the adjoint problem

→ the adjoint solution can also be used to evaluate sensitivity of the QoI with respect to some input model parameters

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- **Theoretical aspects of goal-oriented error estimation in FEM**
- **Some applications**
- **Extensions to modeling error (multiscale analysis, model coupling)**

Goal-oriented error estimation in FEM

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28 juin 2022

We consider the following problem :

$$\boxed{-\operatorname{div}(\mathbb{A}\boldsymbol{\nabla} u) = f \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \Gamma_D, \qquad (\mathbb{A}\boldsymbol{\nabla} u)\cdot \boldsymbol{n} = g \quad \text{on } \Gamma_N} \tag{1}$$

where

- Ω is an open bounded subset of $\mathbb{R}^d$ with Lipschitz boundary $\partial\Omega$
- Γ_D and Γ_N are parts of $\partial\Omega$ such that $\overline{\Gamma_D \cup \Gamma_N} = \partial\Omega$, $\Gamma_D \cap \Gamma_N = \emptyset$ and $|\Gamma_D| \neq 0$.

We assume that $f \in L^2(\Omega)$ and that $\mathbb{A} \in [L^\infty(\Omega)]^{d\times d}$ is a symmetric matrix which is uniformly bounded and positive in the sense that there exists $a_{\max} \geq a_{\min} > 0$ such that

$$\forall \boldsymbol{\xi} \in \mathbb{R}^d, \quad a_{\min}|\boldsymbol{\xi}|^2 \leq \mathbb{A}(x)\boldsymbol{\xi}\cdot\boldsymbol{\xi} \leq a_{\max}|\boldsymbol{\xi}|^2 \quad \text{a.e. in } \Omega. \tag{2}$$

The quantity $\boldsymbol{q} = \mathbb{A}\boldsymbol{\nabla} u$ is the **flux** associated with u.

Considering the Hilbert space $V = \{v \in H^1(\Omega), \quad v = 0 \text{ on } \Gamma_D\}$ equipped with the H^1 norm $\|\cdot\|_1$, we recall that the **weak formulation** of (1) is :

$$\boxed{\text{Find } u \in V \text{ such that, for any } v \in V, \qquad B(u,v) = F(v),} \tag{3}$$

where

$$B(u,v) = \int_\Omega \mathbb{A}\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v, \qquad F(v) = \int_\Omega fv + \int_{\Gamma_N} gv.$$

The well-posedness of (3) of course follows from the **Lax-Milgram theorem**.

The bilinear form B is symmetric, continuous and coercive on V.

It hence defines an inner product and induces the energy norm

$$|||v||| = \sqrt{B(v,v)}$$

which is equivalent to $\|v\|_1$ on V :

$$\forall v \in V, \quad \sqrt{\frac{a_{\min}}{1+C_\Omega^2}}\ \|v\|_1 \leq |||v||| \leq \sqrt{a_{\max}}\ \|v\|_1, \tag{4}$$

where C_Ω is the Poincaré constant of Ω, which satisfies $\|v\|_0 \leq C_\Omega\ |v|_1$.

We see that

$$\forall v, w \in V, \quad |B(v,w)| \leq |||v|||\ |||w|||.$$

We use the notation $|||\boldsymbol{q}^*|||_q = \sqrt{\int_\Omega \mathbb{A}^{-1}\boldsymbol{q}^* \cdot \boldsymbol{q}^*}$ for any field $\boldsymbol{q}^* \in (L^2(\Omega))^d$.

Let $\mathcal{T}_h$ be a partition of Ω.
We introduce the space $V_h^p \subset V$ of continuous and locally supported functions which are polynomials of degree up to p on each element K.

The FE approximation of (3) is

$$\boxed{\text{Find } u_h \in V_h^p \text{ such that, for any } v \in V_h^p, \qquad B(u_h, v) = F(v)} \tag{5}$$

which is a well-posed problem, again in view of the Lax-Milgram theorem.

Let

$$R(v) = F(v) - B(u_h, v)$$

be the so-called **residual** and

$$\|R\|_\star = \sup_{v \in V,\, v \neq 0} \frac{|R(v)|}{|||v|||} \tag{6}$$

be the dual norm of the residual.

The **discretization error** of the approach is $e = u - u_h \in V$. It satisfies the following three properties :

$$\begin{aligned} \forall v \in V, \quad & B(e, v) = R(v) \quad \text{(residual equation)}, \\ \forall v \in V_h^p, \quad & B(e, v) = 0 \quad \text{(Galerkin orthogonality)}, \\ & |||e||| = \|R\|_\star. \end{aligned} \tag{7}$$

Remark

We do not consider errors other than those arising from discretization. In particular, we do not consider

- *geometry error (the partition $\mathcal{T}_h$ is assumed to exactly coincide with Ω)*
- *quadrature error (integrals over any element K are assumed to be exactly computed)*
- *error coming from the use of such iterative solvers (when considering large linear systems)*

Duality-based methods

Recalling that $f \in L^2(\Omega)$, the problem (1) is written, somewhat as for mixed methods, in the form

$$
\begin{aligned}
-\operatorname{div} \boldsymbol{q} &= f \ \text{ in } \Omega, \qquad \boldsymbol{q}\cdot\boldsymbol{n} = g \ \text{ on } \Gamma_N, \qquad \boldsymbol{q} \in H(\operatorname{div},\Omega), && (8)\\
u &= 0 \ \text{ on } \Gamma_D, \qquad u \in H^1(\Omega), && (9)\\
\mathbb{A}\boldsymbol{\nabla} u &= \boldsymbol{q} \ \text{ in } \Omega, && (10)
\end{aligned}
$$

where we recall that $H(\operatorname{div},\Omega) = \left\{\boldsymbol{q} \in [L^2(\Omega)]^d,\ \operatorname{div}\boldsymbol{q} \in L^2(\Omega)\right\}$.

Starting from the residual equation verified by $e \in V$, namely

$$\forall v \in V, \quad B(e, v) = F(v) - B(u_h, v),$$

we observe that e is equivalently the solution of the following (so-called primal) variational problem

$$\boxed{J(e) = \inf \{J(w), \quad w \in V\}}$$

where J is the quadratic functional

$$\begin{aligned} J(w) &= \frac{1}{2} B(w, w) - F(w) + B(u_h, w) \\ &= \frac{1}{2} \int_\Omega \mathbb{A} \boldsymbol{\nabla} w \cdot \boldsymbol{\nabla} w - \int_\Omega f w - \int_{\Gamma_N} g w + \int_\Omega \mathbb{A} \boldsymbol{\nabla} u_h \cdot \boldsymbol{\nabla} w. \end{aligned}$$

We also note that $J(e) = -\frac{1}{2} \int_\Omega \mathbb{A} \boldsymbol{\nabla} e \cdot \boldsymbol{\nabla} e.$

We therefore have

$$\boxed{\forall w \in V, \quad |||e|||^2 = -2J(e) \geq -2J(w)}$$

An interesting consequence is that we can easily compute a lower bound on the error $|||e|||$, namely $\sqrt{-2J(w)}$ for any $w \in V$ such that $J(w) < 0$.

However, this lower bound is usually poor unless w is a suitably chosen representation of e.

Remark

An alternative way to obtain that lower bound is to introduce the potential energy functional J_1 associated with the reference problem

$$J_1(w) = \frac{1}{2}\int_\Omega \mathbb{A}\boldsymbol{\nabla} w \cdot \boldsymbol{\nabla} w - \int_\Omega fw - \int_{\Gamma_N} gw$$

We recall that the solution u to (1) satisfies $J_1(u) = \inf_{w\in V} J_1(w)$.

We then have that $|||e|||^2 = 2(J_1(u_h) - J_1(u))$, and hence the lower bound

$$\forall w \in V, \quad |||e|||^2 \geq -2(J_1(w) - J_1(u_h)) = -2J(w - u_h). \qquad (11)$$

$\Longrightarrow$ *we want to compute w such that $J_1(w)$ is as small as possible.*

In the space V_h^p, we know that u_h is the unique minimizer of J_1.
For (11) to be useful, w should be searched in a space larger than V_h^p.

A complementary variational principle can be associated to the primal variational principle and may be used to get an upper bound on $|||e|||$.

To that aim, we introduce the space

$$W = \{\boldsymbol{p} \in H(\mathrm{div}, \Omega), \quad \mathrm{div}\,\boldsymbol{p} + f = 0 \text{ in } \Omega, \quad \boldsymbol{p}\cdot\boldsymbol{n} = g \text{ on } \Gamma_N\}$$

Consider the quadratic functional

$$G(\boldsymbol{p}) = \frac{1}{2}\int_\Omega \mathbb{A}^{-1}(\boldsymbol{p} - \mathbb{A}\boldsymbol{\nabla} u_h)\cdot(\boldsymbol{p} - \mathbb{A}\boldsymbol{\nabla} u_h) = \frac{1}{2}|||\boldsymbol{p} - \mathbb{A}\boldsymbol{\nabla} u_h|||_q^2$$

and the so-called complementary variational problem

$$\boxed{\inf\{G(\boldsymbol{p}),\ \boldsymbol{p} \in W\}} \tag{12}$$

The minimization problem (12) is well posed, and it is easy to see that the solution flux $\boldsymbol{q} = \mathbb{A}\boldsymbol{\nabla} u$ (where u is the solution to the reference problem (1)) is the solution to (12).

We obviously have $|||e|||^2 = 2G(\boldsymbol{q})$.

We thus deduce the following upper bound :

$$\boxed{\forall \boldsymbol{p} \in W, \quad |||e|||^2 \leq 2G(\boldsymbol{p})} \tag{13}$$

Remark

An alternative way to obtain that upper bound is to introduce the complementary energy functional J_2 associated with the reference problem

$$J_2(\boldsymbol{p}) = \frac{1}{2}\int_\Omega \mathbb{A}^{-1}\boldsymbol{p}\cdot\boldsymbol{p}$$

We recall that the exact flux $\boldsymbol{q} = \mathbb{A}\boldsymbol{\nabla} u$ satisfies $J_2(\boldsymbol{q}) = \inf_{\boldsymbol{p}\in W} J_2(\boldsymbol{p})$.

We then have $|||e|||^2 = 2(J_2(\boldsymbol{q}) + J_1(u_h))$, from which we deduce the upper bound

$$\forall \boldsymbol{p} \in W, \quad |||e|||^2 \leq 2(J_2(\boldsymbol{p}) + J_1(u_h)) = 2G(\boldsymbol{p}). \tag{14}$$

$\Longrightarrow$ *we would like to compute $\boldsymbol{p}$ such that $J_2(\boldsymbol{p})$ is as small as possible.*

A flux field that belongs to W will be referred as **statically admissible** (in the sense that it verifies the equilibrium equations) and denoted $\widehat{\boldsymbol{q}}$ in the following.

For the pair $(u_h, \widehat{\boldsymbol{q}}) \in V_h^p \times W$, we define the constitutive relation error (CRE) functional E_{CRE} by

$$\boxed{E_{\mathrm{CRE}}^2(u_h, \widehat{\boldsymbol{q}}) = \frac{1}{2} |||\widehat{\boldsymbol{q}} - \mathbb{A}\boldsymbol{\nabla} u_h|||_q^2}$$

We of course note that $E_{\mathrm{CRE}}^2(u_h, \widehat{\boldsymbol{q}}) = G(\widehat{\boldsymbol{q}}) = J_1(u_h) + J_2(\widehat{\boldsymbol{q}})$.

In view of (13), we then get that, for any $\widehat{\boldsymbol{q}} \in W$

$$|||e||| \leq \sqrt{2} E_{\mathrm{CRE}}(u_h, \widehat{\boldsymbol{q}})$$

$$|||e||| = \inf_{\widehat{\boldsymbol{q}} \in W} \sqrt{2}\, E_{\mathrm{CRE}}(u_h, \widehat{\boldsymbol{q}})$$

We show in what follows how to obtain more precise relations.

We first have the following result (the so-called Prager-Synge equality).

Lemma

For any $\widehat{\boldsymbol{q}} \in W$, we have

$$2E^2_{\mathrm{CRE}}(u_h, \widehat{\boldsymbol{q}}) = |||e|||^2 + |||\boldsymbol{q} - \widehat{\boldsymbol{q}}|||^2_q. \tag{15}$$

Proof

Let u be the solution to the reference problem (1). We write

$$\begin{aligned} 2E^2_{\mathrm{ERC}}(u_h, \widehat{\boldsymbol{q}}) &= |||\widehat{\boldsymbol{q}} - \mathbb{A}\boldsymbol{\nabla} u_h|||^2_q = |||(\widehat{\boldsymbol{q}} - \mathbb{A}\boldsymbol{\nabla} u) + (\mathbb{A}\boldsymbol{\nabla} u - \mathbb{A}\boldsymbol{\nabla} u_h)|||^2_q \\ &= |||\widehat{\boldsymbol{q}} - \mathbb{A}\boldsymbol{\nabla} u|||^2_q + |||u - u_h|||^2 + 2\int_\Omega (\widehat{\boldsymbol{q}} - \mathbb{A}\boldsymbol{\nabla} u) \cdot \boldsymbol{\nabla}(u - u_h) \end{aligned}$$

The last term in the above right-hand side vanishes by integration by part, using that both $\widehat{\boldsymbol{q}}$ and $\boldsymbol{q} = \mathbb{A}\boldsymbol{\nabla} u$ belong to W and that $u = u_h$ on Γ_D.

We also have the following properties :

$$\boxed{\begin{array}{l}(u_h, \widehat{\boldsymbol{q}}) \in V_h^p \times W \text{ s.t. } E^2_{\mathrm{CRE}}(u_h, \widehat{\boldsymbol{q}}) = 0 \Longleftrightarrow u_h = u \text{ and } \widehat{\boldsymbol{q}} = \boldsymbol{q}, \\ \text{Hypercircle property :} \quad E^2_{\mathrm{CRE}}(u_h, \widehat{\boldsymbol{q}}) = 2 |\!|\!| \boldsymbol{q} - \widehat{\boldsymbol{q}}^m |\!|\!|^2_q \end{array}} \tag{16}$$

where $\widehat{\boldsymbol{q}}^m = \frac{1}{2}(\widehat{\boldsymbol{q}} + \mathbb{A}\boldsymbol{\nabla} u_h)$.

Goal-oriented error estimation

In practical applications, one is often interested in errors on some specific outputs of the computation, i.e. **quantities of interest** $Q(u)$ which are functional of the solution u.

Typical examples include

- the average of the normal flux $q_n = \boldsymbol{q} \cdot \boldsymbol{n} = (\mathbb{A} \boldsymbol{\nabla} u) \cdot \boldsymbol{n}$ through a sub-boundary $\Gamma_Q \subset \partial\Omega$
- the average of the solution u in a local region of interest $\omega_Q \subset \Omega$.

In such cases, energy-norm driven error estimation and mesh adaptation tools fail to provide the required accuracy in the chosen quantity of interest using limited computational resources (e.g. some complex features of the solution might not influence the quantity of interest).

Still using these tools but complementing them with additional information, **goal-oriented error estimation and adaptivity** can be performed.

Goal-oriented error estimation

We consider a linear and continuous functional $Q : V \to \mathbb{R}$, and we define from this a quantity of interest $Q(u)$ (depending linearly on u).

In practice, the functional Q is often defined in a global manner as

$$\boxed{Q(v) = \int_\Omega \left(\widetilde{f}_Q \, v + \widetilde{\boldsymbol{q}}_Q \cdot \boldsymbol{\nabla} v \right) + \int_{\Gamma_N} \widetilde{g}_Q \, v + \int_\Omega \mathbb{A} \boldsymbol{\nabla} \widetilde{u}_Q \cdot \boldsymbol{\nabla} v} \tag{17}$$

$\left(\widetilde{f}_Q, \widetilde{\boldsymbol{q}}_Q, \widetilde{g}_Q, \widetilde{u}_Q \right)$ is a set of **extraction functions** which can be mechanically interpreted in an adjoint problem (see below) as body, pre-flux, traction, and pre-primal field loadings, respectively.

These are defined explicitly or implicitly, depending on the quantity Q.

The last extraction function $\widetilde{u}_Q$, vanishing on Γ_N, is a regular field that enables one to extract components of the normal flux $\boldsymbol{q} \cdot \boldsymbol{n}$ on Γ_D (reaction forces) by imposing a non-homogeneous Dirichlet condition

$$\int_\Omega \mathbb{A} \boldsymbol{\nabla} \widetilde{u}_Q \cdot \boldsymbol{\nabla} u = \int_{\Gamma_D} \widetilde{u}_Q \boldsymbol{q} \cdot \boldsymbol{n} + \int_\Omega \widetilde{u}_Q f$$

Goal-oriented error estimation

The quantity of interest $Q(u)$ can be written $\langle Q, u \rangle$ where Q belongs to the dual space $V^\star$ of V. Consequently, we have

$$\boxed{|Q(u) - Q(u_h)| = |Q(e)| \leq \|Q\|_\star \, |||e|||}$$

where $\|Q\|_\star = \sup_{v \in V,\, |||v|||=1} |Q(v)|$ is the dual norm of Q.

$\Longrightarrow$ A target accuracy ϵ for the error on $Q(u)$ can thus be achieved by ensuring that $|||e||| \leq \epsilon / \|Q\|_\star$.

This method leads to an overestimation (and requires useless computational effort) as norm approximation does not take the locality of Q into account.

We next show, using duality arguments, that the target accuracy ϵ for the error on $Q(u)$ can be achieved by ensuring that $|||e|||$ is of the order $\sqrt{\epsilon}$ only.

We consider in a general setting the problem written in its weak form $B(u,v) = F(v)$ for any $v \in V$.

In order to give an exact representation of the error $Q(u) - Q(u_h) = Q(e)$, the following **adjoint problem** is introduced :

$$\boxed{\text{Find } \widetilde{u} \in V \text{ such that, for any } v \in V, \quad B^\star(\widetilde{u}, v) = Q(v)} \tag{18}$$

where $B^*(u,v)$ is the formal adjoint of the primal form $B(u,v)$, satisfying $B^*(u,v) = B(v,u)$.

Remarque

In the current symmetric case, the forms B and B^* are identical.

We also define the adjoint flux $\widetilde{\boldsymbol{q}} = \mathbb{A}\boldsymbol{\nabla}\widetilde{u}$.

The adjoint solution $\widetilde{u}$ yields the exact representation (primal-dual equivalence) of the error on $Q(u)$:

$$\boxed{Q(e) = B^{\star}(\widetilde{u}, e) = B(e, \widetilde{u}) = R(\widetilde{u}) = \langle R_{|u_h}, \widetilde{u} \rangle}$$

$\Longrightarrow$ This shows that $\widetilde{u}$ provides for the **sensitivity** of the discretization error on $Q(u)$ to the local sources of discretization errors in the whole domain Ω.

Remark

In the case of a nonlinear quantity of interest, the general approach consists in performing a first order linearization $Q(u) - Q(u_h) \approx Q'_{|u_h}(e)$ *and therefore considering* $Q'_{|u_h}(v)$ *as the right-hand side of the adjoint problem.*

A classical numerical approach then consists in computing an approximate solution $\widetilde{u}_h$ of $\widetilde{u}$ using the reference mesh $\mathcal{T}_h$.

We thus get, using the Galerkin orthogonality, that

$$\boxed{Q(e) = B(e, \widetilde{u} - \widetilde{u}_h) = B(e, \widetilde{e})} \tag{19}$$

Remarque

When a different mesh (e.g. with a local enrichment) is used to solve the adjoint problem, yielding an approximate adjoint solution $\widetilde{u}_+$, the relation (19) *should be changed in*

$$Q(e) = B(e, \widetilde{u} - \widetilde{u}_+) + B(e, \widetilde{u}_+) \tag{20}$$

where the second term $B(e, \widetilde{u}_+) = R(\widetilde{u}_+) = F(\widetilde{u}_+) - B(u_h, \widetilde{u}_+)$ is a fully computable correcting term.

A particular case is pointwise quantities of interest, such as $u(\boldsymbol{x}_0)$ for some $\boldsymbol{x}_0 \in \Omega$ (assuming that $u \in \mathcal{H}^1(\Omega)$ is continuous at point $\boldsymbol{x}_0$).

A classical approach then consists in using a regularized functional, i.e. defining a modified quantity of interest

$$Q(u) \approx \int_\Omega k_{\delta,\boldsymbol{x}_0} u(\boldsymbol{x})$$

$k_{\delta,\boldsymbol{x}_0}$ is a smooth function (characterized by the length-scale $\delta > 0$ and such that $\int_\Omega k_{\delta,\boldsymbol{x}_0} = 1$) which performs a weighted average over a small neighborhood of the point $\boldsymbol{x}_0$.

Remark

A local enrichment technique for the solution of the adjoint problem (using analytical Green's functions) can also be performed (see later).

An error indicator may be derived from (20) using the **dual weighted residual** (DWR) method, based on hierarchical *a posteriori* error analysis.

After computing an approximate adjoint solution $\widetilde{u}_+$ from a hierarchically refined FE space $V_+ \supset V_h^p$ (higher-order basis functions, refined mesh), and assuming that the error between $\widetilde{u}$ and $\widetilde{u}_+$ is small, the DWR method then consists in writing

$$\boxed{Q(u) - Q(u_h) \approx R(\widetilde{u}_+)} \tag{21}$$

so that the quantity $R(\widetilde{u}_+)$ is taken as an error indicator on Q.

Remark

Due to the Galerkin orthogonality, choosing $V_+ = V_h^p$ would of course lead to a meaningless indicator (in that case, we would have $R(\widetilde{u}_+) = 0$). Consequently, a convenient approximation of the adjoint solution should involve a subspace in $(V_h^p)^\perp$.

The previous argument can be somewhat quantified.

Let $u_+ \in V_+$ be the approximation (in the refined space) of u.
Assume that $|Q(u) - Q(u_+)| \leq \beta |Q(u) - Q(u_h)|$ (saturation assumption) is satisfied for some $0 \leq \beta < 1$.

Using the fact that $u_+ - u_h \in V_+$ and next the fact that $\widetilde{u}_+ \in V_+$, we obtain

$$Q(u_+) - Q(u_h) = B(u_+ - u_h, \widetilde{u}_+) = B(u - u_h, \widetilde{u}_+) = R(\widetilde{u}_+).$$

From the triangle inequality, we eventually get

$$\boxed{\frac{|R(\widetilde{u}_+)|}{1+\beta} \leq |Q(u) - Q(u_h)| \leq \frac{|R(\widetilde{u}_+)|}{1-\beta}}$$

The indicator $R(\widetilde{u}_+)$ may be used to drive adaptive algorithms as it gives a clear and accurate distribution of error sources, but it does not provide for *guaranteed* error bounds on Q.

In the following, we bound the error on $Q(u)$ using (19).

A first possibility is to directly use the Cauchy-Schwarz inequality :

$$\boxed{|Q(u) - Q(u_h)| = |B(e, \widetilde{e})| \leq |||e||| \; |||\widetilde{e}||| \leq \eta \; \widetilde{\eta}} \tag{22}$$

where η and $\widetilde{\eta}$ are upper error bounds (in the energy norm) for the primal and adjoint problems, respectively.

$\Longrightarrow$ Any global error estimate can be used to assess the error on $Q(u)$.
$\Longrightarrow$ The error on $Q(u)$ decreases with a rate which is **twice larger than that for the error on u in the energy norm**.

However, the previous estimate may be crude (and may not exploit the locality of $Q(u)$) due to the use of the Cauchy-Schwarz inequality.

It is also possible, still starting from (19), to use a local Cauchy-Schwarz inequality, writing that

$$|Q(u) - Q(u_h)| = \left| \sum_{K \in \mathcal{T}_h} B_K(e, \widetilde{e}) \right| \leq \sum_{K \in \mathcal{T}_h} |||e|||_{|K} \; |||\widetilde{e}|||_{|K}, \tag{23}$$

but bounds on $|||e|||_{|K}$ and $|||\widetilde{e}|||_{|K}$ (using for instance local error indicators η_K and $\widetilde{\eta}_k$) are heuristic and this version is again very conservative (in the sense that it does not take into account possible cancellation of errors over the domain).

Remark

A quantitative evaluation of $Q(e)$ involving the elementary error components (but not providing for an upper error bound), can also be exhibited when using the DWR method.

$$Q(u) - Q(u_h) \approx R(\widetilde{u}_+) = R(\widetilde{e}_+) = \sum_{K \in \mathcal{T}_h} \left[\int_K r_K \, \widetilde{e}_+ + \int_{\partial K} R_{\partial K} \, \widetilde{e}_+ \right],$$

where $\widetilde{e}_+ = \widetilde{u}_+ - \widetilde{u}_h$ is an approximation of $\widetilde{e}$, and r_K and $R_{\partial K}$ are local residuals. Consequently, an error indicator can be defined as

$$|Q(u) - Q(u_h)| \approx \sum_{K \in \mathcal{T}_h} \rho_K \, \omega_K \quad \text{with} \quad \left\{ \begin{array}{l} \rho_K = \|r_K\|_{0,K} + h_K^{-1/2} \|R_{\partial K}\|_{0,\partial K}, \\ \omega_K = \|\widetilde{e}_+\|_{0,K} + h_K^{1/2} \|\widetilde{e}_+\|_{0,\partial K}. \end{array} \right. \tag{24}$$

Note that ρ_K and ω_K are computable terms.

An alternative technique consists in using the parallelogram identify to get an upper bound on the error.

$$B(e,\widetilde{e}) = B\left(se, \frac{1}{s}\widetilde{e}\right) = \frac{1}{4}\left[\left|\left|\left|se + \frac{1}{s}\widetilde{e}\right|\right|\right|^2 - \left|\left|\left|se - \frac{1}{s}\widetilde{e}\right|\right|\right|^2\right] = \frac{1}{4}\left[\chi_+ - \chi_-\right]$$

where $s \in \mathbb{R}$ is a scaling factor (to be optimized) and

$$\chi_+ = \left|\left|\left|se + \frac{1}{s}\widetilde{e}\right|\right|\right|^2, \qquad \chi_- = \left|\left|\left|se - \frac{1}{s}\widetilde{e}\right|\right|\right|^2,$$

$$\Longrightarrow \boxed{\frac{1}{4}\left[\chi_+^{\text{low}} - \chi_-^{\text{upp}}\right] \leq Q(u) - Q(u_h) \leq \frac{1}{4}\left[\chi_+^{\text{upp}} - \chi_-^{\text{low}}\right]} \qquad (25)$$

where χ_-^{upp} and χ_-^{low} (resp. χ_+^{upp} and χ_+^{low}) are upper and lower bounds on χ_- (resp. χ_+), derived from classical approaches.

$\Longrightarrow$ more accurate error bounds compared to (22), but error cancellations over the domain are still not captured.

Another alternative bounding technique is based on properties of duality-based approaches (CRE).

Introduce the space of equilibrated fluxes (for the adjoint problem) :

$$\widetilde{\mathcal{S}} = \left\{ \widetilde{\boldsymbol{p}} \in \mathcal{H}(div, \Omega); \quad \forall v \in V, \quad \int_\Omega \widetilde{\boldsymbol{p}} \cdot \boldsymbol{\nabla} v = Q(v) \right\}.$$

After constructing admissible flux fields $\widehat{\boldsymbol{q}}_h \in \mathcal{S}$ and $\widehat{\widetilde{\boldsymbol{q}}}_h \in \widetilde{\mathcal{S}}$ as a post-processing of $\boldsymbol{q}_h$ and $\widetilde{\boldsymbol{q}}_h$ (as detailed before), a direct consequence of (22) and (13) is

$$\boxed{|Q(u) - Q(u_h)| \leq 2.E_{CRE}(u_h, \widehat{\boldsymbol{q}}_h)\, E_{CRE}(\widetilde{u}_h, \widehat{\widetilde{\boldsymbol{q}}}_h)} \tag{26}$$

An *a posteriori* error estimate on Q which is more accurate than (26) can be obtained using the hypercircle property (16) verified by $\widehat{\boldsymbol{q}}_h^m = \frac{1}{2}(\widehat{\boldsymbol{q}}_h + \boldsymbol{q}_h)$.

Indeed, we infer from (19) and from $\widehat{\widetilde{\boldsymbol{q}}}_h \in \widetilde{\mathcal{S}}$ that

$$Q(u) - Q(u_h) = B\left(u - u_h, \widetilde{u} - \widetilde{u}_h\right) = \int_\Omega \boldsymbol{\nabla}(u - u_h) \cdot (\widetilde{\boldsymbol{q}} - \mathbb{A}\boldsymbol{\nabla}\widetilde{u}_h)$$
$$= \int_\Omega \boldsymbol{\nabla}(u - u_h) \cdot \left(\widehat{\widetilde{\boldsymbol{q}}}_h - \mathbb{A}\boldsymbol{\nabla}\widetilde{u}_h\right)$$

We consequently obtain

$$Q(u) - Q(u_h) = \int_\Omega \mathbb{A}^{-1}(\boldsymbol{q} - \boldsymbol{q}_h) \cdot \left(\widehat{\widetilde{\boldsymbol{q}}}_h - \mathbb{A}\boldsymbol{\nabla}\widetilde{u}_h\right)$$
$$= \int_\Omega \mathbb{A}^{-1}\left(\boldsymbol{q} - \widehat{\boldsymbol{q}}_h^m\right) \cdot \left(\widehat{\widetilde{\boldsymbol{q}}}_h - \mathbb{A}\boldsymbol{\nabla}\widetilde{u}_h\right) + C_h$$

where $C_h = \frac{1}{2}\int_\Omega \mathbb{A}^{-1}\left(\widehat{\boldsymbol{q}}_h - \boldsymbol{q}_h\right) \cdot \left(\widehat{\widetilde{\boldsymbol{q}}}_h - \widetilde{\boldsymbol{q}}_h\right)$ is a computable term.

From the Cauchy-Schwarz inequality and the use of (16), we eventually obtain the bound

$$\boxed{|Q(u) - Q(u_h) - C_h| \leq E_{CRE}(u_h, \widehat{\boldsymbol{q}}_h)\, E_{CRE}(\widetilde{u}_h, \widehat{\widetilde{\boldsymbol{q}}}_h)} \tag{27}$$

which is twice sharper than (26), and partially takes into account error cancellations (through the term C_h).

The quantity $Q(u_h) + C_h$ can be interpreted as a corrected approximate value of the quantity of interest.

Remarque

Furthermore, the estimate (27) *can also be written as*

$$|Q(u) - Q(u_h)| \leq \eta^Q := \max_{\theta=\pm 1} \left| C_h + \theta . E_{CRE}(u_h, \widehat{\boldsymbol{q}}_h)\, E_{CRE}(\widetilde{u}_h, \widehat{\widetilde{\boldsymbol{q}}}_h) \right| . \tag{28}$$

Remark

A still sharper bound can of course be obtained from the previous approach, when using an enriched adjoint solution $\widetilde{u}_+$.

$$Q(u) - Q(u_h) - R(\widetilde{u}_+) = \int_\Omega \boldsymbol{\nabla}(u - u_h) \cdot \left(\widehat{\widetilde{\boldsymbol{q}}}_+ - \mathbb{A}\boldsymbol{\nabla}\widetilde{u}_+\right)$$
$$= \int_\Omega \mathbb{A}^{-1}\left(\boldsymbol{q} - \widehat{\boldsymbol{q}}_h^m\right) \cdot \left(\widehat{\widetilde{\boldsymbol{q}}}_+ - \mathbb{A}\boldsymbol{\nabla}\widetilde{u}_+\right) + C_+$$

with $C_+ = \frac{1}{2}\int_\Omega \mathbb{A}^{-1}\left(\widehat{\boldsymbol{q}}_h - \boldsymbol{q}_h\right) \cdot \left(\widehat{\widetilde{\boldsymbol{q}}}_+ - \widetilde{\boldsymbol{q}}_+\right)$. *This leads to the bound :*

$$\boxed{|Q(u) - Q(u_h) - \overline{C}_+| \leq E_{CRE}(u_h, \widehat{\boldsymbol{q}}_h)\, E_{CRE}(\widetilde{u}_+, \widehat{\widetilde{\boldsymbol{q}}}_+)}$$

where $\overline{C}_+ = R(\widetilde{u}_+) + C_+$ *is a new computable correction term.*

Once the error on $Q(u)$ has been estimated, an adaptive strategy similar to the one presented before can be used to reach a given error tolerance.

The adaptive algorithm, which should now be based on local error contributions given by (23), (24) or (25), enables one to recover **optimal convergence rates**.

For instance, when using (27) and denoting θ_{max} the maximizer, we have :

$$|Q(u) - Q(u_h)| \leq \left| C_h + \theta_{max} E_{CRE}(u_h, \widehat{\boldsymbol{q}}_h) E_{CRE}(\widetilde{u}_h, \widehat{\widetilde{\boldsymbol{q}}}_h) \right|$$

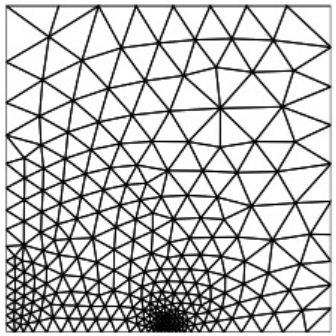
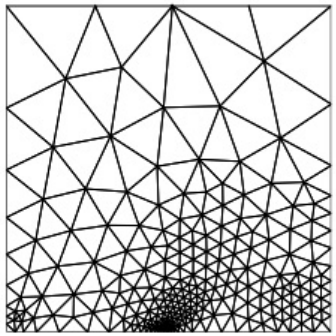
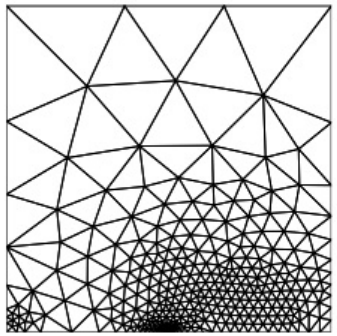
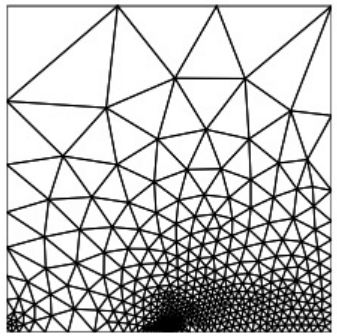
$$= \left| \sum_K C_h^K + \theta_{max} \sqrt{\sum_K \eta_K^2} \right|$$

with

$$C_h^K = \frac{1}{2} \int_K \mathbb{A}^{-1}(\widehat{\boldsymbol{q}}_h - \boldsymbol{q}_h) \cdot (\widehat{\tilde{\boldsymbol{q}}}_h - \tilde{\boldsymbol{q}}_h)$$

$$\eta_K^2 = \frac{1}{2} E_{CRE}^2 \widetilde{E}_{CRE,K}^2 + \frac{1}{2} E_{CRE,K}^2 \widetilde{E}_{CRE}^2$$

Goal-oriented error estimation
Adaptive strategy

Outline

- Motivation
- Theoretical aspects of goal-oriented error estimation in FEM
- Some applications
- Extensions to modeling error (multiscale analysis, model coupling)

Getting Guaranteed Bounds

General technique for linear elasticity

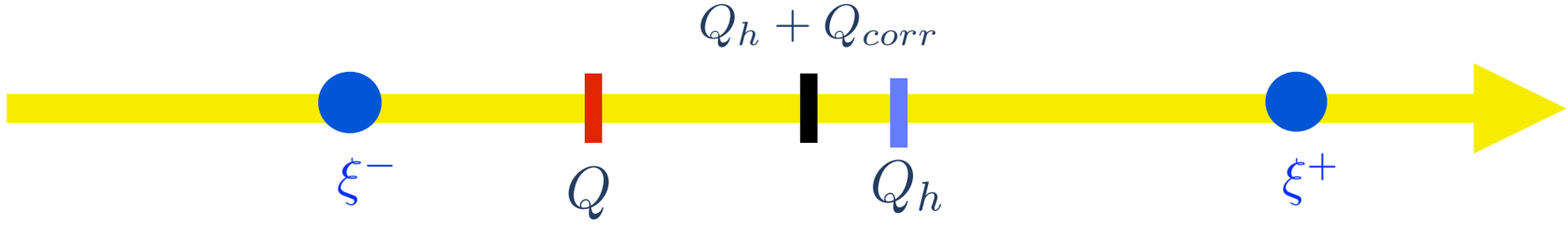
→ based on properties of admissible fields

$$Q(u) - Q(u_h) - \underbrace{Q_{corr}(\hat{s}_h, \hat{\tilde{s}}_h)}_{\text{correction term}} = \left(q - \hat{q}_h^m, \hat{\tilde{q}}_h - \tilde{q}_h\right)_{A^{-1},\Omega}$$

$$\left|Q(u) - Q(u_h) - Q_{corr}(\hat{s}_h, \hat{\tilde{s}}_h)\right| \leq E_{CRE} \cdot \tilde{E}_{CRE}$$

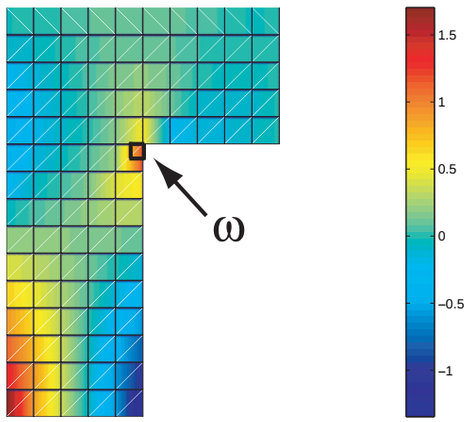
- $Q(u_h) + Q_{corr}(\hat{s}_h, \hat{\tilde{s}}_h)$ is a **new approximation** of $Q(u)$
- **guaranteed** bounds of $Q(u)$ (or $Q(u) - Q(u_h)$)
- still true for **independent discretizations** (no need for orthogonality conditions)

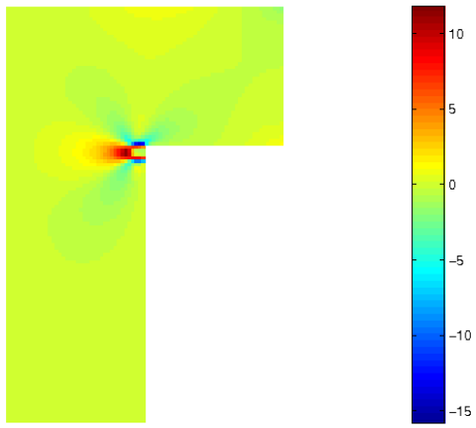
→ accurate bounds provided the adjoint solution is solved accurately



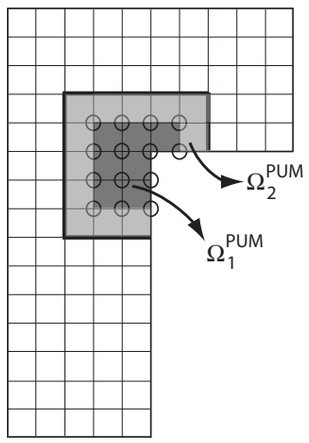
Getting Practical Bounds

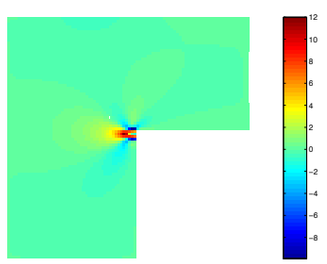
Non-intrusive adjoint solution [Chamoin & Ladevèze 08]





→ enrichment using *handbook techniques* [Strouboulis *et al.* 00]





handbook function (numerical/analytical

$$\tilde{u} = \phi.\tilde{u}^{hand} + \tilde{u}^{res}$$

weight function $\left(\sum_{j=1}^{n^{PUM}} \phi_j(\underline{x})\right)$

$$\tilde{S} = \tilde{S}^{hand}_{PUM} + \tilde{S}^{res}$$

represents local high gradients — enables to verify BC

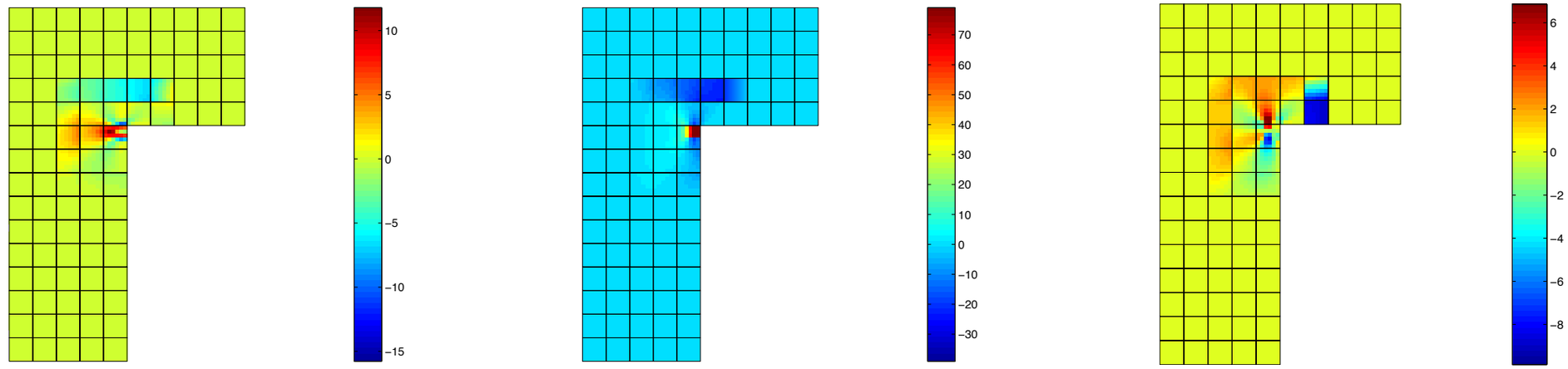
$$\int_\Omega k\boldsymbol{\nabla}\tilde{u}_{res}\cdot\boldsymbol{\nabla}v d\Omega = -\int_{\partial\Omega_1^{PUM}} \tilde{\mathbf{q}}^{hand}\cdot\mathbf{n}_{12}v ds - \int_{\Omega_2^{PUM}} \tilde{\mathbf{q}}^{hand}_{PUM}\cdot\boldsymbol{\nabla}v d\Omega \quad \forall v\in V$$

→ accurate approximation with the **initial coarse mesh**

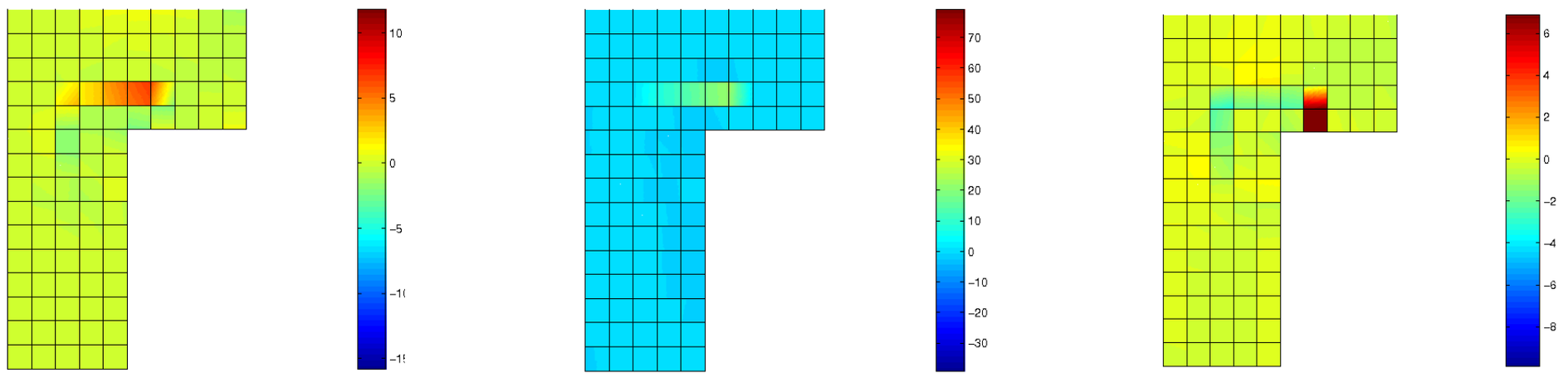
Non-Intrusive Framework

xx yy xy

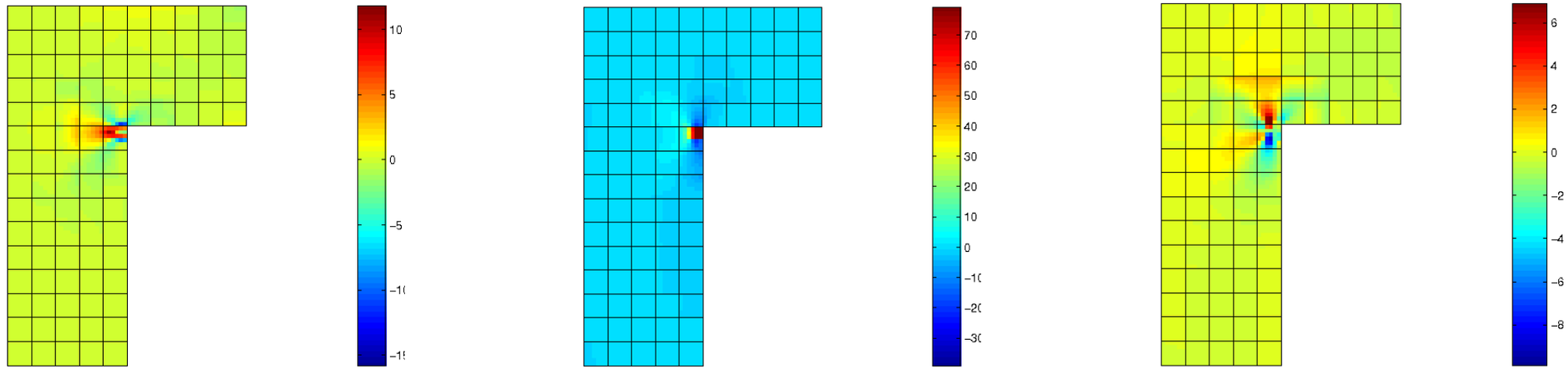
$\tilde{\sigma}^{hand}_{PUM|t=T}$



$\tilde{\sigma}^{r}_{h|t=T}$



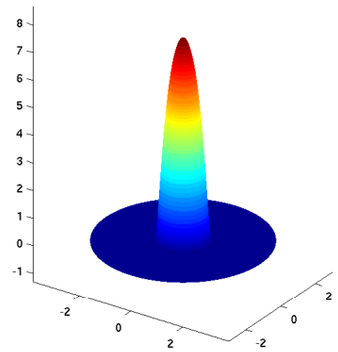
$\tilde{\sigma}_{h|t=T}$



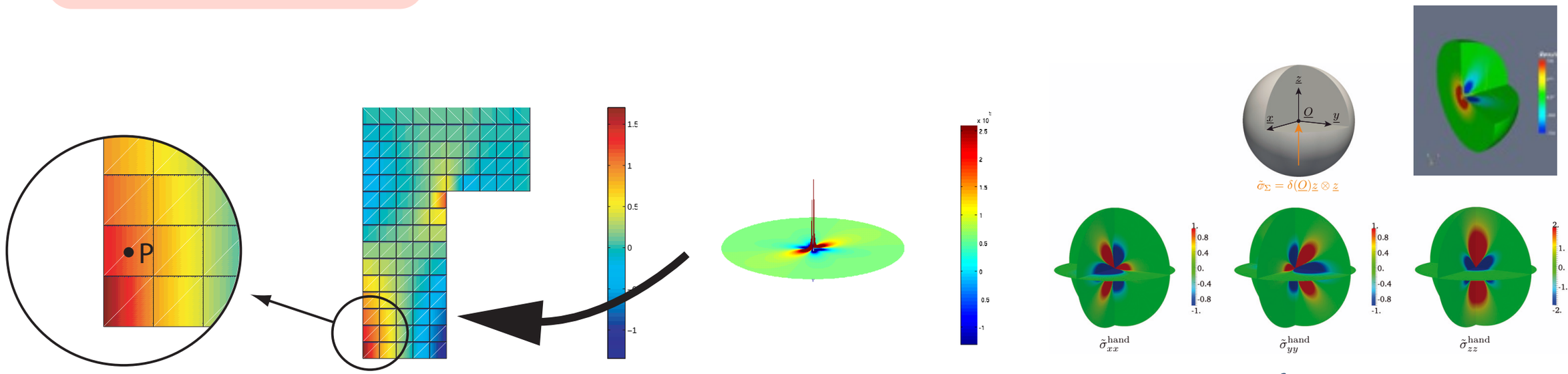
Non-Intrusive Framework

Application to pointwise quantities [Ladevèze & Chamoin 10]

Classical procedure : use of molifier function to regularize
[Prudhomme & Oden 99]



$$Q = \sigma_{yy}(P)$$



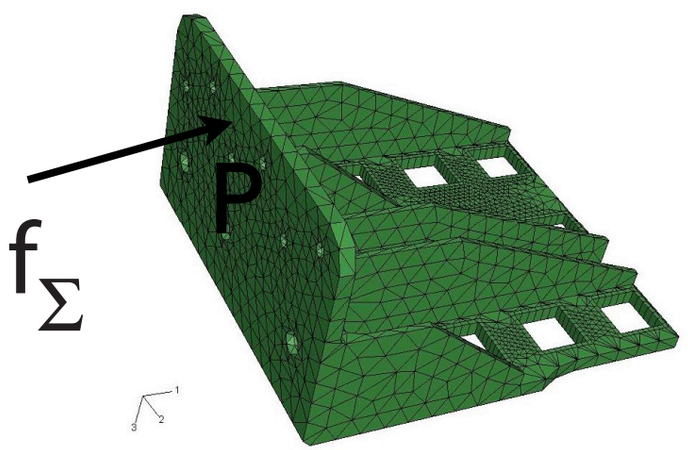
Green's function
[Mindlin 36, Sneddon & Hill 64]

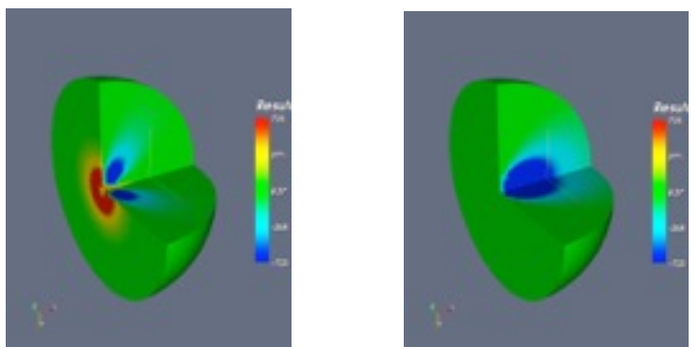
χ_{inf} Q χ_{sup} Q_h

12.09 12.41 12.85 12.98

Non-Intrusive Framework

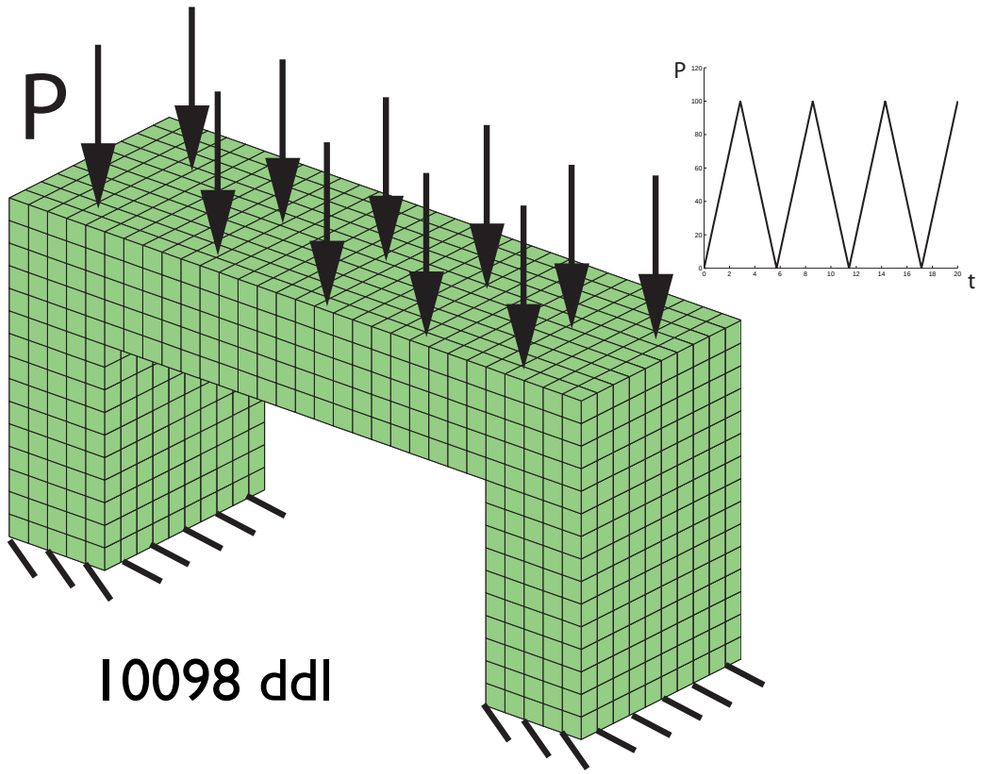
$$I = u_x(P)$$

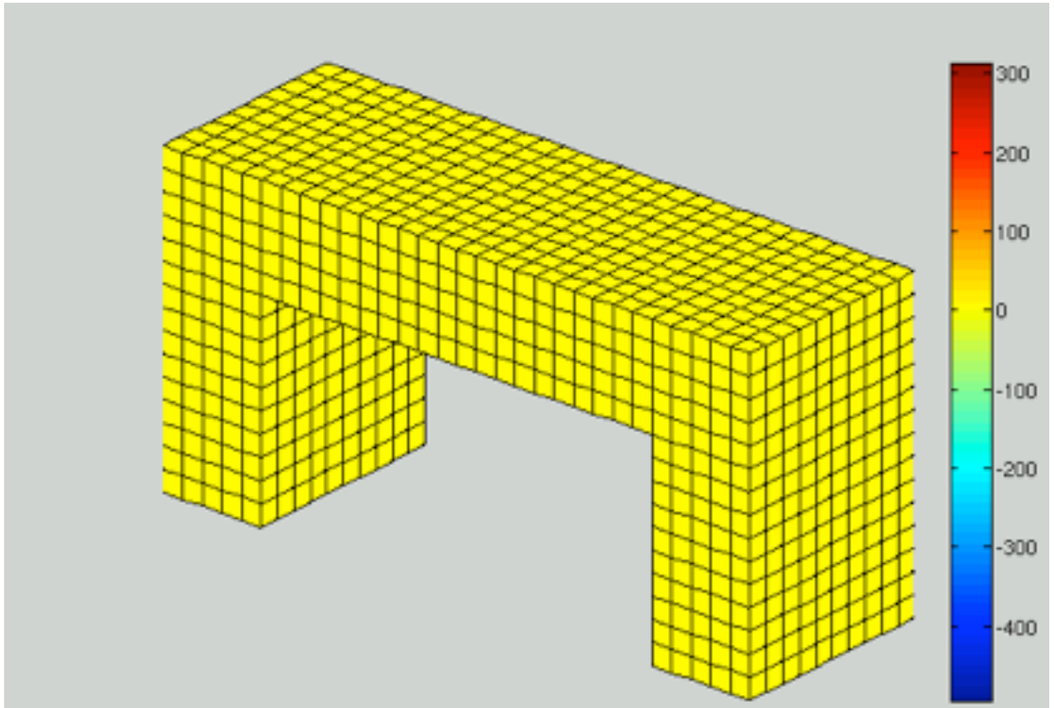


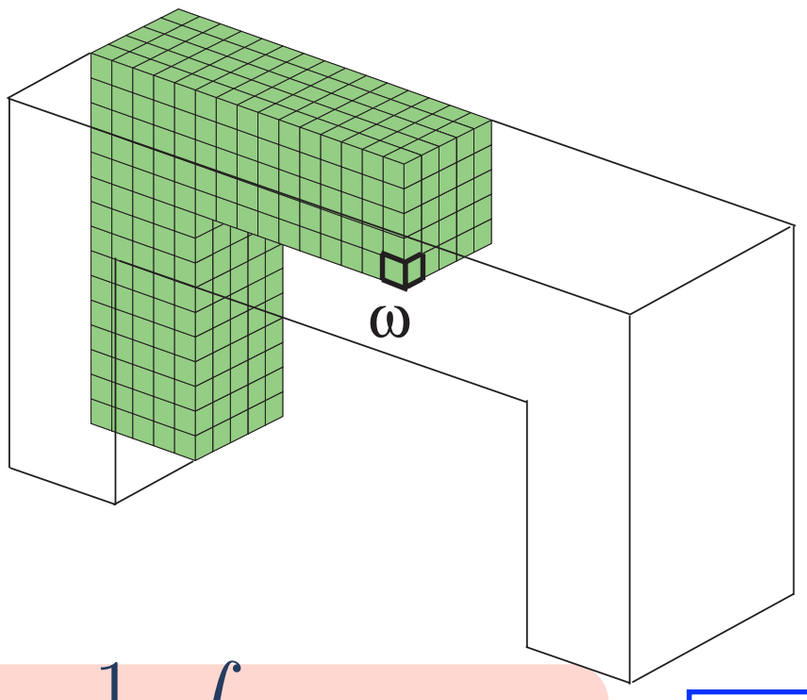


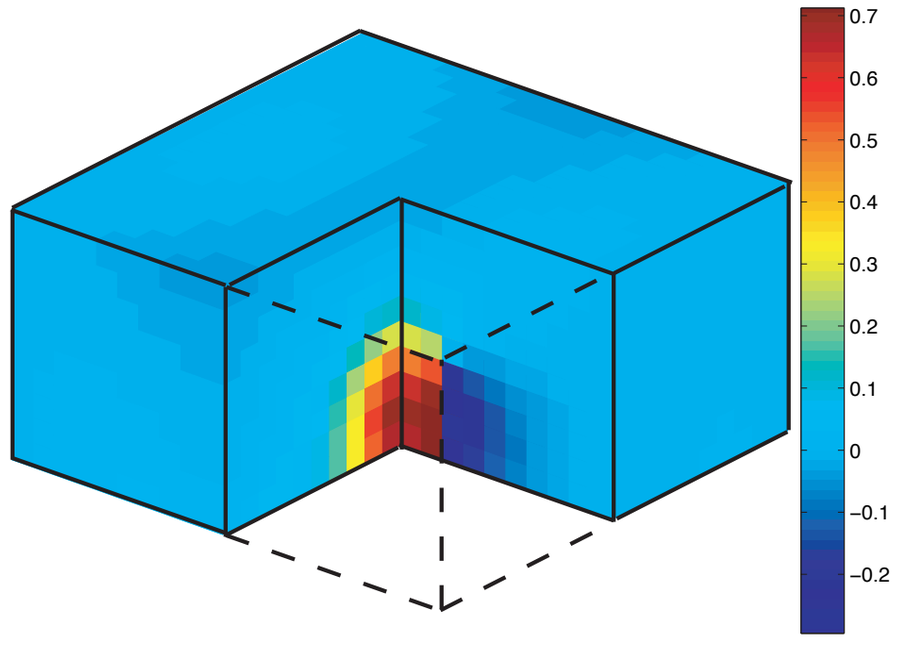
$$\frac{\chi_{inf}}{I_{ex}} = 0.95 \qquad \frac{\chi_{sup}}{I_{ex}} = 1.06$$

Non-Intrusive Framework







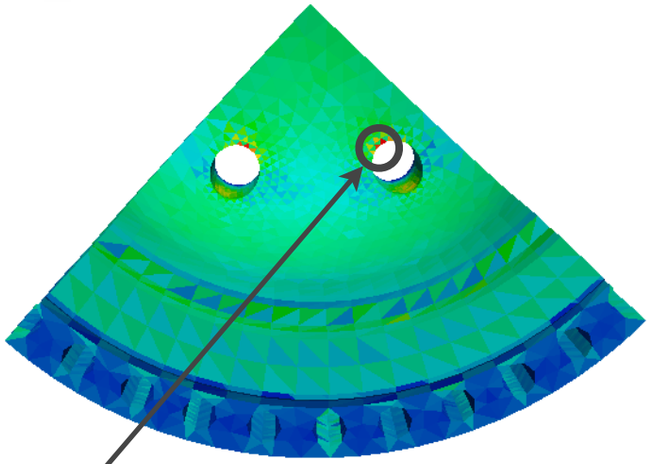


$$Q = \frac{1}{\omega}\int_{\omega} \sigma_{xx|T} d\omega$$

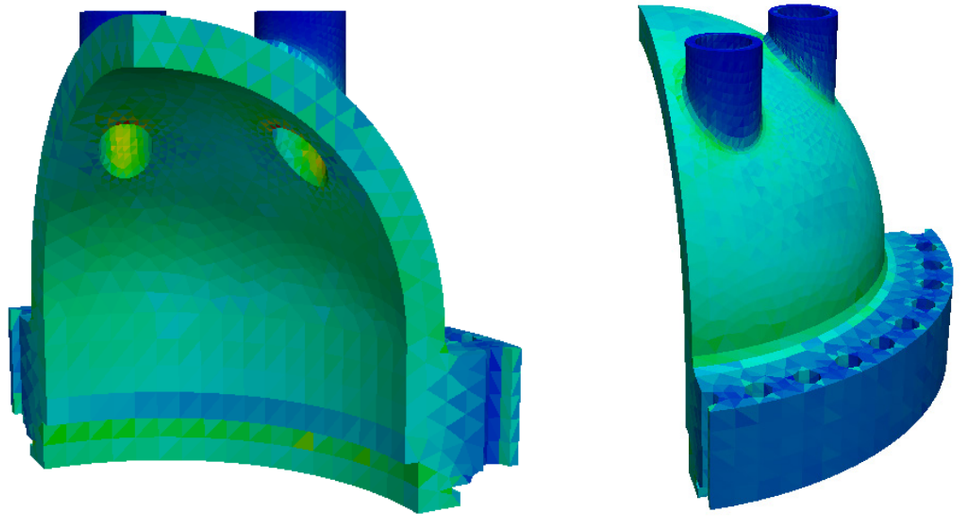
$$Q^- = 498.57 \qquad Q^+ = 506.28$$

Practical Applications

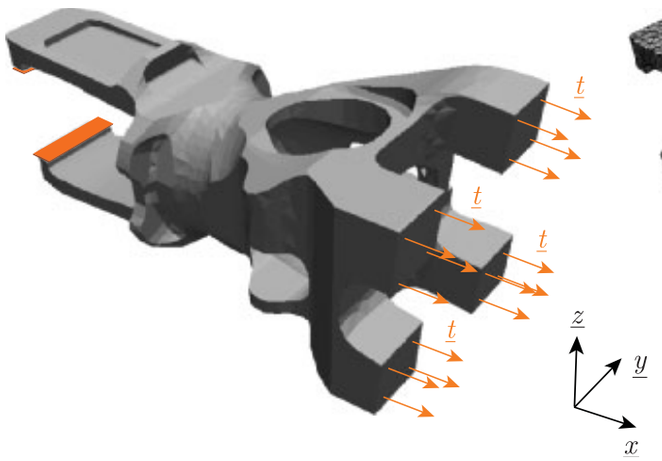
Industrial cases

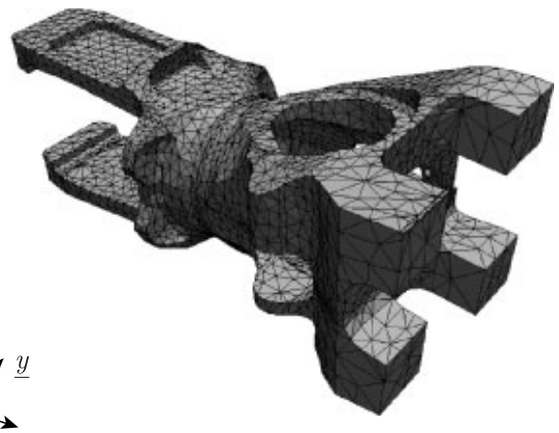


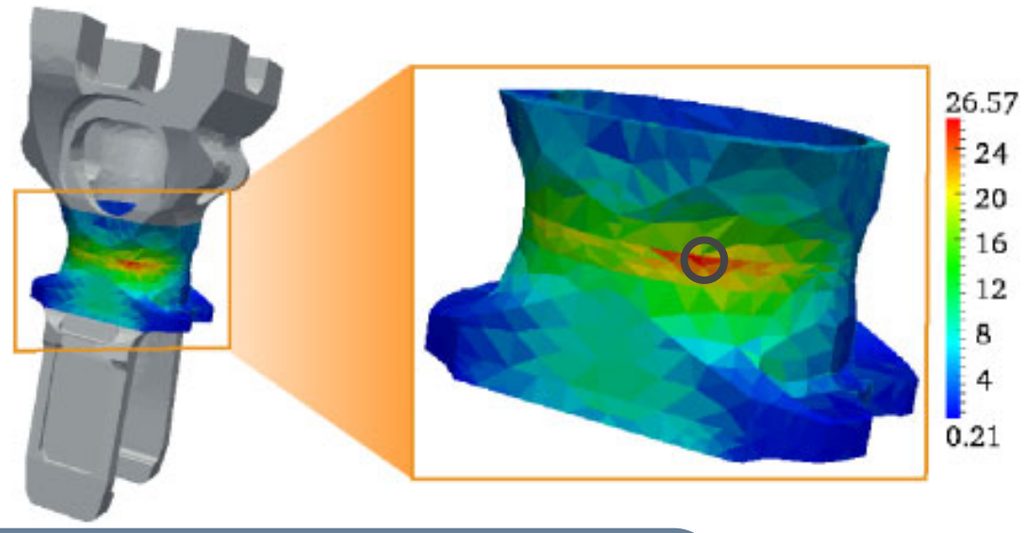
$$Q = \frac{1}{|\omega|}\int_{\omega} \sigma_{VM} d\omega$$



$$14.08 \leq Q \leq 14.93$$

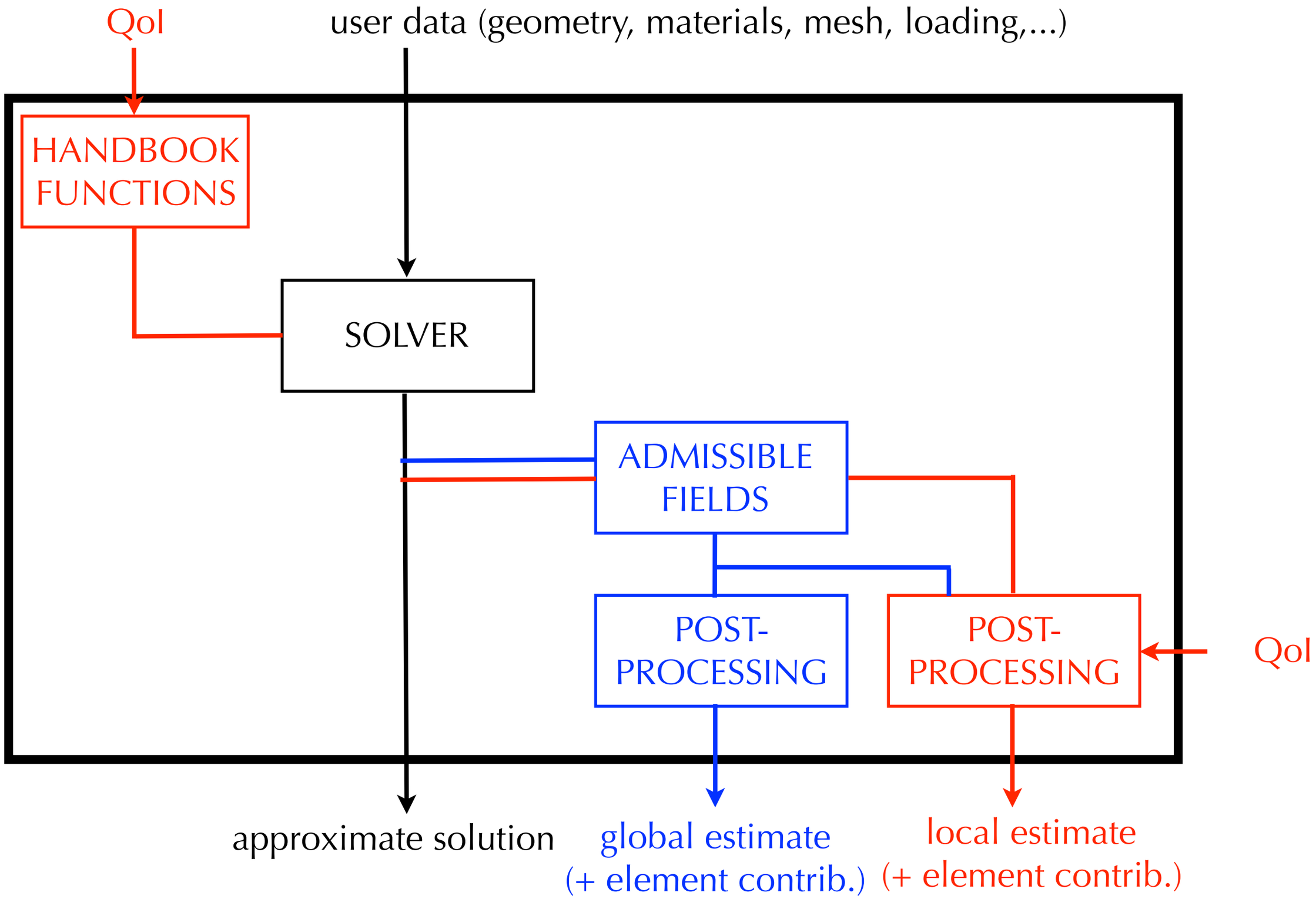






$$25.32 \leq Q \leq 28.24$$

Non-Intrusive Framework



procedure for goal-oriented error estimation = black box for the user

Outline

- **Motivation**
- **Theoretical aspects of goal-oriented error estimation in FEM**
- **Some applications**
- **Extensions to modeling error (multiscale analysis, model coupling)**

Outline

- Motivation
- Theoretical aspects of goal-oriented error estimation in FEM
- Some applications
- Extensions to modeling error (**multiscale analysis**, model coupling)

Context

Model problem

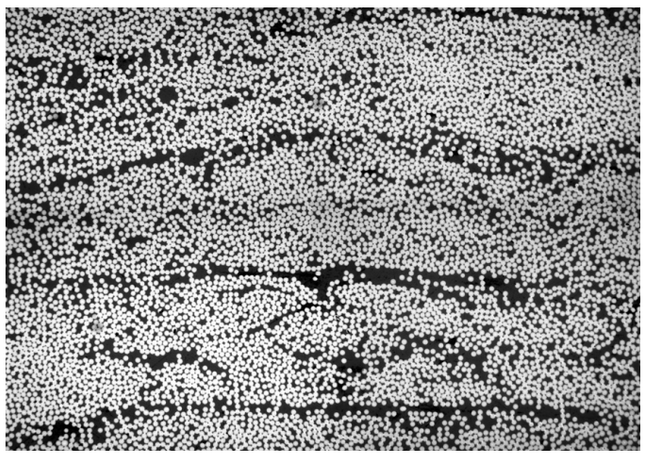
Linear elliptic multiscale problems (heterogeneous microstructure)

$$-\boldsymbol{\nabla} \cdot [\mathbb{A}^{\varepsilon}(\boldsymbol{x};\mu)\boldsymbol{\nabla} u^{\varepsilon}] = f \text{ in } \Omega \subset \mathbb{R}^d \quad + \text{boundary conditions}$$

$\mathbb{A}^{\varepsilon}$: highly oscillatory quantity ⟶ small scale variations (length scale ε)

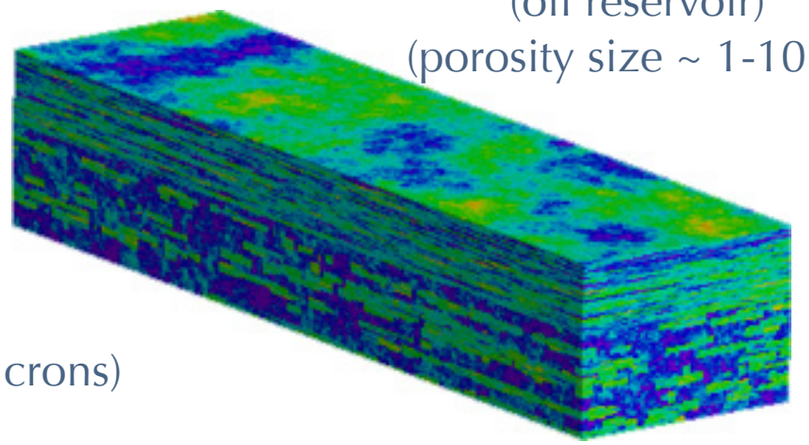
⟶ high contrast

Applications: porous media, composite materials,….

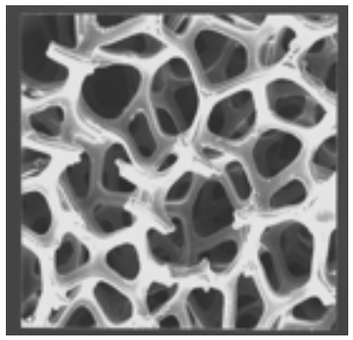


composite
(fiber size = 10 microns)

two-phase porous medium
(oil reservoir)
(porosity size ~ 1-10 m)

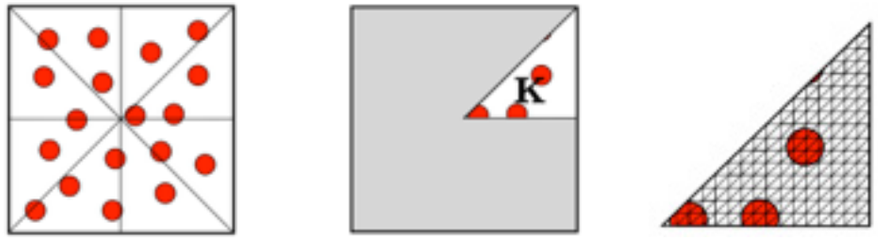


Nickel foam
(hole size: 200 microns)



Multiscale Analysis

Multiscale FEM (MsFEM)



IDEA: encode small scale information in multiscale basis functions

↳ Galerkin approximation with suitably chosen basis functions

offline stage: basis functions $\{\phi_i^\varepsilon\}$ are pre-computed solving fine-scale local problems

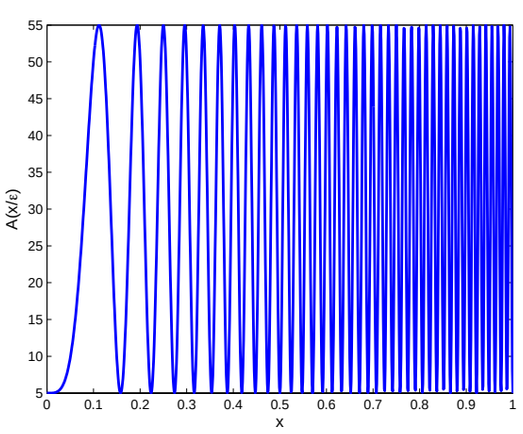
$$\boldsymbol{\nabla} \cdot (\mathbb{A}^\varepsilon \boldsymbol{\nabla} \phi_i^\varepsilon) = 0 \quad \text{in } K \quad + \text{BC}$$

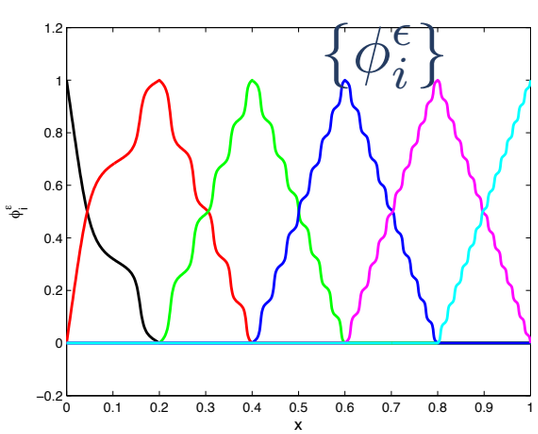
→ independent of f

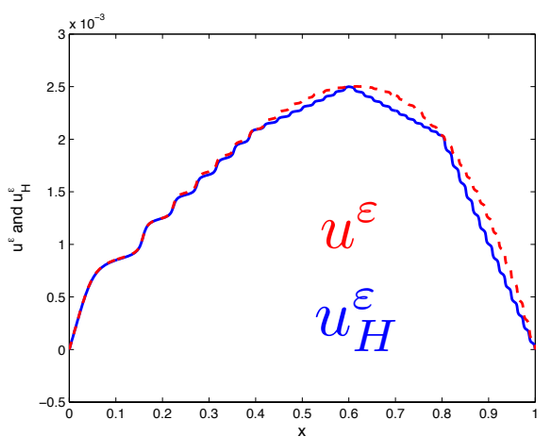
↳ $V_H^\varepsilon = \text{Span}\{\phi_i^\varepsilon\}$ (finite dimensional space)

online stage: a cheap (Petrov) Galerkin approximation is solved on the coarse mesh $\mathcal{T}_H$

$$\forall v \in V_H^\varepsilon, \quad B^\varepsilon(u_H^\varepsilon, v) = F(v)$$







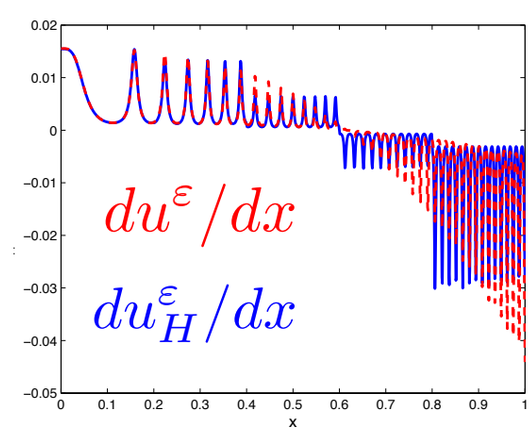


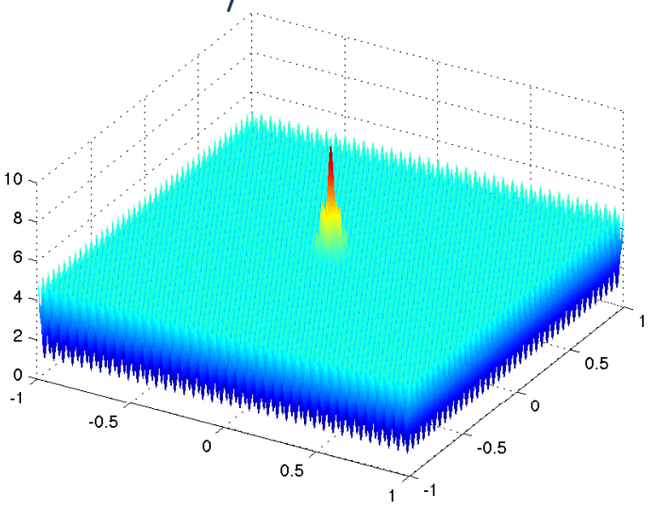
Illustration 1

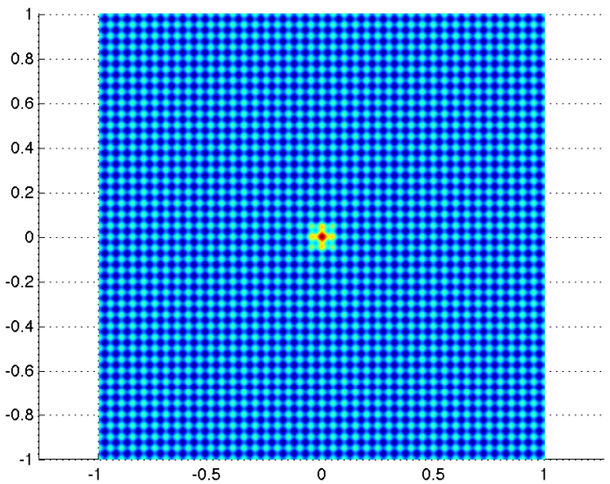
Structure with local defect [Blanc *et al.* 12]

$\Omega = (-1,1)^2$ homogeneous Dirichlet BC $f(x_1,x_2) = \sin(\pi x_1)\cos(\pi x_2)$

$\mathbb{A}^\varepsilon(\boldsymbol{x}) = A^\varepsilon(\boldsymbol{x})\mathbb{I}$ $A^\varepsilon(\boldsymbol{x}) = A_{per}(\frac{x_1}{\varepsilon},\frac{x_2}{\varepsilon}) + B_{defect}(\frac{x_1}{\varepsilon},\frac{x_2}{\varepsilon})$

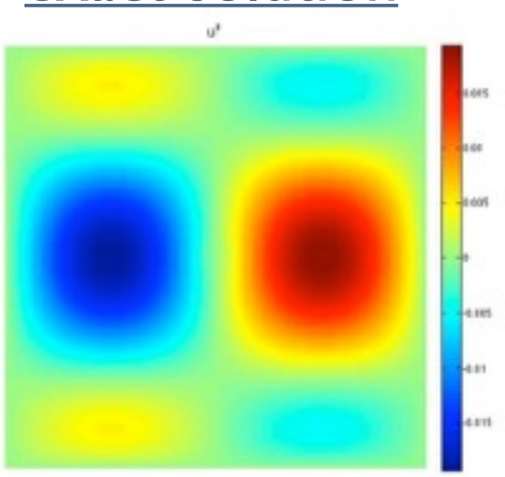
$\varepsilon = 1/20$ $A_{per}(x_1,x_2) = 3 + \cos(2\pi x_1) + \cos(2\pi x_2)$ $B_{defect}(x_1,x_2) = 5.exp(-(x_1^2+x_2^2))$



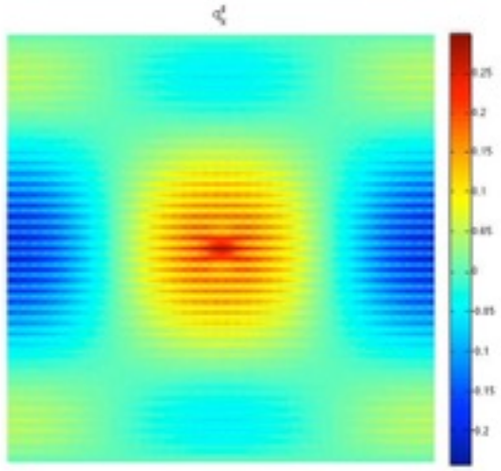


the defect might not modify the macroscopic solution, but it affects the solution locally (at scale εx close to the defect)

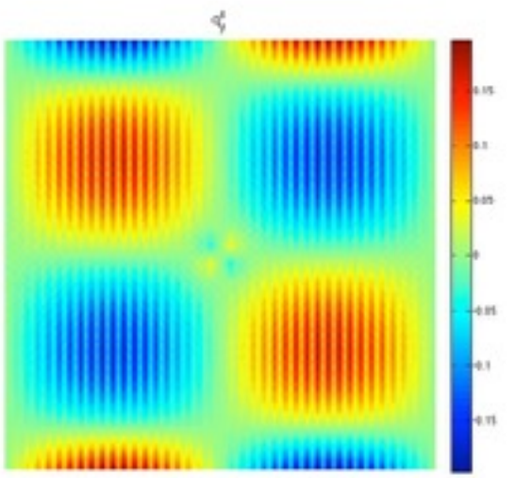
exact solution



u^ε



$\boldsymbol{q}^\varepsilon \cdot \boldsymbol{e}_1$



$\boldsymbol{q}^\varepsilon \cdot \boldsymbol{e}_2$

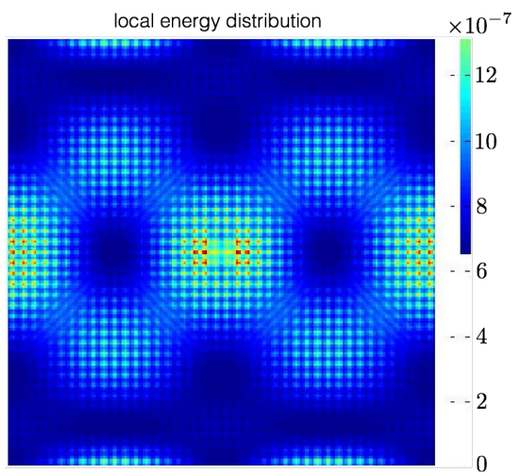
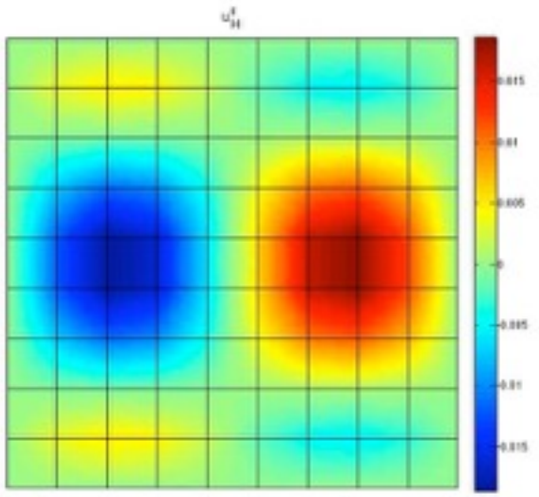
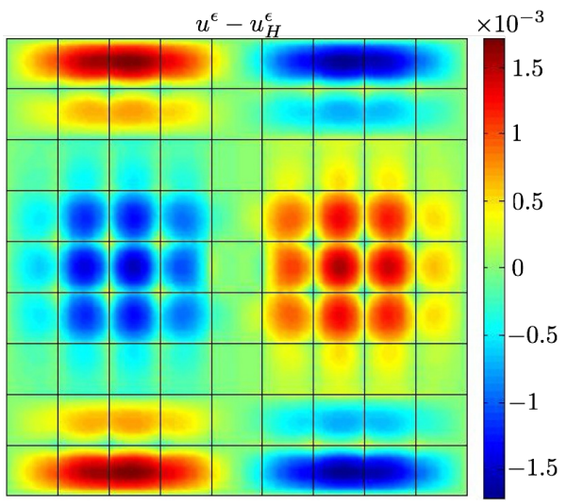


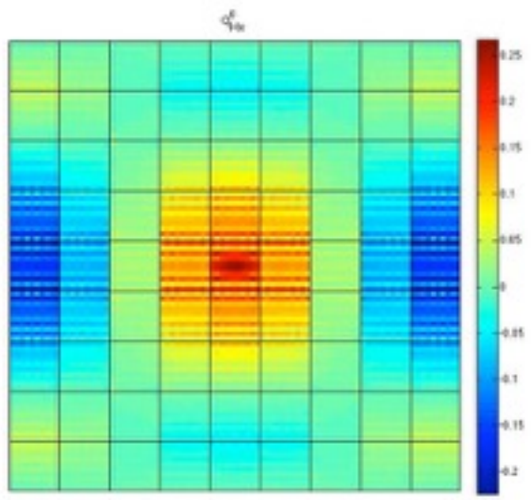
Illustration 1

MsFEM solution

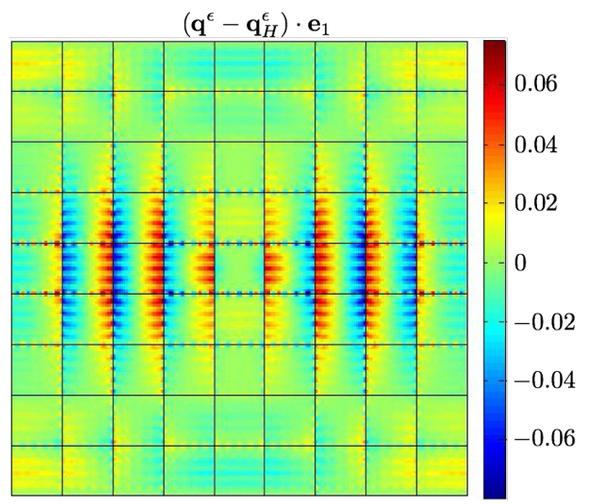


u_H^ε



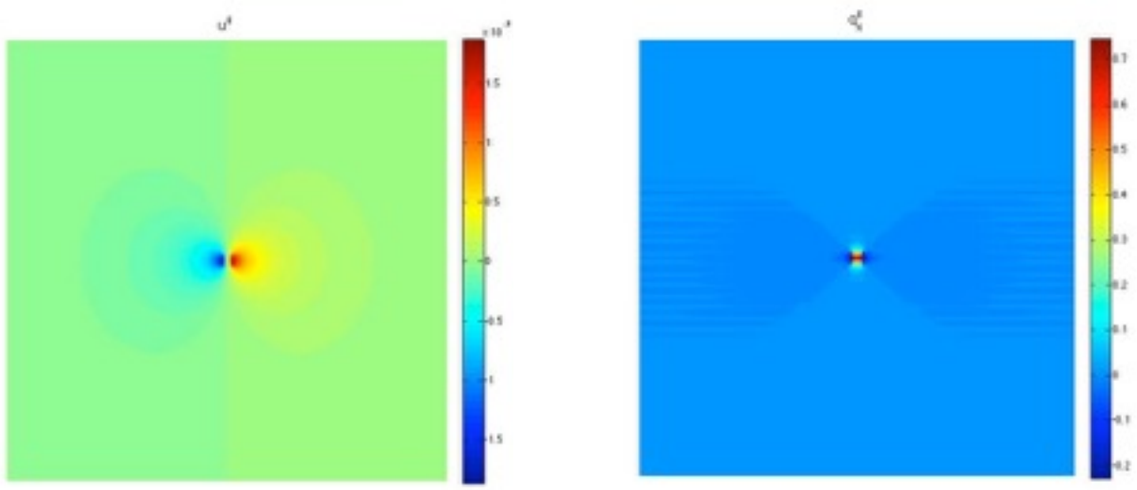


$\boldsymbol{q}_H^\varepsilon \cdot \boldsymbol{e}_1$

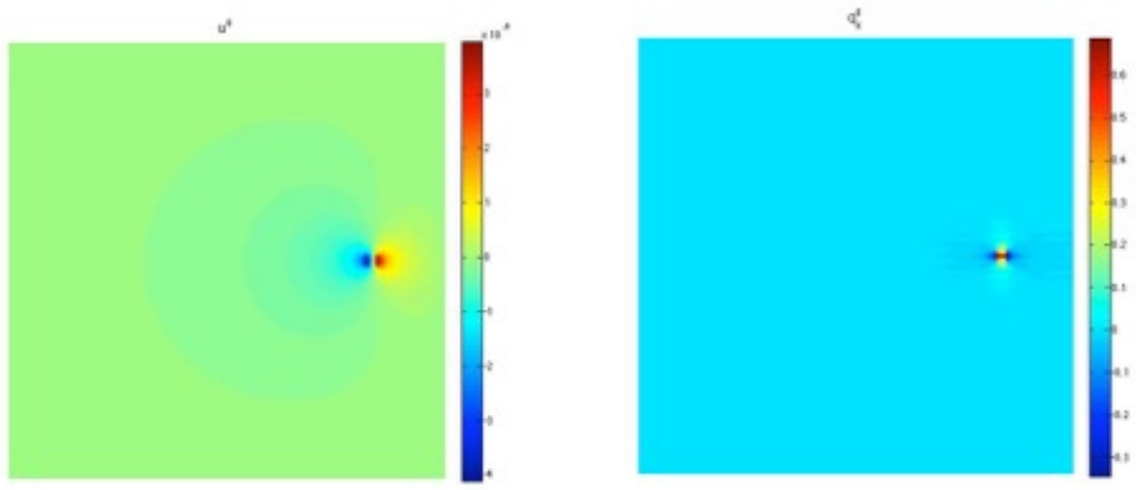


$$Q = \frac{1}{|\omega|}\int_\omega q_1 \qquad |\omega| = 4\varepsilon \times 4\varepsilon$$

Adjoint solution



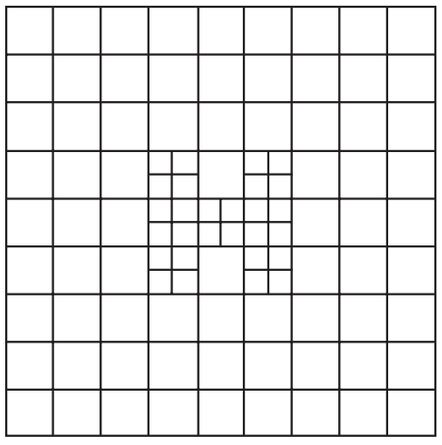
Case 1

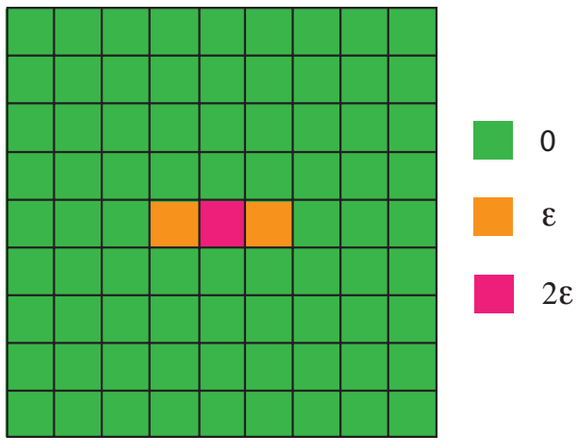


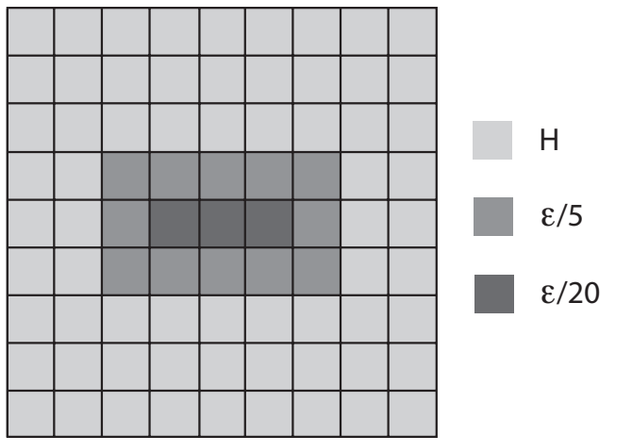
Case 2

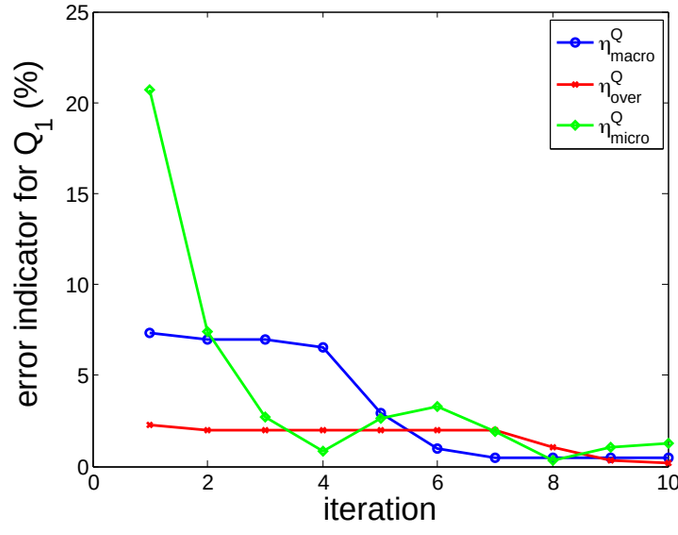
Illustration 1

Goal-oriented error control: case 1

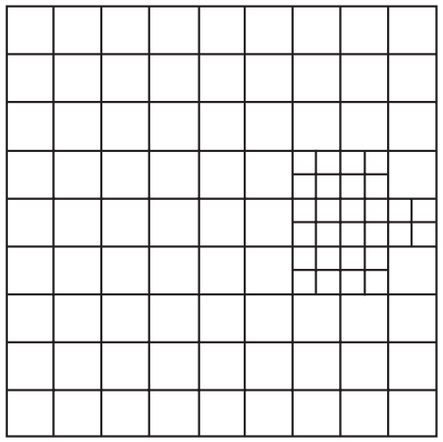


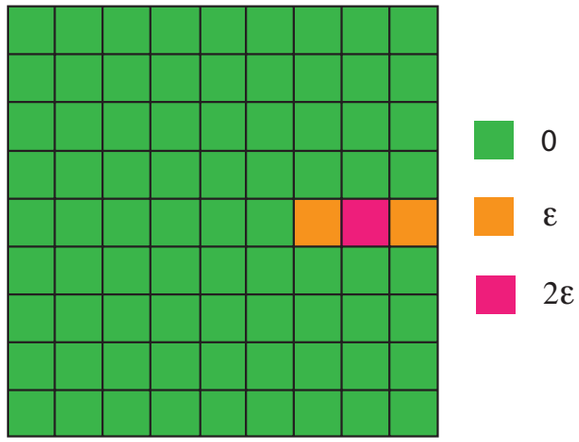


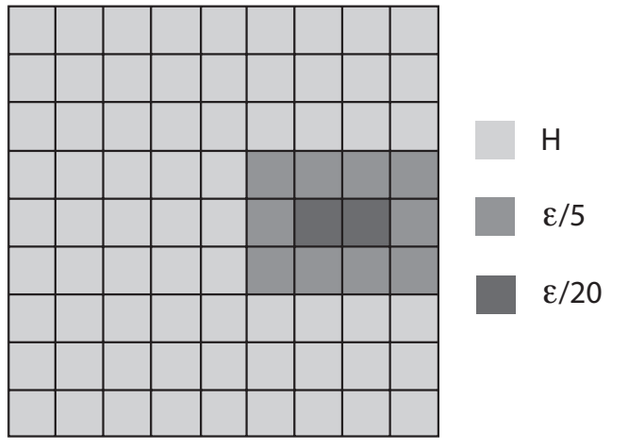


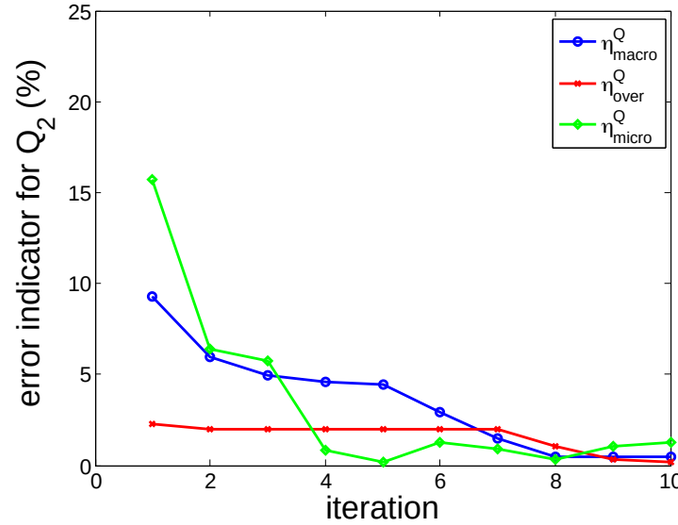


Goal-oriented error control: case 2

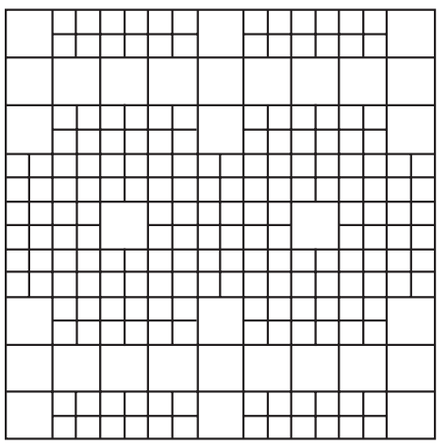


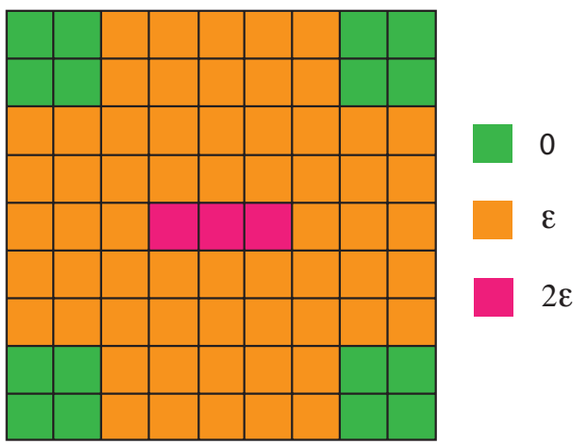






Global error control (error 5%)





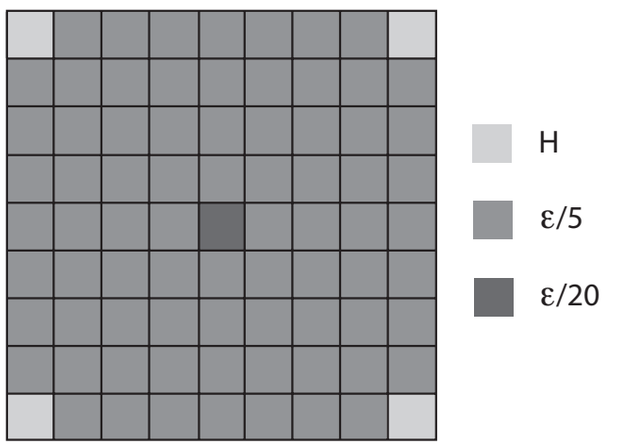
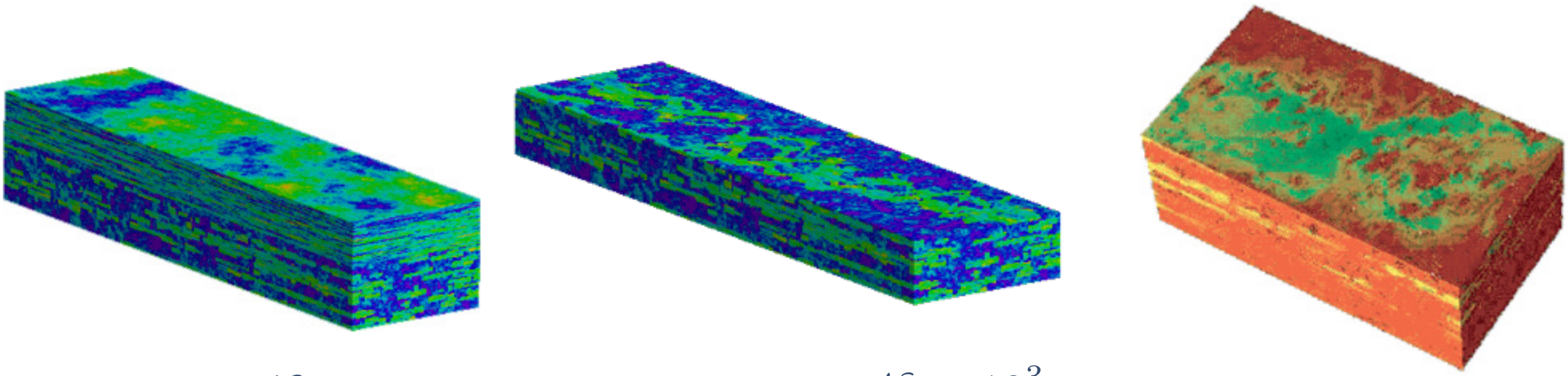


Illustration 2

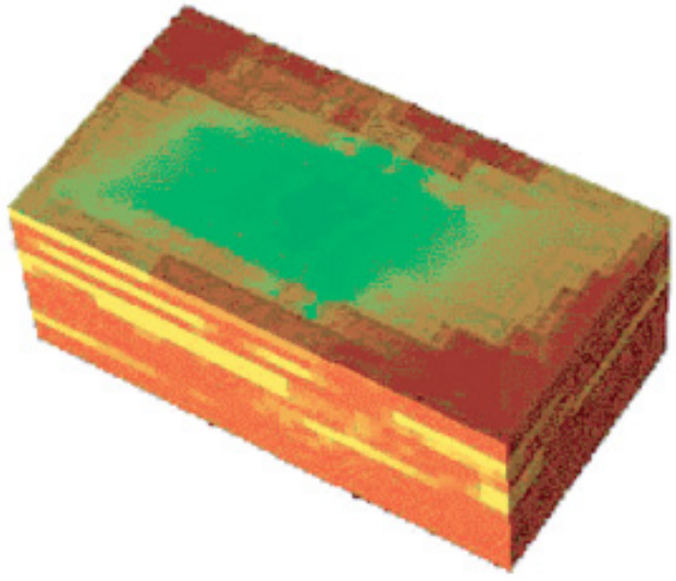
Gas injection in a two-phase (oil, gas) medium [Society of Petroleum Engineers]

- Flow problem (Darcy) in a fractured porous medium
- 1.1 million-cell geostatistical model (60x220x85 cells, 20x10x2 ft/cell)



high contrast: $A^\varepsilon = 1$ in brightest (yellow) zones, $A^\varepsilon = 10^3$ in darkest (blue) zones

water injected from a central sink, oil produced on 3 wells W_i



initial coarse mesh (10x25x

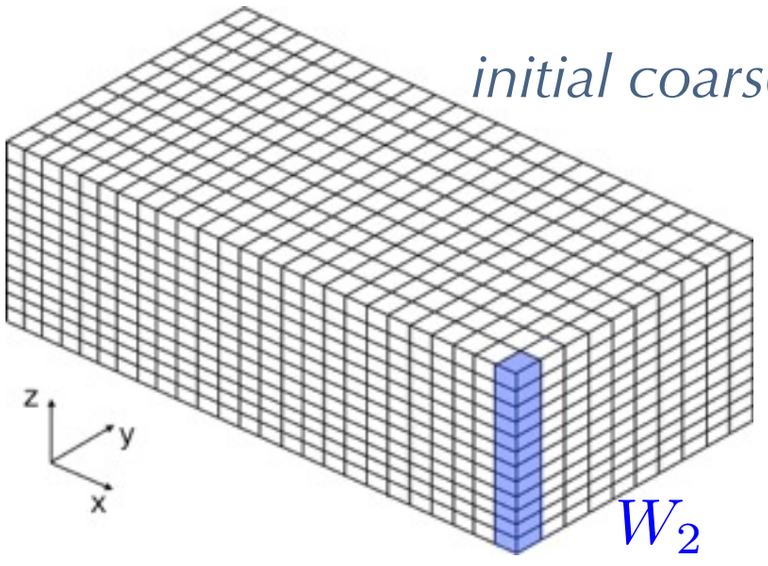
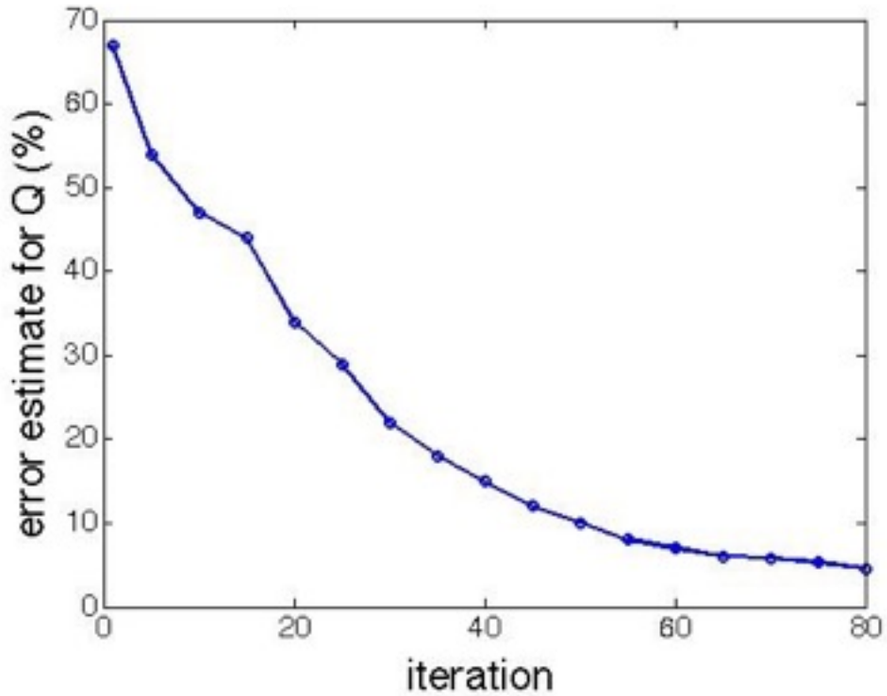


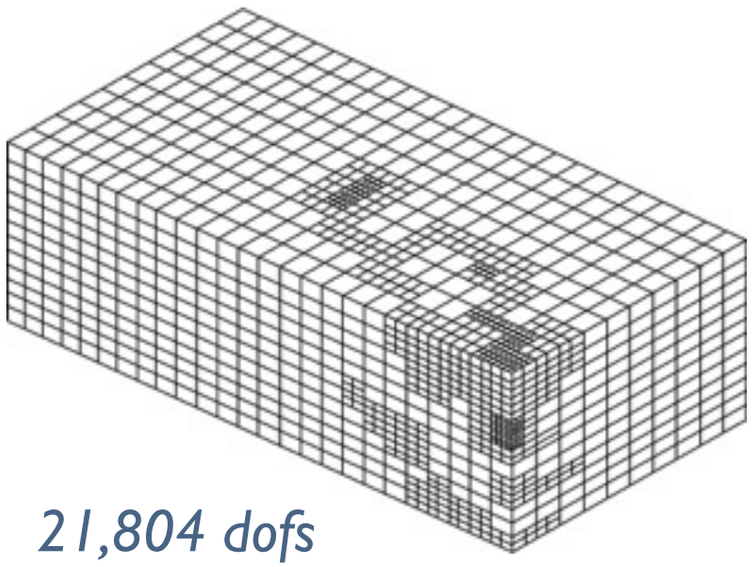
Illustration 2

$$Q = \frac{1}{|W_2|} \int_{W_2} u^{\varepsilon}$$ local pressure average

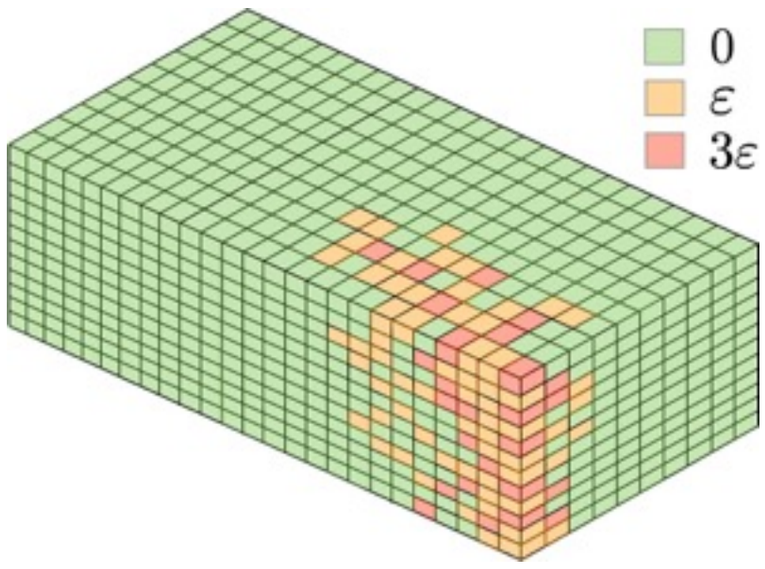
initial error: 67% ⟶ reduced to 6% (speed-up of 37)

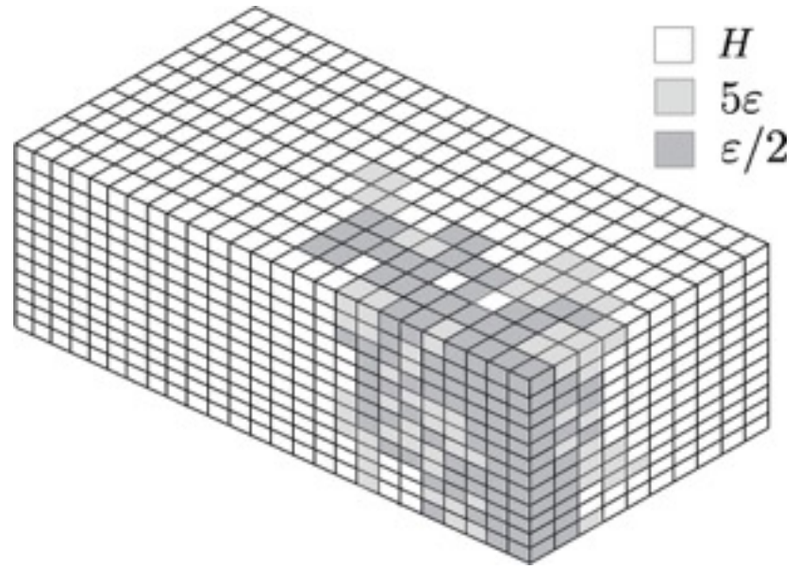
effectivity index between 1.18 and 1.11





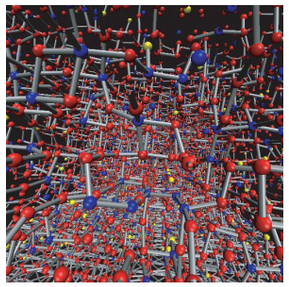
21,804 dofs

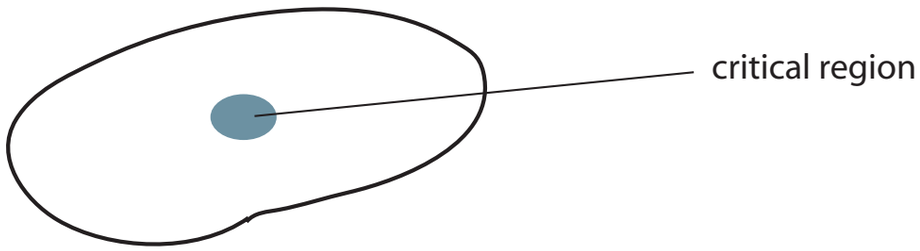




Outline

- **Motivation**
- **Theoretical aspects of goal-oriented error estimation in FEM**
- **Some applications**
- **Extensions to modeling error (multiscale analysis, model coupling)**

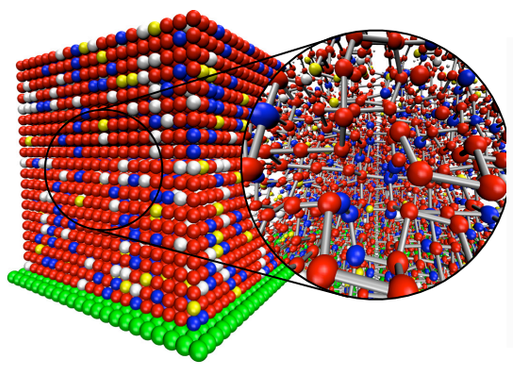


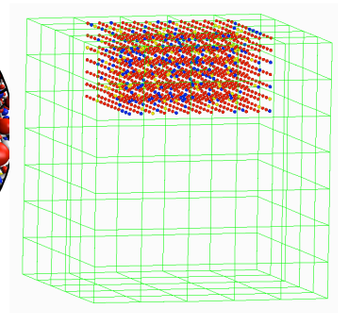


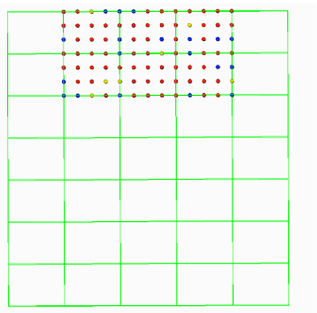
Model Upscaling

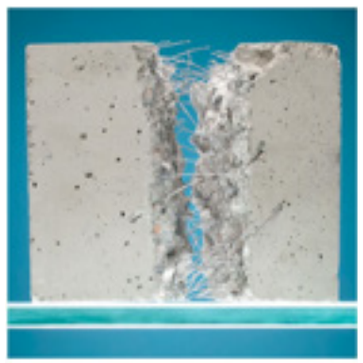
→ reduction of the complexity of the model

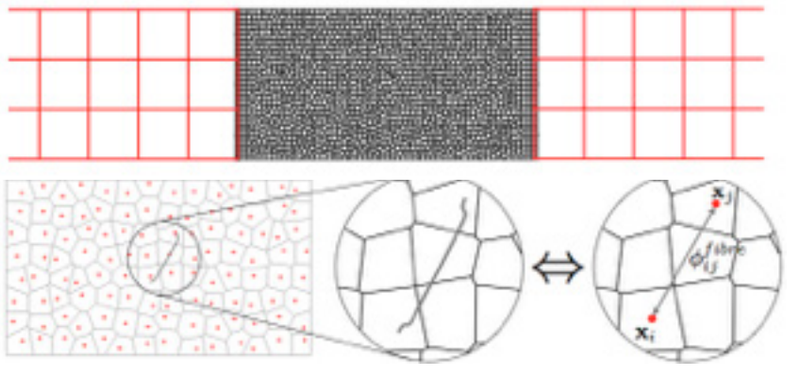
Example : particle/continuum coupling [Oden *et al.* 10, Marchais *et al.* 14]











reference model : $u \in V \quad ; \quad B(u;v) = F(v) \quad \forall v \in V$

surrogate model : $u_0 \in V \quad ; \quad B_0(u_0;v) = F(v) \quad \forall v \in V$

reference adjoint model : $p \in V \quad ; \quad B'(u;v,p) = Q'(u;v) \quad \forall v \in V$

$$e_0 = u - u_0$$
$$\epsilon_0 = p - p_0$$

→

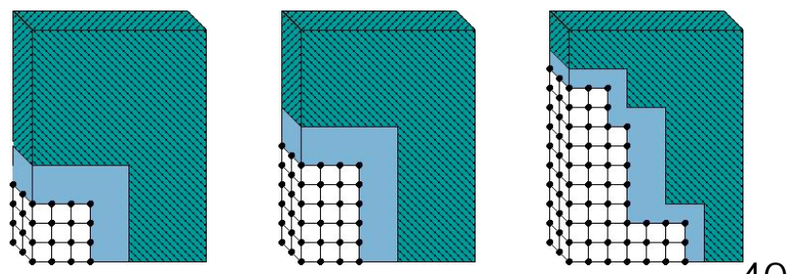
$$Q(u) - Q(u_0) = \underbrace{R(u_0;p)}_{F(p) - B(u_0;p)} + \Delta$$

error indicator

higher order terms

[Oden *et al.* 02]

→ adaptive modeling

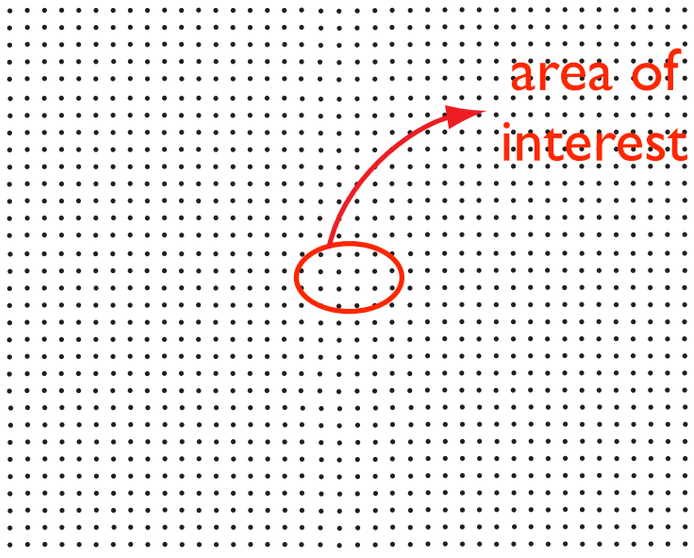


Rem: error estimation strategy depends on the problem…

$$Q(u) - Q(u_0^h) = [Q(u) - Q(u_0)] + [Q(u_0) - Q(u_0^h)]$$

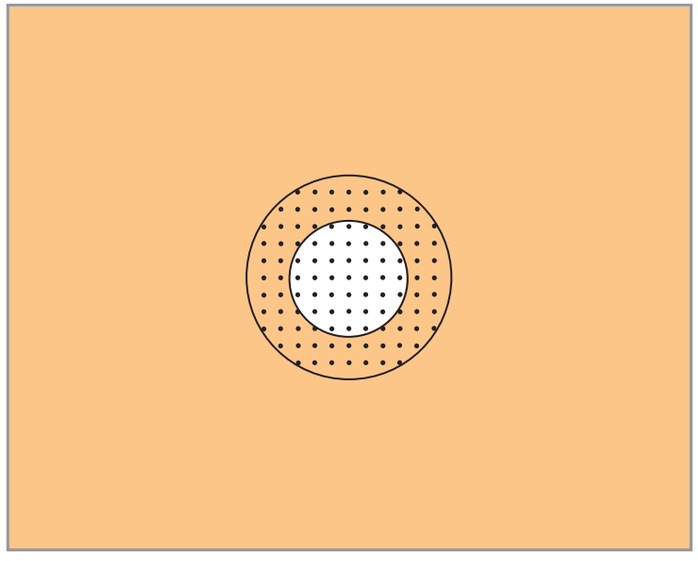
Models

particle scale (intractable)



upscaling

surrogate model (particle+continuum)



$$B(\mathbf{z};\mathbf{w}) = F(\mathbf{w}) \quad \forall \mathbf{w} \in V$$

$$\sum_{i=1}^{N_p} \frac{\partial E(\mathbf{z})}{\partial \mathbf{z}_i} \cdot \mathbf{w}_i \qquad E(\mathbf{z}) = \frac{1}{2}\sum_{i=1}^{N_p}\sum_{j=1}^{N_p} V_{ij}(\mathbf{z}_i,\mathbf{z}_j) \approx \frac{1}{2}\sum_{i=1}^{N_p}\sum_{j\in\mathcal{N}_i} V_{ij}(\mathbf{z}_i,\mathbf{z}_j)$$

$$B_0(\mathbf{z}_0;\mathbf{w}) = F_0(\mathbf{w}) \quad \forall \mathbf{w} \in V$$

coupling using the Arlequin method
[Ben Dhia 2005]

Adjoint problem (linear)

Hessian →

$$B'(\mathbf{z};\mathbf{q},\mathbf{p}) = Q'(\mathbf{z};\mathbf{q}) \quad \forall \mathbf{q} \in V$$

→ approximated using a (richer) surrogate model ⟶ $\mathbf{p}_0$

Adaptive Algorithm

1. Set γ_{tol} (tolerance)
   γ_a (adaptation parameter)

2. Initiate $k = 1$

3. Solve the primal surrogate pb $\longrightarrow u_0^{(k)}$

4. Solve the adjoint surrogate pb $\longrightarrow p_0^{(k)}$

5. Compute the estimate $\eta_{est}^{(k)} = \mathcal{R}(u_0^{(k)}, p_0^{(k)})$

$$\left| \frac{\eta_{est}^{(k)}}{Q(u_0^{(k)})} \right| > \gamma_{tol}$$

Insert the fine model in zones for which contribution to $\eta_{est}^{(k)}$ is $\geq \gamma_a$

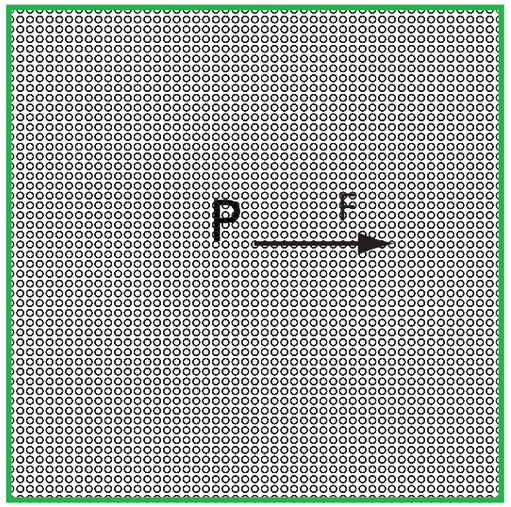
$k = k + 1$

$$\left| \frac{\eta_{est}^{(k)}}{Q(u_0^{(k)})} \right| \leq \gamma_{tol}$$

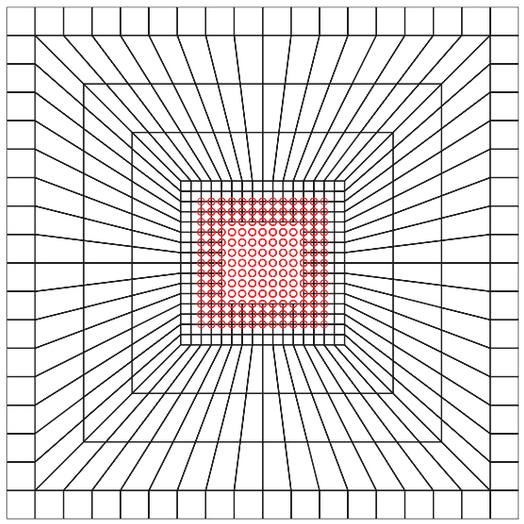
Keep surrogate model k

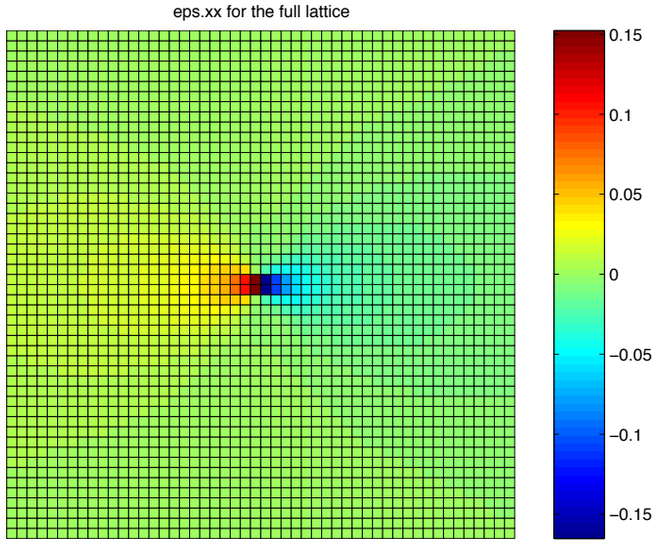
Control of modeling error

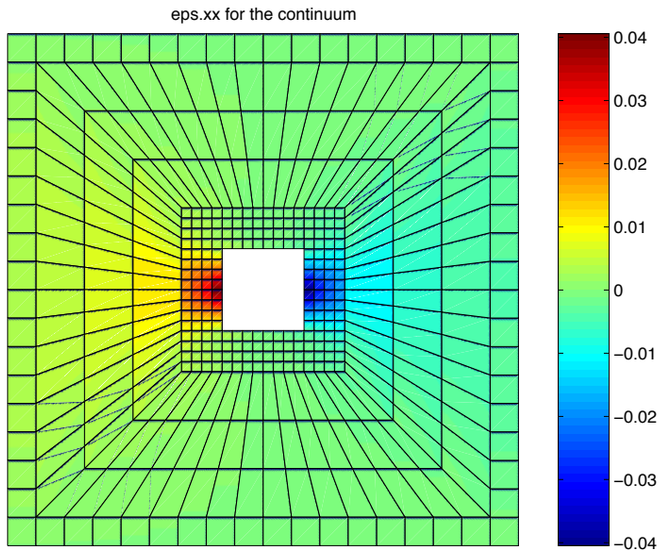
Reference model



Numerical model



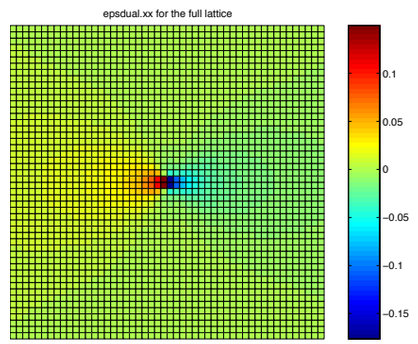


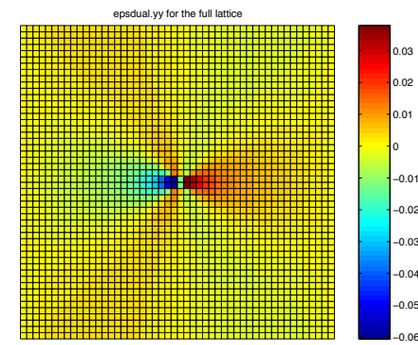


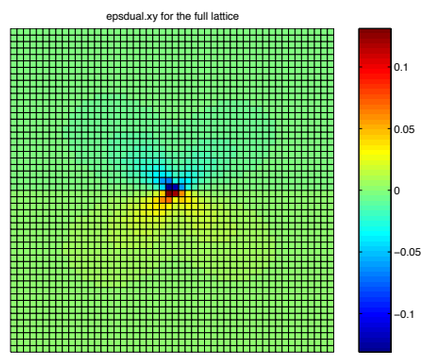
local error

$$Q(\mathbf{z}) = \mathbf{z}_P \cdot \mathbf{x}$$

adjoint solution



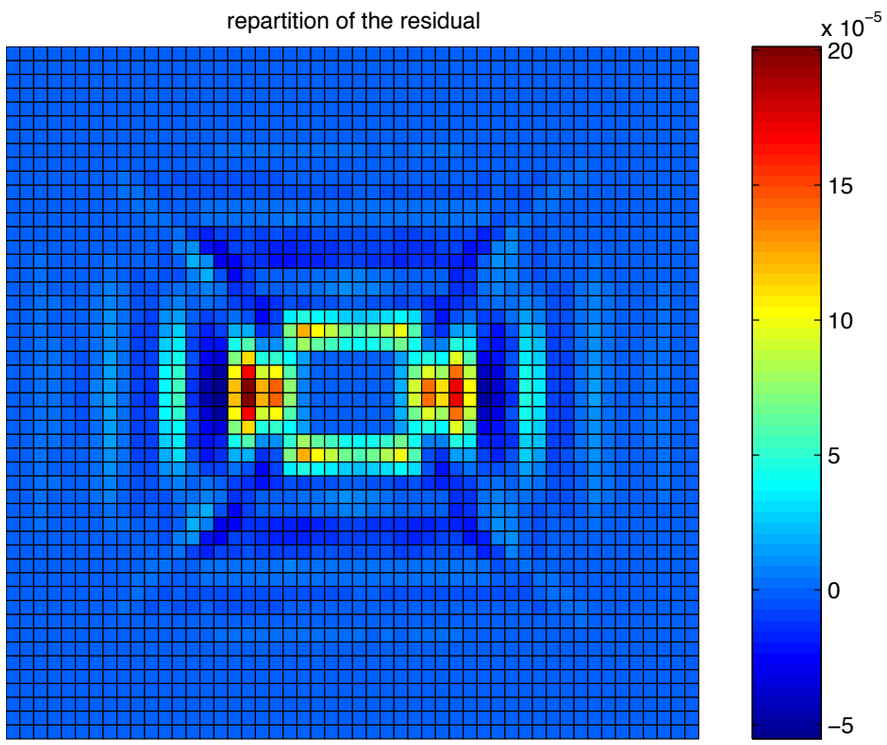




Control of modeling error

Error estimate [Oden & Prudhomme 02]

$$\varepsilon = Q(\mathbf{z}) - Q(\mathbf{z}_0) = R(\mathbf{z}_0; \mathbf{p}) + \Delta$$



$$Q(\mathbf{z}) = 0.1017 \qquad Q(\mathbf{z}_0) = 0.0941$$

$$\longrightarrow \varepsilon = 7\% \text{ of } Q(\mathbf{z})$$

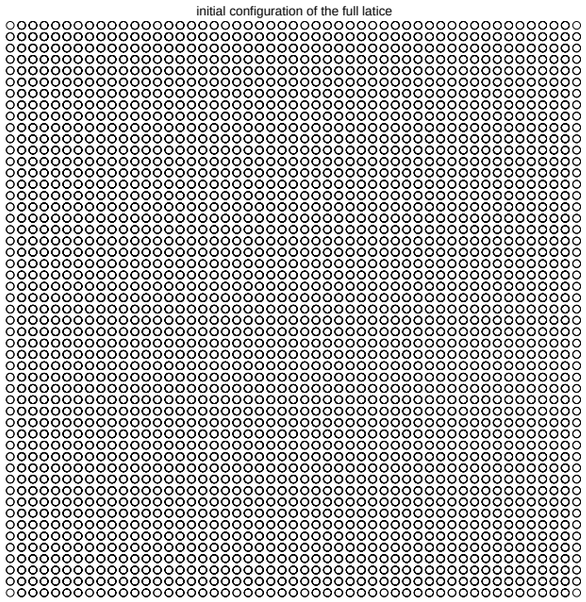
$$R(\mathbf{z}_0; \mathbf{p}) = 0.0076$$

$$\Delta = -7.71.10^{-8} = 0.001\% \text{ of } \varepsilon$$

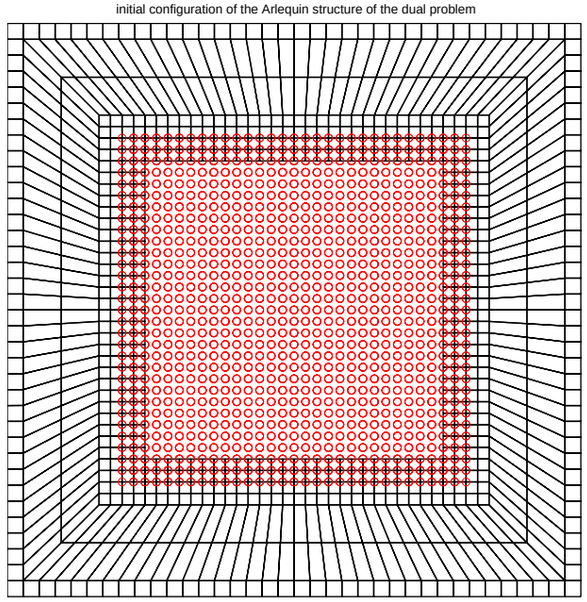
Control of modeling error

Approximate adjoint solution

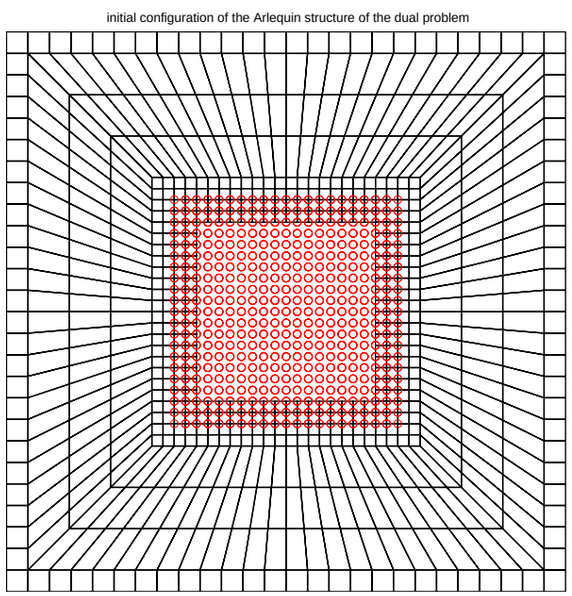
In practice, we approximate $\mathbf{p}$ with $\mathbf{p}_0^+$ $\Rightarrow$ $\varepsilon \approx R(\mathbf{z}_0; \mathbf{p}_0^+)$



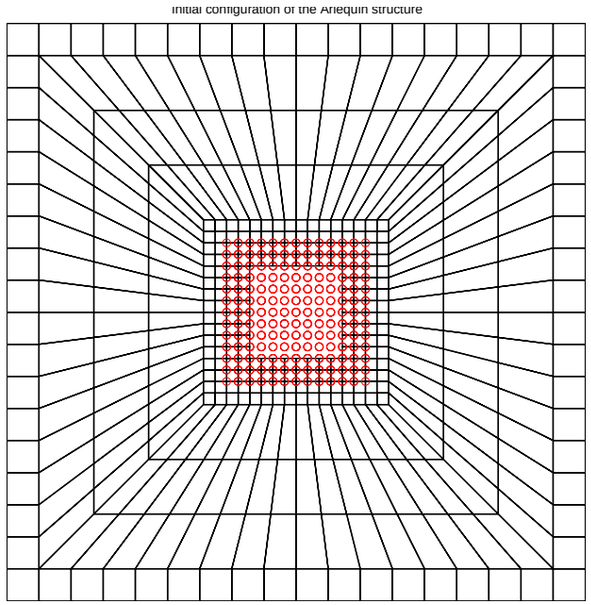
$R(\mathbf{z}_0; \mathbf{p}) = 0.0076$



$R(\mathbf{z}_0; \mathbf{p}_0^+) = 0.0073$



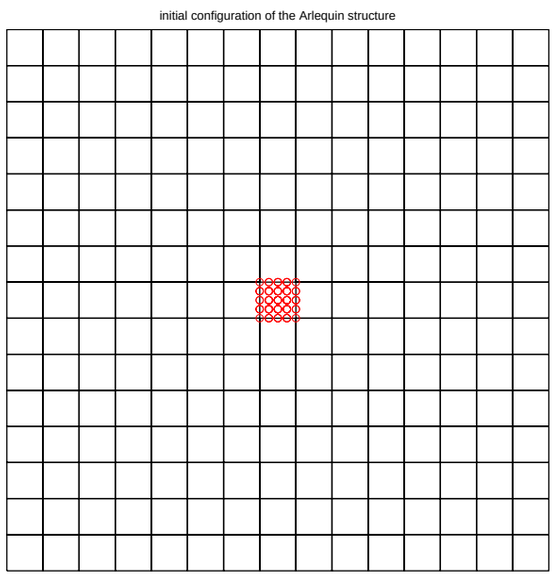
$R(\mathbf{z}_0; \mathbf{p}_0^+) = 0.0066$



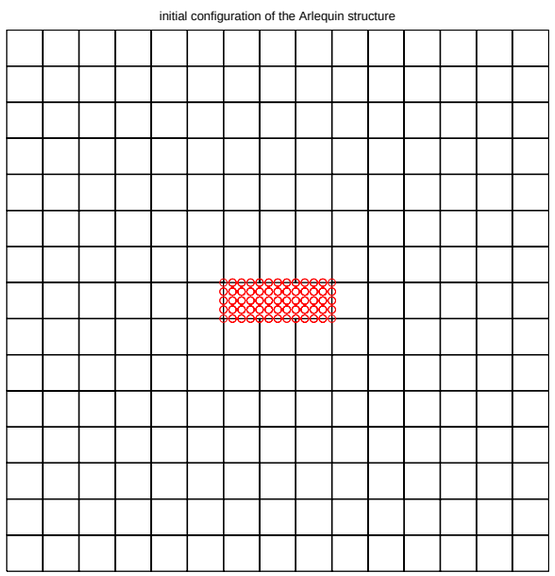
$R(\mathbf{z}_0; \mathbf{p}_0^+) = 0.0052$

Control of modeling error

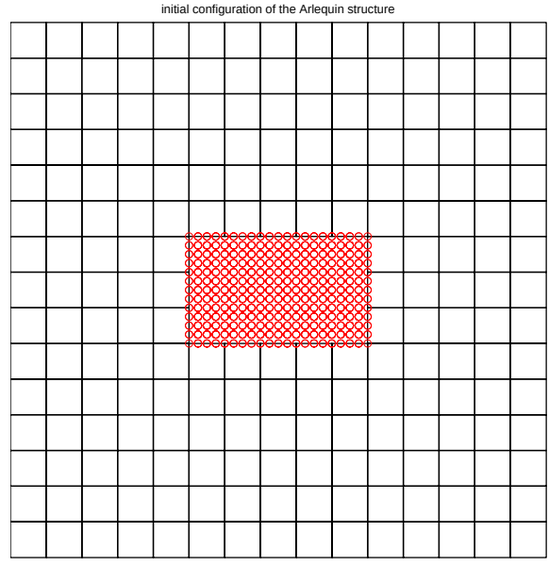
Implementation of the algorithm



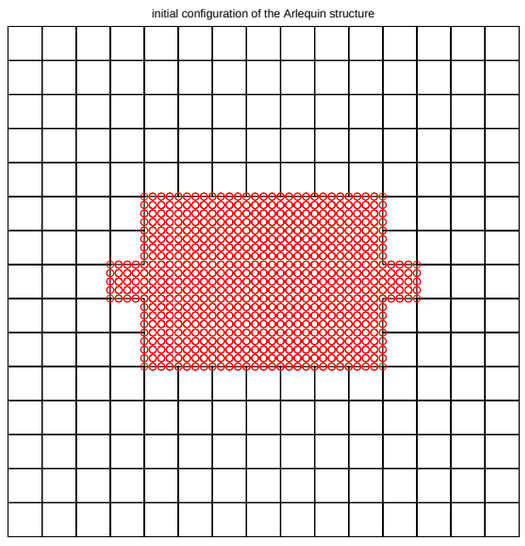
$\varepsilon = 1.71\%$



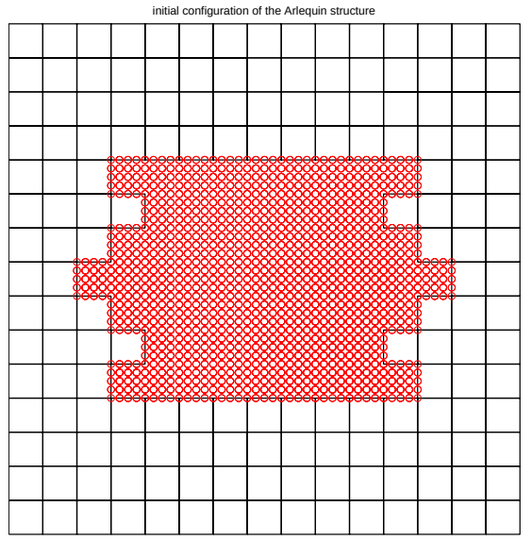
$\varepsilon = 6.13\%$



$\varepsilon = 3.33\%$



$\varepsilon = 2.03\%$

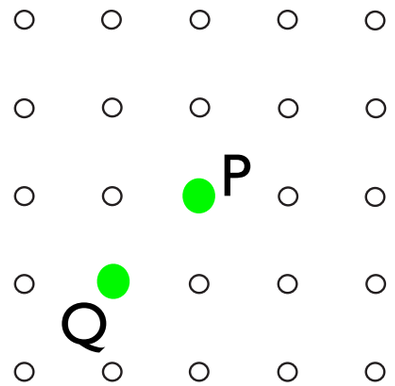


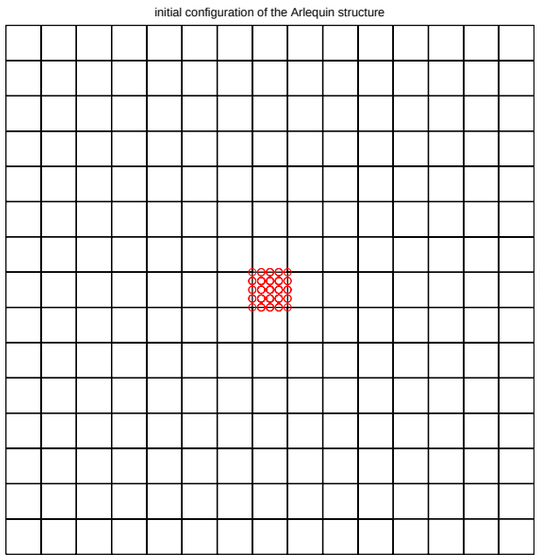
$\varepsilon = 1.21\%$

Control of modeling error

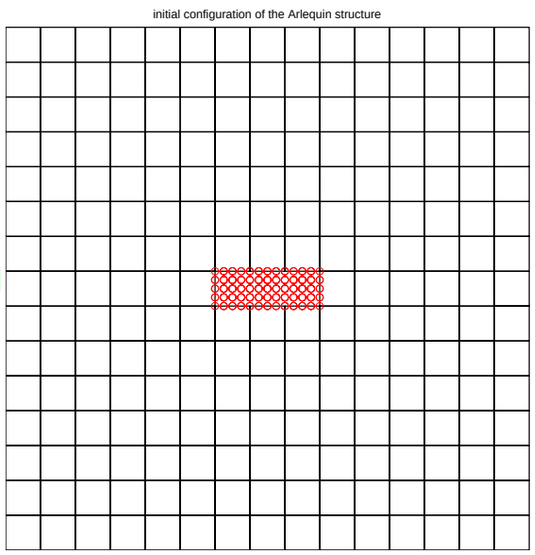
Implementation of the algorithm

QoI = stretch of the connexion PQ

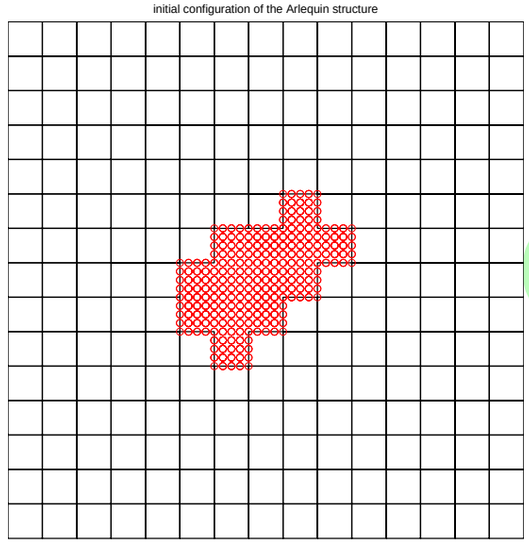




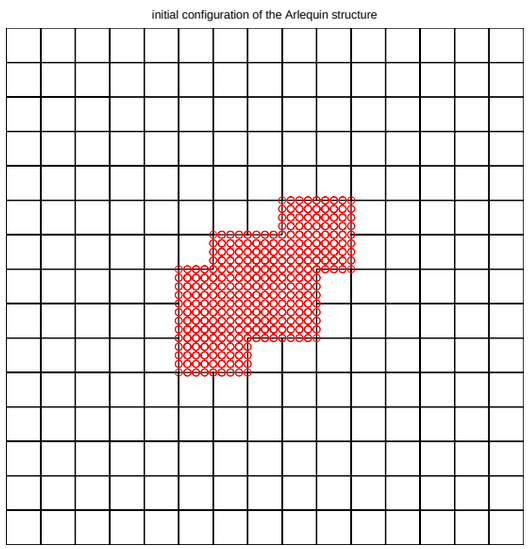
$\varepsilon = 2.98\%$



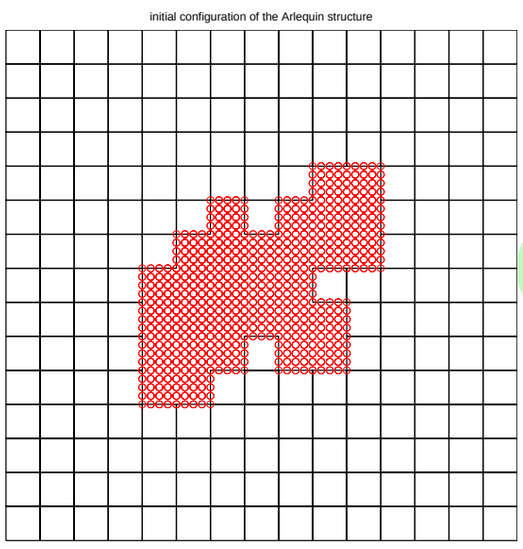
$\varepsilon = 0.74\%$



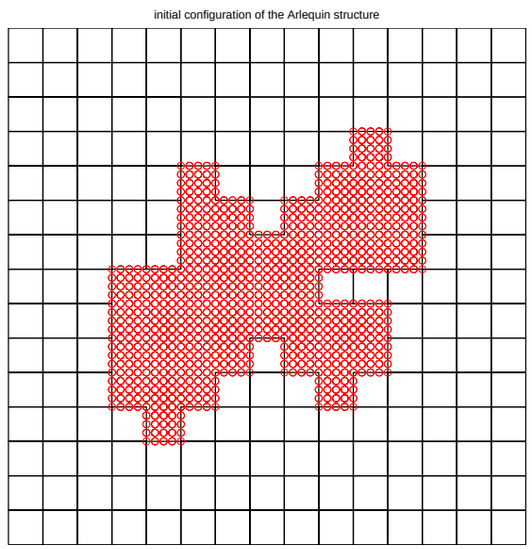
$\varepsilon = 0.11\%$



$\varepsilon = 0.064\%$



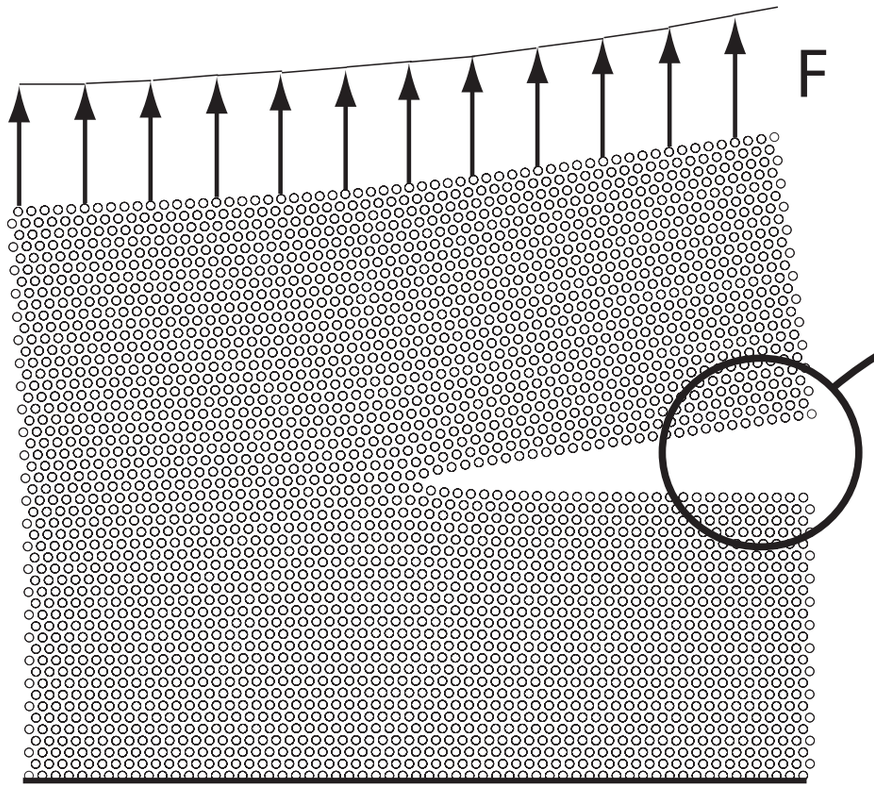
$\varepsilon = 0.034\%$

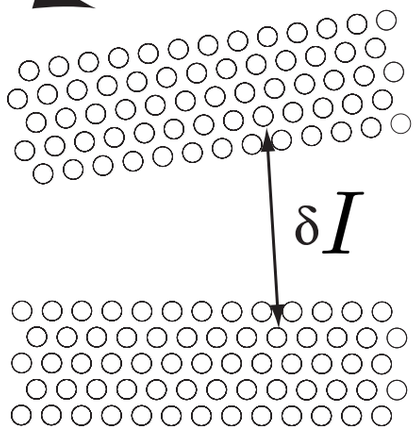


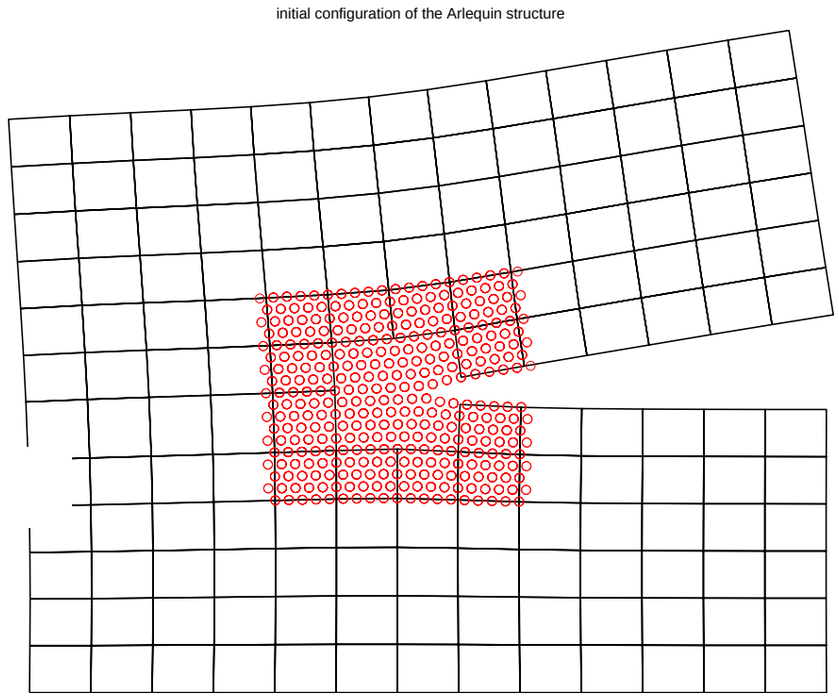
$\varepsilon = 0.003\%$

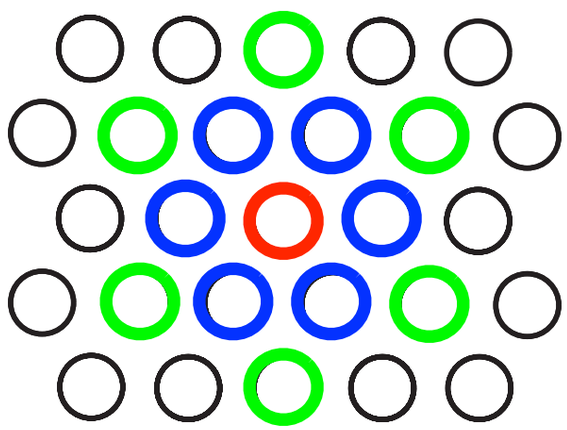
Other examples

Crack opening [Prudhomme et al. 09]





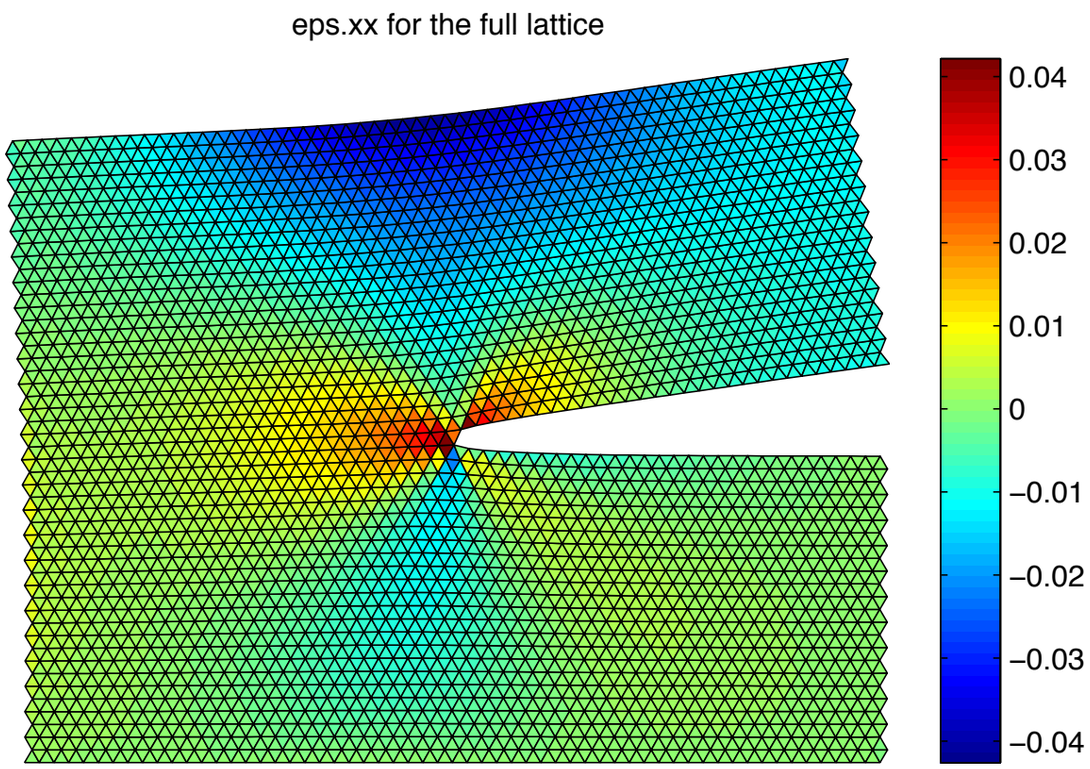




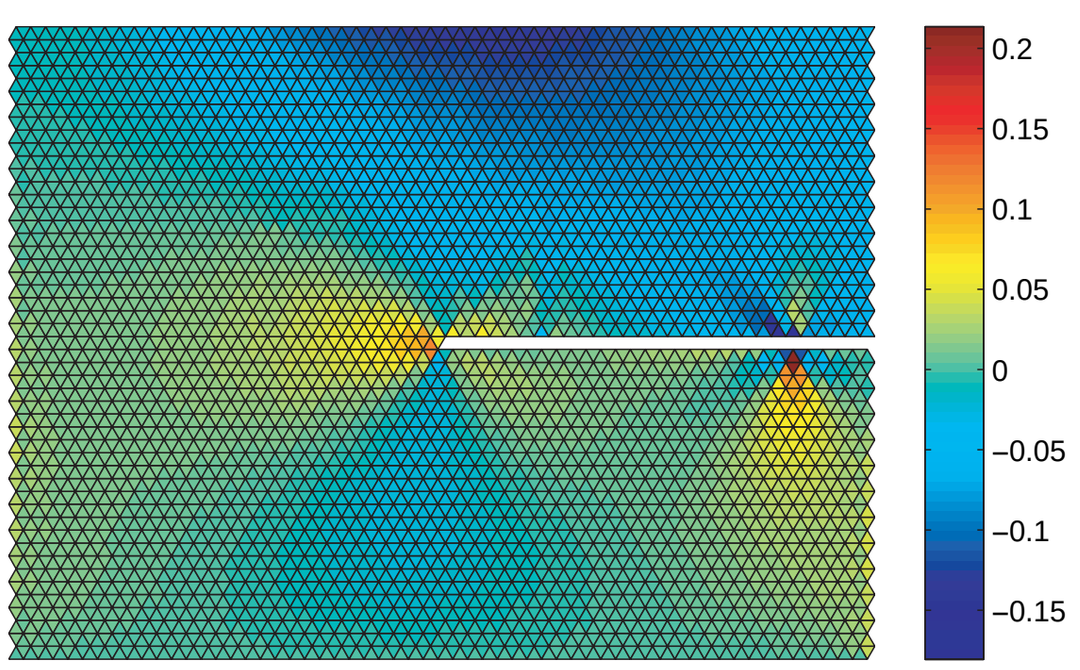
Other examples

Crack opening

Exact solution of both problems



reference problem

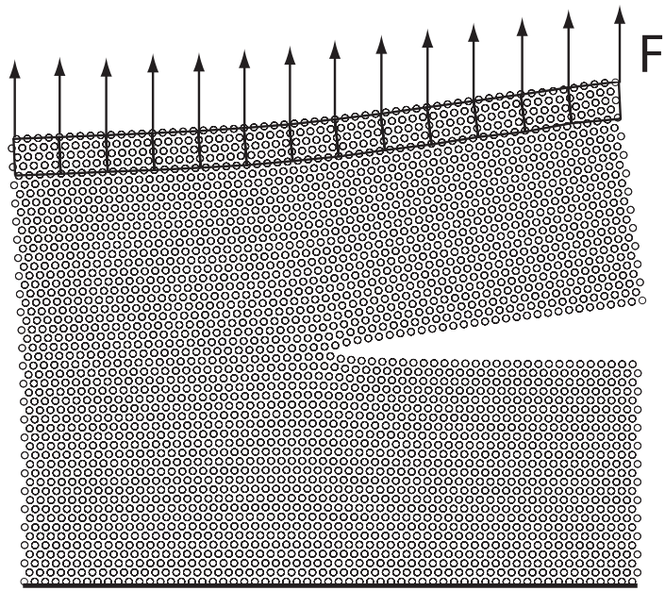


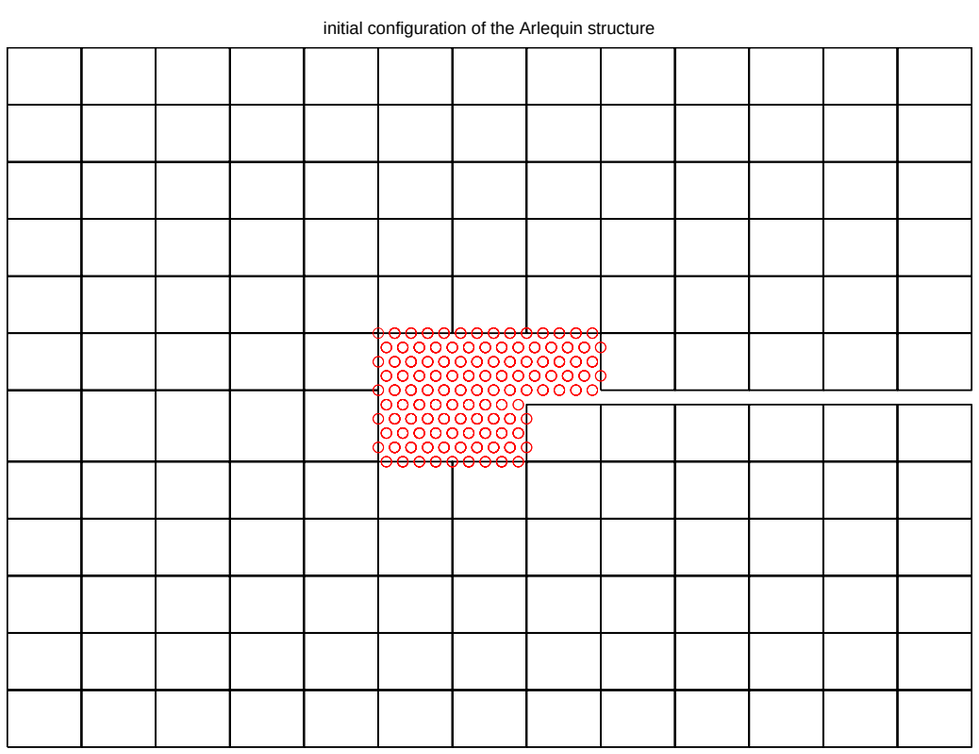
adjoint problem

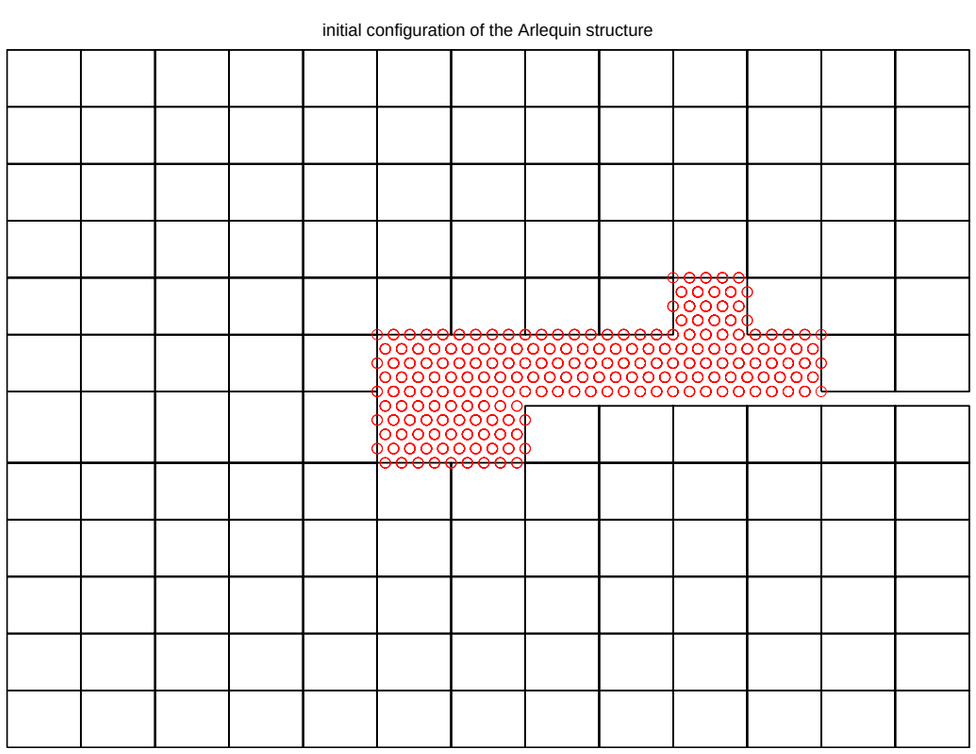
Other examples

Crack opening

Adaptive procedure



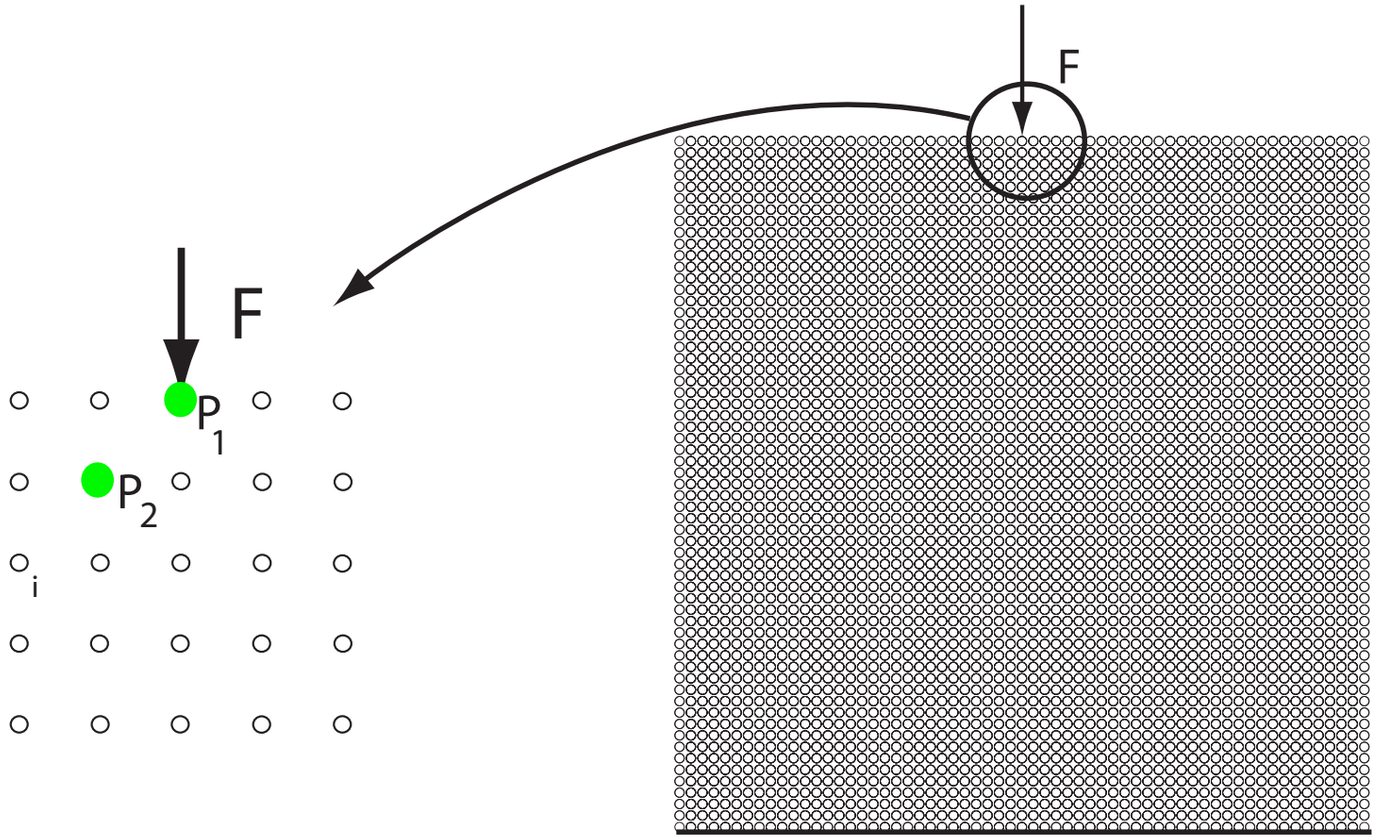


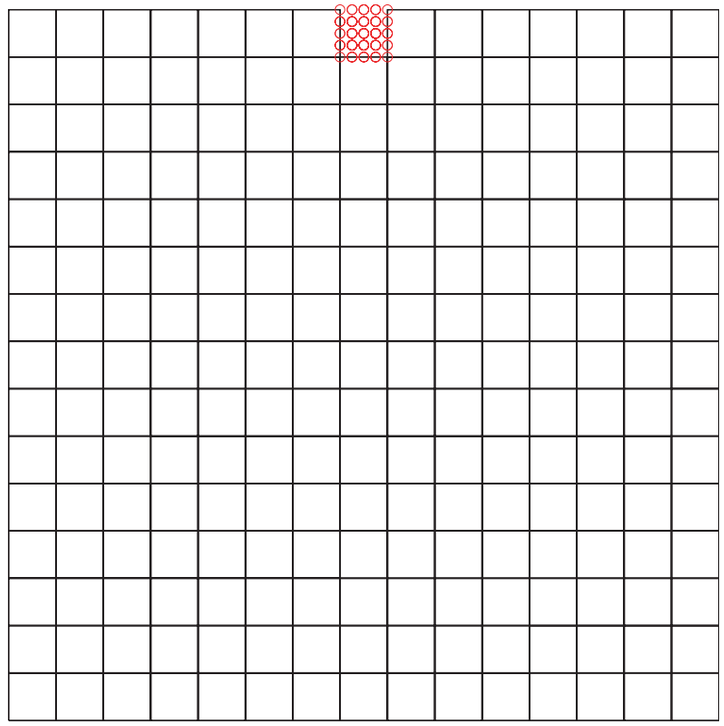


Error decreases from $\varepsilon = 12.4\%$ to $\varepsilon = 1.2\%$

Other examples

Nano-indentation [Prudhomme et al. 09]





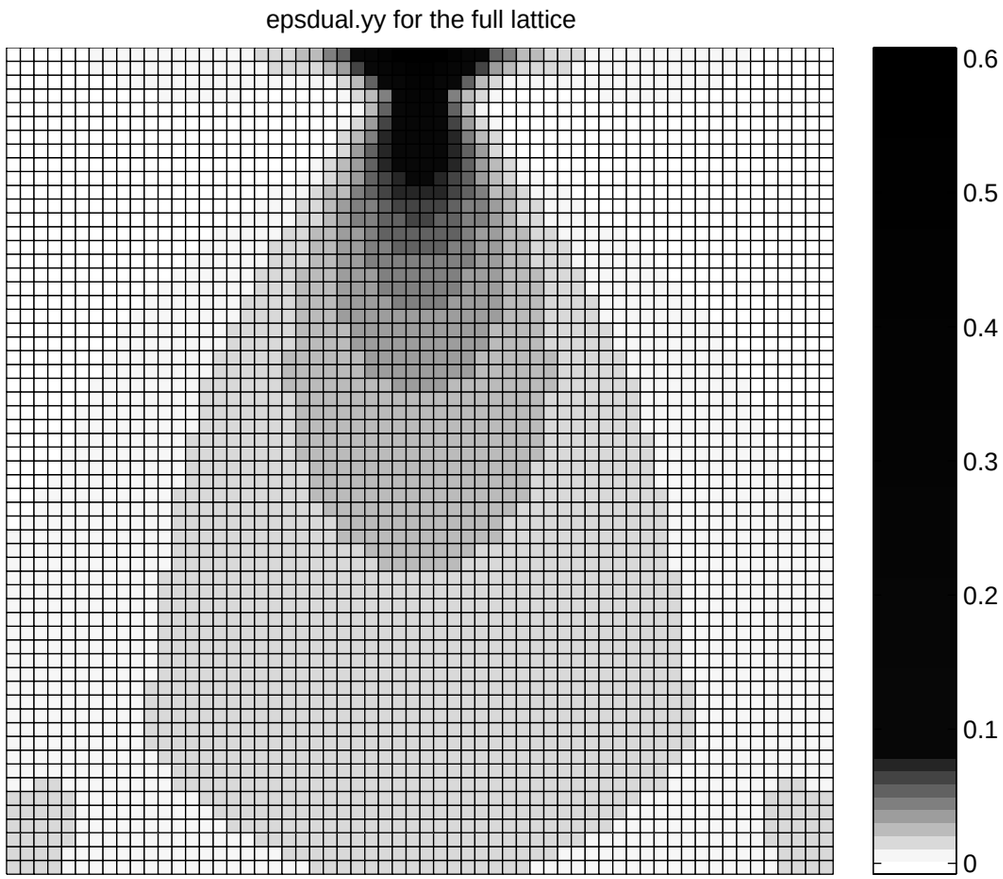
$Q_1 =$ vertical displacement of point P_1

$Q_2 =$ stretching of connexion $P_1 P_2$

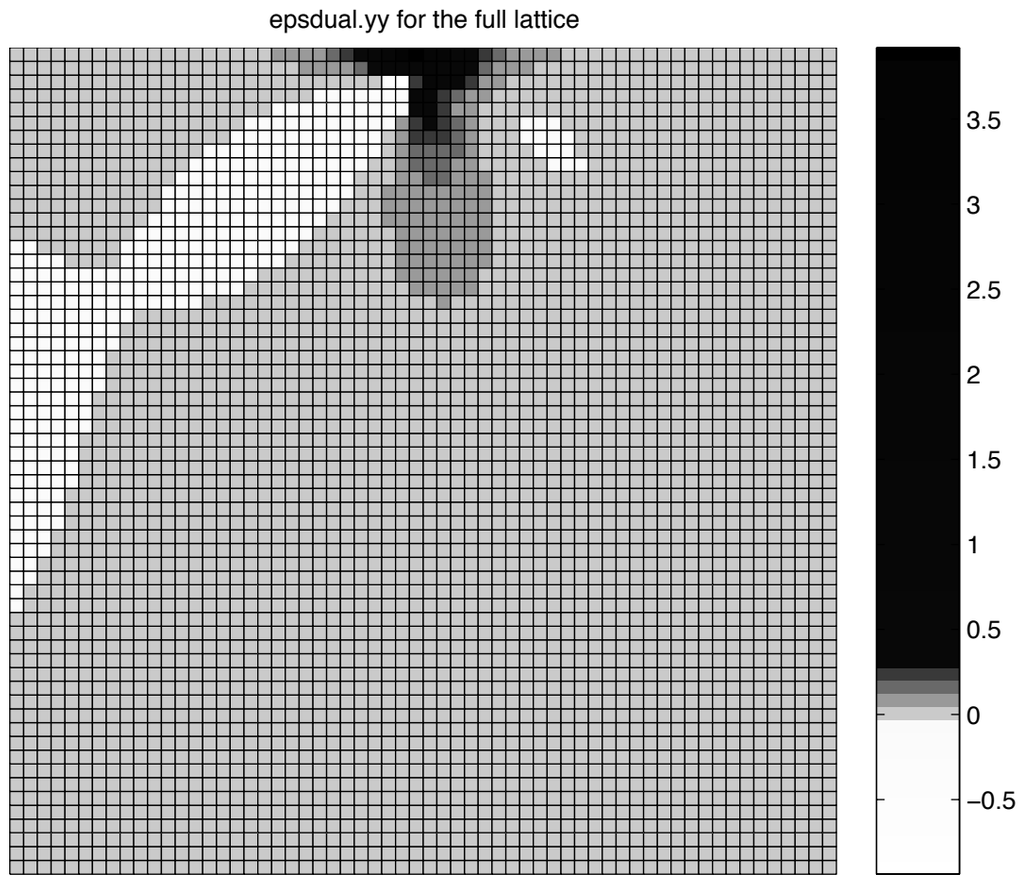
Other examples

Nano-indentation

Adjoint problem solution



for Q_1

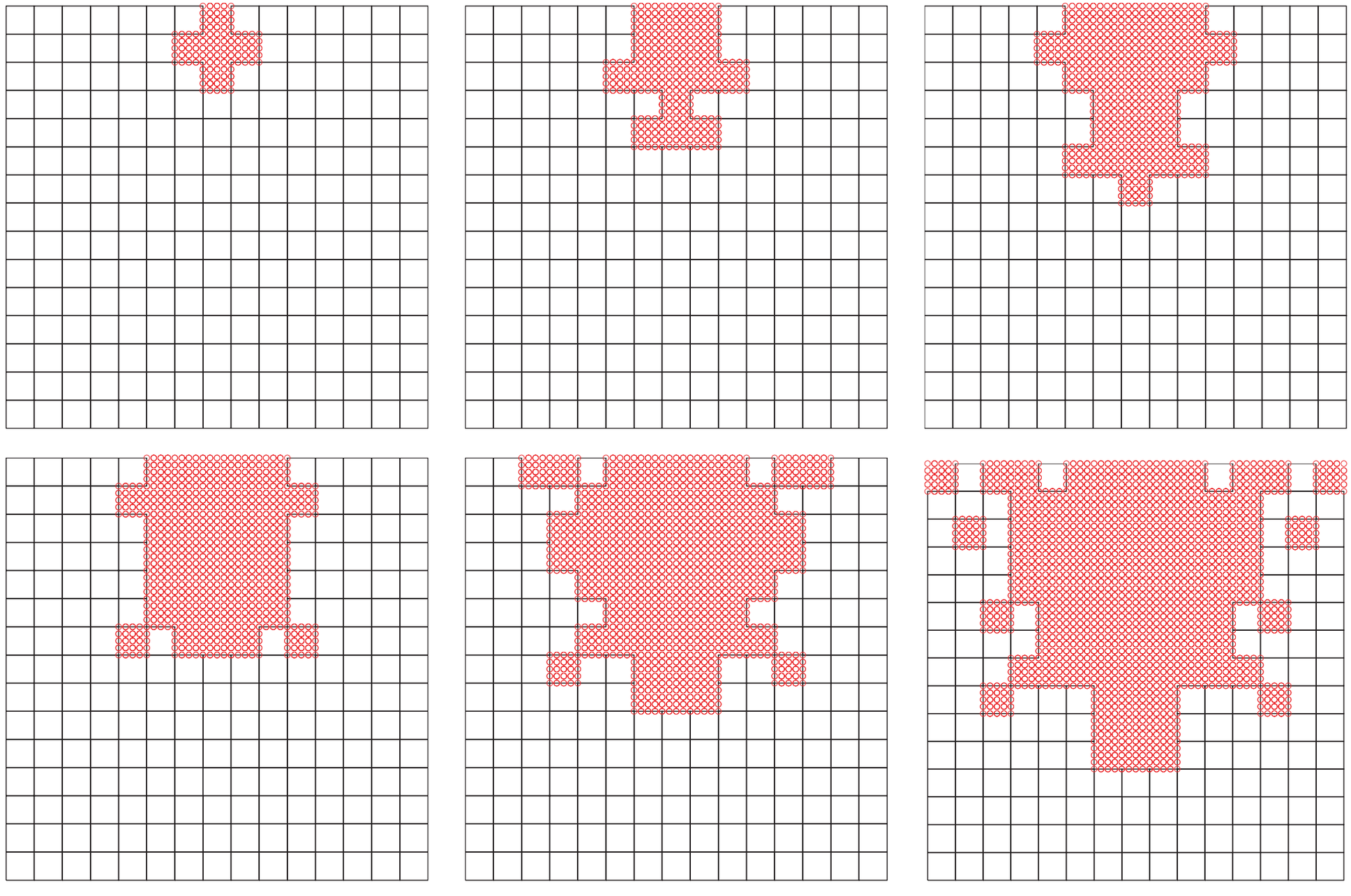


for Q_2

Other examples

Nano-indentation

Adaptivity for Q_1

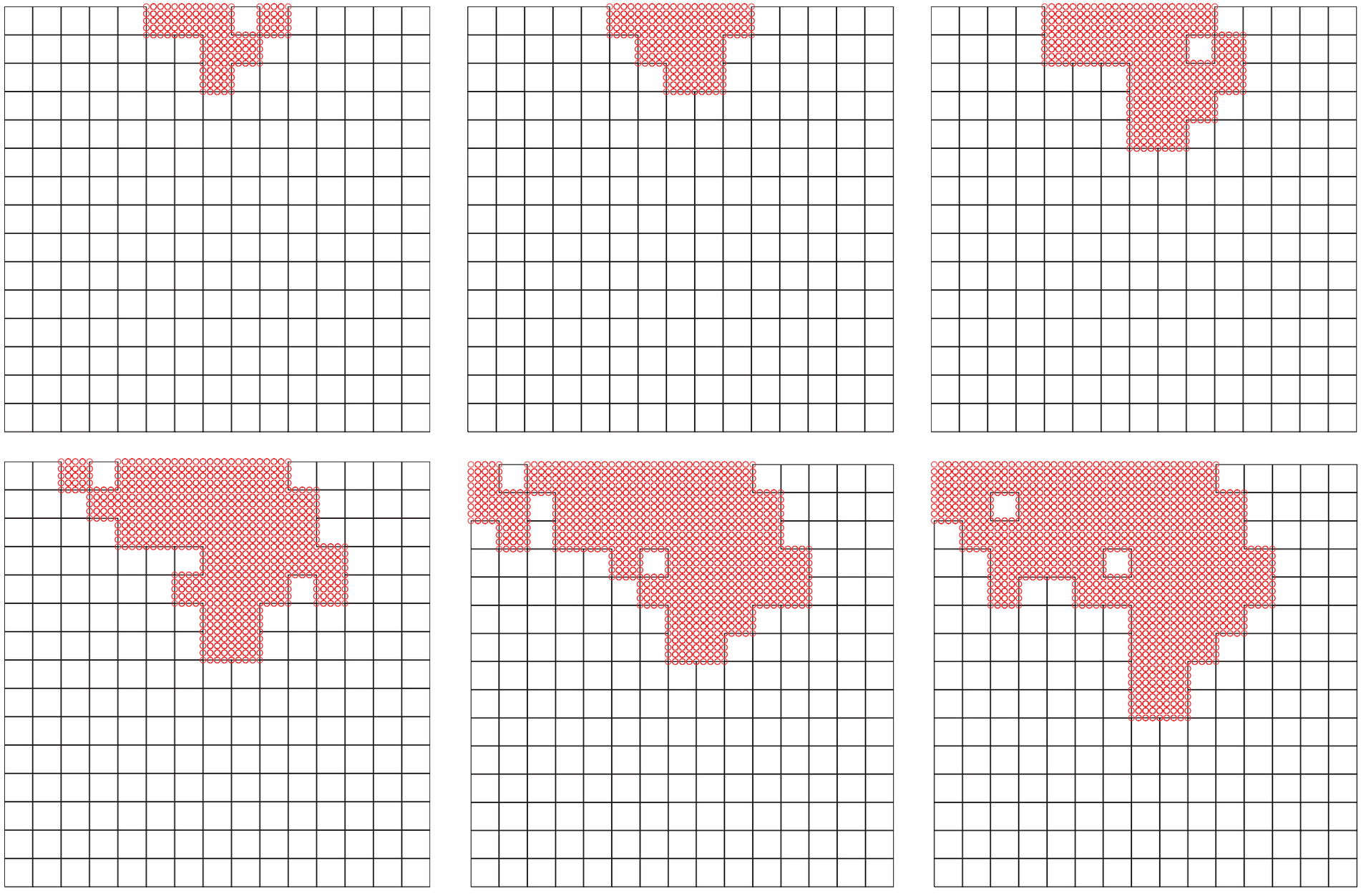


Error decreases from $\varepsilon = 7.4\%$ to $\varepsilon = 2.4\%$

Other examples

Nano-indentation

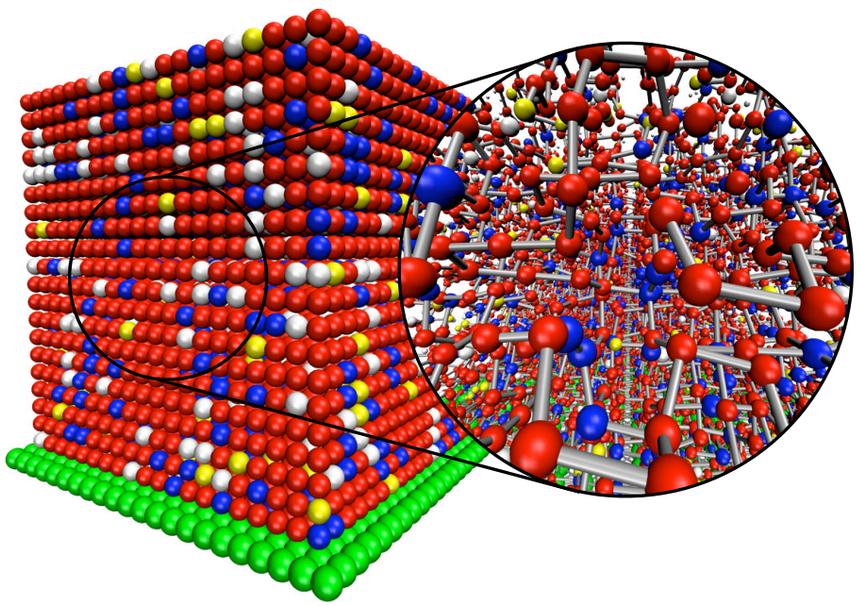
Adaptivity for Q_2

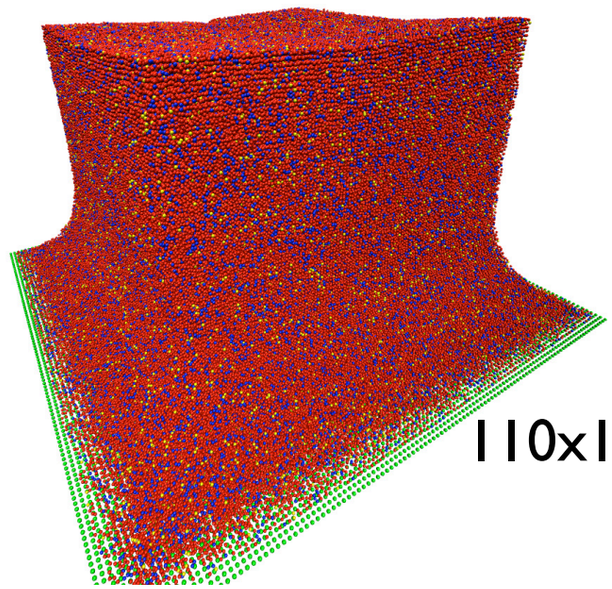


Error decreases from $\varepsilon = 3.9\%$ to $\varepsilon = 0.4\%$

Other examples

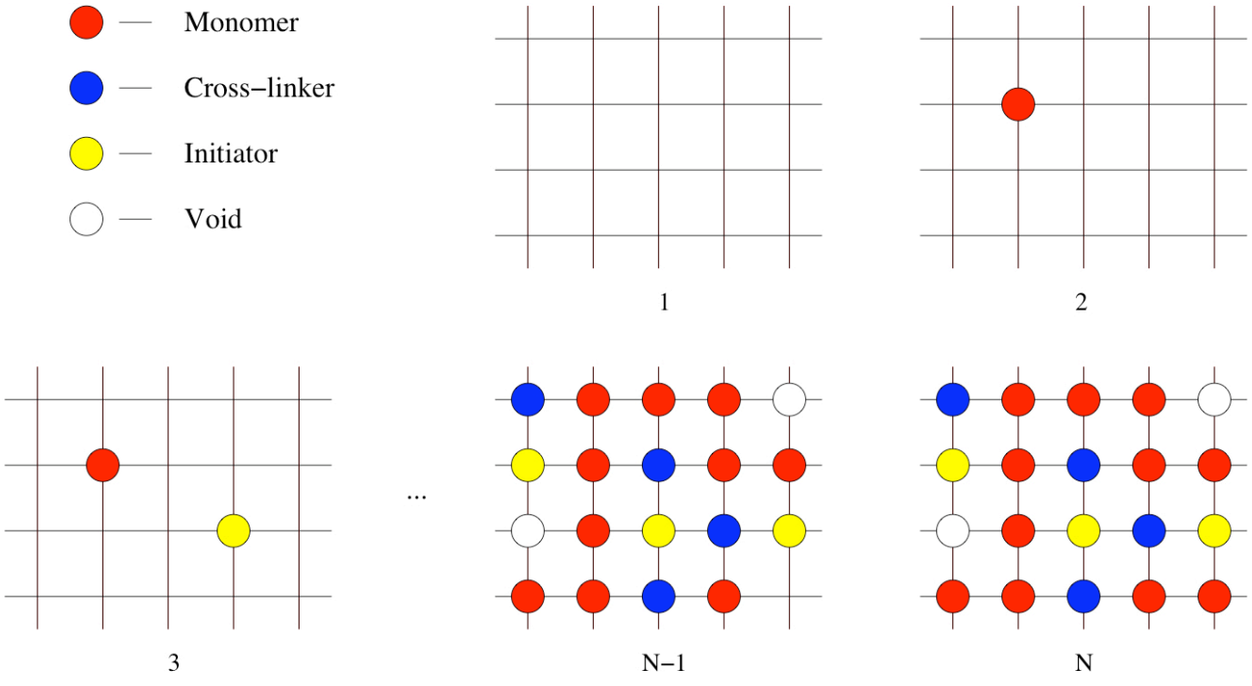
3D polymer structure [Bauman *et al.* 08]

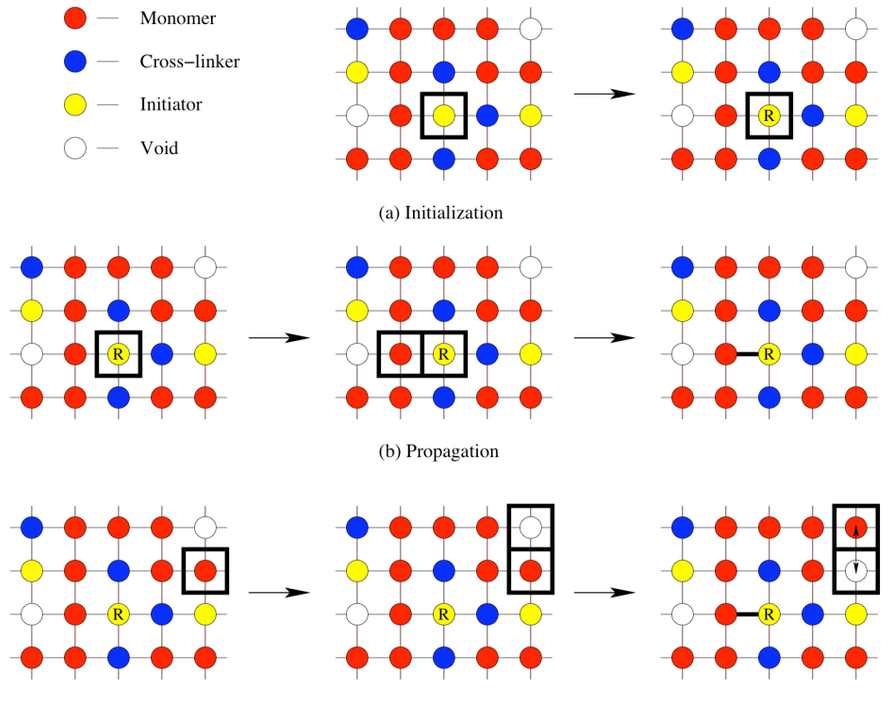




110x110x110 particles

simulation of polymerization using kinetic MC approach



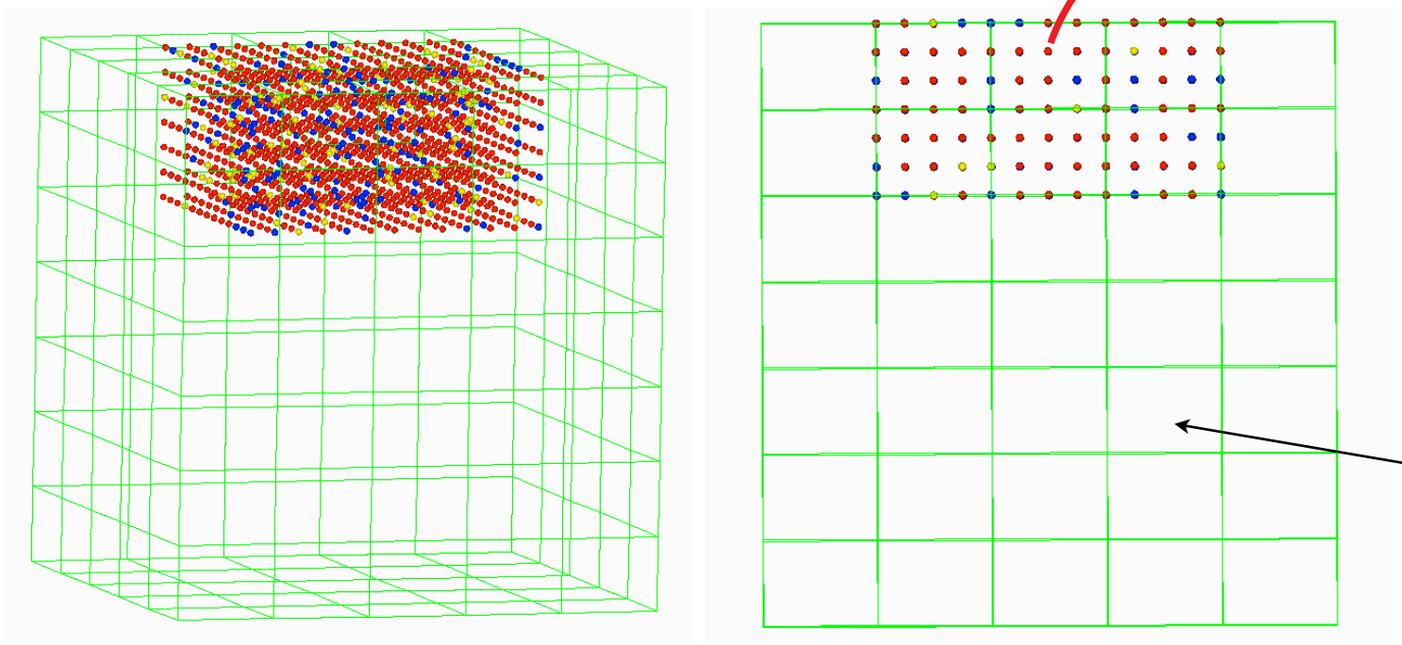


Other examples

3D polymer structure

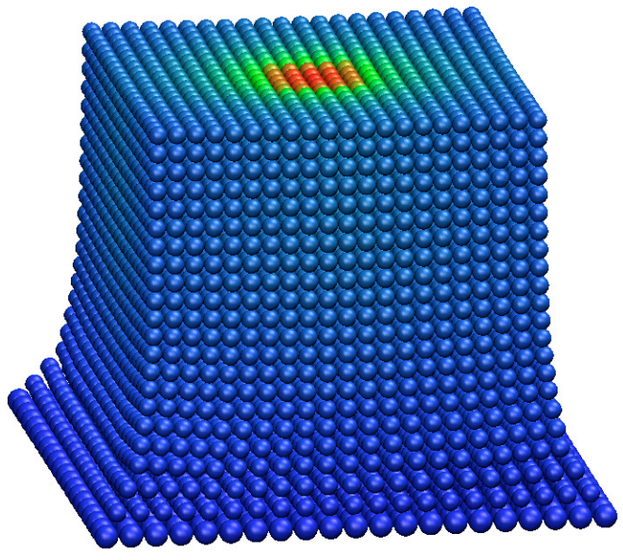
$$Q = \frac{1}{N} \sum_{i=1}^{N} \mathbf{z}_i \cdot \mathbf{y}$$

Simulation model



Mooney-Rivlin model

Adjoint problem solution

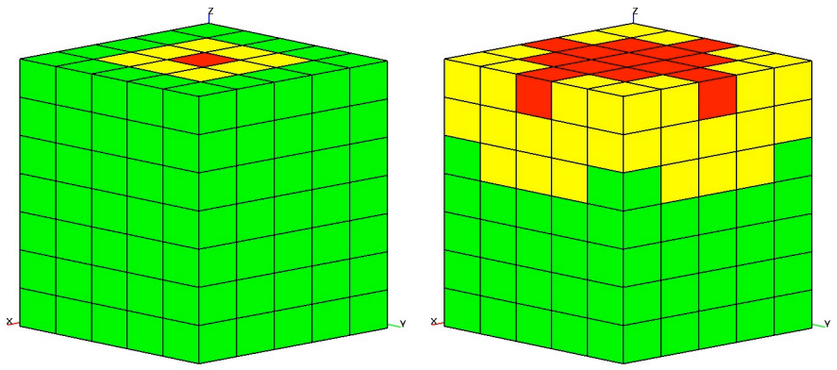


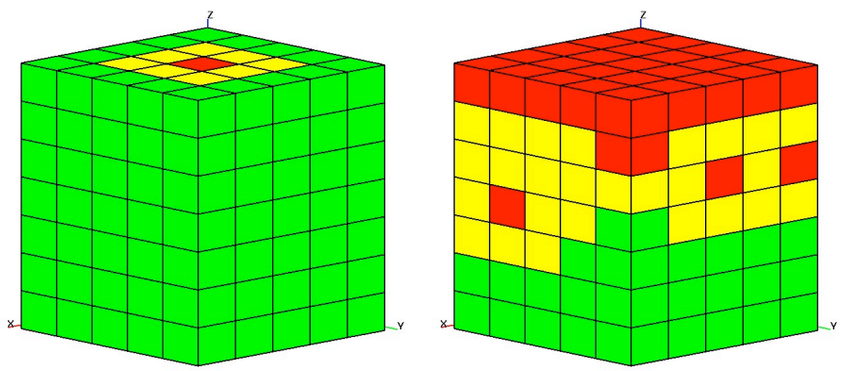
computation with dedicated algorithms (line search/trust region)

Other examples

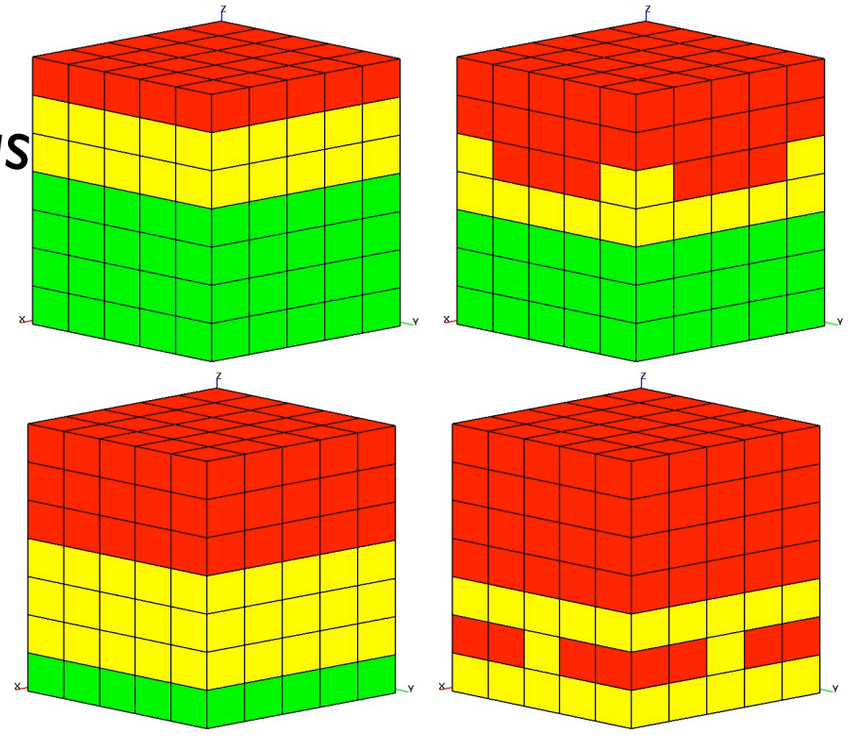
3D polymer structure

Adaptive procedure

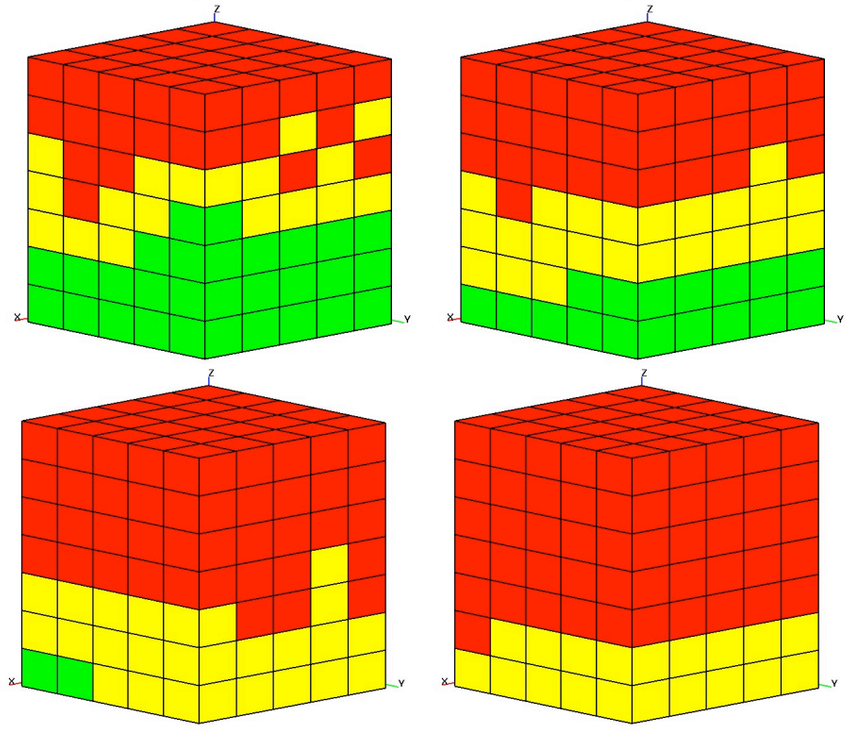




homogeneous network



polymer



$$\varepsilon = 31.8\% \longrightarrow \varepsilon = 4.1\%$$

$$\varepsilon = 42.2\% \longrightarrow \varepsilon = 5.3\%$$

Other examples

3D polymer structure

CPU cost

- 50x50x50 network : 375 000 dofs, 1.4 h CPU with 32 proc. (*particle model*)
  18 228 dofs, 5 min with 1 proc. (*coupled model*)

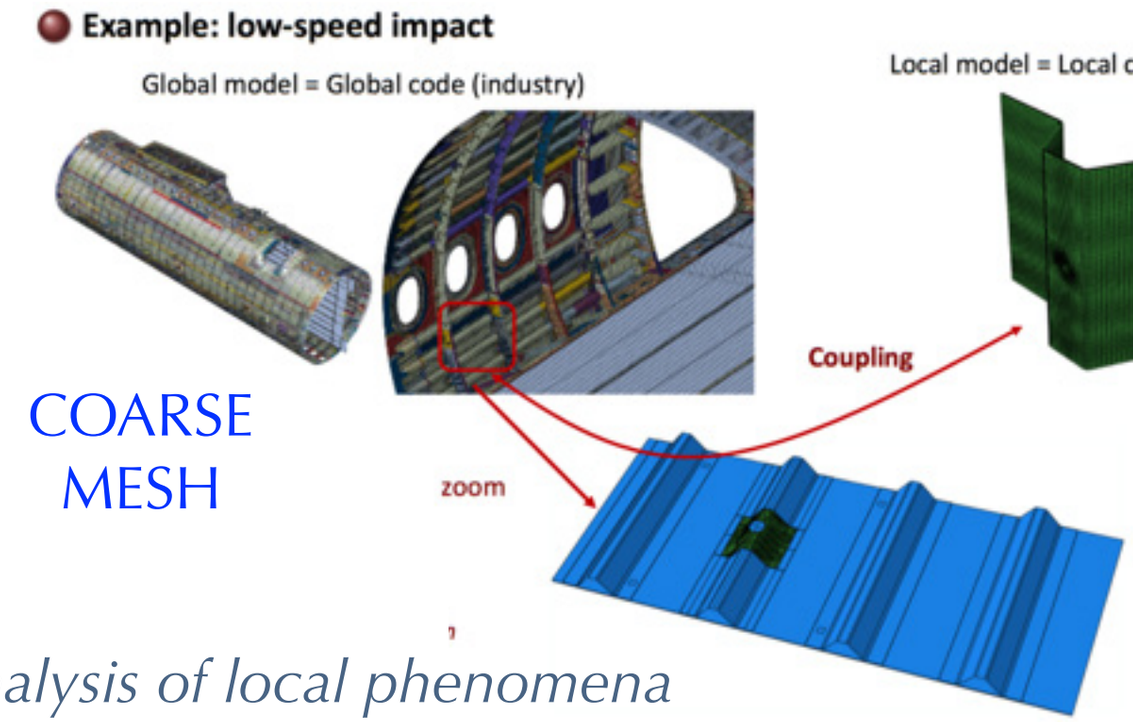
Model Coupling

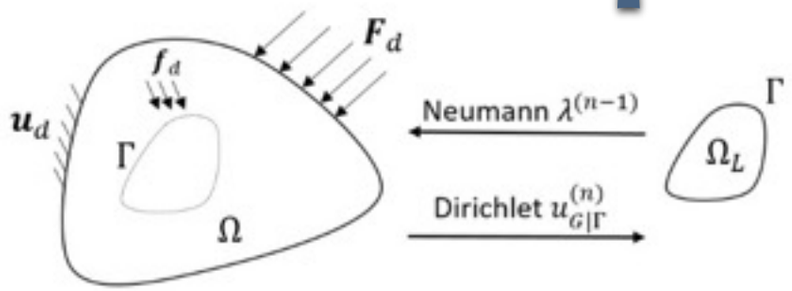
Non-intrusive coupling

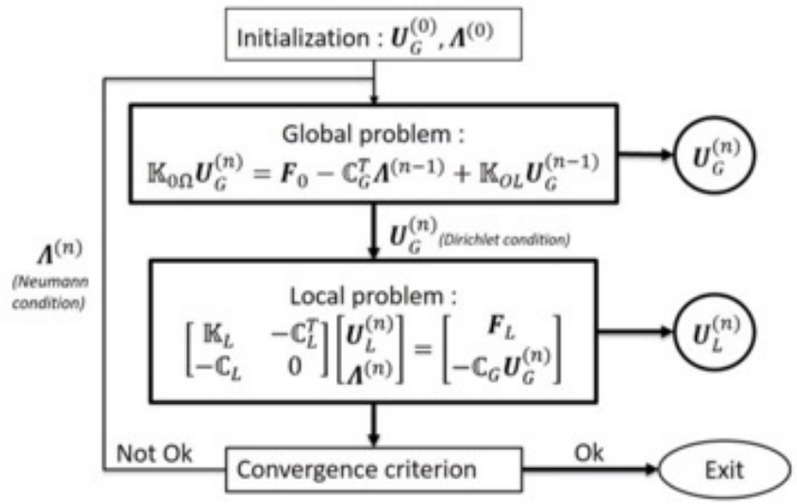
[Gendre *et al.* 09, Passieux *et al.* 13]

FINE MESH

COARSE MESH



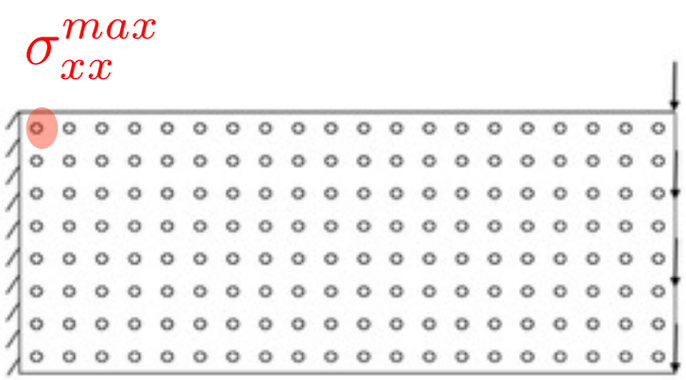


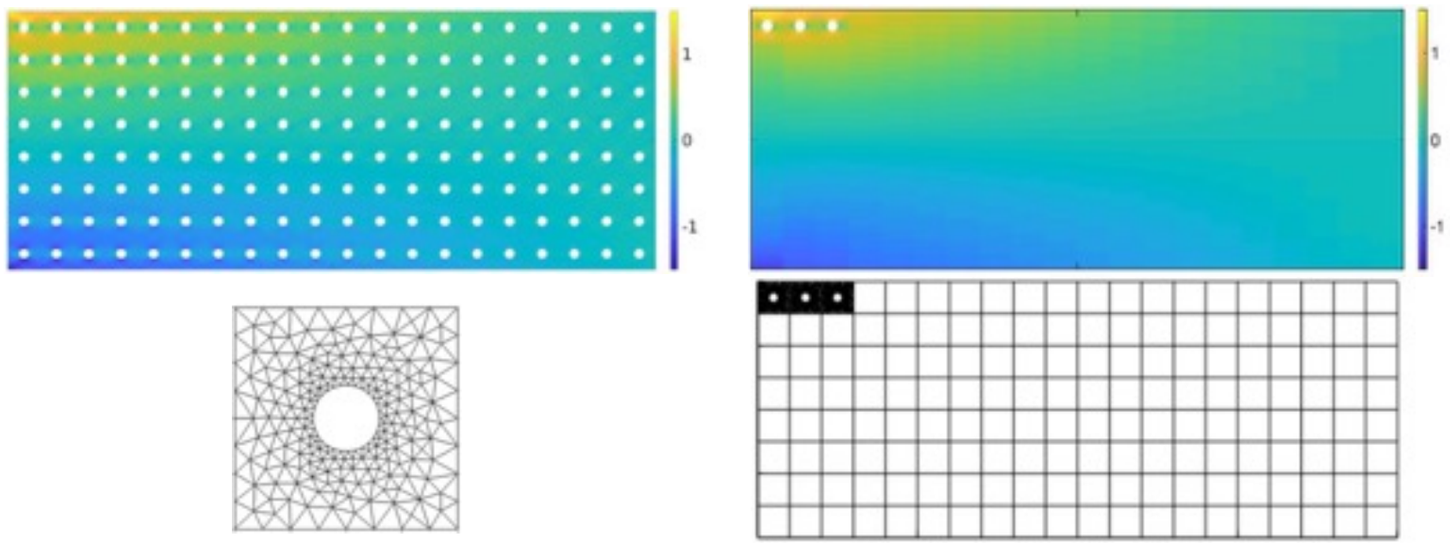


- *analysis of local phenomena*
- ***non-intrusive*** *= no modification of the global model (stiffness matrix, mesh,…)*

Certification & adaptivity [Chamoin *et al.* 19]

only 1 iteration required!!!





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Other GO error control applications (ROM, multiscale, model coupling, parameter estimation…)

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