Workshop «Numerical methods for high-dimensional problems»
15/04/2014 - ENPC

Control of PGD-based approximations
-
A posteriori error estimation and adaptive strategies

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LMT-Cachan

Outline

- PGD solution and post-processing
- A posteriori error estimation using the concept of CRE
- Application to PGD computations - adaptive strategy
- Goal-oriented error estimation

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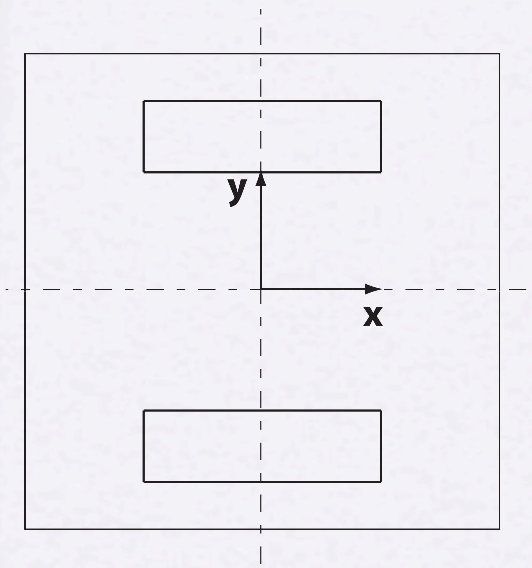
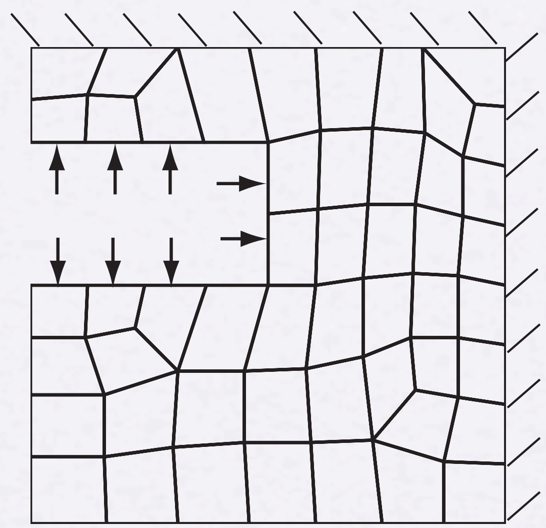
Context

Transient thermal problem





$$u = 0 \quad \text{on } \partial_u\Omega \times \mathcal{I}$$
$$u_{|t=0} = 0$$
$$c\frac{\partial u}{\partial t} - \underline{\nabla} \cdot \underline{q} = f_d$$
$$\underline{q} \cdot \underline{n} = q_d \quad \text{on } \partial_q\Omega \times \mathcal{I}$$
$$\underline{q} = k\underline{\nabla} u$$

multi-parameter problem : $\underline{x}, t, \cancel{\underline{p}}$

$$\boxed{B(u,v) = L(v) \quad \forall v \in L^2(\mathcal{I}) \otimes H^1_0(\Omega)}$$

«classical» approach : space mesh $\mathcal{M}_h$, time mesh $\mathcal{M}_{\Delta t}$ $\longrightarrow$ $N_h \times N_{\Delta t}$ dof

Model reduction using PGD

[Chinesta *et al.* 2010, 2011] [Nouy 2010]

$$\boxed{u(\underline{x},t) \approx u_m(\underline{x},t) = \sum_{i=1}^{m} \psi_i(\underline{x})\lambda_i(t)}$$

$\longrightarrow$ $m \times (N_h + N_{\Delta t})$ dof

$\longrightarrow$ computation/storage costs $\searrow$

<u>«progressive Galerkin» approach</u>

$$u_m = u_{m-1} + \psi\lambda \quad \text{s.t.} \quad B(u_m, \psi^*\lambda + \psi\lambda^*) = L(\psi^*\lambda + \psi\lambda^*) \quad \forall \psi^*, \lambda^*$$

problem in space $\psi = S_m(\lambda)$

$$B(u_m, \psi^*\lambda) = L(\psi^*\lambda) \quad \forall \psi^*$$

$$\Downarrow$$

$$(\alpha_S \mathbb{M} + \beta_S \mathbb{K})\underline{X} = \underline{F}$$

problem in time $\lambda = T_m(\psi)$

$$B(u_m, \psi\lambda^*) = L(\psi\lambda^*) \quad \forall \lambda^*$$

$$\Downarrow$$

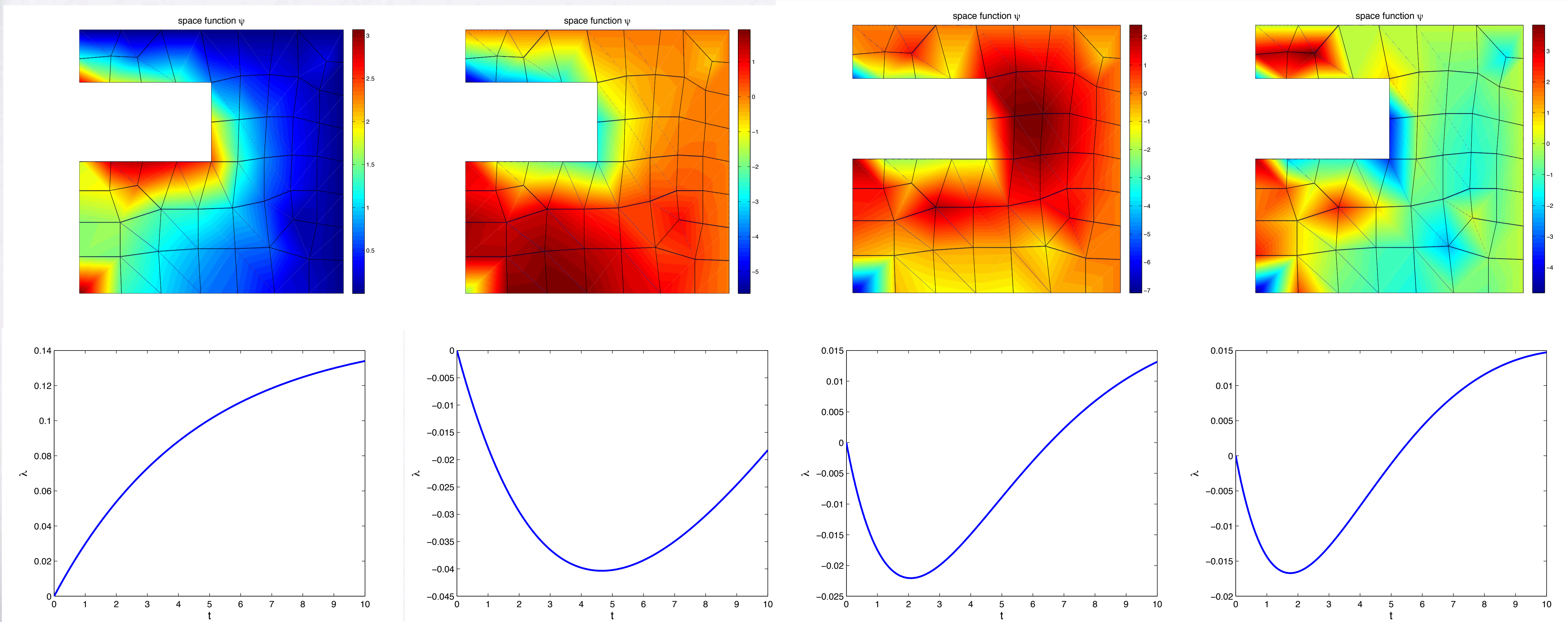
$$\alpha_T \frac{\lambda^{(k+1)} - \lambda^{(k)}}{\Delta t} + \beta_T \lambda^{(k)} = \delta_T^{(k)} \qquad \lambda^{(0)} = 0$$

<u>variants :</u> convergence, orthogonalization of modes, updating of time functions, ...

PGD modes

$$q_d(\underline{x},t) = -1\ ,\ f_d(\underline{x},t) = 200xy$$
$$N_e = 50, N_p = 1000$$

$m=1$ $\quad$ $m=2$ $\quad$ $m=3$ $\quad$ $m=4$



accuracy of solution $u_m(\underline{x},t)$? of quantities of interest $I(u_m)$?

(guaranteed) estimation of the global/local error

adaptivity criteria

Bibliography

Large litterature for error estimation and adaptive strategies (greedy) in reduced basis methods [Machiels *et al.* 2001, Grepl & Patera 2005,...]

specific case of PGD

[Ladevèze 1998] → *a priori* error estimation for separated variables representations (LATIN method)

[Ammar *et al.* 2010] → *a posteriori* error estimation for outputs of interest indicators based on residuals

[Moitinho de Almeida 2013] → goal-oriented error estimation using complementary solutions

Post-processing

[Ladevèze & Chamoin 2012]

We stop PGD sub-iterations with a problem in space

for each PGD mode $m_0 \in [1, m]$

$$\boxed{B(u_{m_0}, \psi^* \lambda_{m_0}) = L(\psi^* \lambda_{m_0}) \quad \forall \psi^* \in \mathcal{V}_h}$$

assumption : radial loading $\underline{f}_d = \sum_{j=1}^{J} \alpha_j(t) \underline{f}_d^j(\mathbf{x}) \qquad \underline{q}_d = \sum_{j=1}^{J} \alpha_j(t) \underline{q}_d^j(\mathbf{x})$

$$\underline{q}_0 = \sum_{j=1}^{J} \left[\alpha_j(t) \underline{q}_{0,f}^j(\mathbf{x}) + \beta_j(t) \underline{q}_{0,q}^j(\mathbf{x}) \right]$$

is equilibrated in a FE sense with $(\underline{f}_d, \underline{q}_d)$, for all t

$$\boxed{\int_\Omega \underbrace{\left[\int_{\mathcal{I}} \lambda_{m_0} (k \underline{\nabla} u_{m_0} - \underline{q}_0) dt \right]}_{\underline{Q}_{m_0}} \underline{\nabla} \psi^* d\Omega = - \int_\Omega \sum_{i=1}^{m_0} \underbrace{\left[\int_{\mathcal{I}} c \lambda_{m_0} \dot{\lambda}_i dt \right]}_{G_{m_0 i}} \psi_i \psi^* d\Omega \quad \forall \psi^* \in \mathcal{V}_h}$$

Post-processing

$\underline{Q}_{m_0}$ is equilibrated with $\sum_{i=1}^{m_0} G_{m_0 i}\psi_i$ in a FE sense, $\forall t$

$\sum_{j=1}^{m} R_{ij}\underline{Q}_j$ is equilibrated with ψ_i in a FE sense, $\forall t$

$$\left| \begin{aligned} u_m &= \sum_{i=1}^{m} \lambda_i \psi_i \\ \underline{q}_m &= \underline{q}_0 - \sum_{i=1}^{m}\sum_{j=1}^{m} c\dot{\lambda}_i R_{ij}\underline{Q}_j \end{aligned} \right.$$

verify balance equations in a FE sense

$$\boxed{\int_\Omega (\underline{q}_m - \underline{q}_0)\cdot \underline{\nabla} u^* d\Omega = -\int_\Omega c\frac{\partial u_m}{\partial t} d\Omega \quad \forall u^* \in \mathcal{V}_h, \forall t}$$

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Constitutive relation error (CRE)

getting guaranteed and computable a posteriori error bounds

→ one way which can be described with different words
(CRE, equilibrated residuals, flux-free,...)

Steady thermal problem

$$\int_\Omega k\underline{\nabla}u\cdot\underline{\nabla}u^*d\Omega=\int_\Omega f_d u^* d\Omega+\int_{\partial_q\Omega}F_d u^* dS \quad \forall u^*\in\mathcal{V}$$

Primal approach (Ritz-Galerkin) : yields an upper bound to the potential energy

$$||\hat{u}-u||_u^2=||\hat{u}||_u^2-||u||_u^2-2\int_\Omega k\underline{\nabla}u\cdot\underline{\nabla}(\hat{u}-u)d\Omega=2[E_p(\hat{u})-E_p(u)]$$

Dual approach: produces a lower bound to the potential energy

$$||\underline{\hat{q}}-\underline{q}||_q^2=||\underline{\hat{q}}||_q^2-||\underline{q}||_q^2-2\int_\Omega\frac{1}{k}\underline{q}\cdot(\underline{\hat{q}}-\underline{q})d\Omega=2[E_c(\underline{\hat{q}})-E_c(\underline{q})]$$

$-E_p(u)$

Constitutive relation error (CRE)

Prager-Synge equality

$$||\hat{u} - u||_u^2 + ||\underline{\hat{q}} - \underline{q}||_q^2 = 2[E_c(\underline{\hat{q}}) + E_p(\hat{u})] = ||\underline{\hat{q}} - k\underline{\nabla}\hat{u}||_q^2$$

$$E_{CRE}^2(\hat{u}, \underline{\hat{q}})$$

Hypercircle property

$$||\underline{\hat{q}}^* - \underline{q}||_q^2 = \frac{1}{2} E_{CRE}^2(\hat{u}, \underline{\hat{q}}^*)$$

- Technical point: construction of $\underline{\hat{q}}$

post-processing of the approximate solution $\hat{u}$

(use of Galerkin properties in the FE context)

provides for asymptotic convergence properties [Ladevèze & Pelle 2004]

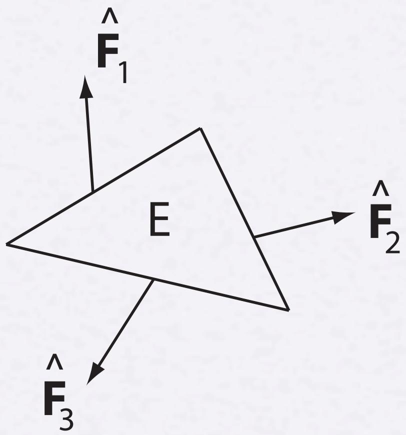
$$||\hat{u} - u||_u \leq E_{CRE}(\hat{u}, \underline{\hat{q}}) \leq C||\hat{u} - u||_u$$

Construction of $\underline{\hat{q}}$

[Ladevèze 75, Ladevèze *et al* 10, Pled *et al* 11]

Use of classical techniques (hybrid flux - EET - EESPT) for FEM with two steps:

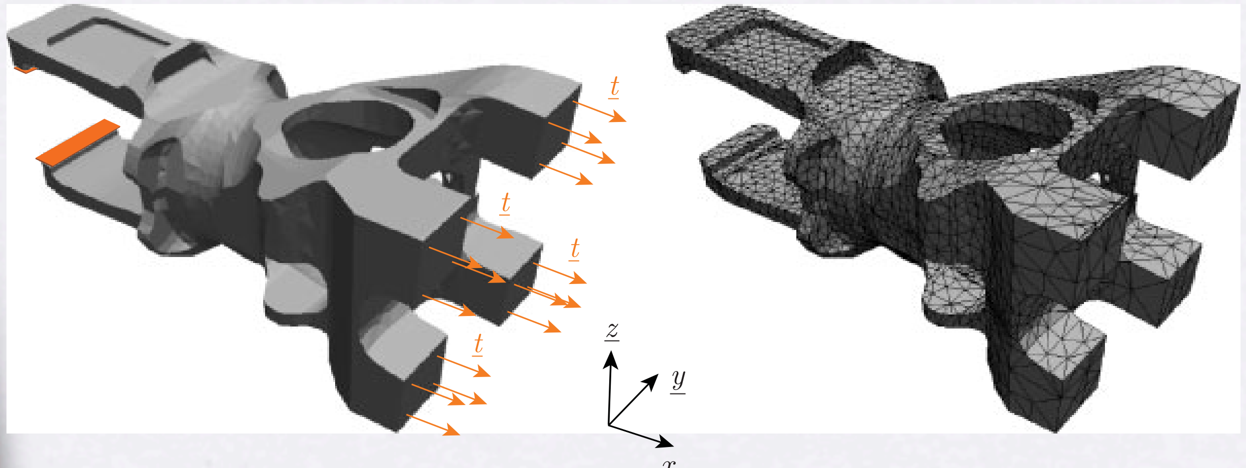
1) Definition of equilibrated fluxes on element edges (by means of prolongation condition with $\underline{q}_h = k\underline{\nabla} u_h$)

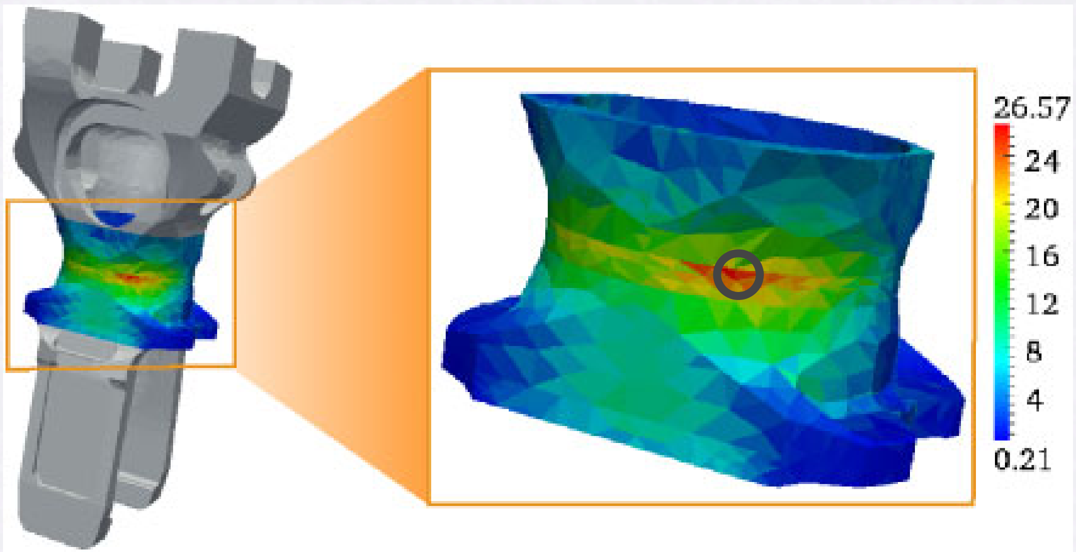


local systems around each FE node

2) Solution of a local problem at the element level (use of PGD (offline))

implemented in a C++ plateform





Extension of CRE

Definition in the unsteady case

$$\boxed{E_{CRE}(\hat{u},\underline{\hat{q}}) = |||\underline{\hat{q}} - k\underline{\nabla}\hat{u}|||_q} \longrightarrow \sqrt{\int_0^T \int_\Omega \frac{1}{k}\bullet\cdot\bullet \, d\Omega dt}$$

Fundamental results

$$|||u^{ex}-\hat{u}|||_u^2 + |||\underline{q}^{ex}-\underline{\hat{q}}|||_q^2 + \int_\Omega c(u^{ex}-\hat{u})^2_{|T} d\Omega = E^2_{CRE}(\hat{u},\underline{\hat{q}})$$

$$|||\underline{q}^{ex} - \underbrace{\underline{\hat{q}}^*}_{\underline{\hat{q}}^* = \frac{1}{2}(\underline{\hat{q}} + k\underline{\nabla}\hat{u})}|||^2 + \int_\Omega c(u_{ex}-\hat{u})^2_{|T} d\Omega = \frac{1}{2}E^2_{CRE}(\hat{u},\underline{\hat{q}}^*)$$

→ guaranteed bounding of global and local errors

Rem : can be generalized to time-dependent nonlinear problems with dissipation

→ dissipation error [Ladevèze & Moës 98, Chamoin *et al.* 07]

$$e^2_{dis}(\dot{X},Y) = \varphi(\dot{X}) + \varphi^*(Y) - \dot{X}\cdot Y$$

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CRE applied to PGD solution

$(\hat{u}, \underline{\hat{q}})$ is admissible (compatible+equilibrated) if :

- $\hat{u}$ is KA $\quad \hat{u} = 0 \quad \text{on } \partial_u\Omega \times \mathcal{I} \qquad \hat{u}_{|t=0} = 0$

  → we choose $\hat{u} = u_m$

- $(\hat{u}, \underline{\hat{q}})$ is SA

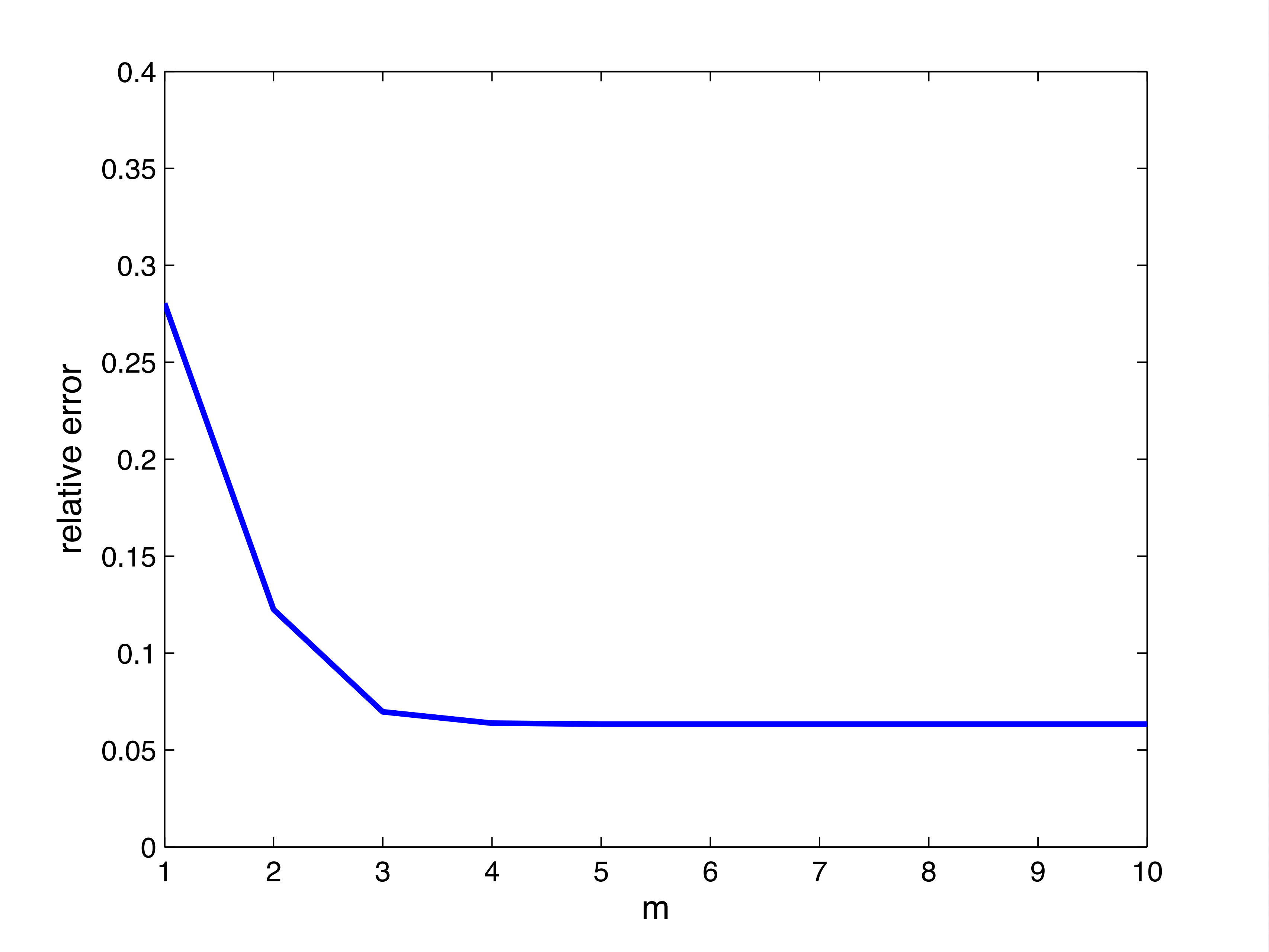
$$\int_\Omega \underline{\hat{q}} \cdot \boldsymbol{\nabla} u^* d\Omega = \int_\Omega (f_d - c\frac{\partial \hat{u}}{\partial t}) u^* d\Omega - \int_{\partial_q\Omega} q_d u^* dS \quad \forall u^*, \forall t$$

→ technical point

→ $(u_m, \underline{q}(u_m))$ is not SA in a FE sense, but (u_m, q_m) is!!!

Error estimate

$$\frac{E_{CRE}}{|||\hat{q}|||_q}$$



- convergence for m=3
- asymptotic value = discretization error

Splitting of error sources

$$u^{ex} - u_m^{h,\Delta t} = (u^{ex} - u^{h,\Delta t}) + (u^{h,\Delta t} - u_m^{h,\Delta t})$$

$$\underbrace{|||u^{ex} - u_m^{h,\Delta t}|||_u^2}_{\text{total error}} = \underbrace{|||u^{h,\Delta t} - u_m^{h,\Delta t}|||_u^2}_{\text{PGD truncation error}} + \underbrace{|||u^{ex} - u^{h,\Delta t}|||_u^2}_{\text{discretization error}}$$

estimated with a discretized reference model

post-processing of $(u_m, \underline{q}_m)$ to get an admissible solution $(\hat{u}^{h,\Delta t}, \hat{\underline{q}}^{h,\Delta t})$

in the sense of the new reference problem (weaker sense in space and time)

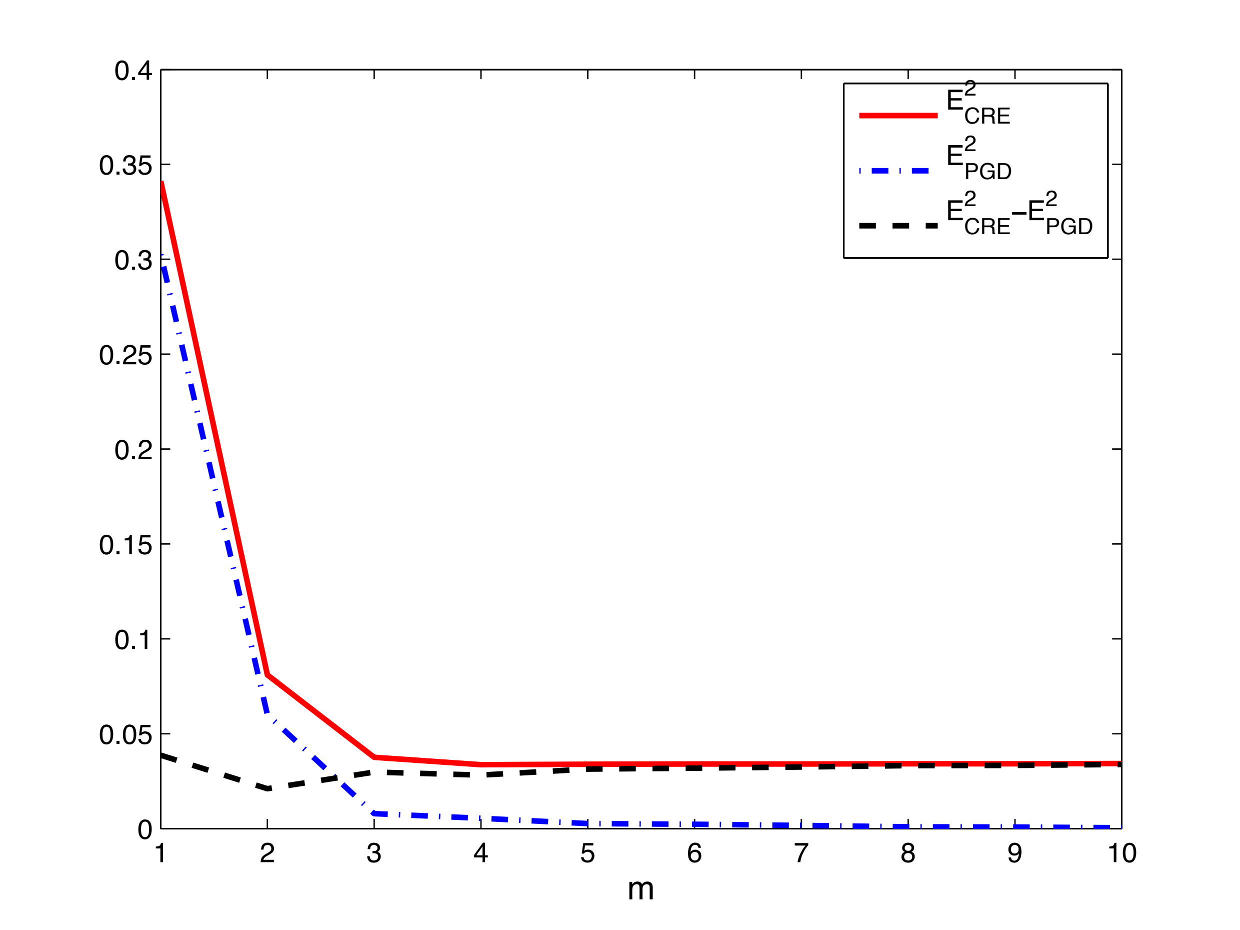
$$\hat{\underline{q}}^{h,\Delta t} = \mathbf{N}^T [\int_0^T \mathbf{N}\mathbf{N}^T dt]^{-1} [\underline{R}_1, \ldots, \underline{R}_k]$$

$$\underline{R}_i = \int_0^T \underline{q}_m N_i dt$$

$$E_{CRE,PGD} = |||\hat{\underline{q}}^{h,\Delta t} - k\underline{\nabla}\hat{u}^{h,\Delta t}|||_q$$

$$E_{CRE,dis} = \sqrt{E_{CRE}^2 - E_{CRE,PGD}^2}$$

Splitting of error sources



after 3 modes, discretization error is dominating

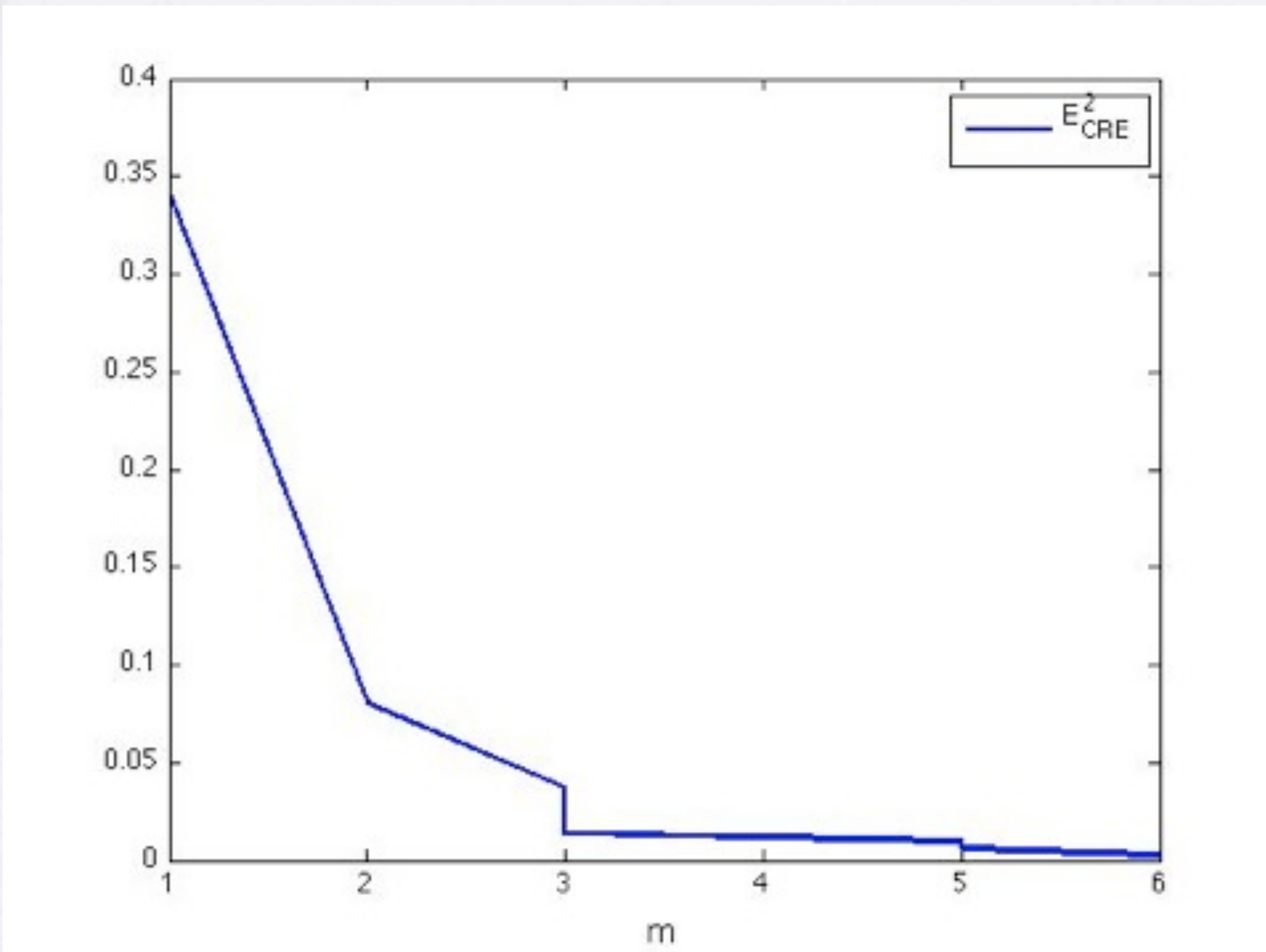
Possible to split space/time discretization errors

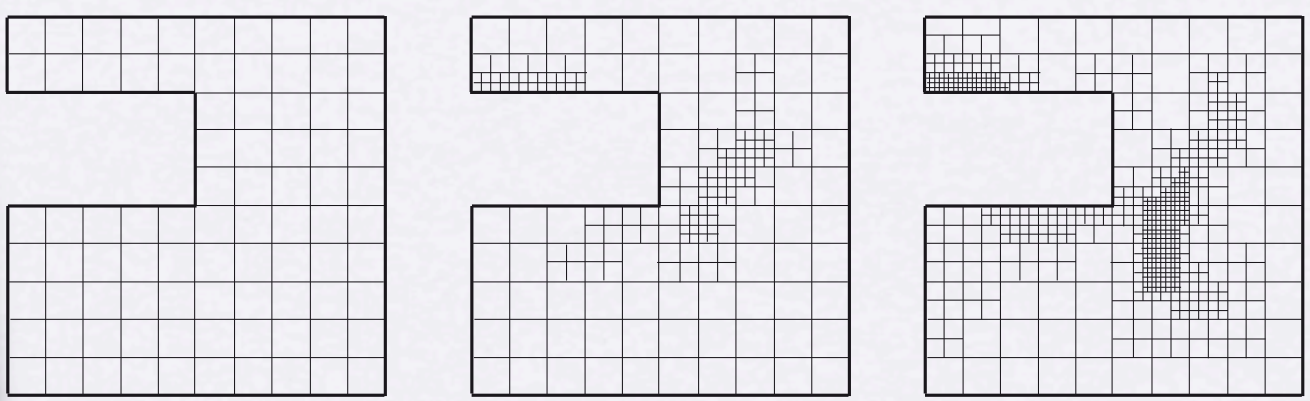
$$E^2_{CRE,dis} = \underbrace{E^2_{CRE,h}}_{|||\underline{\hat{q}} - \underline{\hat{q}}^h|||^2_q} + \underbrace{E^2_{CRE,\Delta t}}_{|||\underline{\hat{q}}^h - \underline{\hat{q}}^{h,\Delta t}|||^2_q}$$

discretization error in space : 83%

Adaptivity

<u>IDEA</u> : the model is adapted mode after mode by comparing contributions of error sources





compute mode 1

↓ PGD error dominant

compute mode 2

↓ PGD error dominant

compute mode 3

↓ discretization error dominant

local refinement of mode 3 mesh

↓ PGD error dominant

compute mode 4

- first PGD modes give general aspects : coarse approximation is sufficient
- next modes need more accuracy : fine discretization required

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Error on a QoI

An optimal PGD decomposition for u_m is usually not optimal for $I(u_m)$

use of goal-oriented techniques

Adjoint problem

$$I(u) = \int_0^T \int_\Omega (\underline{q}_\Sigma \cdot \underline{\nabla} u + f_\Sigma u) d\Omega dt$$

$$\tilde{u} = 0 \quad \text{on } \partial_u \Omega \times \mathcal{I}$$

$$\tilde{u}_{|t=T} = 0$$

$$-c \frac{\partial \tilde{u}}{\partial t} - \underline{\nabla} \cdot \underline{\tilde{q}} = f_\Sigma$$

$$\underline{\tilde{q}} \cdot \underline{n} = 0 \quad \text{on } \partial_q \Omega \times \mathcal{I}$$

$$\underline{\tilde{q}} = k \underline{\nabla} \tilde{u}$$

solution $\tilde{u}$ = **influence function** (impact of global error on local error)

Goal-oriented error estimation

From an admissible solution $(\hat{\tilde{u}}, \underline{\hat{\tilde{q}}})$

$$I(u^{ex}) - I(u_m) = \int_0^T \int_\Omega \left\{ c \frac{\partial (u^{ex} - u_m)}{\partial t} \hat{\tilde{u}} + \underline{\nabla}(u^{ex} - u_m) \cdot \underline{\hat{\tilde{q}}} \right\} d\Omega dt$$

$$= \int_0^T \int_\Omega (\underline{q}^{ex} - \underline{\hat{q}}) \frac{1}{k} (\underline{\hat{\tilde{q}}} - k \underline{\nabla} \hat{\tilde{u}}) d\Omega dt + I_{corr}(\underline{\hat{q}}, \underline{\hat{\tilde{q}}})$$

$$|I(u^{ex}) - I(u_m) - I_{corr}(\underline{\hat{q}}, \underline{\hat{\tilde{q}}})| \leq E_{CRE} \times \tilde{E}_{CRE}$$

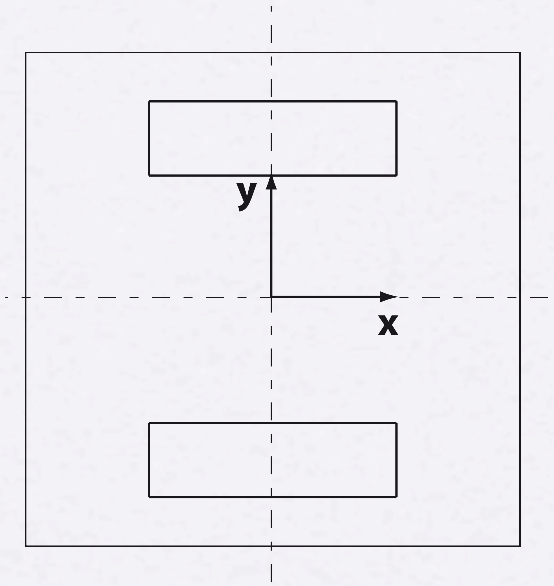
optimized bounding possible
[Chamoin *et al* 08, Pled *et al* 12]

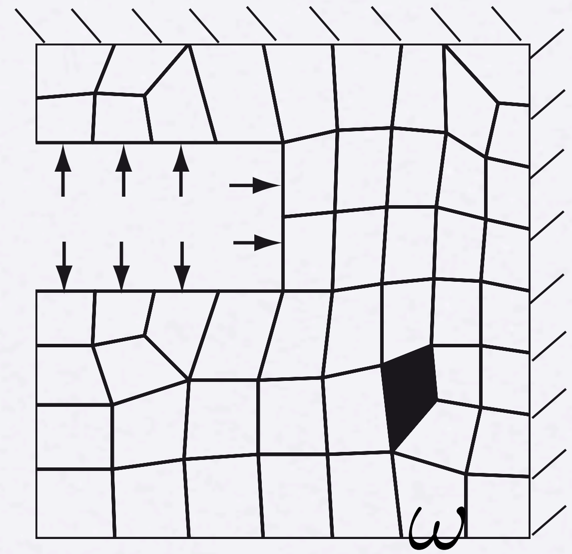
Sources splitting

$$I(u^{ex}) - I(u_m^{h,\Delta t}) = \underbrace{[I(u^{ex}) - I(u^{h,\Delta t})]}_{\text{discretization error}} + \underbrace{[I(u^{h,\Delta t}) - I(u_m^{h,\Delta t})]}_{\text{PGD truncation error}}$$

indicators are computed after changing reference problem

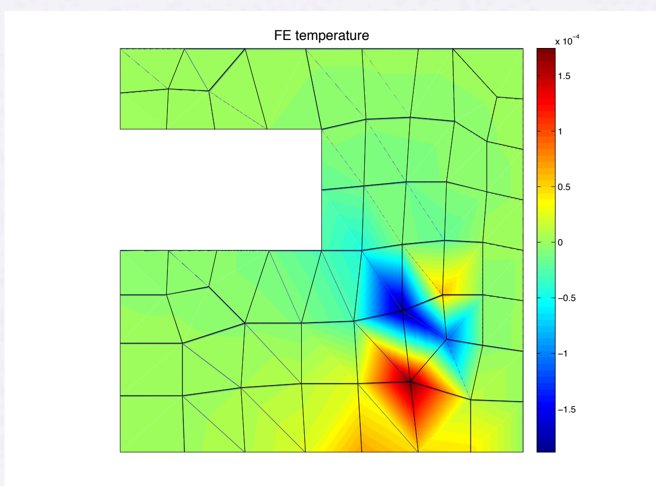
Solving the adjoint problem





$$I = < u >_{\omega,T}$$

$$\hookrightarrow f_\Sigma = \frac{\delta_T}{|\omega|} \quad \text{in } \omega$$



→ localized solution, with high gradients

→ *a priori* enrichment + PGD comput.

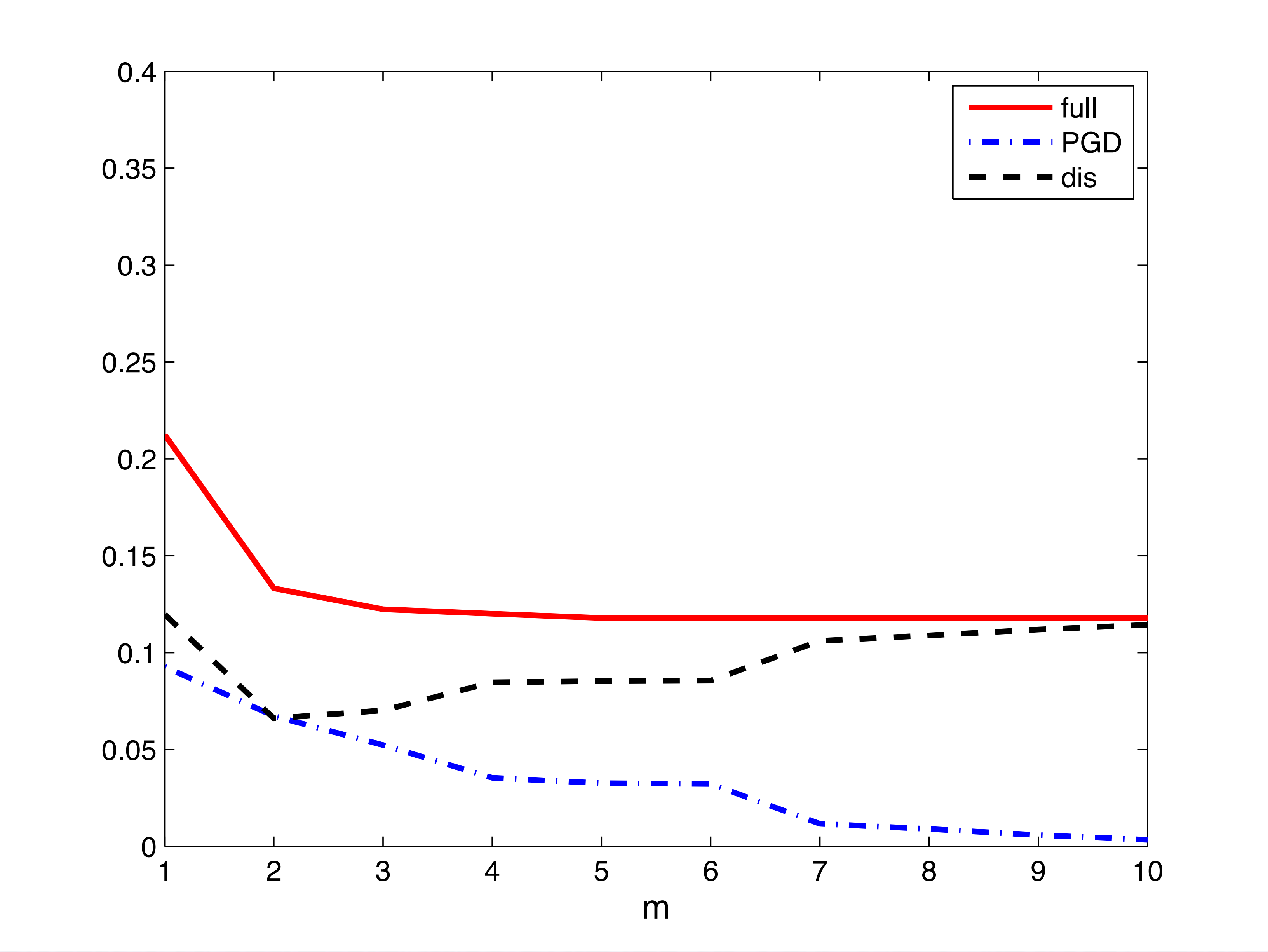
[Chamoin & Ladevèze 2008]

$$\tilde{u}(\underline{x},t) = \underbrace{\sum_{j=1}^{n^{PUM}} \varphi_j(\underline{x})\tilde{u}^{hand}(\underline{x},t)}_{\substack{\text{local enrichment} \\ \text{(generalized Green's function)}}} + \underbrace{\tilde{u}^{res}(\underline{x},t)}_{\text{residual term, computed with PGD}}$$

$$\approx \sum_{i=1}^{m} \psi_i^{res}(\underline{x})\lambda_i^{res}(t)$$

Error on the QoI

$$\frac{E_{CRE} \cdot \tilde{E}_{CRE}}{|I(u_m) + I_{corr}|}$$

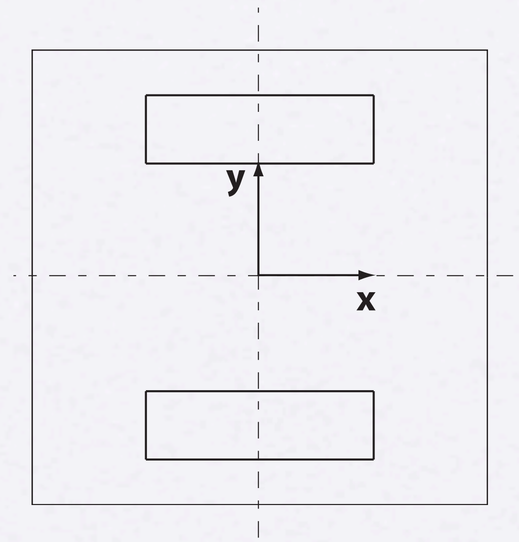


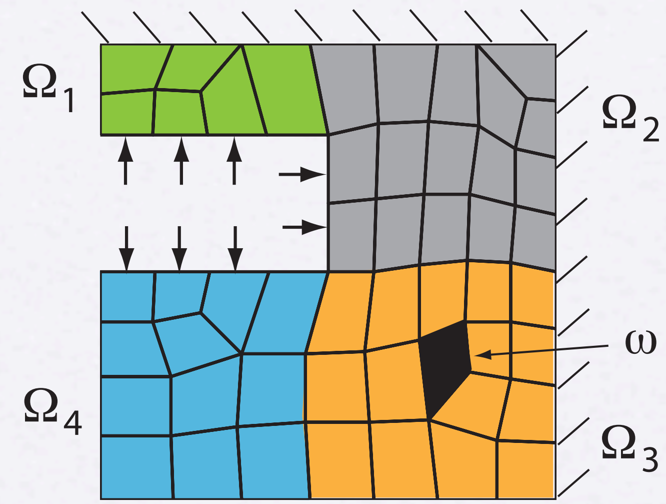
→ requires more PGD modes than for global adaptation

→ discretization error becomes rapidly dominating

→ space-time refinement different from the global case

With unknown parameters

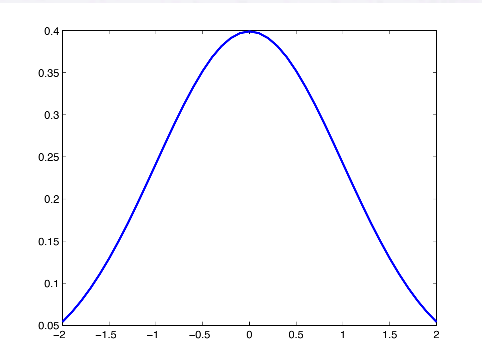




- $k(\mathbf{x}, \theta_i) = 1 + \sum_{i=1}^{4} g_i I_{\Omega_i}(\mathbf{x})\theta_i$ ⟶ piecewise homogeneous

  $[g_1, g_2, g_3, g_4] = [0.1, 0.1, 0.2, 0.05]$

- $c(\mathbf{x}, \theta_5) = 1 + 0,2\theta_5$ ⟶ homogeneous



5 extra-coordinates

$\theta_i \in [-2, 2]$

$$\boxed{u(\mathbf{x}, t, \mathbf{p}) \approx u_m(\mathbf{x}, t, \mathbf{p}) \equiv \sum_{i=1}^{m} \psi_i(\mathbf{x})\lambda_i(t)\underbrace{\Gamma_i(\mathbf{p})}_{\prod_{n=1}^{N} \gamma_{i,n}(p_n)}}$$

$$\longrightarrow B(u, v) = \int_\Theta \dots \qquad L(v) = \int_\Theta \dots$$

SA solution

[Ladevèze & Chamoin 2012]

Equilibrium in a FE sense $\forall(t,\underline{p}) \in \mathcal{I} \times \Theta$

$$\boxed{\int_\Omega \underline{q}_m \cdot \underline{\nabla} u^* d\Omega = \int_\Omega \left(f_d - c\frac{\partial \hat{u}_m}{\partial t}\right) u^* d\Omega - \int_{\partial_q \Omega} q_d u^* dS \quad \forall u^* \in \mathcal{V}_h}$$

$$\int_\Omega (\underline{q}_m - \underline{q}_0) \cdot \boldsymbol{\nabla} u^* d\Omega = -\int_\Omega c \frac{\partial \hat{u}_m}{\partial t} u^* d\Omega = -\sum_{i=1}^{m} c \dot{\lambda}_i \Gamma_i \underbrace{\int_\Omega \psi_i u^* d\Omega}_{\text{loading}} \quad \forall u^* \in \mathcal{V}_h$$

At the end of sub-iterations to compute each PGD mode $m_0 \in [1, m]$

$$B(u_{m_0}, \psi^* \lambda_{m_0} \Gamma_{m_0}) = L(\psi^* \lambda_{m_0} \Gamma_{m_0}) \quad \forall \psi^* \in \mathcal{V}_h$$

$$\int_\Omega \overbrace{\left[\int_\Theta \int_{\mathcal{I}} \lambda_{m_0} \Gamma_{m_0} (k \underline{\nabla} u_{m_0} - \underline{q}_0) dt d\underline{p}\right]}^{\underline{Q}_{m_0}} \underline{\nabla} \psi^* d\Omega = -\int_\Omega \sum_{i=1}^{m_0} \overbrace{\left[\int_\Theta \int_{\mathcal{I}} c \lambda_{m_0} \Gamma_{m_0} \dot{\lambda}_i dt d\underline{p}\right]}^{A_{m_0 i}} \psi_i \psi^* d\Omega \quad \forall \psi^* \in \mathcal{V}_h$$

SA solution

$$\int_\Omega \mathbb{A}\boldsymbol{\Psi}_m \psi^* d\Omega + \int_\Omega \{\underline{Q}\}_1^m \underline{\nabla}\psi^* d\Omega = 0 \quad \forall \psi^* \in \mathcal{V}_h$$

$$\int_\Omega c\boldsymbol{\Gamma}_m \otimes \dot{\boldsymbol{\Lambda}}_m \otimes \boldsymbol{\Psi}_m \psi^* d\Omega + \int_\Omega c(\boldsymbol{\Gamma}_m \otimes \dot{\boldsymbol{\Lambda}}_m \otimes \mathbb{A}^{-1}\{\underline{Q}\}_1^m)\underline{\nabla}\psi^* d\Omega = 0 \quad \forall \psi^* \in \mathcal{V}_h$$

$(u_m, -c\boldsymbol{\Gamma}_m \otimes \dot{\boldsymbol{\Lambda}}_m \otimes \mathbb{A}^{-1}\{\underline{Q}\}_1^m + \underline{q}_0)$ satisfies FE equilibration

$\boxed{(u_m, -c\boldsymbol{\Gamma}_m \otimes \dot{\boldsymbol{\Lambda}}_m \otimes \mathbb{A}^{-1}\{\underline{\hat{Q}}\}_1^m + \underline{q}_0) \text{ is SA}}$

Bounding result for outputs of interest

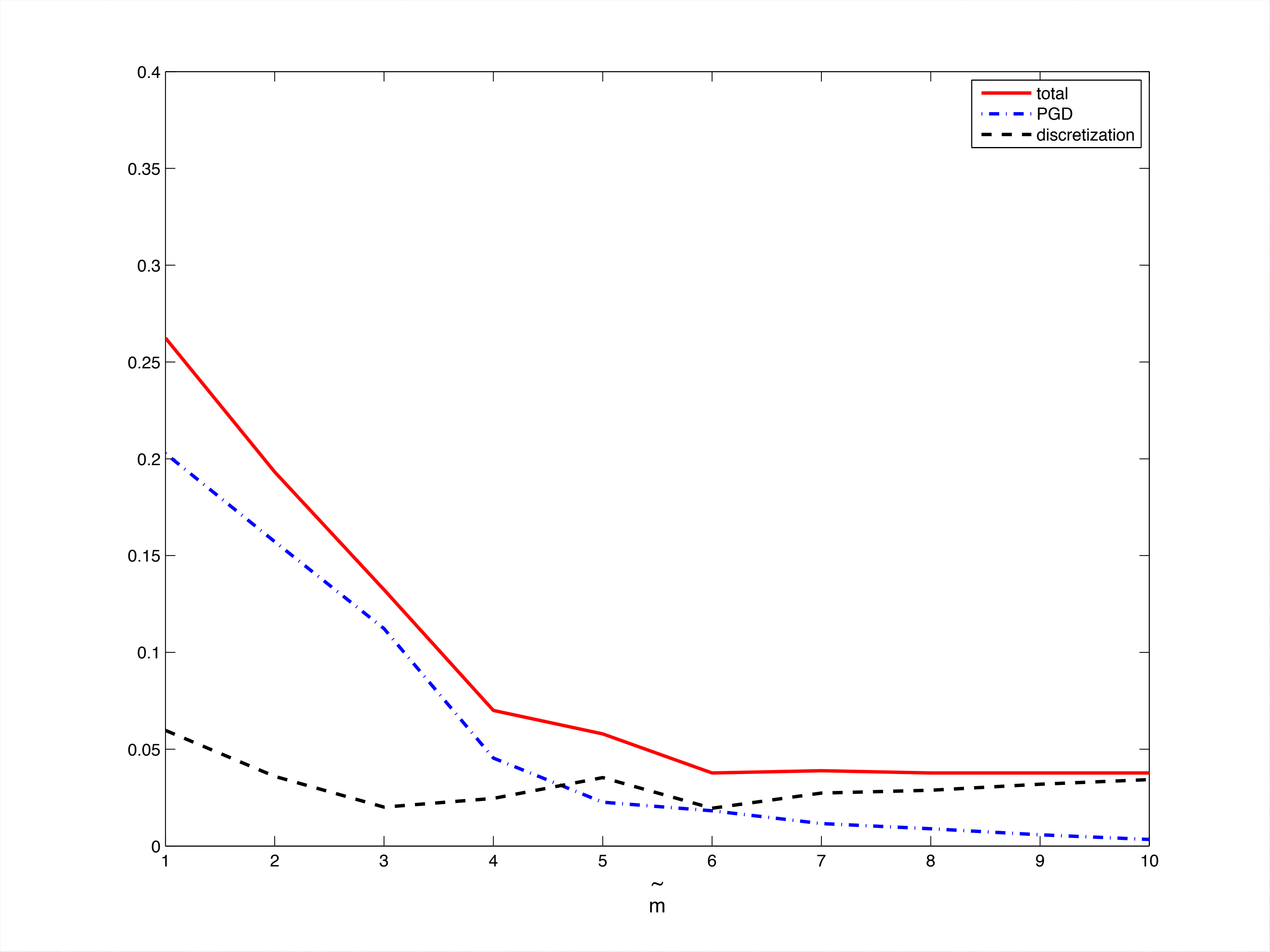
$$|I(\underline{p}) - I_m(\underline{p}) - I_{corr}(\underline{p})| \leq E_{CRE}(\underline{p})\tilde{E}_{CRE}(\underline{p})$$

$$\eta_{inf}(\underline{p}) \leq I(\underline{p}) \leq \eta_{sup}(\underline{p})$$

Goal-oriented error estimate

- $$I_1 = E[\frac{1}{|\omega|}\int_\omega u_{|T} d\omega]$$

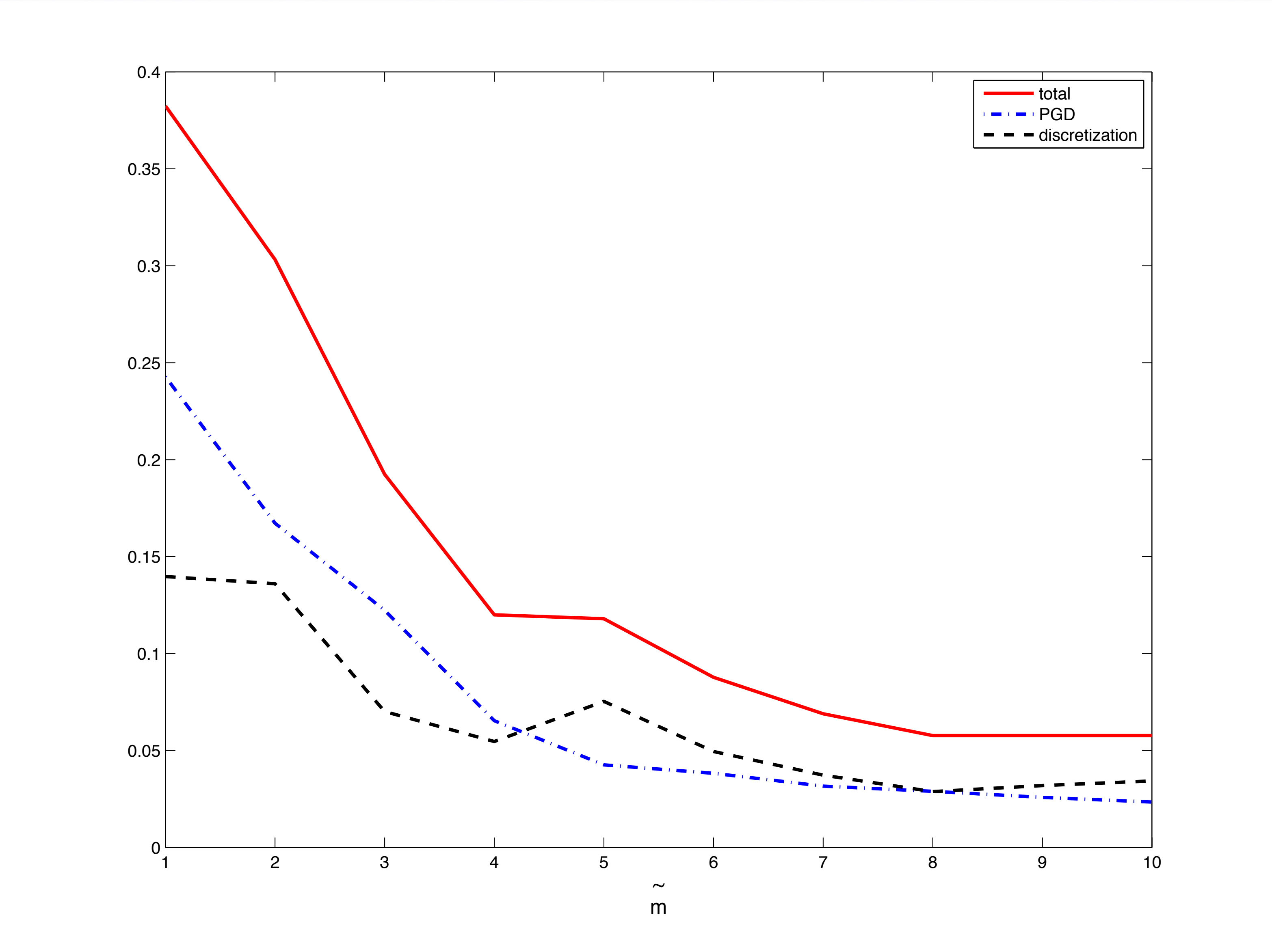
$$\frac{\int_\Theta E_{CRE} \cdot \tilde{E}_{CRE} dP}{|I(u_m) + I_{corr}|}$$



Goal-oriented error estimate

- $$I_2 = \sup_{\theta_i} \frac{1}{|\omega|} \int_\omega u_{|T} d\omega$$

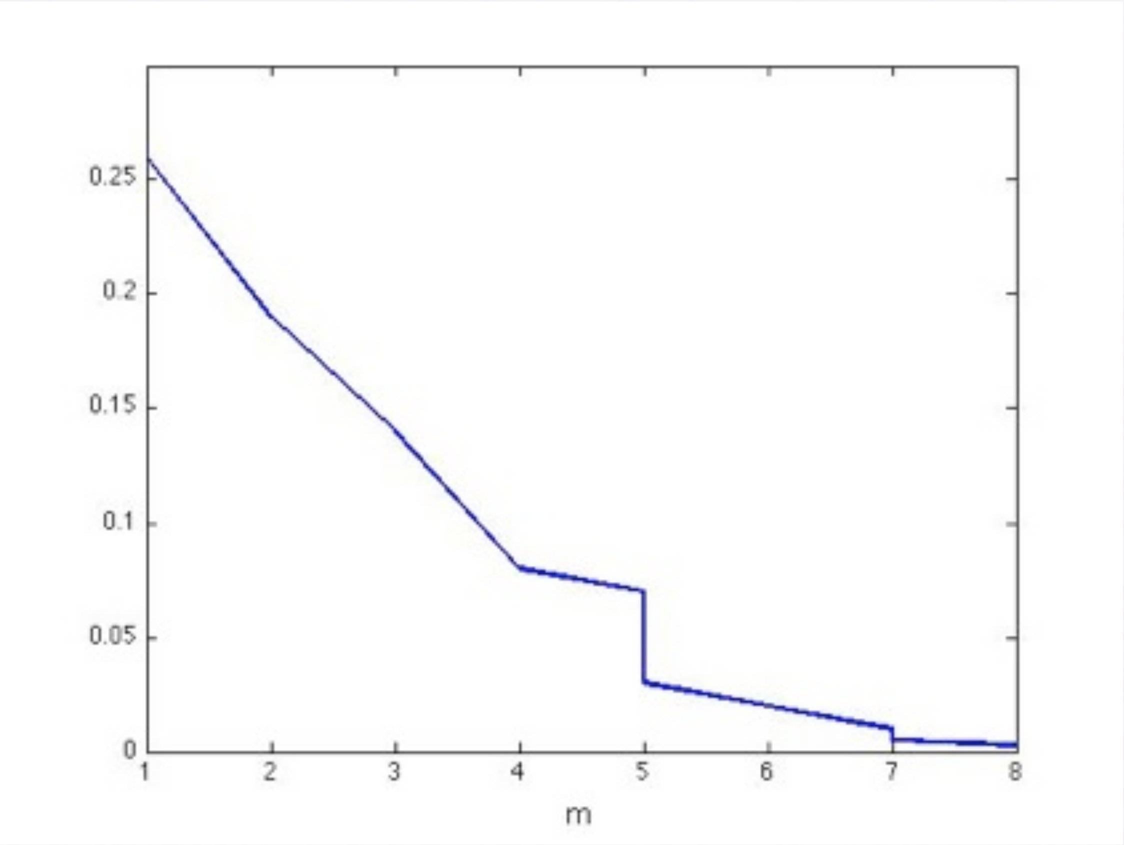
$$\frac{\sup_{\theta \in \Theta} E_{CRE} \cdot \tilde{E}_{CRE}}{|I(u_m) + I_{corr}|}$$

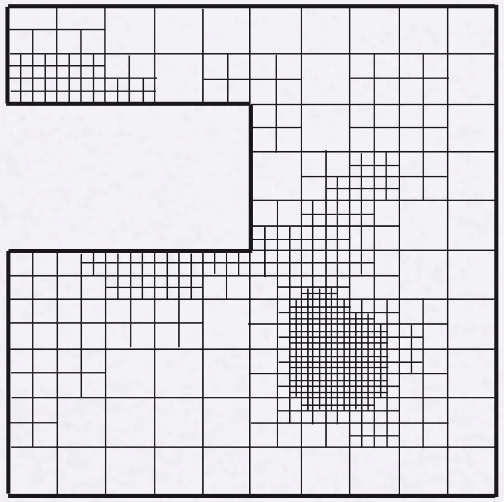


Adaptivity

$$\frac{\int_{\Theta} E_{CRE} \cdot \tilde{E}_{CRE} dP}{|I(u_m) + I_{corr}|}$$

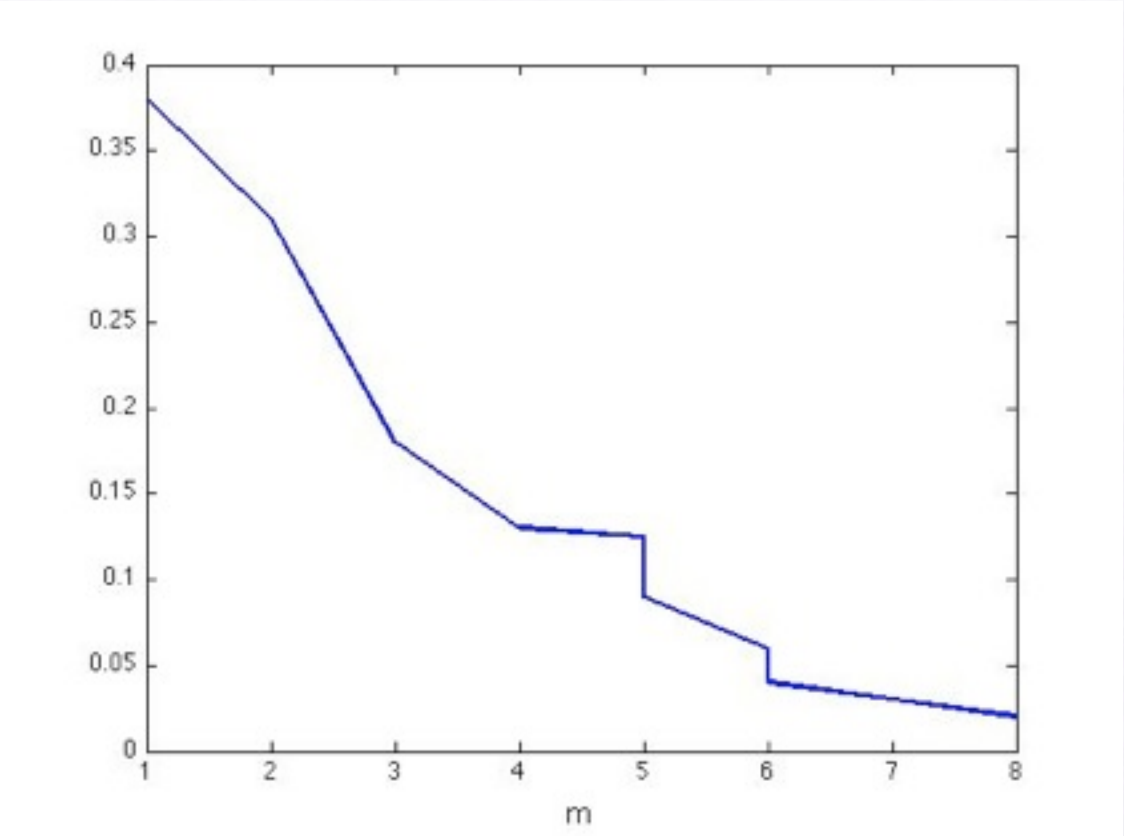
For I_1

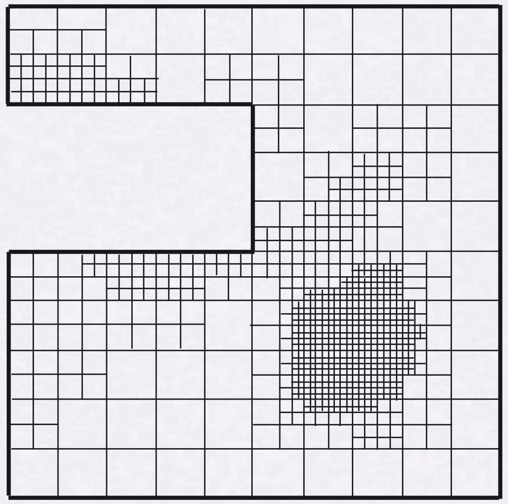




$$\frac{\sup_{\theta \in \Theta} E_{CRE} \cdot \tilde{E}_{CRE}}{|I(u_m) + I_{corr}|}$$

For I_2





Optimization with PGD

- Steady state case

$$B(u_{m_0}, \psi^* \Gamma_{m_0}) = L(\psi^* \Gamma_{m_0}) \quad \forall \psi^* \in \mathcal{V}_h$$

$$\int_\Omega \left[\int_{\mathcal{I}} \Gamma_{m_0} (k \underline{\nabla} u_{m_0} - \underline{q}_0) d\underline{p} \right] \underline{\nabla} \psi^* d\Omega = 0$$

$\underline{Q}_{m_0}$ auto-equilibrated (in a FE sense)

$$\boxed{\hat{\underline{q}}_m(\mathbf{x}, \underline{p}) = \hat{\underline{q}}_0(\mathbf{x}) + \sum_{m_0=1}^{m} \beta_{m_0}(\underline{p}) \hat{\underline{Q}}_{m_0}(\mathbf{x})}$$

with β_{m_0} minimizing $\displaystyle\int_\Theta E^2_{CRE}(\underline{p}) d\underline{p}$

Conclusions and prospects

- reliable control/adaptation of PGD approximation for global/local error based on CRE $\longrightarrow$ robust virtual charts
- guaranteed bounds to assess performances of PGDs (pb dependent) and various error sources
- case of numerous parameters : integration issues (reference points)
- various 3D & complex multi-parameter pb (PhD P.E. Allier)
- nonlinear problems
- optimal PGD strategy based on CRE

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Thank you !!!