Verification and effectivity of PGD model reduction

L. Chamoin, P. Ladevèze, P.E. Allier

LMT-Cachan (ENS Cachan / CNRS / Univ. Paris-Saclay)
INRIA Rocquencourt - CERMICS

MORE Workshop
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Proper Generalized Decomposition
Radial approximation
Generalized spectral decomposition
....

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Outline

- Basics on Proper Generalized Decomposition (PGD)
- Illustrations of PGD applications
- A posteriori error estimation: the CRE concept
- Control and adaptivity in PGD computations
- PGD performances and limits

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General ideas

[Chinesta *et al.* 2010, 2011]

Context: multiparameter EDPs (stochastic, optimization): $u(x, t, p_1, p_2, \ldots, p_n)$

- exponential growth of the number of dof with brute force approaches (curse of dimensionality)
- issues of computation cost / storage
- model order reduction: RB, POD, PGD,...

Idea of PGD: *a priori* representation using linear combination of modes with variable separation (tensor product space, low-rank structure, canonical format)

$$u(x, t, p_1, p_2, \ldots, p_n) \approx \sum_{m=1}^{M} \psi_m(x)\lambda_m(t)\phi_{1m}(p_1)\phi_{2m}(p_2)\ldots\phi_{nm}(p_n)$$

main features of the solution

- decrease of computation/storage costs (linear growth of the number of dof)
- no need of *a priori* information on the solution (no snapshot)
- modes are computed offline and on the fly solving simple problems
- first used to solve NL time-dependent problems with LATIN [Ladeveze 99]
- growing interest in the Computational Mechanics community

Computation of modes

When the **solution is known** (at least partially): an optimal low-rank separated representation may be searched by minimizing the distance with respect to a given metric on the tensor product

→ classical POD (SVD) approach with L2 norm and 2 variables

When the **solution is unknown**: several techniques (minimal residuals, (Petrov-) Galerkin formulation,...) [Nouy 2010]

→ we concentrate on progressive Galerkin-based method

$$B(u,v) = L(v) \quad \forall v \qquad u_m = u_{m-1} + \psi(x)\lambda(t)\phi_1(p_1)\phi_2(p_2)\dots\phi_n(p_n)$$

$$B(u_m, \psi^*\lambda\phi_1\dots\phi_n) = L(\psi^*\lambda\phi_1\dots\phi_n) \quad \forall\psi^* \longrightarrow \psi = F(\lambda,\phi_1,\dots,\phi_n)$$

$$B(u_m, \psi\lambda^*\phi_1\dots\phi_n) = L(\psi\lambda^*\phi_1\dots\phi_n) \quad \forall\lambda^* \longrightarrow \lambda = G(\psi,\phi_1,\dots,\phi_n)$$

$$B(u_m, \psi\lambda\phi_1^*\dots\phi_n) = L(\psi\lambda\phi_1^*\dots\phi_n) \quad \forall\phi_1^* \longrightarrow \phi_1 = J_1(\psi,\lambda,\phi_2,\dots,\phi_n)$$

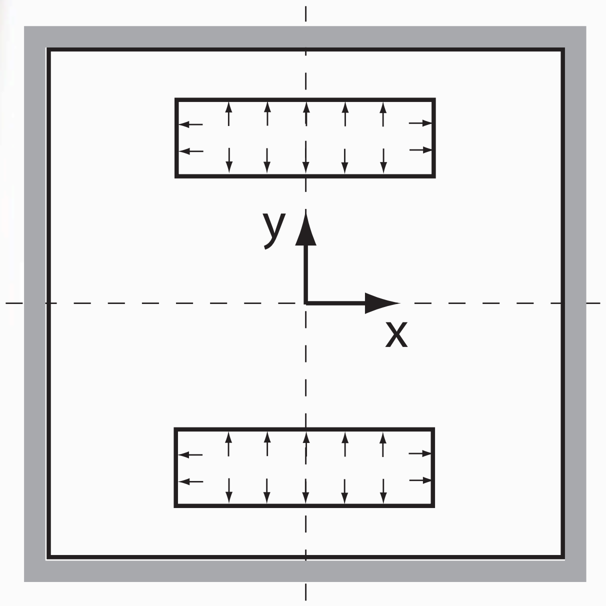
$$\vdots \qquad\qquad \vdots$$

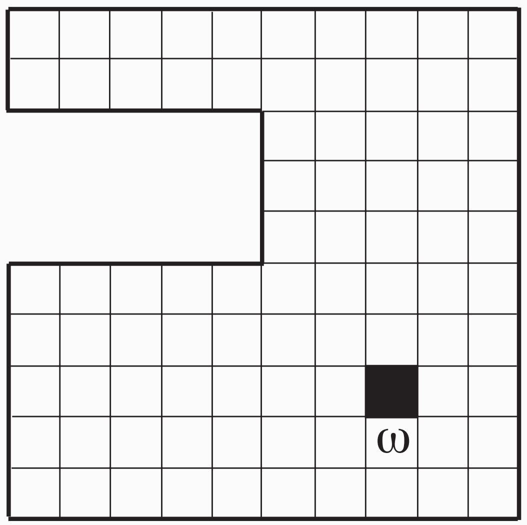
→ NL eigenvalue problem, solved with dedicated iterative strategies (fixed point)

<u>variants</u> : convergence, mode orthogonalization, mode updating, ...

Example

Transient thermal problem





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

$$u_{|t=0} = 0$$

$$c\frac{\partial u}{\partial t} - \boldsymbol{\nabla} \cdot \mathbf{q} = f_d$$

$$\mathbf{q} \cdot \mathbf{n} = q_d \quad \text{on } \partial_q\Omega \times \mathcal{I}$$

$$\mathbf{q} = k\boldsymbol{\nabla} u$$

Example

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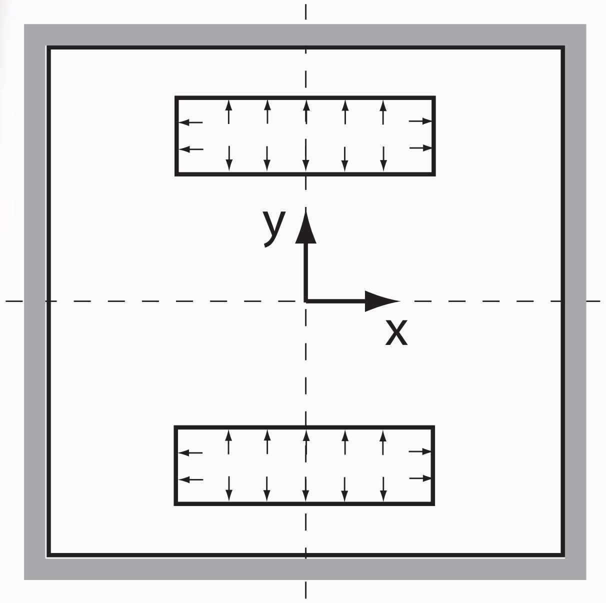

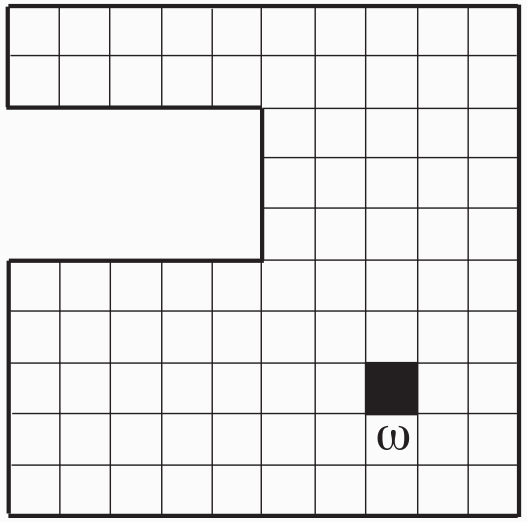

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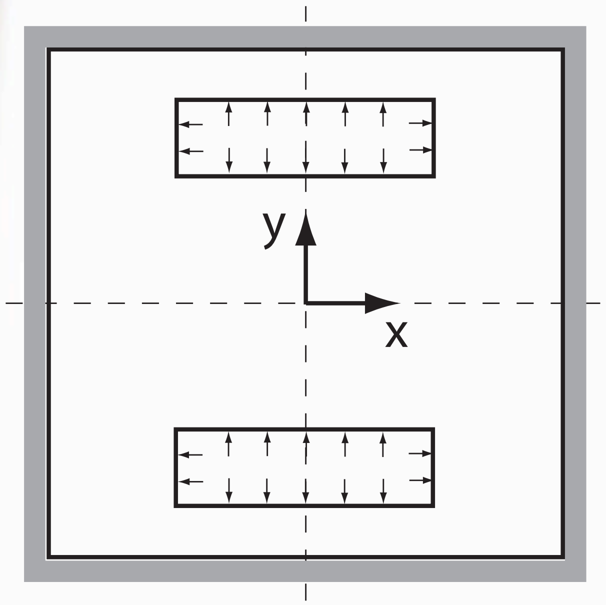
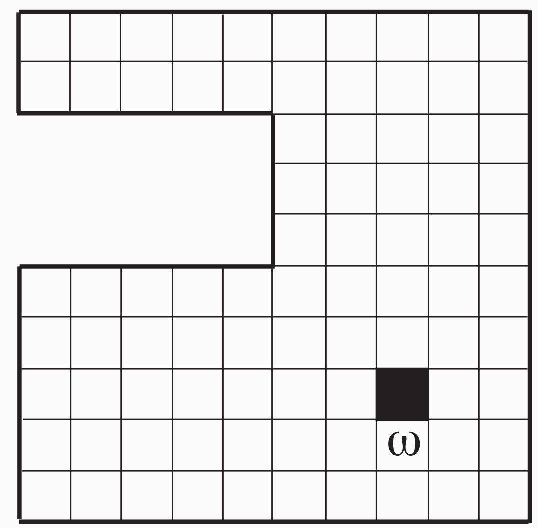
multi-parameter problem : $\mathbf{x}, t, \mathbf{p}$

Example

Transient thermal problem





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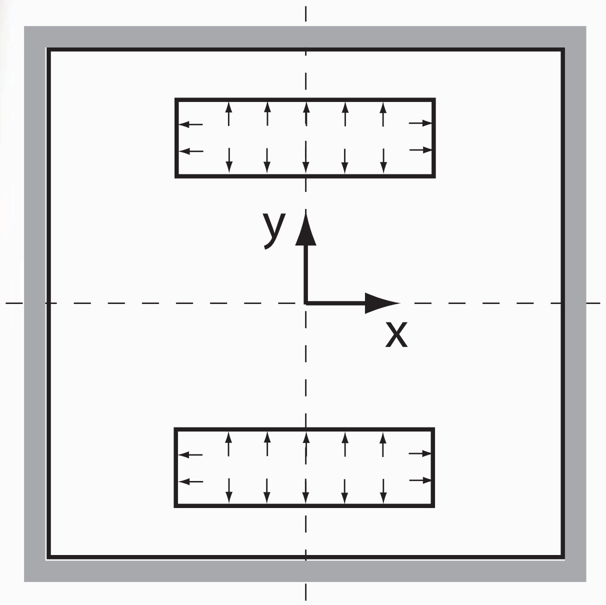

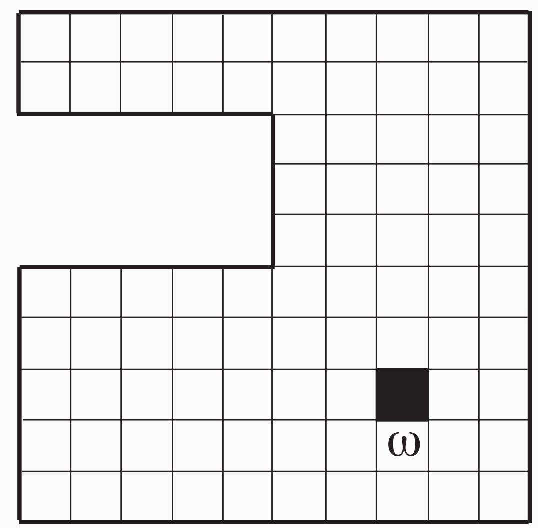

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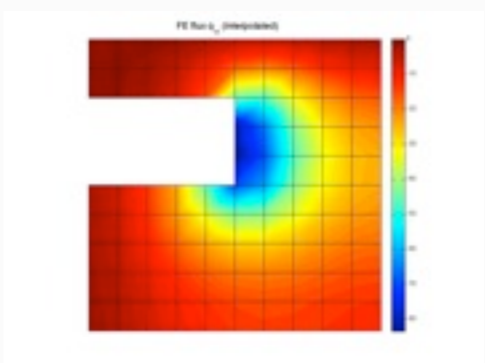
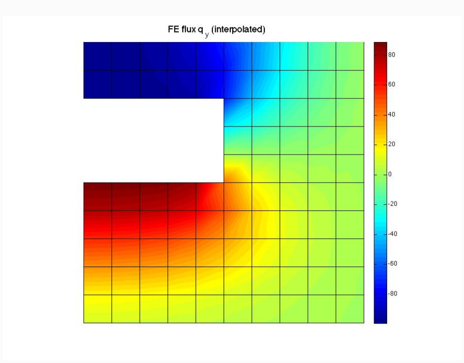
multi-parameter problem : $\mathbf{x}, t, \cancel{\mathbf{p}}$

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

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





Example

$$\boxed{u(\underline{x},t) \approx u_m(\underline{x},t) = \sum_{i=1}^{m} \psi_i(\underline{x})\lambda_i(t)} \longrightarrow m \times (N_h + N_{\Delta t}) \text{ dof}$$

«progressive Galerkin» approach

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

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

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

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

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

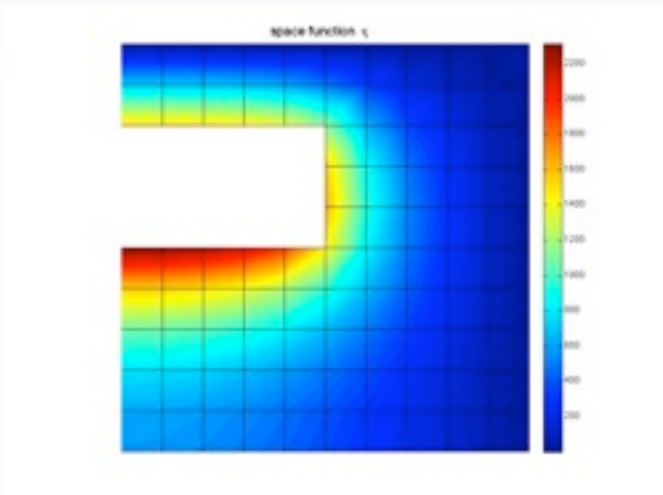
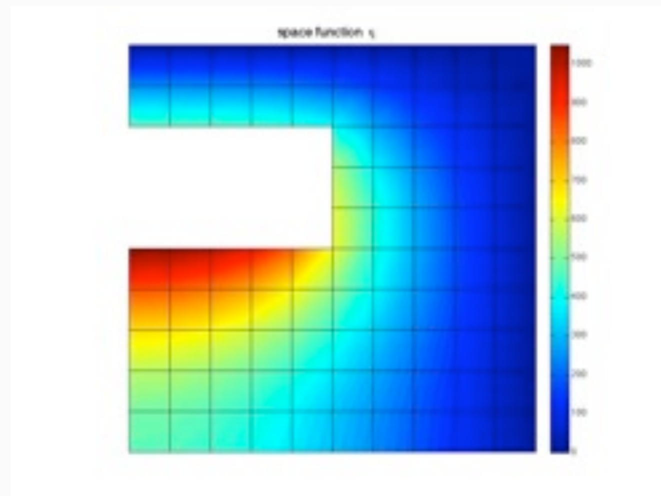
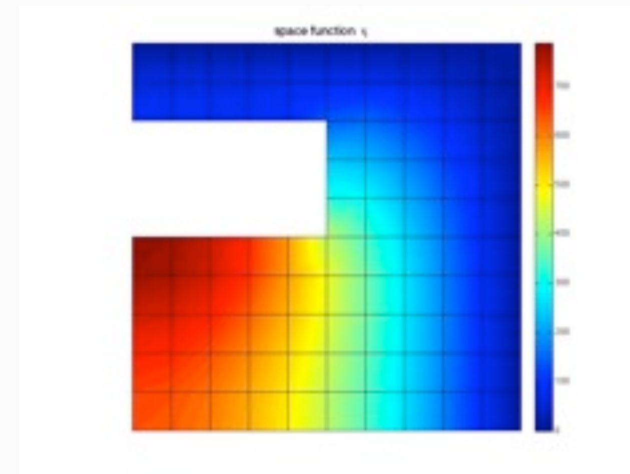
$$B(u_m, \psi\lambda^*) = L(\psi\lambda^*) \quad \forall \lambda^*$$

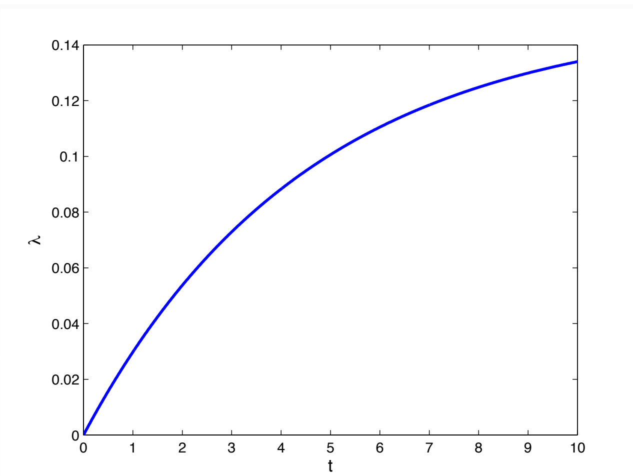
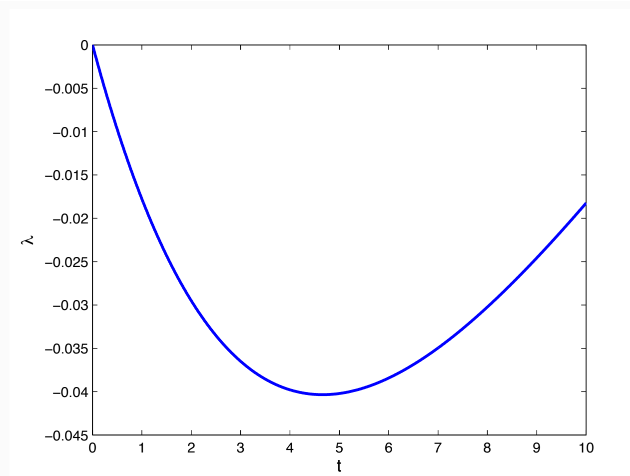
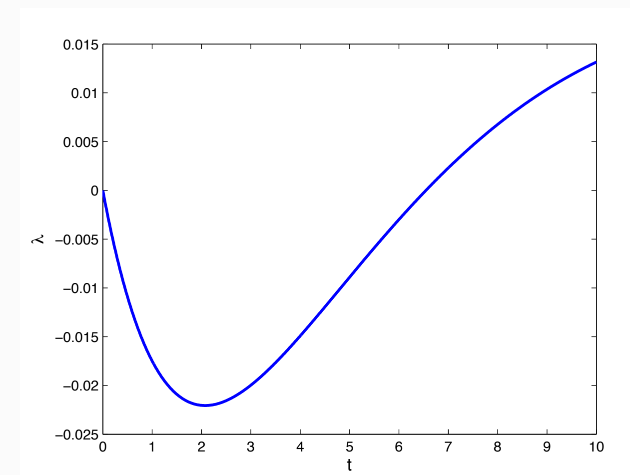
$$\alpha_T \frac{\lambda^{(k+1)} - \lambda^{(k)}}{\Delta t} + \beta_T \lambda^{(k)} = \delta_T^{(k)} \qquad \lambda^{(0)} = 0$$

Example

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

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

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

→ (guaranteed) estimation of the global/local error

→ adaptivity criteria

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- **Illustrations of PGD applications**
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PGD strategy

model parameters are seen as extra-coordinates [Chinesta *et al.* 2011]

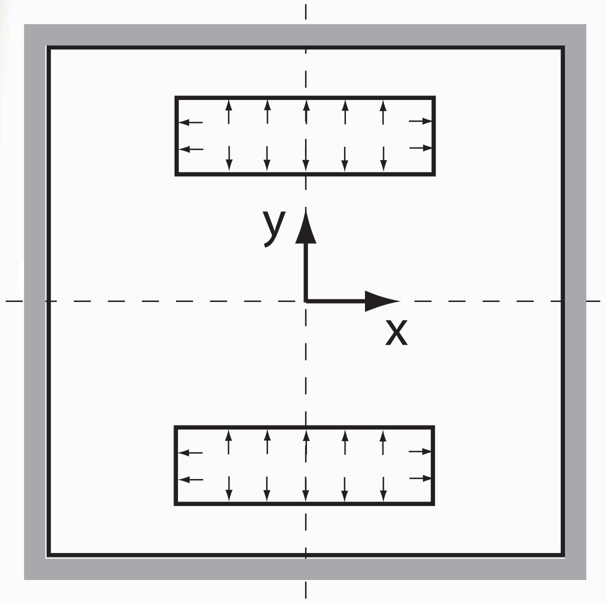
→ enables to address many engineering problems:
- variations of material parameters
- changes in boundary/initial conditions
- changes in loading
- geometry variations
- data assimilation (PGD+Kalman filter) [Marchand *et al.* submitted]

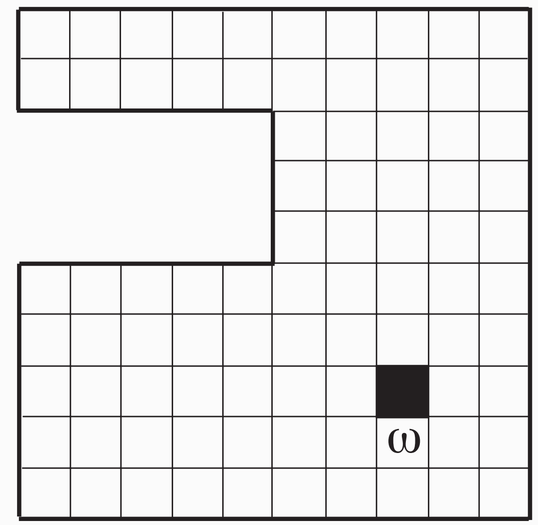
→ PGD modes are computed offline and used online for inverse analysis, optimization with cheap and fast computations on light computing platforms

→ concept of virtual charts

Material parameters

Transient thermal problem





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

$$\boxed{B(u,v) = L(v) \quad \forall v \in H^1_{0,\Gamma_D}(\Omega) \otimes L^2(\mathcal{I}) \otimes_j L^2(\mathcal{P}_j)}$$

$$B(u,v) = \int_\Theta \int_\mathcal{I} \int_\Omega (c\frac{\partial u}{\partial t}v + k\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v)d\Omega dt d\mathbf{p}$$

$$L(v) = \int_\Theta \int_\mathcal{I} \left(\int_\Omega f_d v d\Omega + \int_{\Gamma_N} q_d v ds \right) dt d\mathbf{p}$$

PGD modes

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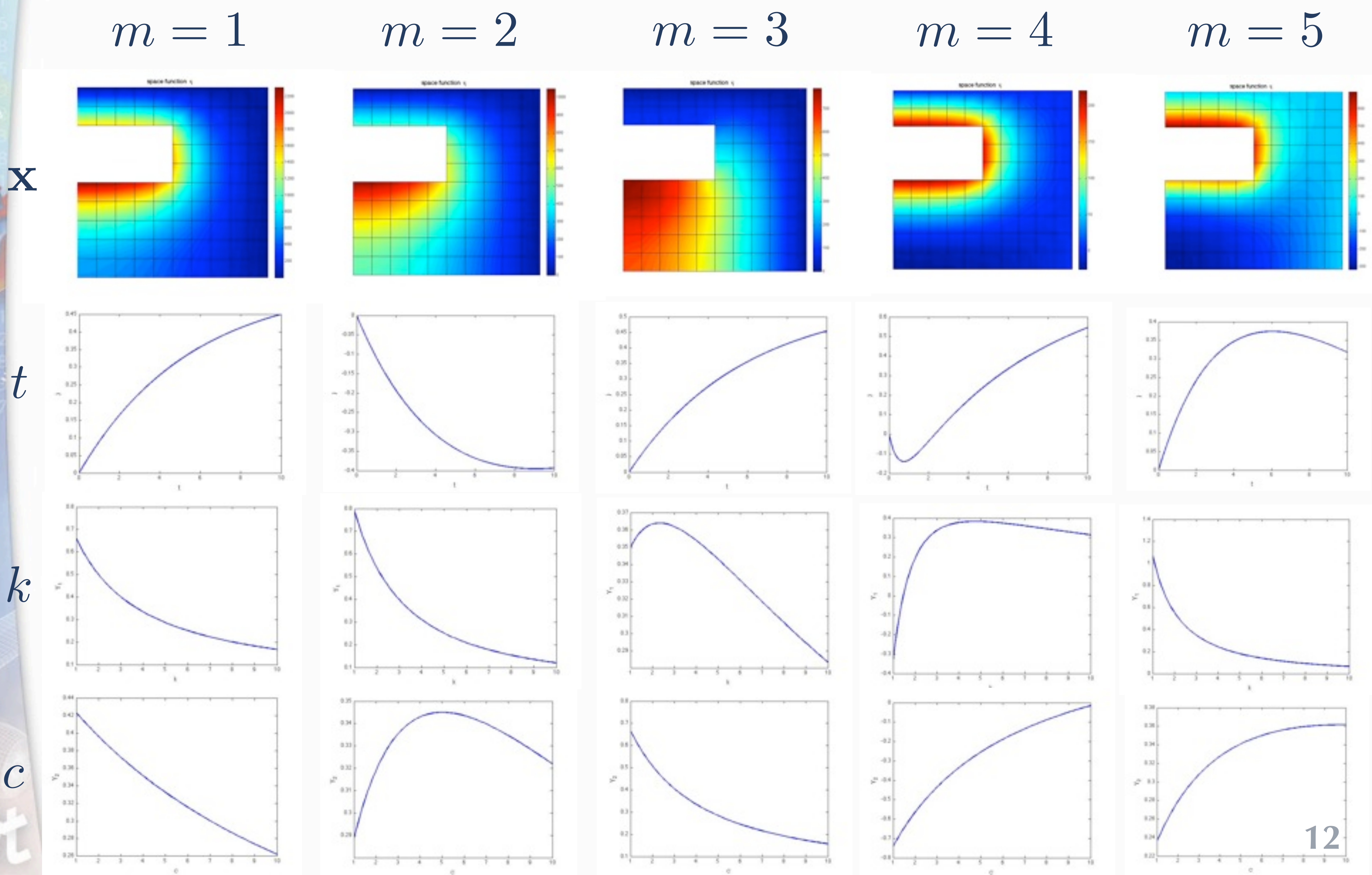
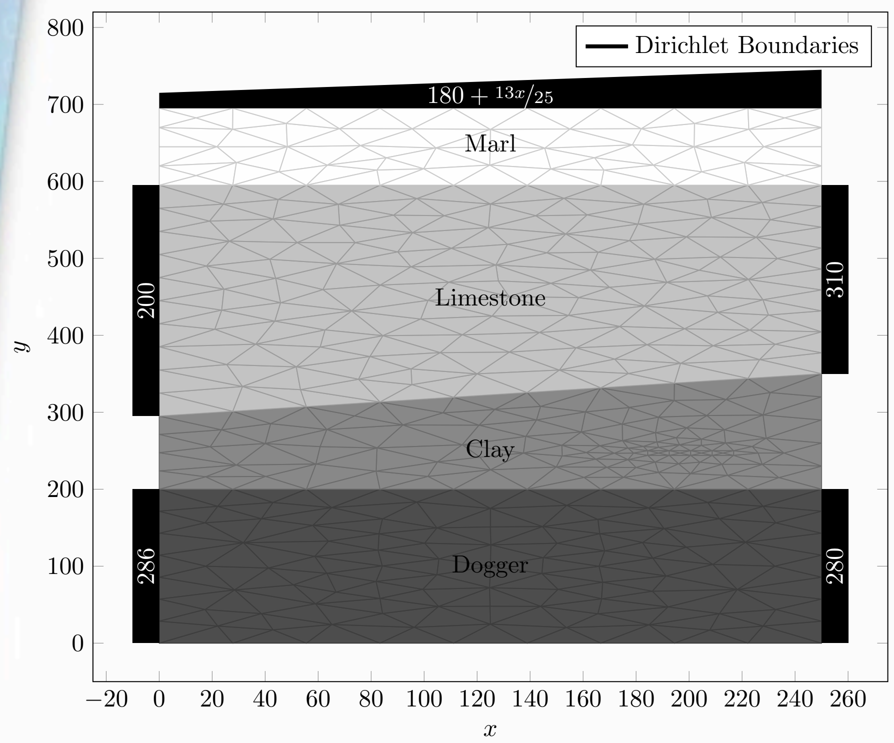


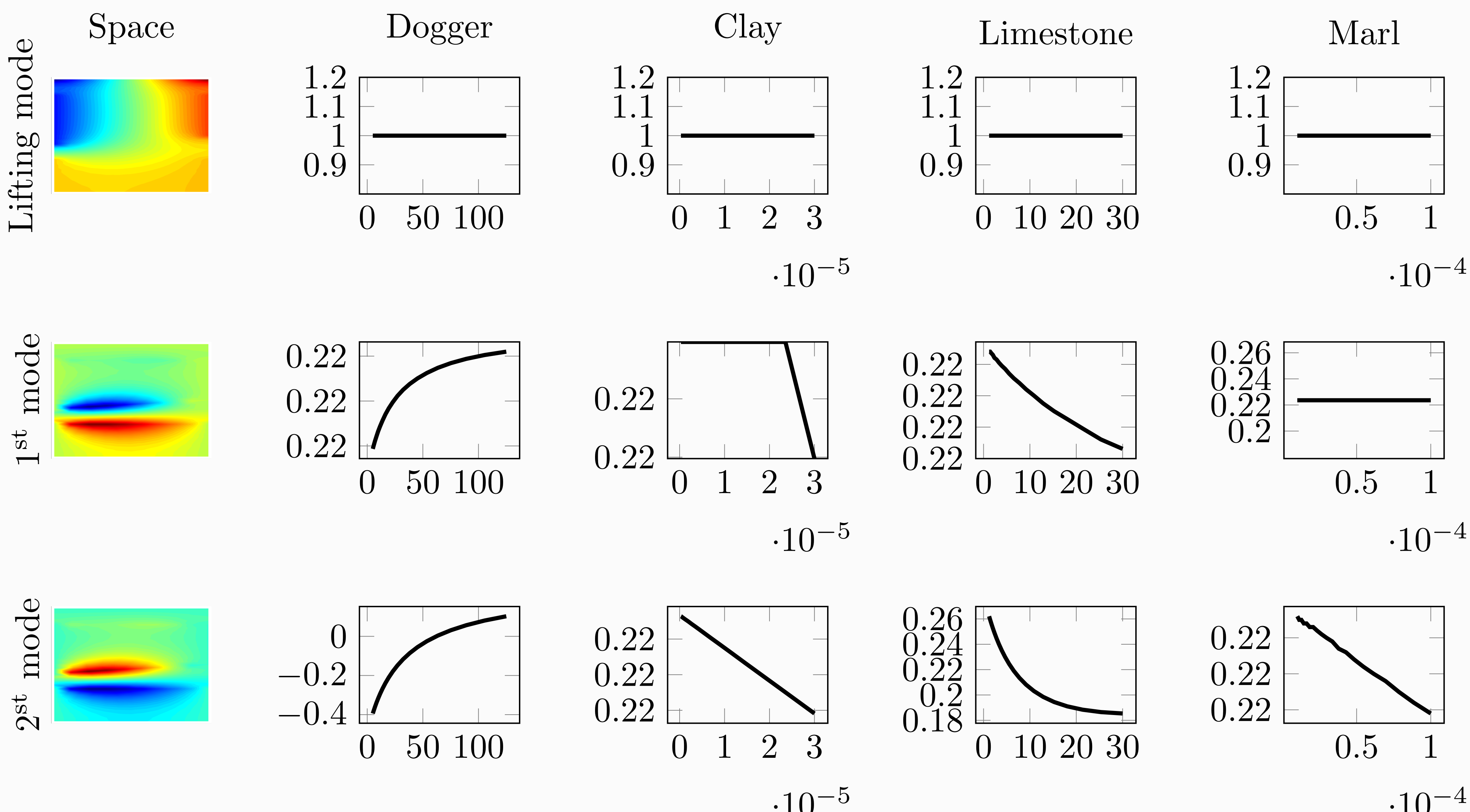
Another 2D example



- porous medium

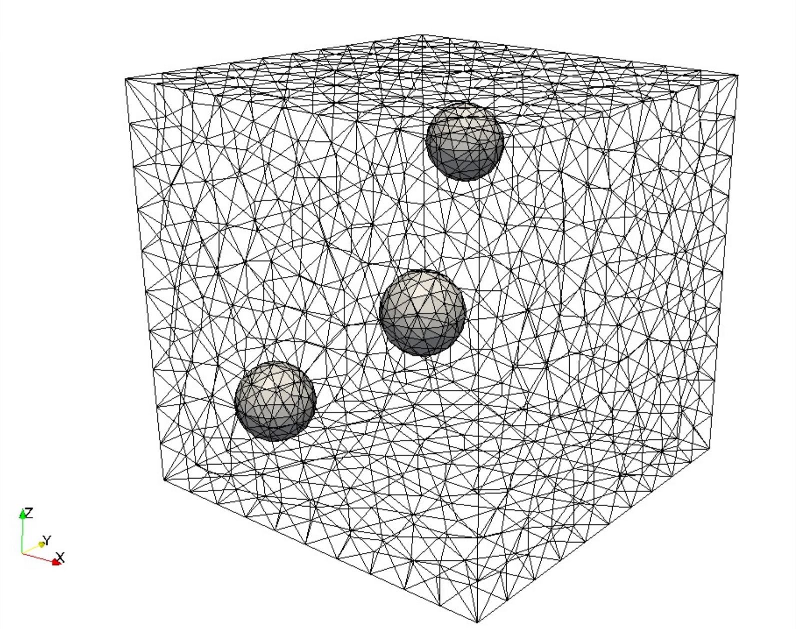
- Darcy's law: $\mathbf{u} = -k\nabla p$

- extra-parameters: k (piecewise constant)



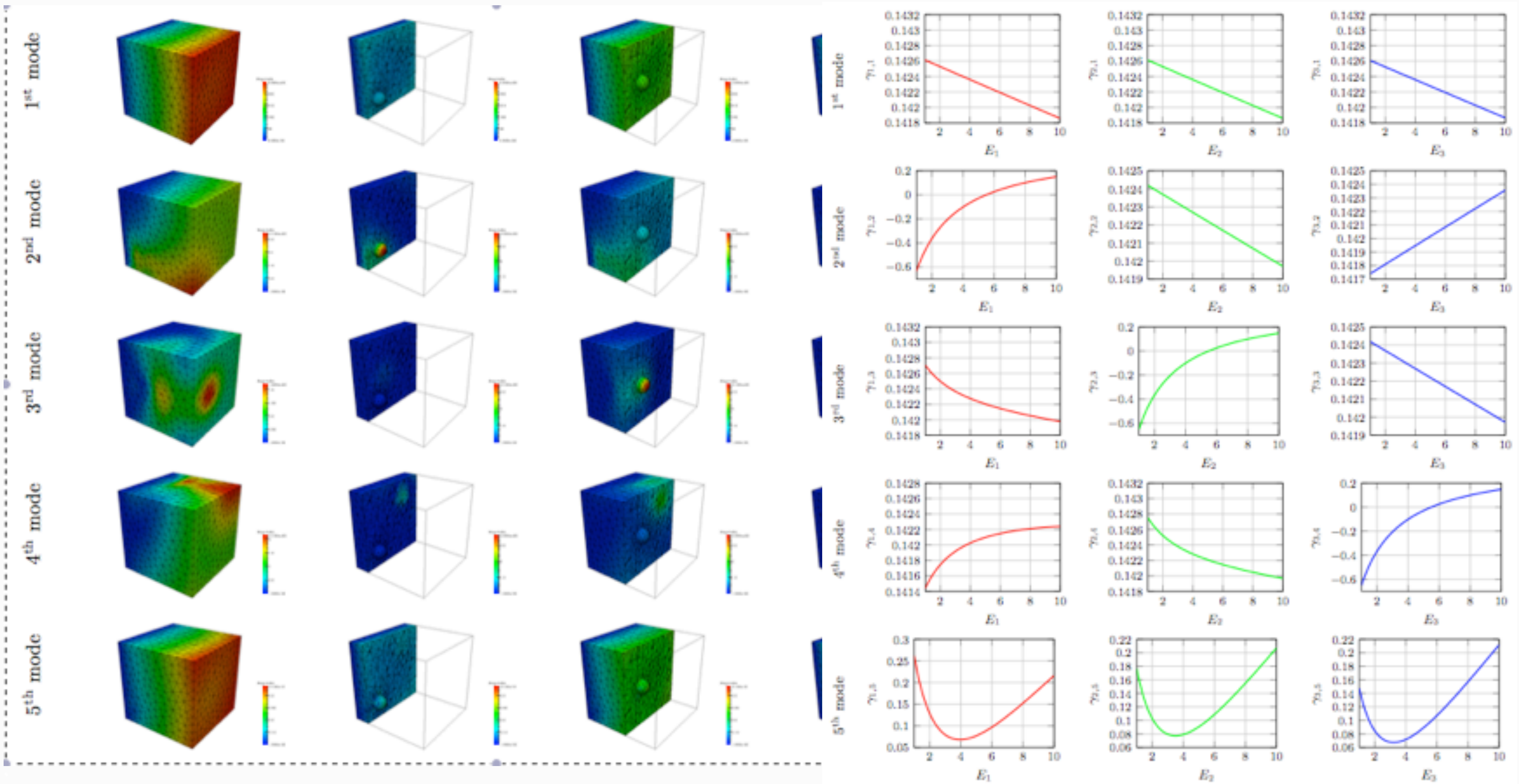
3D case

[Chamoin *et al* 2015]



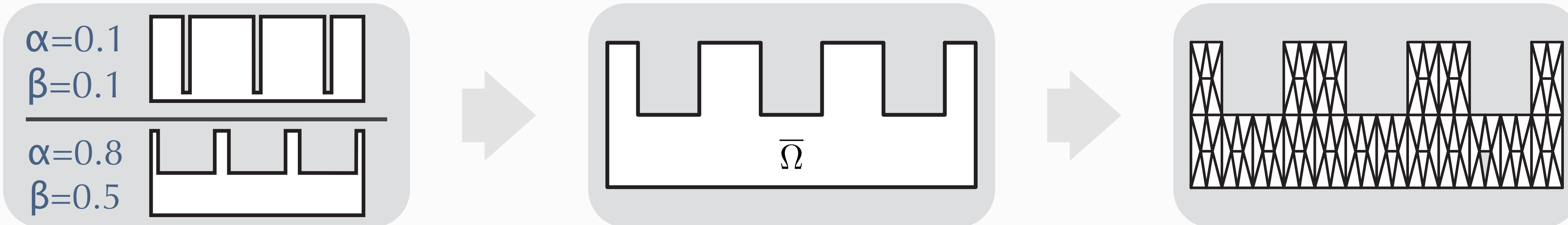
- linear elastic material (small perturbations)

- extra-parameters: E (in each inclusion)



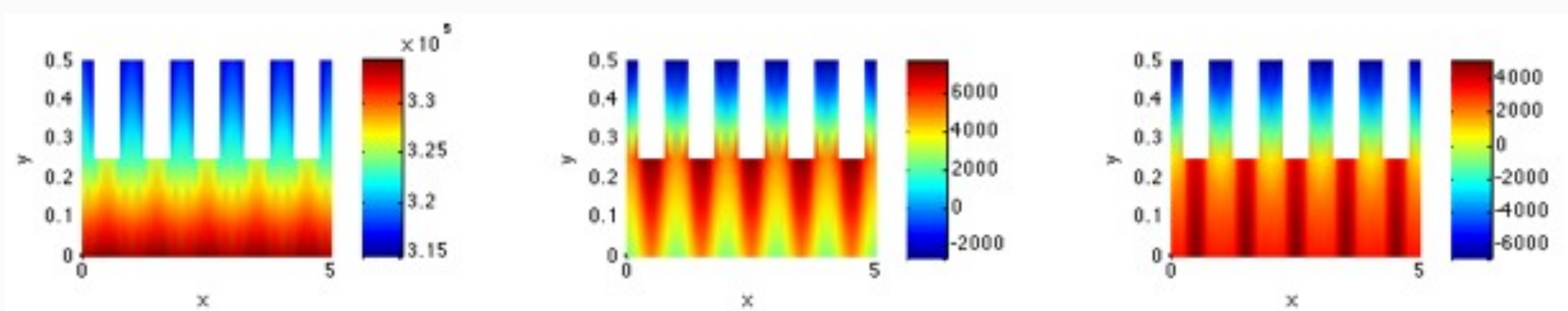
Geometry variations

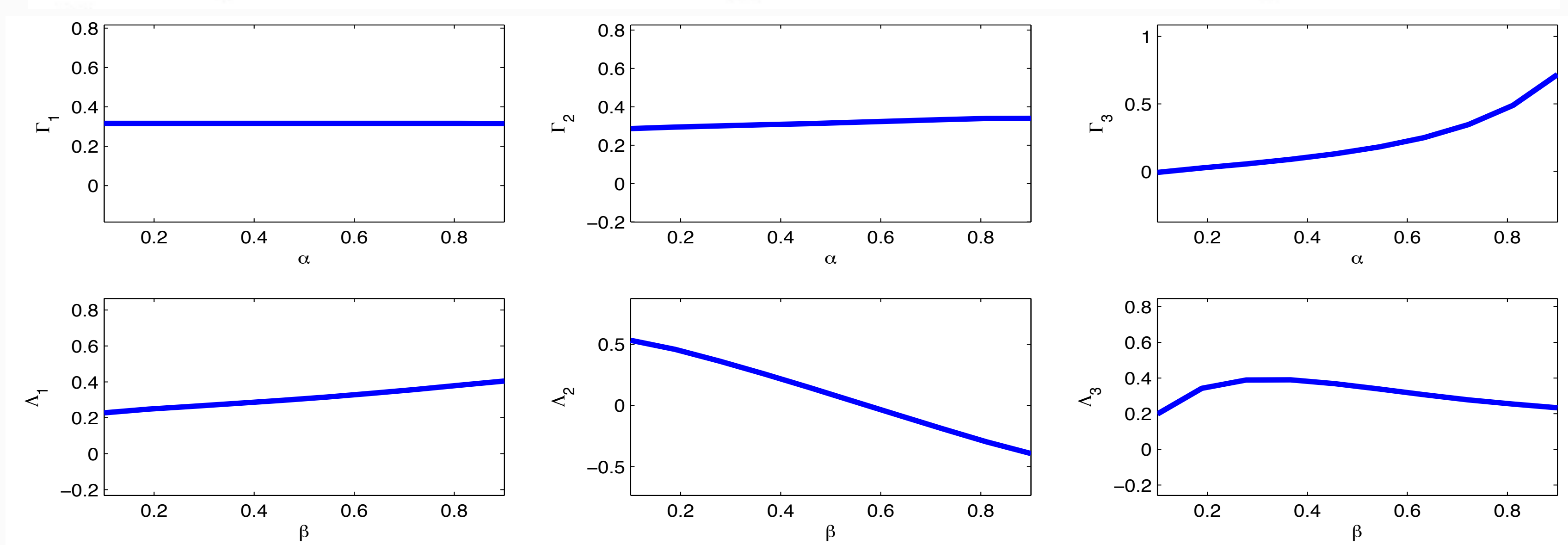
- **Reference domain**



- **Leading to an equivalent material**
  - Use of Jacobian transformation

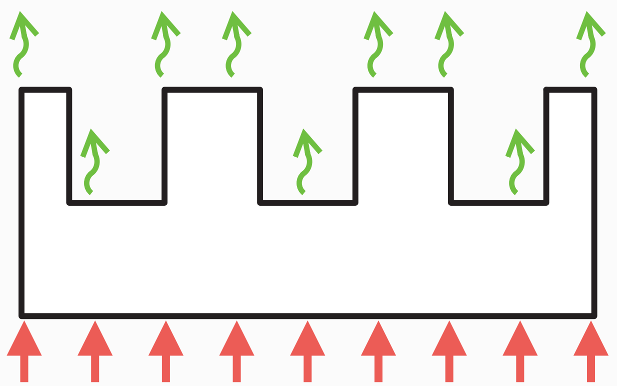
$$\int_{\Omega} k \nabla v \cdot \nabla u \; \mathrm{d}\Omega = \int_{\overline{\Omega}} (\nabla v)^T \left(k \mathbb{J}^{-1^T} \mathbb{J}^{-1} |\mathbb{J}| \right) \nabla u \; \mathrm{d}\Omega$$





Geometry variations

- **Problem: heater**
  - convection on the top border
  - imposed flux on the bottom



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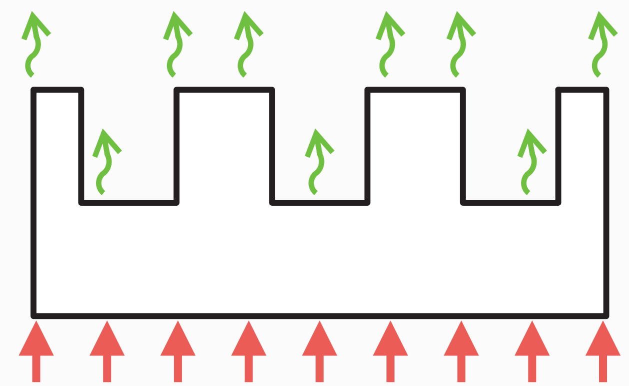
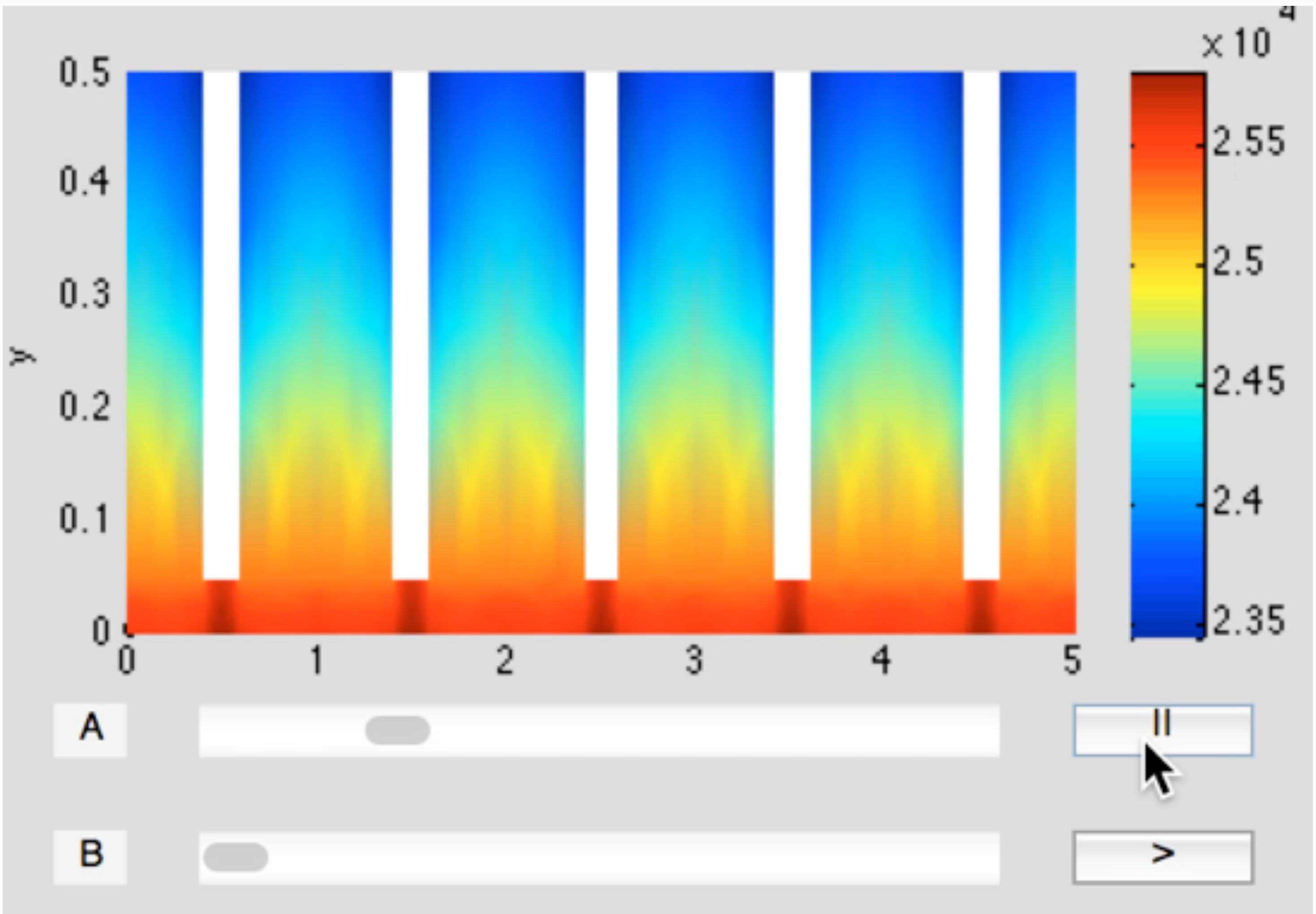




Nonlinear parametrized problems

APPRoFI project

- supported by the French National Research Agency
- collaboration between 7 industrials and academics
- driven by SAFRAN

Problematic

- development of probabilistic approaches for the **robust design in fatigue**
- **taking into account variability** in durability simulations to guarantee the robustness and reliability of the design

Typical example

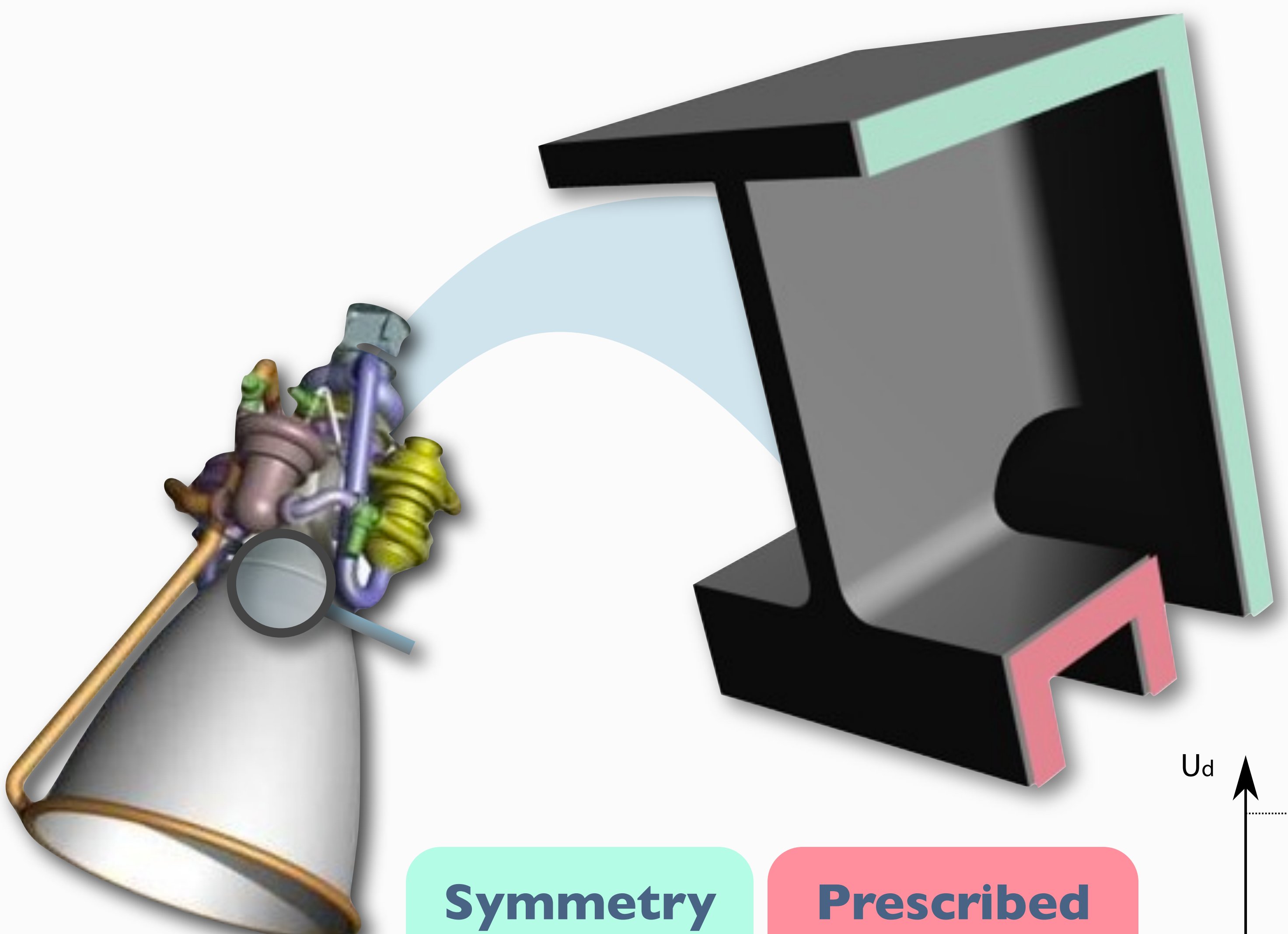
- blade of the Vulcain engine booster
- elasto-viscoplastic model
- variability of material properties
- variability of loadings

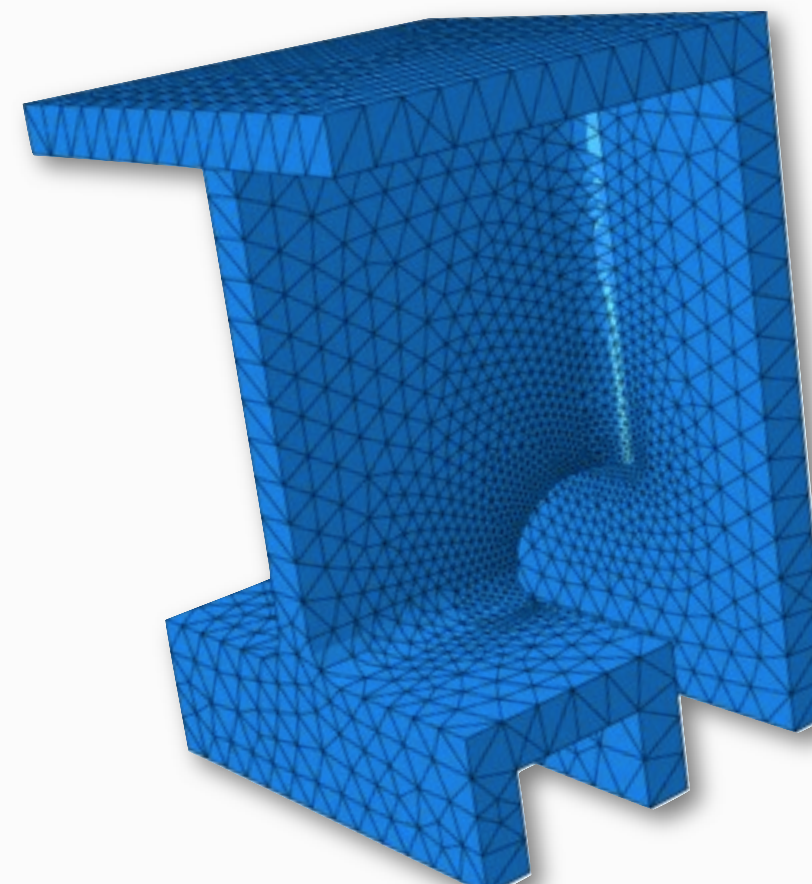
Engine blade

Description of the test-case

- ANR project APPROFI
- elasto-viscoplastic material

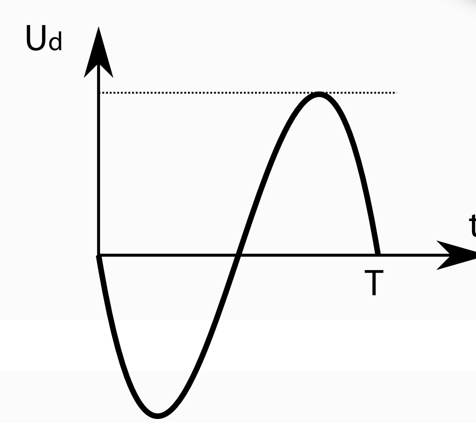
SAFRAN Snecma





Symmetry conditions

Prescribed displacement



740,000 DOFs
60 time steps

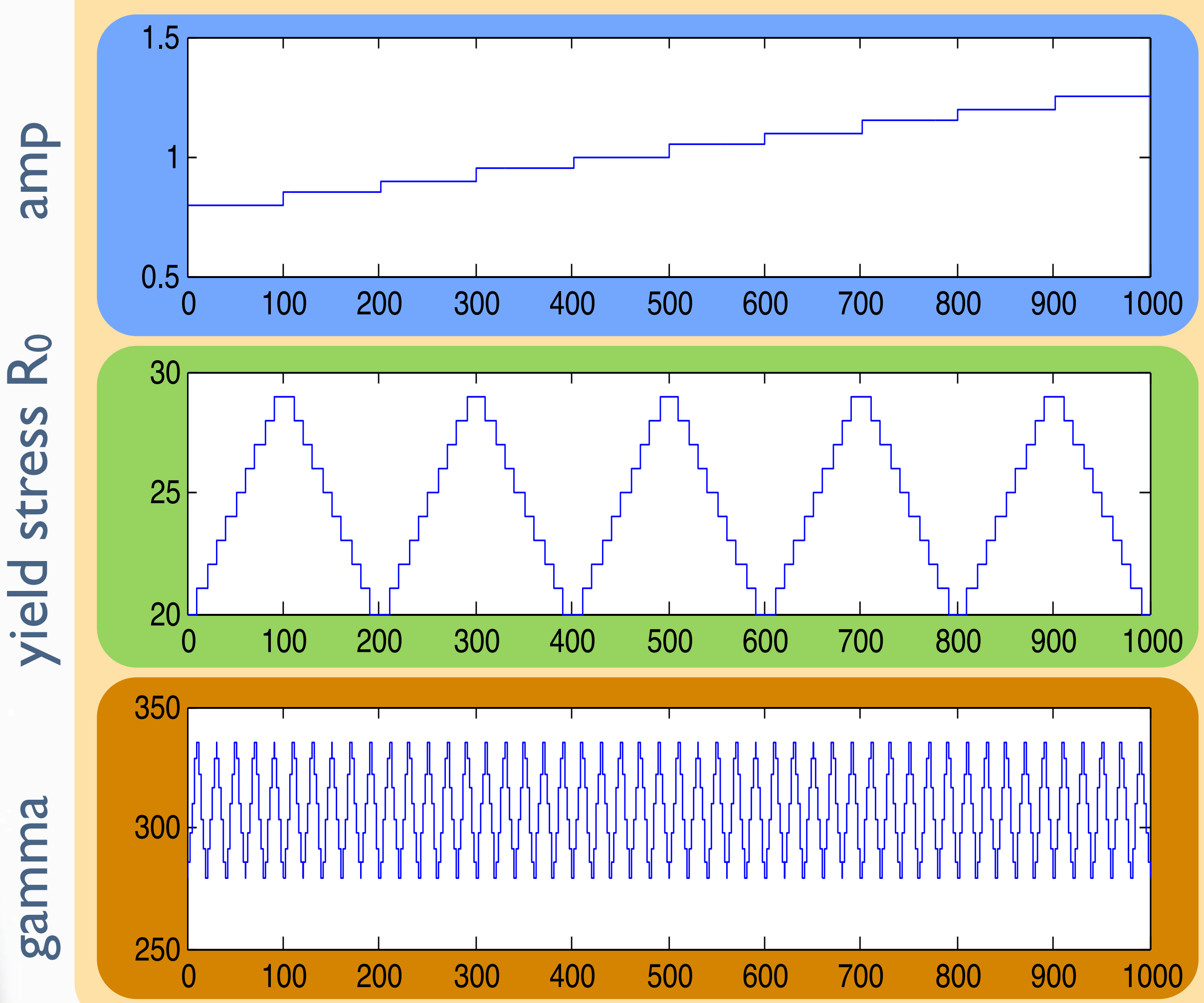
Parametric study

Parametric study

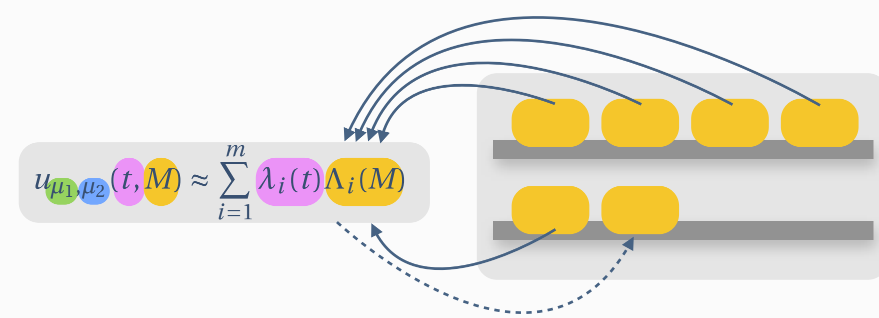
- 3 parameters: loading amplitude and material characteristics (R_0, γ)
- 10 x 10 x 10 = 1,000 sets of parameters (range of variation ±30%)
- influence on the maximum value of the σ_{mises}

µPDE: $\mathscr{L}(u(t,M),\mu_1,\mu_2) = 0$

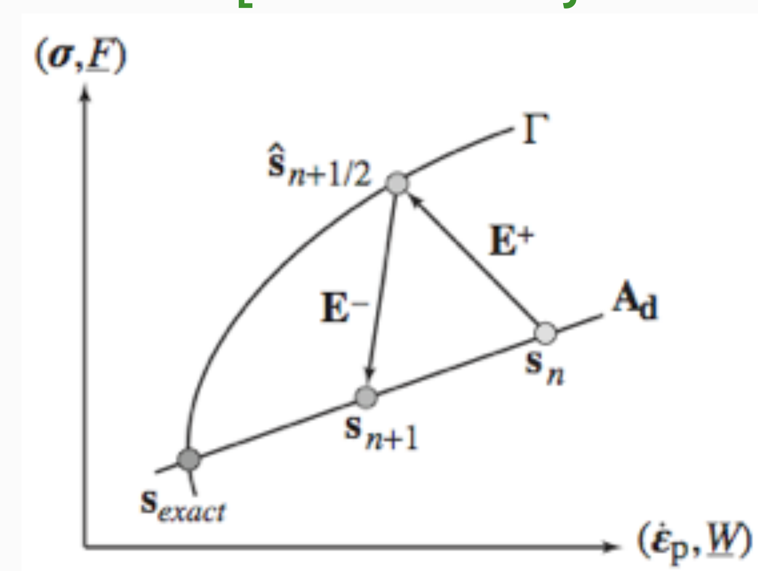
1,000 sets of parameters



Idea:
to build a library of modes common to all sets using the LATIN solver

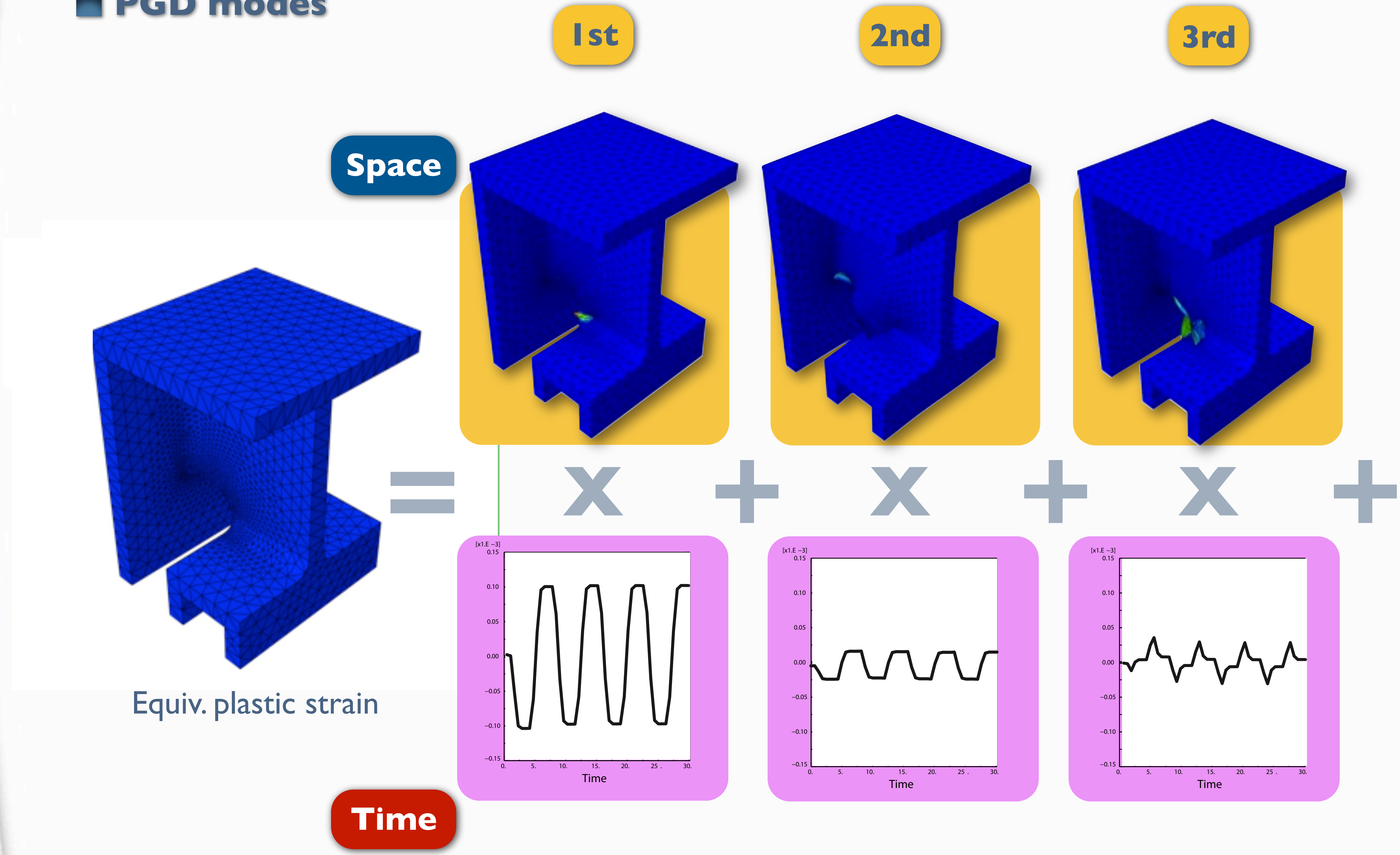


[Néron et al. IJNME 2015]



For a given set of parameters

- **PGD modes**



Virtual chart

Parametric study

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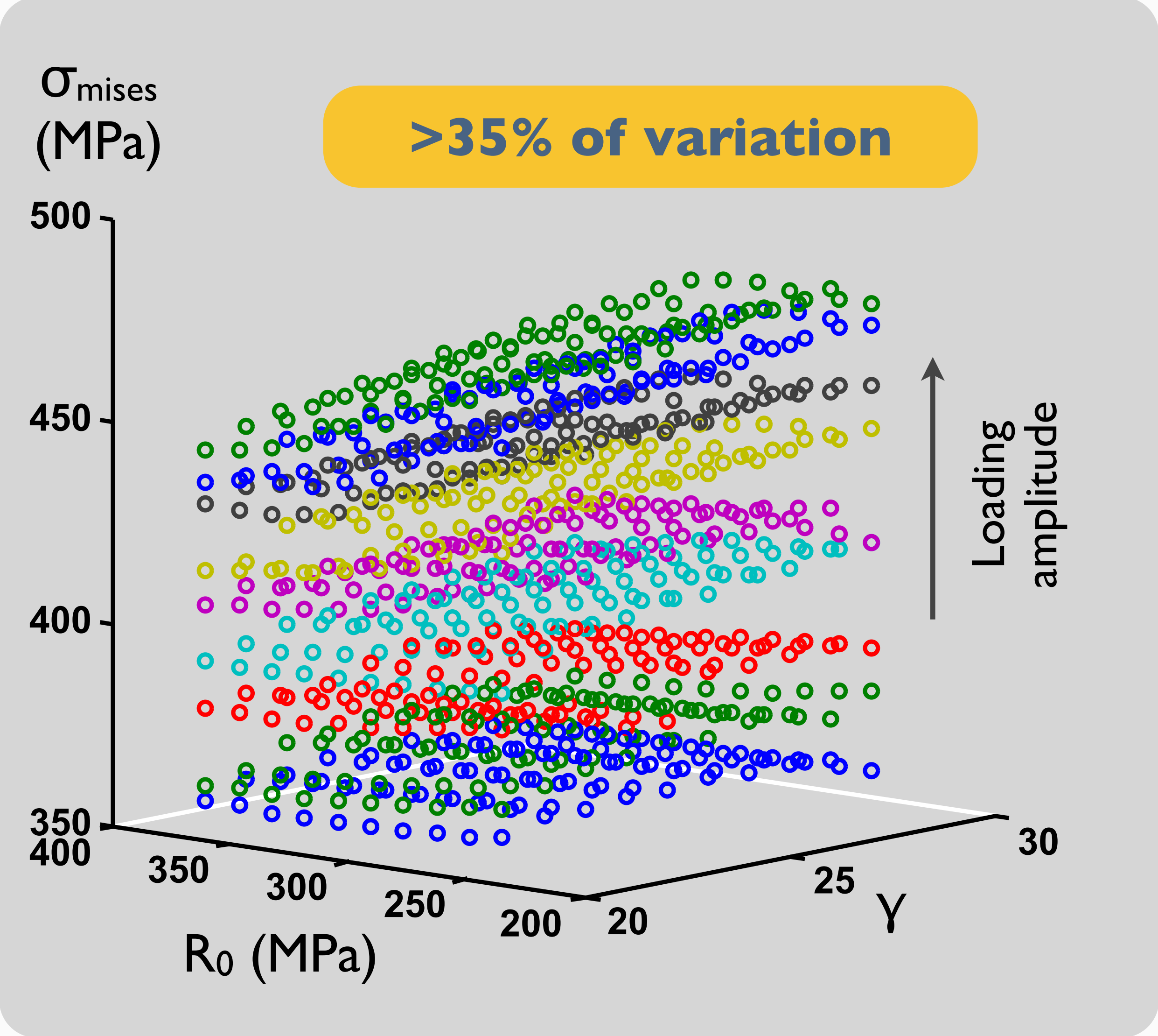
- influence on the maximum value of the σ_{mises}



4 months with ABAQUS

LATIN+PGD
3 days (gain: 40)

``True" complexity: ***50 modes***
(SVD of the ROB)

PGD based approach: ***67 modes***
(few needless computations)

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- A posteriori error estimation: the CRE concept
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Objectives

Goal: design a PGD algorithm such that:
- a given precision is attained
- as small as possible amount of computational work is needed

The designed error estimation method should:
- give a **fully computable upper bound** on the overall error (error control)
- enable to **distinguish** and **estimate** separately the **different error components**
- allow to **adjust optimally** the calculation parameters

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

Proposed estimate

PGD control, for linear elliptic or parabolic problems, with robust bounds
[Allier *et al.* 2015, Ladevèze & L.C. 2011, 2012]

→ use of the Constitutive Relation Error (CRE) concept

- widely used in the Computational Mechanics community for many years
  [Ladevèze & Leguillon 83, Destuynder & Métivet 99, Ladevèze & Pelle 04]
- guaranteed and fully computable a posteriori error estimate on the energy norm

method based on dual analysis, with recovery of equilibrated fluxes (verifying equilibrium in a strong sense) from the FEM solution

- estimate split into several indicators to drive adaptive procedures

↓

robust virtual charts that can be used for industrial design

Basics on CRE

$$\begin{aligned} -\boldsymbol{\nabla}\cdot(k\boldsymbol{\nabla}u) &= f \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \Gamma_D \\ k\boldsymbol{\nabla}u\cdot\mathbf{n} &= g \quad \text{on } \Gamma_N \end{aligned}$$

(equilibrium of flux $\mathbf{q} = k\boldsymbol{\nabla}u$)

$f \in L^2(\Omega) \quad ; \quad g \in L^2(\Gamma_N)$

k : unif. bounded, strictly positive function

Find $u \in V$ such that

$$a(u,v) = l(v) \quad \forall v \in V$$

CONFORMING FEM

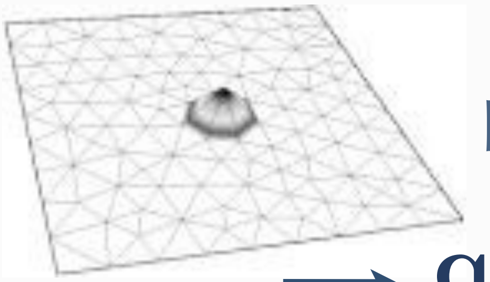
Find $u_h \in V_h^p$ such that

$$a(u_h,v_h) = l(v_h) \quad \forall v_h \in V_h^p$$

$$a(u,v) = \int_\Omega k\boldsymbol{\nabla}u\cdot\boldsymbol{\nabla}v d\Omega$$

$$l(v) = \int_\Omega fvd\Omega + \int_{\Gamma_N} gvds$$

$$V = H^1_{\Gamma_D,0}(\Omega)$$



partition $\mathcal{T}_h$

$\longrightarrow \mathbf{q}_h = k\boldsymbol{\nabla}u_h$

Basics on CRE

$$\boxed{\begin{aligned} -\boldsymbol{\nabla}\cdot(k\boldsymbol{\nabla}u) &= f \quad \text{in } \Omega \quad \text{(equilibrium of flux } \mathbf{q}=k\boldsymbol{\nabla}u\text{)} \\ u &= 0 \quad \text{on } \Gamma_D \\ k\boldsymbol{\nabla}u\cdot\mathbf{n} &= g \quad \text{on } \Gamma_N \end{aligned}}$$

$f \in L^2(\Omega) \quad ; \quad g \in L^2(\Gamma_N)$

k : unif. bounded, strictly positive function

Find $u \in V$ such that

$$a(u,v) = l(v) \quad \forall v \in V$$

CONFORMING FEM

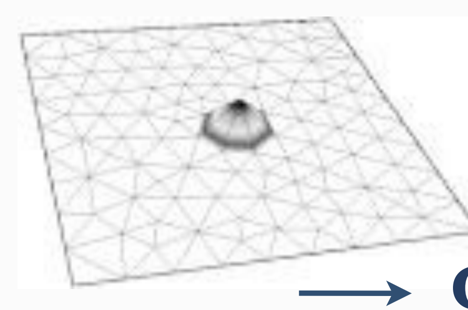
Find $u_h \in V_h^p$ such that

$$a(u_h,v_h) = l(v_h) \quad \forall v_h \in V_h^p$$

$$a(u,v) = \int_\Omega k\boldsymbol{\nabla}u\cdot\boldsymbol{\nabla}v\,d\Omega$$

$$l(v) = \int_\Omega fv\,d\Omega + \int_{\Gamma_N} gv\,ds$$

$$V = H^1_{\Gamma_D,0}(\Omega)$$



partition $\mathcal{T}_h$

$\longrightarrow \mathbf{q}_h = k\boldsymbol{\nabla}u_h$

discretization error $e = u - u_h$

$\sqrt{\int_\Omega k^{-1}\bullet\cdot\bullet\,d\Omega}$

global measure: $|||e||| := \sqrt{a(e,e)} = |||\mathbf{q}-\mathbf{q}_h|||_{\mathbf{q}}$

Basics on CRE

Space of equilibrated fluxes:

$$W := \{\mathbf{p} \in H(div, \Omega), \boldsymbol{\nabla} \cdot \mathbf{p} + f = 0 \text{ in } \Omega, \mathbf{p} \cdot \mathbf{n} = g \text{ on } \partial_2\Omega\}$$

$\rightarrow \int_\Omega \mathbf{p} \cdot \boldsymbol{\nabla} v d\mathbf{x} = \int_\Omega f v d\mathbf{x} + \int_{\partial_2\Omega} g v d\mathbf{s} \quad \forall v \in H^1_{0,\partial_1\Omega}(\Omega)$ (weak form of equilibrium)

$\rightarrow$ $\mathbf{p} \in W$ is said statically admissible (SA)

$$\boxed{J_2(\mathbf{q}) = \min_{\mathbf{p} \in W} J_2(\mathbf{p}) \quad ; \quad J_2(\mathbf{p}) := \frac{1}{2}\int_\Omega k^{-1}\mathbf{p} \cdot \mathbf{p} d\mathbf{x}}$$

For any approximation $\hat{u}_h$ of u which is kinematically admissible (KA), we define:
$(\hat{u}_h \in H^1(\Omega) \quad ; \quad \hat{u}_{h|\partial_1\Omega} = 0)$
flux field $\mathbf{p}$ which is SA

CRE functional

$$E^2_{CRE}(\hat{u}_h, \mathbf{p}) := \int_\Omega k^{-1}(\mathbf{p} - k\boldsymbol{\nabla}\hat{u}_h)^2 d\mathbf{x} \equiv |||\mathbf{p} - k\boldsymbol{\nabla}\hat{u}_h|||^2_{\mathcal{F}} = 2(J_1(\hat{u}_h) + J_2(\mathbf{p}))$$

$$\rightarrow |||u - \hat{u}_h||| = E_{CRE}(\hat{u}_h, \mathbf{q}) \leq E_{CRE}(\hat{u}_h, \mathbf{p}) \quad \forall \mathbf{p} \in W$$

Basics on CRE

Properties

- Prager-Synge equality:

$$|||u - \hat{u}_h|||^2 + |||\mathbf{q} - \mathbf{p}|||_{\mathcal{F}}^2 = E_{CRE}^2(\hat{u}_h, \mathbf{p}) \quad \forall \mathbf{p} \in W$$

→ easily obtained from $\int_\Omega (\mathbf{q} - \mathbf{p}) \cdot \boldsymbol{\nabla}(u - \hat{u}_h) d\mathbf{x} = 0$

- Hypercircle equality:

$$4|||\mathbf{q} - \mathbf{p}^*|||_{\mathcal{F}}^2 = E_{CRE}^2(\hat{u}_h, \mathbf{p}) \quad \forall \mathbf{p} \in W$$

with $\mathbf{p}^* = \frac{1}{2}(\mathbf{p} + k\boldsymbol{\nabla}\hat{u}_h)$

→ used for goal-oriented error estimation

- Technical point: construction of a relevant admissible flux $\hat{\mathbf{q}}_h \in W$

→ post-processing of the approximate solution u_h (use of Galerkin properties in the FE context no full dual computation)

[Ladevèze & Leguillon 83, Destuynder & Métivet 99, Vohralik 12, Pares & Diez 06, Pled *et al.* 11,12]

→ provides for asymptotic convergence properties [Ladevèze & Pelle 2004]

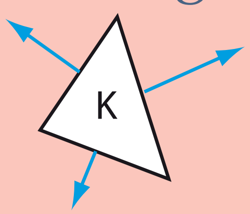
$$|||u - u_h||| \leq E_{CRE}(u_h, \hat{\mathbf{q}}_h) \leq C|||u - u_h||$$

Construction of $\hat{\mathbf{q}}_h$

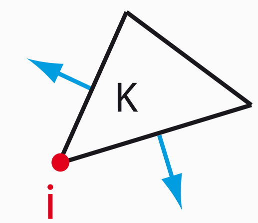
Hybrid approach (domain decomposition)[Ladevèze 75, Ladevèze *et al* 10]

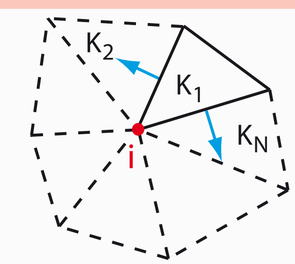
Step 1 : construction of equilibrated tractions $\hat{g}_K = \sigma_K \hat{g}_\gamma$ on element edges γ

$$\int_K f d\Omega + \int_{\partial K} \hat{g}_K ds = 0 \quad \forall K \quad ; \quad \hat{g}_K = g \quad \text{on } \Gamma_N$$



condition $\int_{\partial K} \hat{g}_K \varphi_i ds = \int_K (\mathbf{q}_h \cdot \boldsymbol{\nabla} \varphi_i - f \varphi_i) d\Omega = Q_i^K$



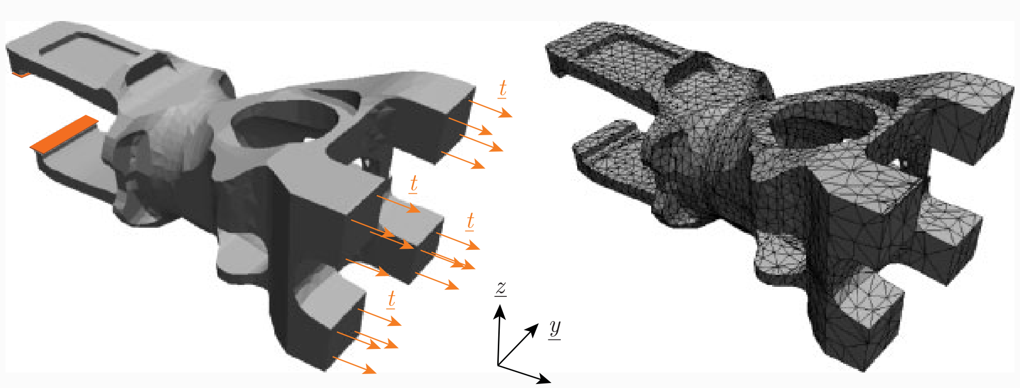


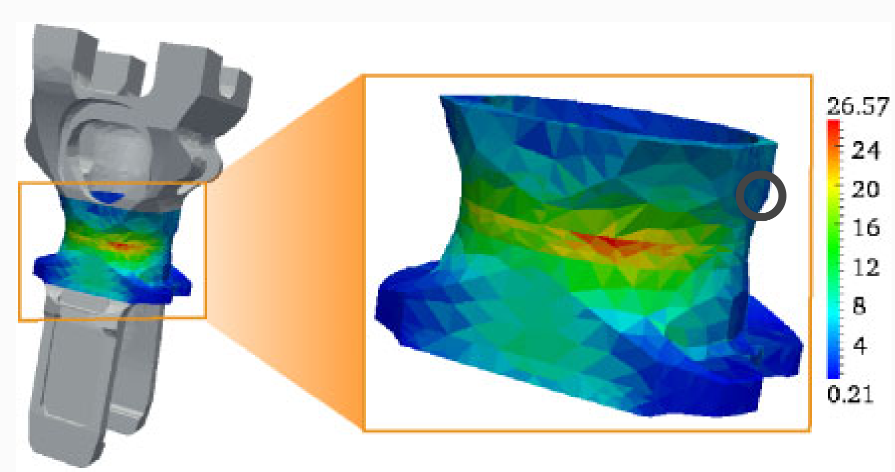
Step 2 : local construction of $\hat{\mathbf{q}}_{h|K}$ at the element level, verifying:

$$-\boldsymbol{\nabla} \cdot \hat{\mathbf{q}}_{h|K} = f \quad \text{in } K \quad ; \quad \hat{\mathbf{q}}_{h|K} \cdot \mathbf{n}_K = \hat{g}_K \quad \text{on } \partial K$$

solved using PGD (offline)

implemented in a C++ plateform





Extension of CRE

Definition in the unsteady case

$$\boxed{E^2_{CRE}(u_h,\hat{\mathbf{q}}_h) = |||\hat{\mathbf{q}}_h - k\boldsymbol{\nabla} u_h|||^2_q}$$

$$\int_0^T \int_\Omega k^{-1} \bullet \cdot \bullet \, d\Omega dt$$

Fundamental result

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

→ guaranteed bounding on global and local errors

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

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

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

convex pseudo-potentials (with Fenchel's duality)

Outline

- Basics on Proper Generalized Decomposition (PGD)
- Illustrations of PGD applications
- A posteriori error estimation: the CRE concept
- Control and adaptivity in PGD computations
- PGD performances and limits

Use of the CRE concept

Example: thermal problem solved with PGD

$$u_m(\mathbf{x},t,k,c)=\sum_{i=1}^{m}\psi_i(\mathbf{x})\lambda_i(t)f_i(k)g_i(c) \quad ; \quad \mathbf{q}(u_m)=k\boldsymbol{\nabla}u_m$$

- $\hat{u}$ should be compatible (KA) : $\hat{u}=0 \text{ on } \Gamma_D\times\mathcal{I}\ ;\ \hat{u}_{|t=0}=0 \quad \forall\mathbf{p}$

→ we choose $\hat{u}=u_m$

- $(\hat{u},\hat{\mathbf{q}})$ should be equilibrated (SA) :

$$\int_\Omega \hat{\mathbf{q}}\cdot\boldsymbol{\nabla}u^* d\Omega=\int_\Omega (f_d-c\frac{\partial\hat{u}}{\partial t})u^* d\Omega+\int_{\Gamma_N} q_d u^* ds \quad \forall u^*\in V,\forall t,\forall\mathbf{p}$$

→ $(u_m,\mathbf{q}(u_m))$ is not SA in a FE sense

→ necessary to post-process to get $(u_m,\mathbf{q}_m)$ SA in a FE sense

→ then, use of classical FE techniques (prolongation condition)

Post-processing

[Ladevèze & Chamoin 11,12]

We stop PGD sub-iterations with a problem in space

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

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

assumption : radial loading $f_d = \sum_{j=1}^{J} \alpha_j(t) f_d^j(\mathbf{x}) \qquad q_d = \sum_{j=1}^{J} \beta_j(t) q_d^j(\mathbf{x})$

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

is equilibrated in a FE sense with (f_d, q_d) , for all t

$$\int_\Omega \underbrace{\left(\int_\Theta \int_{\mathcal{I}} \lambda_{m_0} \Gamma_{m_0} (k \nabla u_{m_0} - \mathbf{q}_0) dt d\mathbf{p} \right)}_{\mathbf{Q}_{m_0}} \cdot \nabla \psi^* d\Omega + \int_\Omega \sum_{i=1}^{m_0} \underbrace{\left[\int_\Theta \int_{\mathcal{I}} c \lambda_{m_0} \Gamma_{m_0} \dot{\lambda}_i dt d\mathbf{p} \right]}_{A_{m_0 i}} \psi_i \psi^* d\Omega = 0 \quad \forall \psi^* \in V_h$$

Post-processing

$$\int_\Omega \mathbb{A}\boldsymbol{\Psi}_m \psi^* d\Omega + \int_\Omega \{\mathbf{Q}\}_1^m \cdot \boldsymbol{\nabla}\psi^* d\Omega = 0 \quad \forall \psi^* \in V_h$$

$$\int_\Omega \boldsymbol{\Psi}_m \psi^* d\Omega + \int_\Omega \mathbb{A}^{-1}\{\mathbf{Q}\}_1^m \cdot \boldsymbol{\nabla}\psi^* d\Omega = 0 \quad \forall \psi^* \in V_h$$

$$\int_\Omega \underbrace{c\boldsymbol{\Gamma}_m \otimes \dot{\boldsymbol{\Lambda}}_m \otimes \boldsymbol{\Psi}_m}_{\dot{u}_m} \psi^* d\Omega + \int_\Omega \underbrace{c\boldsymbol{\Gamma}_m \otimes \dot{\boldsymbol{\Lambda}}_m \otimes \mathbb{A}^{-1}\{\mathbf{Q}\}_1^m}_{-\bar{\mathbf{q}}_m} \cdot \boldsymbol{\nabla}\psi^* d\Omega = 0 \quad \forall \psi^* \in V_h, \forall t, \forall \mathbf{p}$$

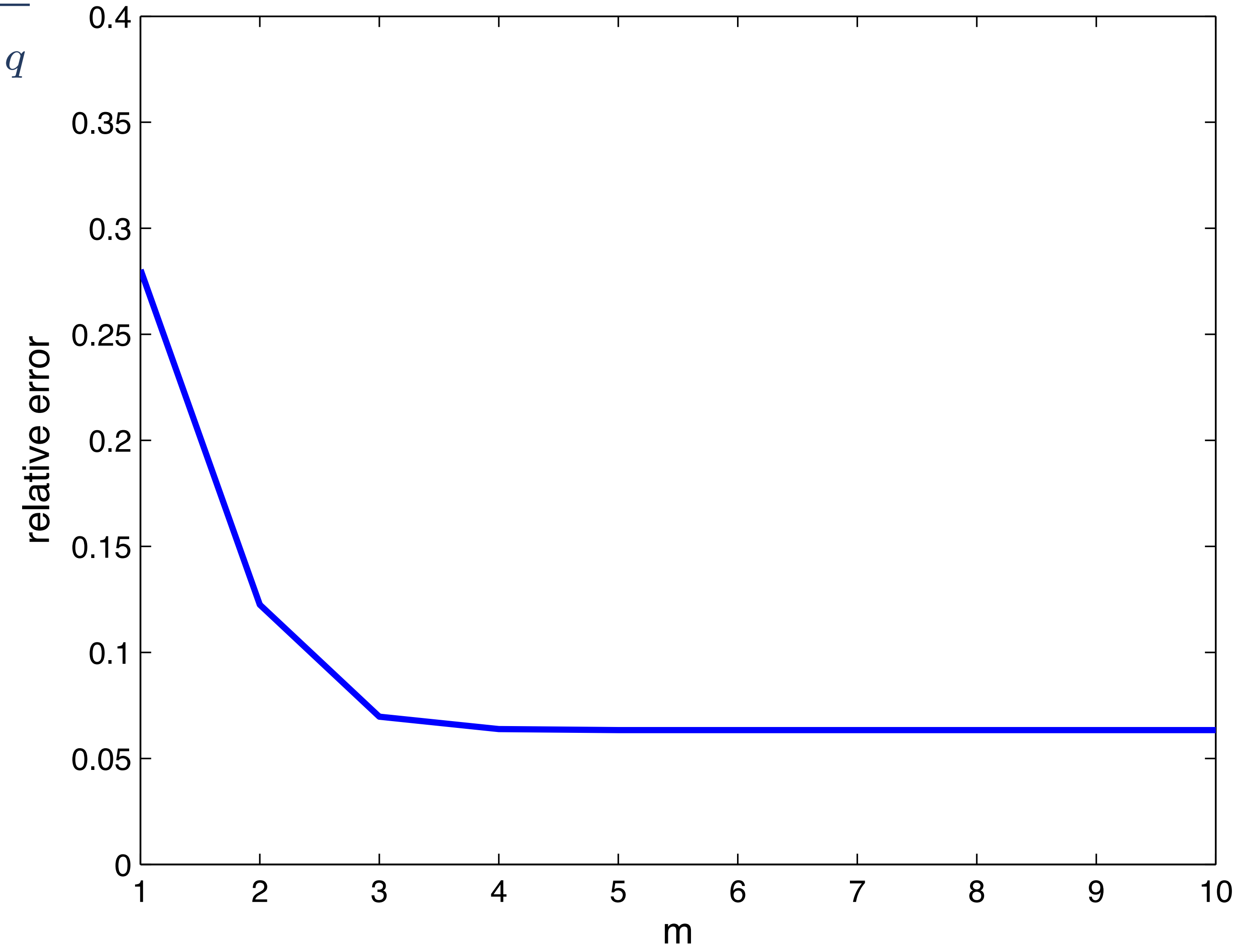
$\left(u_m, \bar{\mathbf{q}}_m + \mathbf{q}_0\right)$ satisfies FE equilibration

we construct a SA field following the standard procedure

$$\boxed{\hat{\mathbf{q}}_m = \mathbf{q}_0 - c\boldsymbol{\Gamma}_m \otimes \dot{\boldsymbol{\Lambda}}_m \otimes \mathbb{A}^{-1}\{\hat{\mathbf{Q}}\}_1^m}$$

CRE estimate

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



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

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

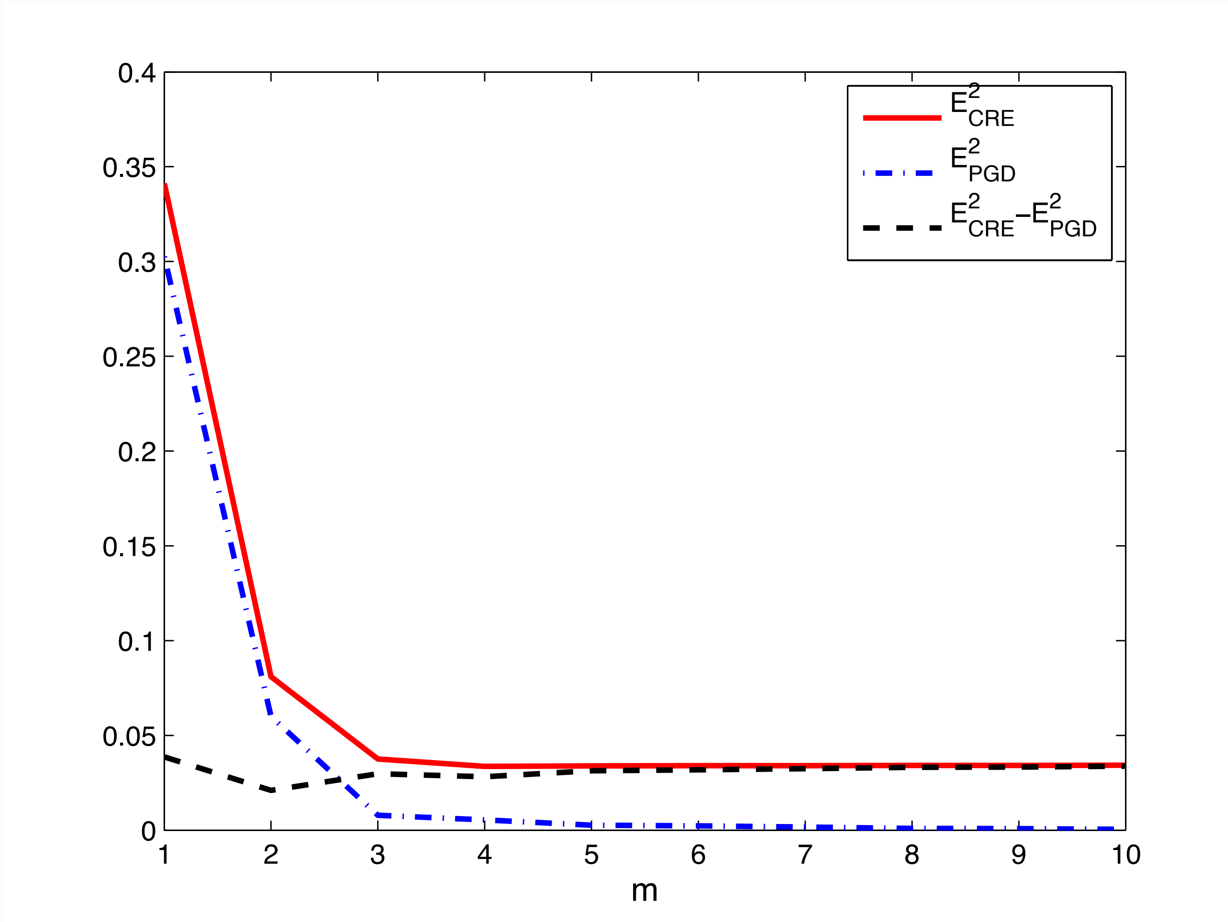
$$\hat{\mathbf{q}}^{h,\Delta t} = \mathbf{N}^T [\int_0^T \mathbf{N}^T \mathbf{N} dt]^{-1} [\mathbf{R}_1, \dots, \mathbf{R}_k]$$

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

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

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

Splitting of error sources



→ after 3 modes, discretization error is dominating

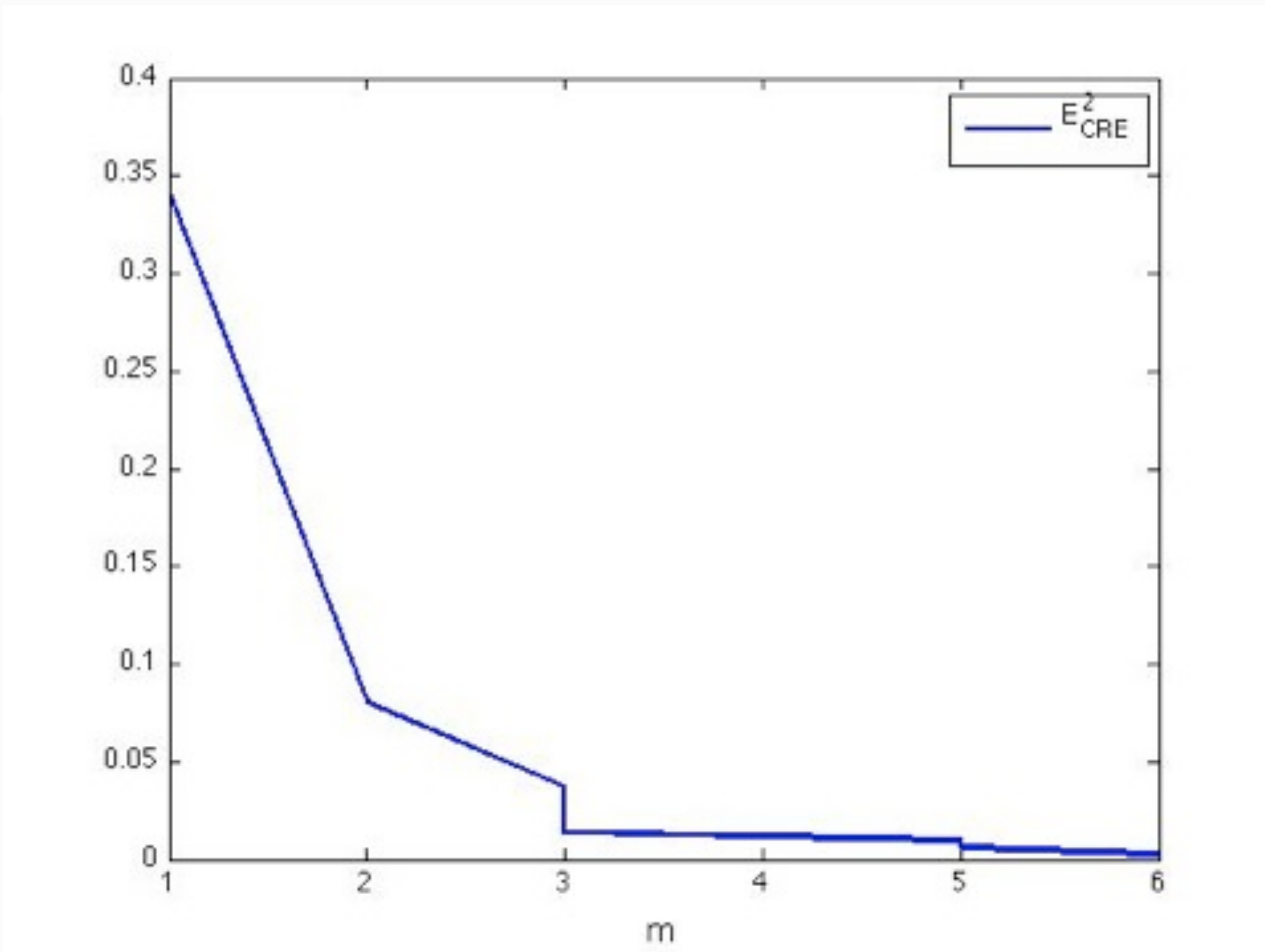
Possible to split space/time discretization errors

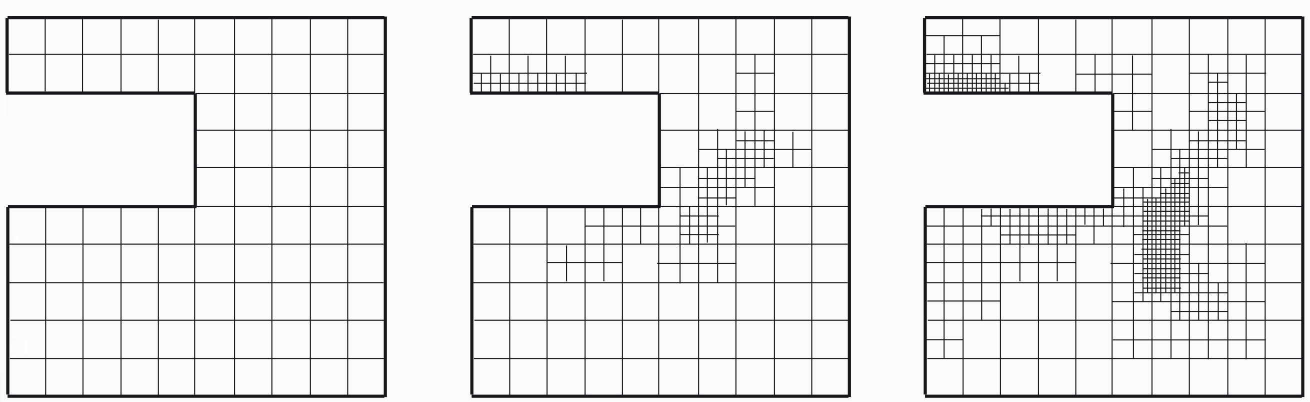
$$E^2_{CRE,dis} = \underbrace{E^2_{CRE,h}}_{|||\hat{\mathbf{q}} - \hat{\mathbf{q}}^h|||_q} + \underbrace{E^2_{CRE,\Delta t}}_{|||\hat{\mathbf{q}}^h - \hat{\mathbf{q}}^{h,\Delta t}|||_q}$$

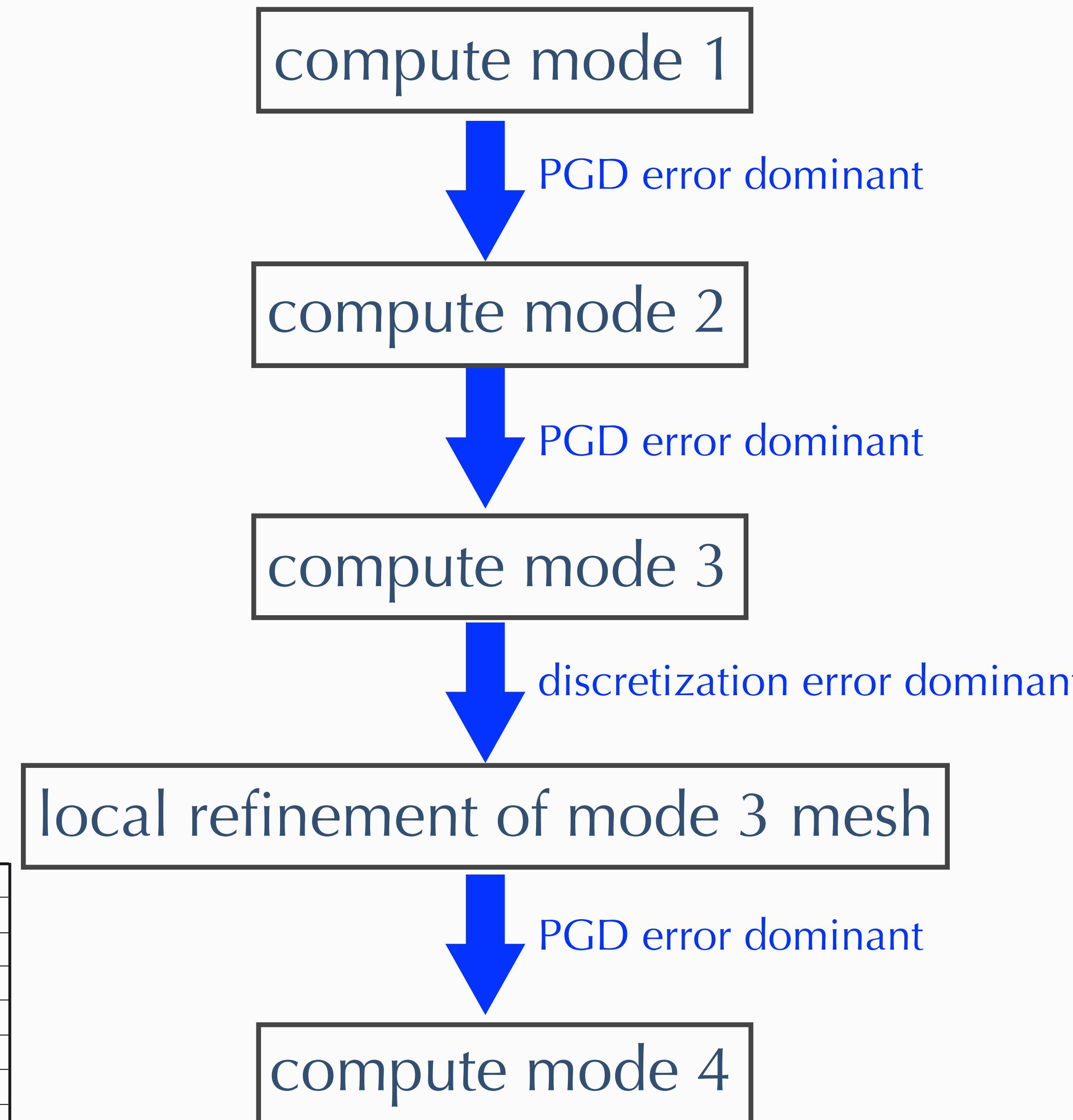
→ discretization error in space : 83%

Adaptivity

IDEA : the model is adapted mode after mode by comparing contributions of error sources (greedy algorithm)







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

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

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

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

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

$$-c \frac{\partial \tilde{u}}{\partial t} - \boldsymbol{\nabla} \cdot (\tilde{\mathbf{q}} - \mathbf{q}_\Sigma) = f_\Sigma$$

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

$$\tilde{\mathbf{q}} = k \boldsymbol{\nabla} \tilde{u}$$

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

Goal-oriented error estimation

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

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

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

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

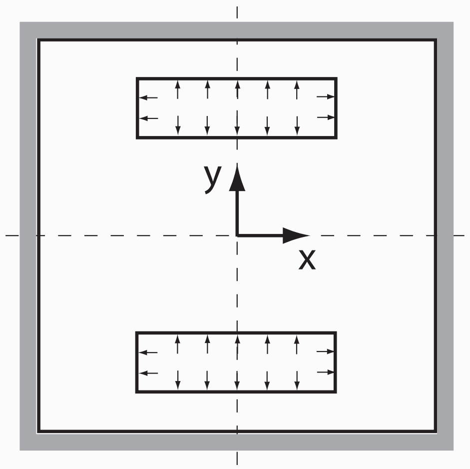
optimized bounding possible
[Chamoin *et al* 08, Pled *et al* 12]

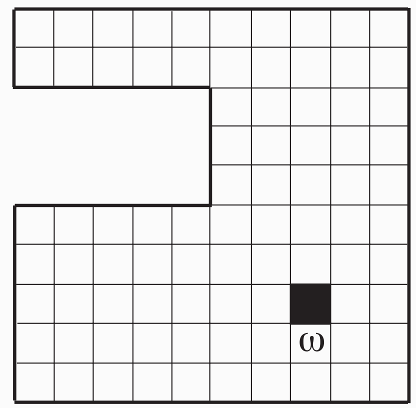
Sources splitting

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

→ indicators are computed after changing reference problem

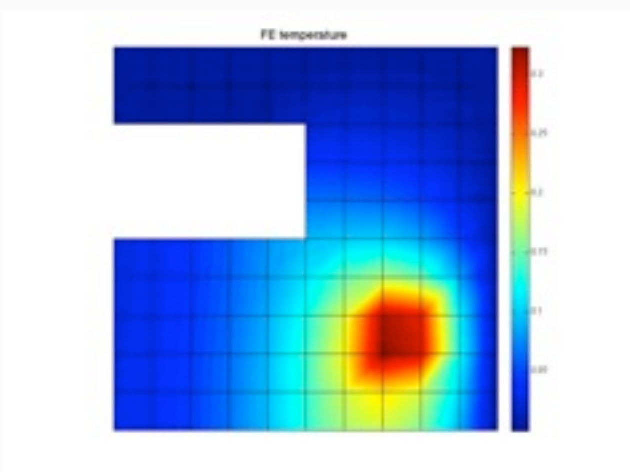
Solving the adjoint problem

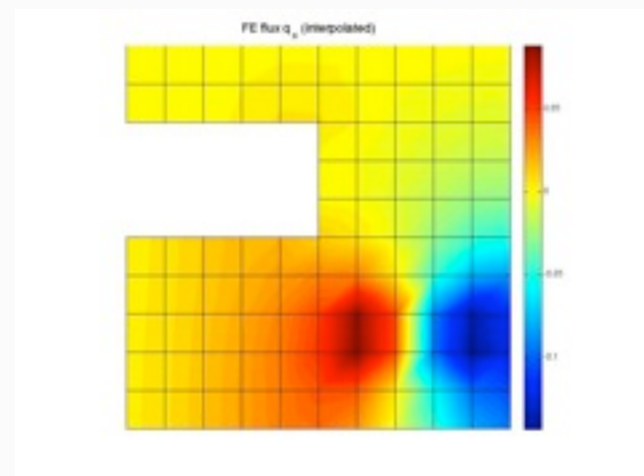


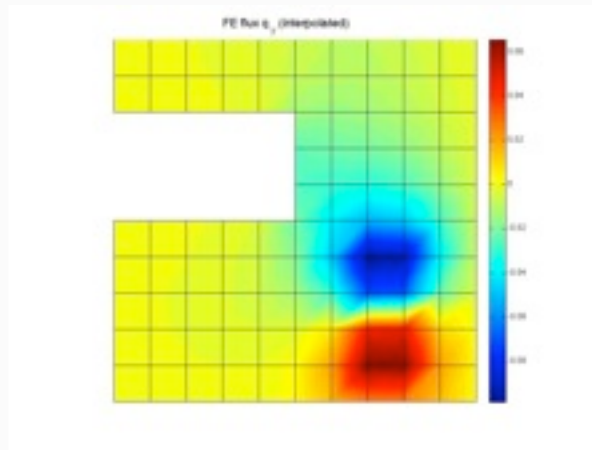


$$I = < u >_{\omega,T}$$

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







[Chamoin & Ladevèze 2008]

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

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

Goal-Oriented Error Estimation

From adjoint-based techniques + CRE properties

$$|I_{ex}(\mathbf{p}) - I_m(\mathbf{p}) - I_{corr}(\mathbf{p})| \leq E_{CRE}(\mathbf{p}) \cdot \tilde{E}_{CRE}(\mathbf{p})$$

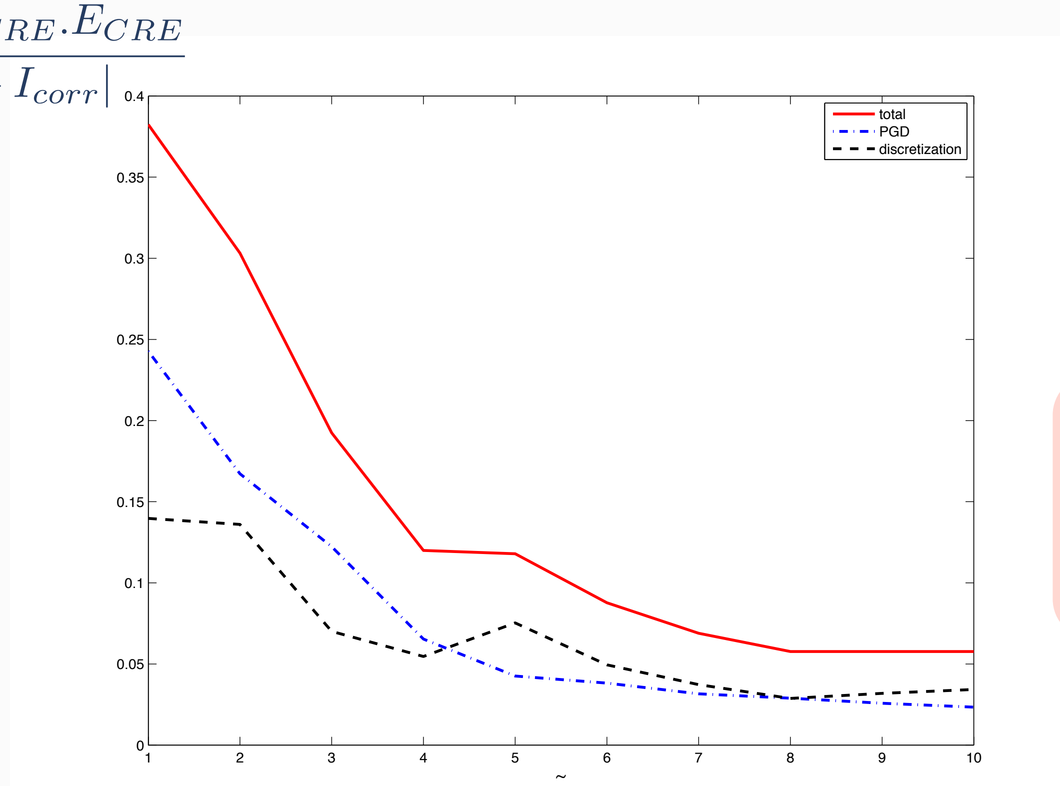
$$I^-(\mathbf{p}) \leq I_{ex}(\mathbf{p}) \leq I^+(\mathbf{p})$$

Sources splitting

$$I_{ex} - I_m^{h,\Delta t} = \underbrace{[I_{ex} - I^{h,\Delta t}]}_{\text{discretization error}} + \underbrace{[I^{h,\Delta t} - I_m^{h,\Delta t}]}_{\text{PGD truncation error}}$$

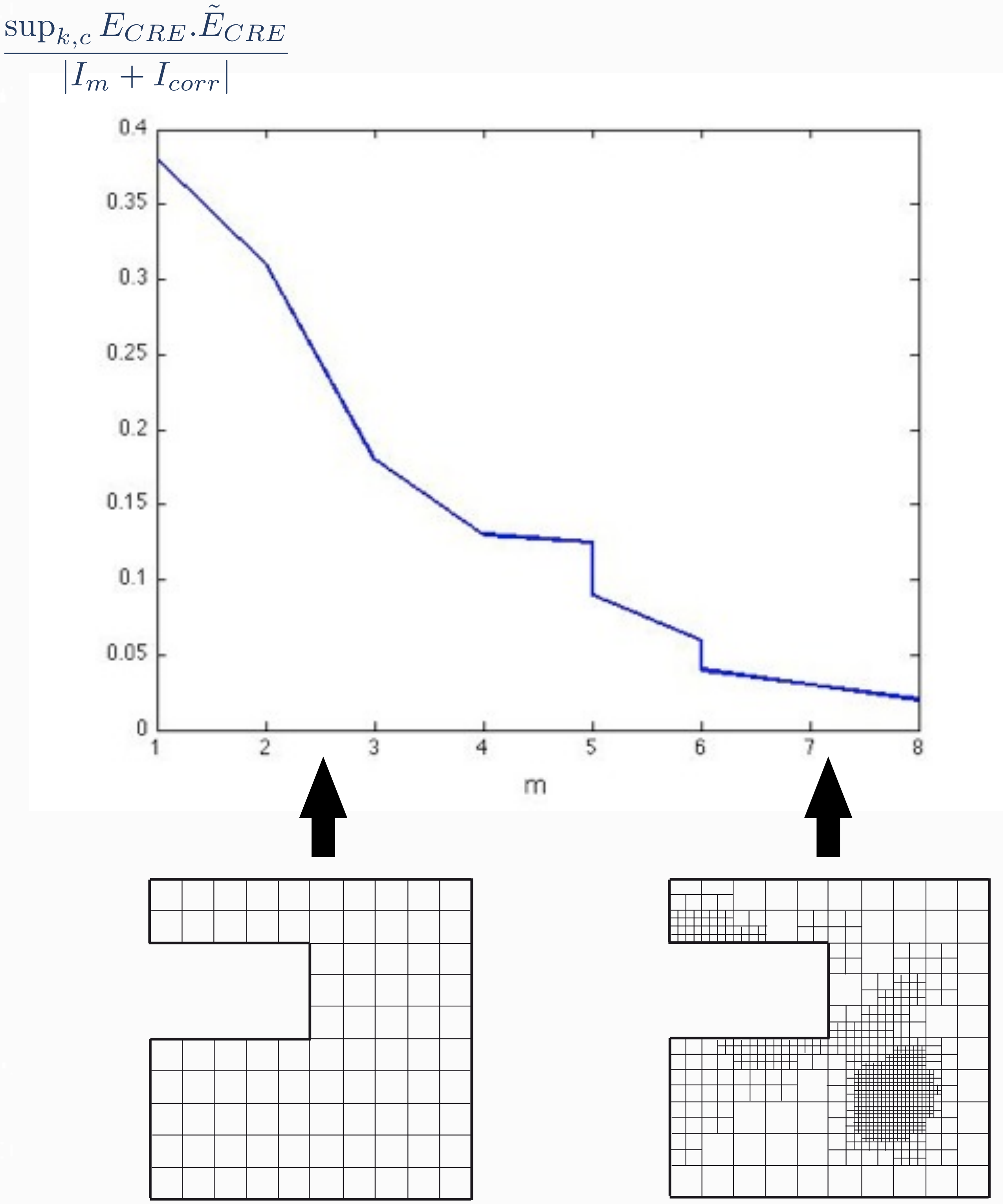
estimated with a discretized reference model

$$\frac{\sup_{k,c} E_{CRE}.\tilde{E}_{CRE}}{|I_m + I_{corr}|}$$



$$I = \sup_{k,c} \frac{1}{\omega} \int_\omega u_{|T} d\omega$$

Adaptivity



compute mode 1

↓ PGD error dominant

compute mode 2

↓ PGD error dominant

⋮

compute mode 5

↓ discretization error dominant

local refinement of mode 5 mesh

↓ PGD error dominant

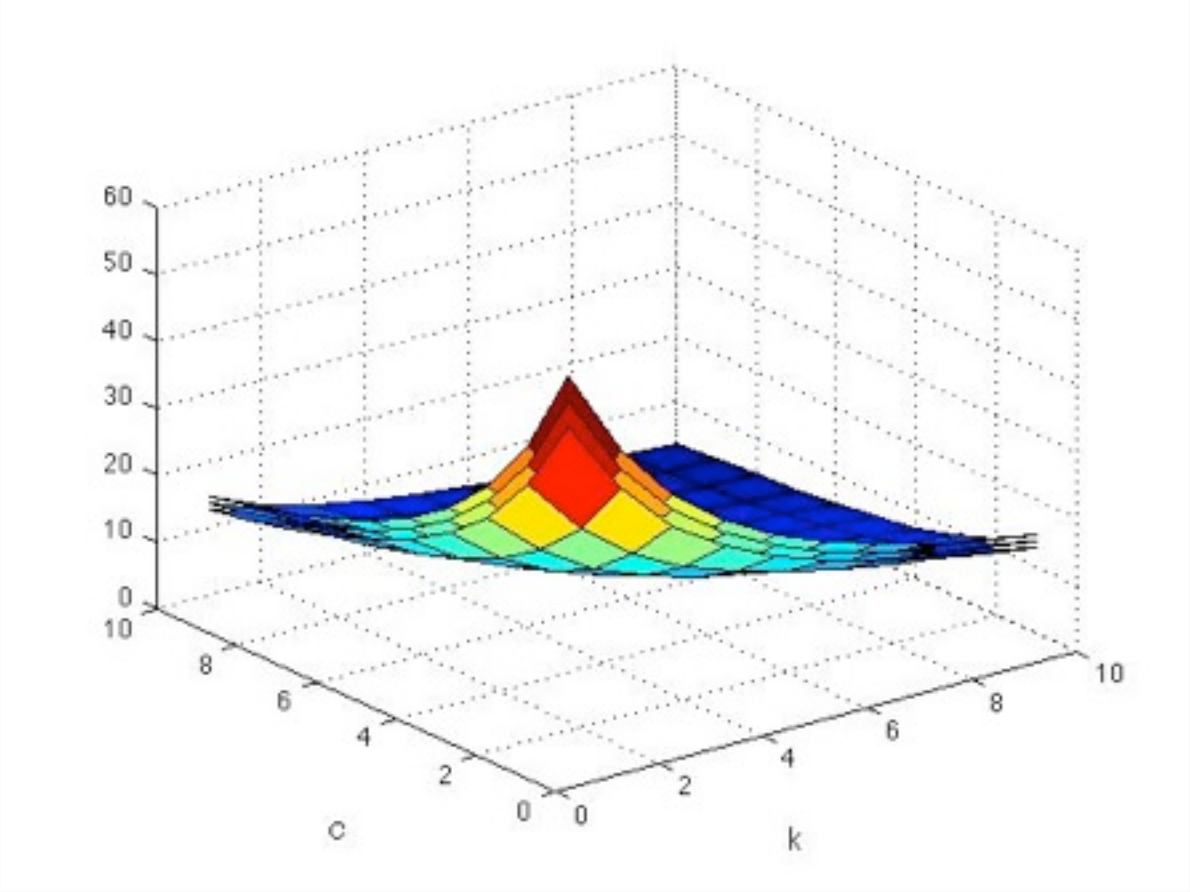
compute mode 6

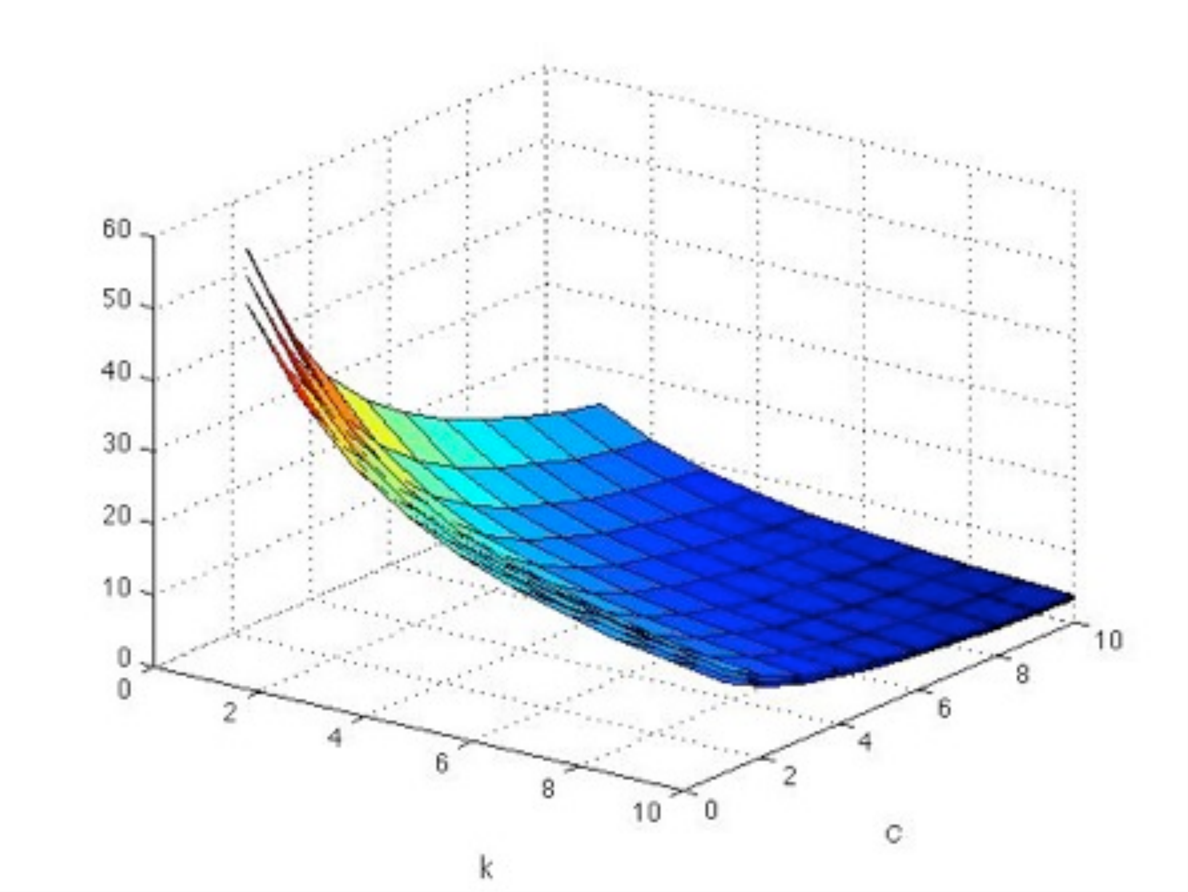
⋮

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

Guaranteed virtual chart

$$I(k,c) = < u(x,t,k,c) >_{\omega,T}$$





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- Basics on Proper Generalized Decomposition (PGD)
- Illustrations of PGD applications
- A posteriori error estimation: the CRE concept
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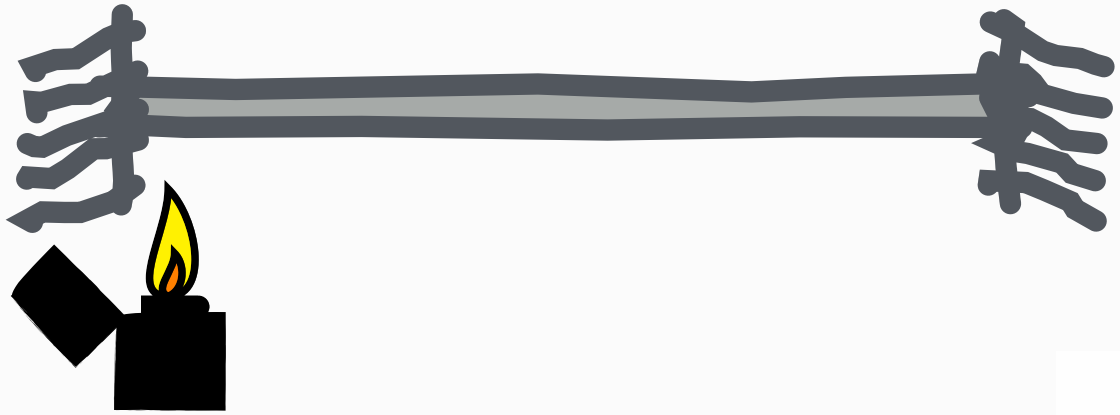
Idelsohn's benchmark



$$\begin{cases} c\dfrac{\partial u}{\partial t}(x,t) - \dfrac{\partial \sigma}{\partial x}(x,t) = \delta(x - vt) \\ u(0,t) = u(L,t) = 0 \\ u(x,0) = 0 \end{cases}$$

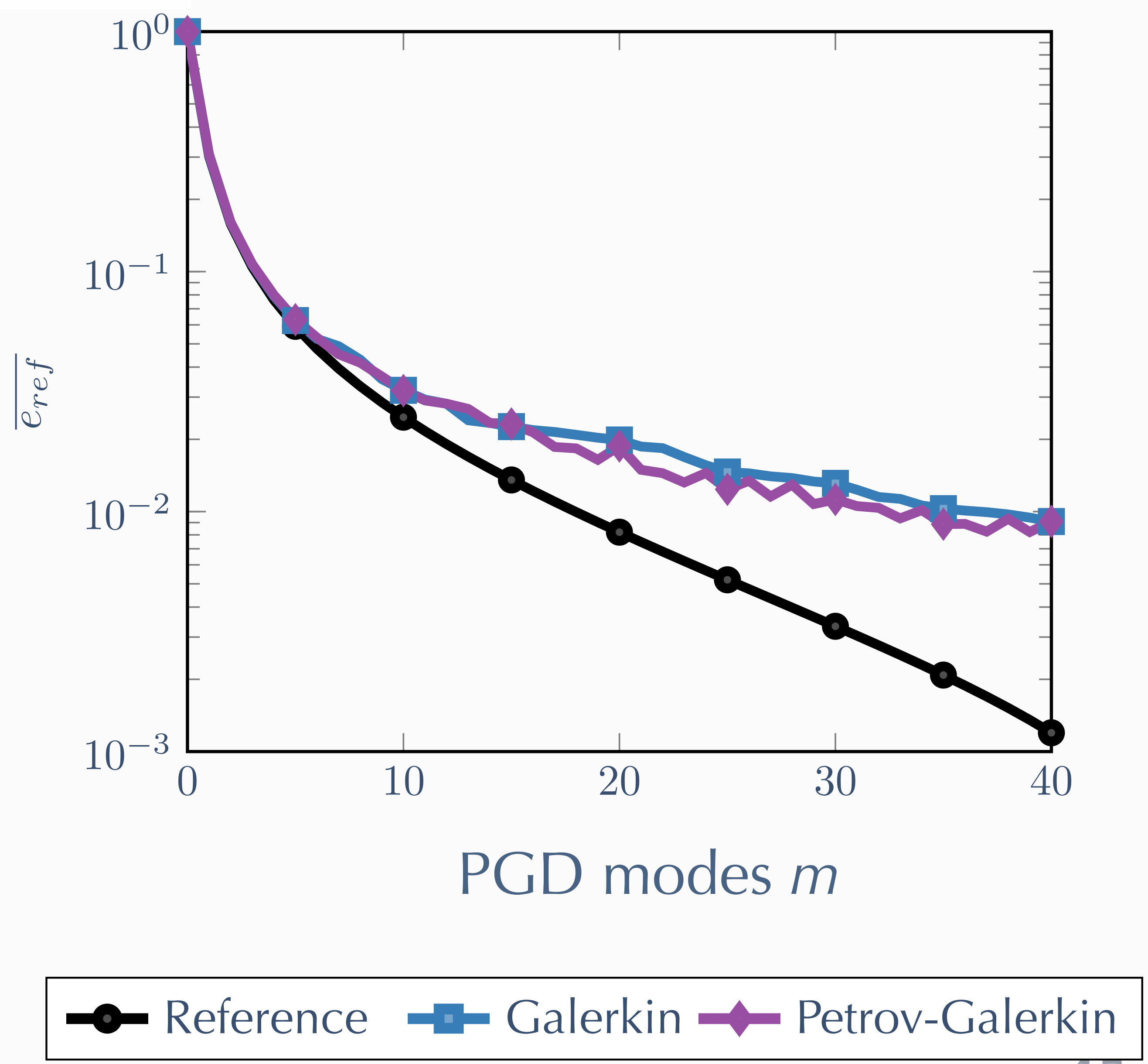
Reference solution

- brute force FEM solution
- SVD decomposition according to energy norm
- optimal one

Reference reduction error

- neglect the discretization error

$$\overline{e_{ref}} = \frac{\|u_h - u_m\|_E}{\|u_h\|_E}$$

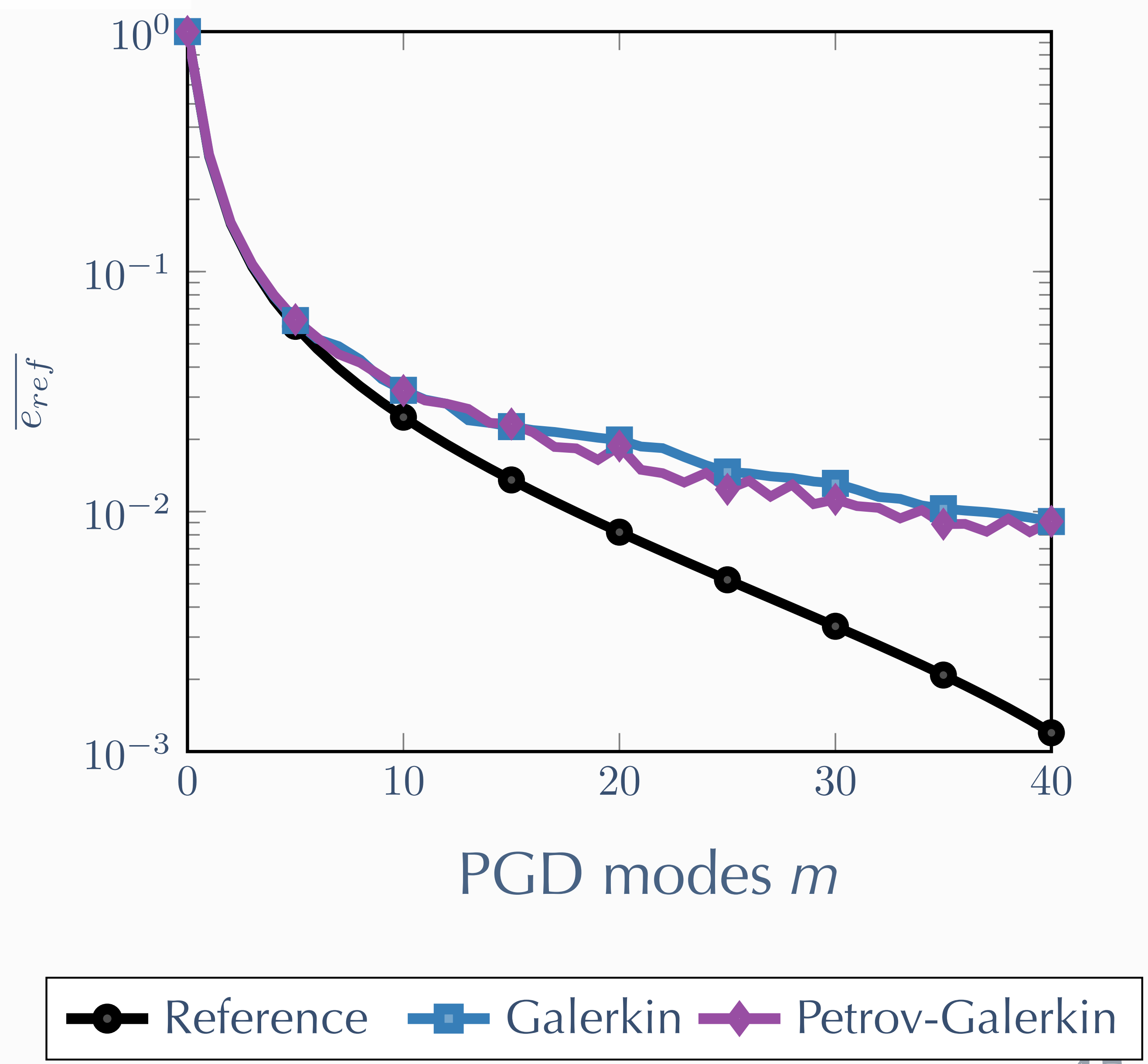


Idelsohn's benchmark

$$\begin{cases} c\dfrac{\partial u}{\partial t}(x,t) - \dfrac{\partial \sigma}{\partial x}(x,t) = \delta(x - vt) \\ u(0,t) = u(L,t) = 0 \\ u(x,0) = 0 \end{cases}$$

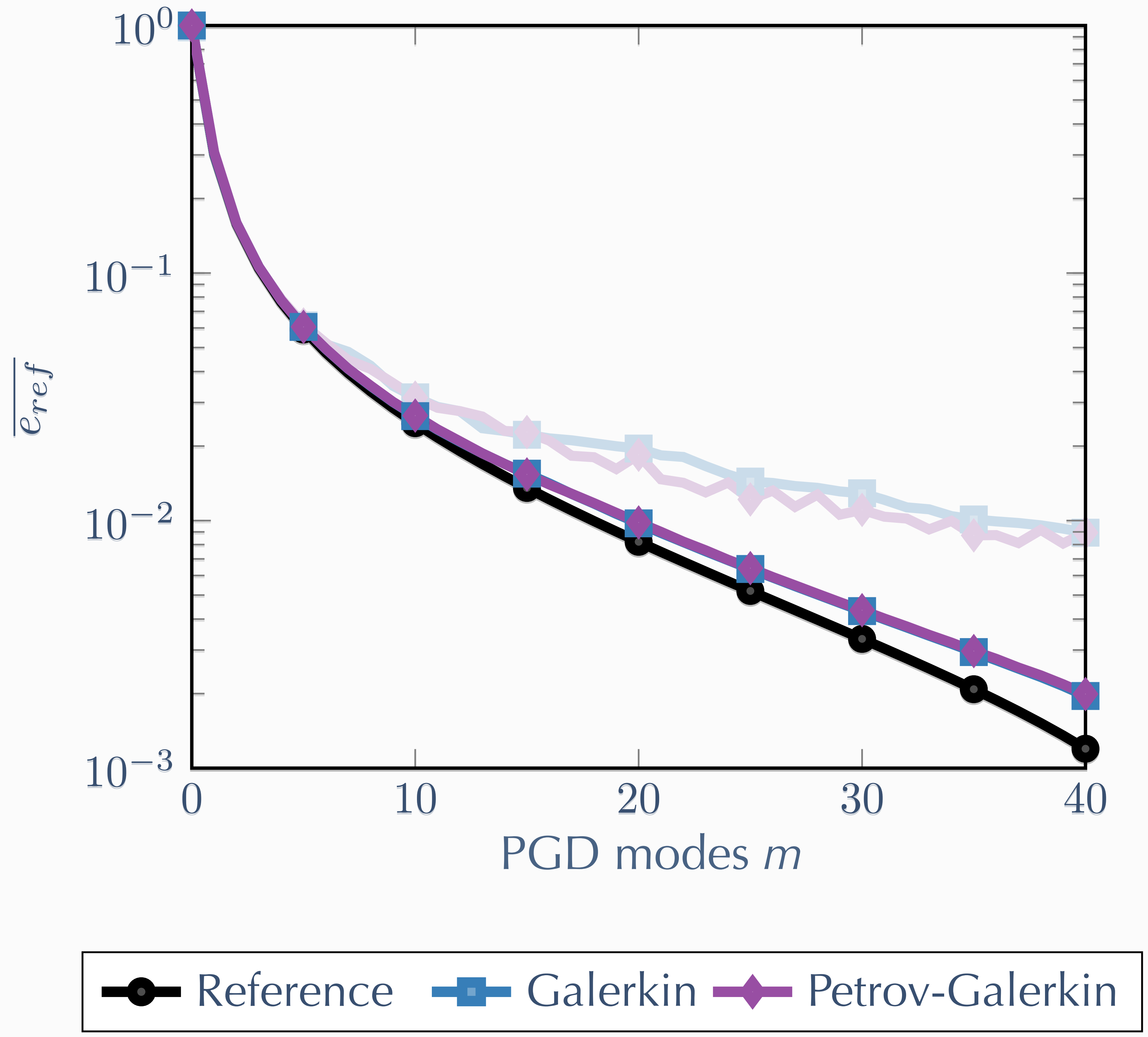
- **Reference solution**
  - brute force FEM solution
  - SVD decomposition according to energy norm
  - optimal one
- **Reference reduction error**
  - neglect the discretization error

$$\overline{e_{ref}} = \frac{\|u_h - u_m\|_E}{\|u_h\|_E}$$



Convergence of PGD strategies

Update of time fonctions (LMT method)



Minimal CRE in PGD

[Allier *et al* 2015]

Idea

- Minimizing the CRE indicator: $\arg\min_{u,\sigma} \|e_{CRE}(u,\sigma)\|_E$
- Under the condition of equilibrium (**without the constitutive relation**)

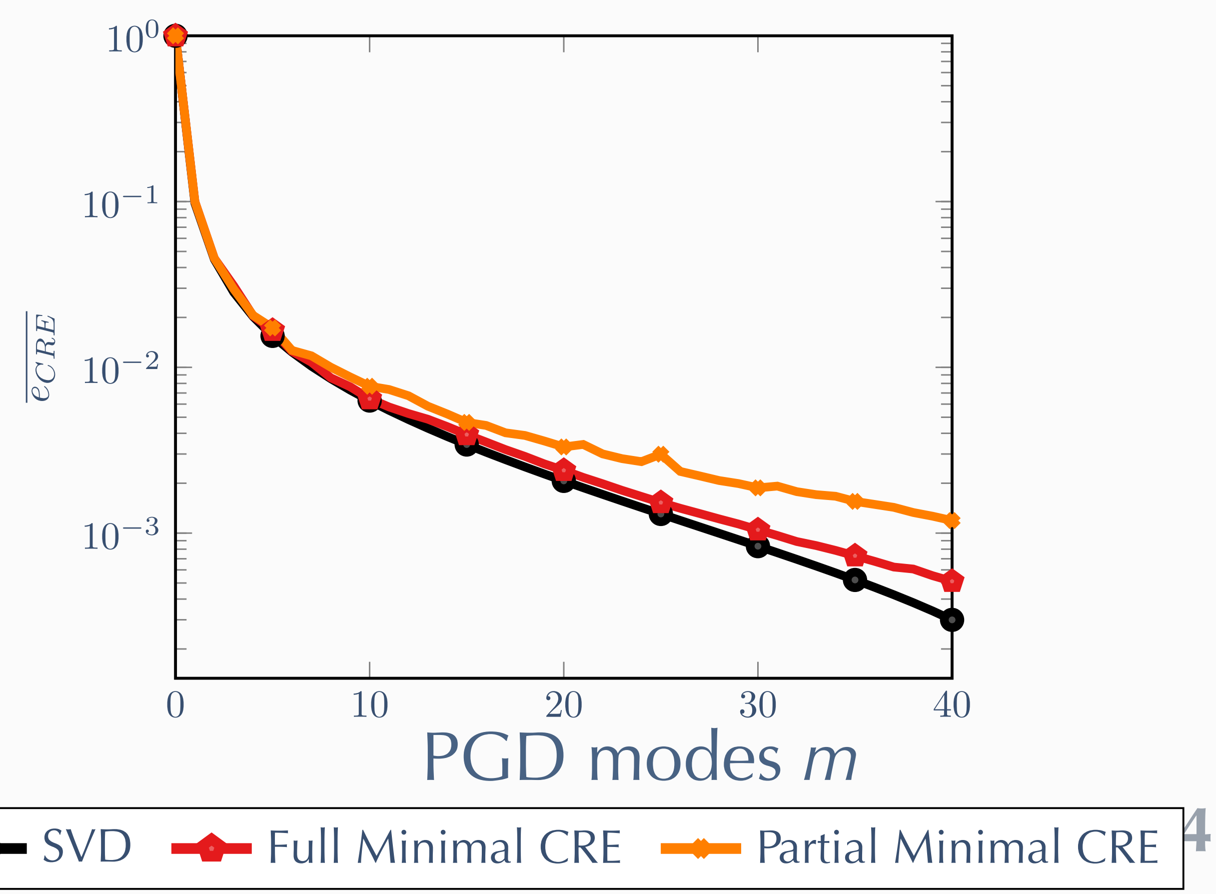
$$B(u,\sigma;v) = L(v) \quad \forall v \in \mathcal{V} \otimes \mathcal{T}$$

Advantages

- Immediate reduction error estimator;
- Pilots the progressive algorithm;
- Easy access to full error estimator through classical FEM CRE methods.

Minimisation

- partial
- full



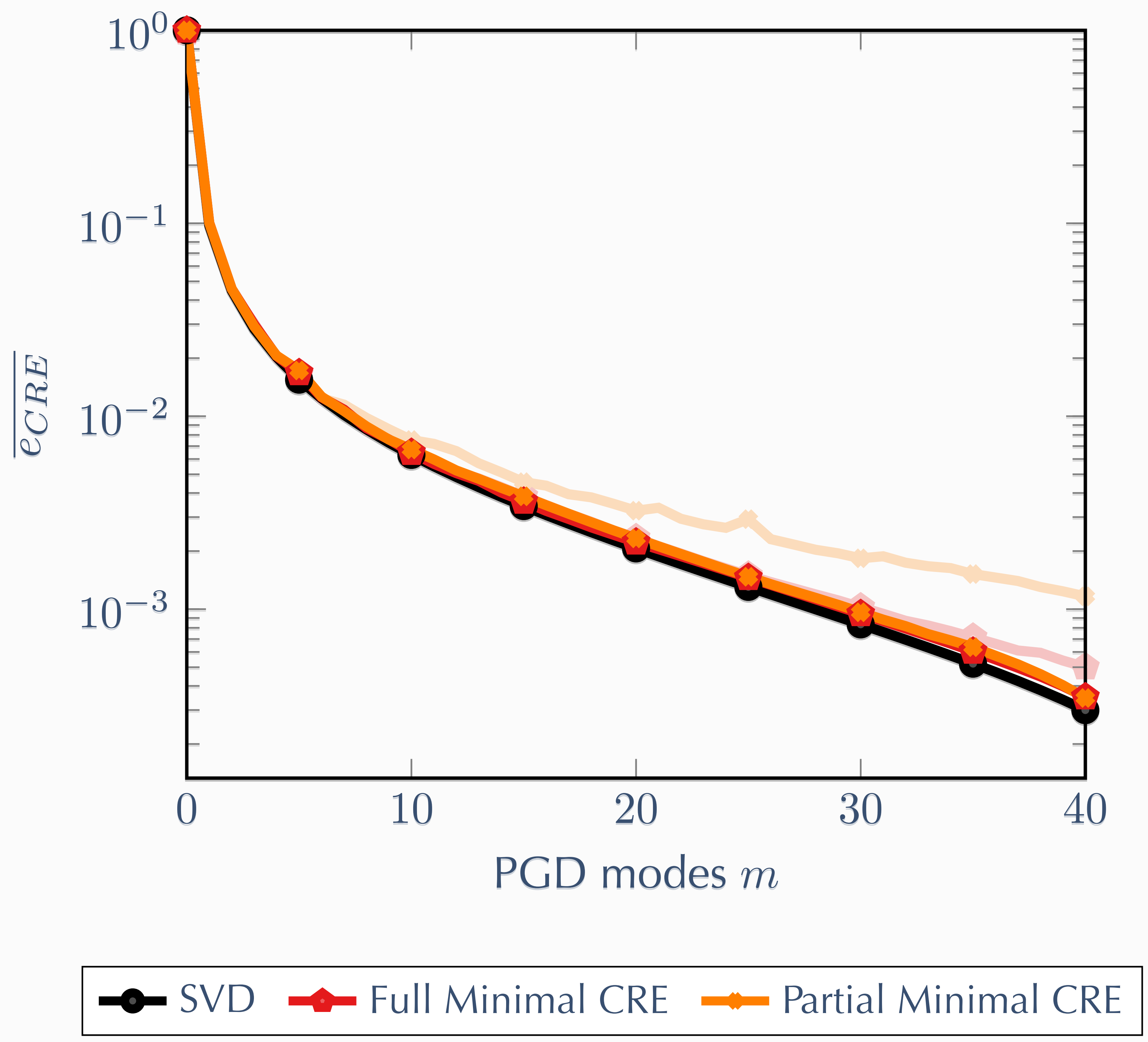
Estimation through CRE

- Only an estimation !

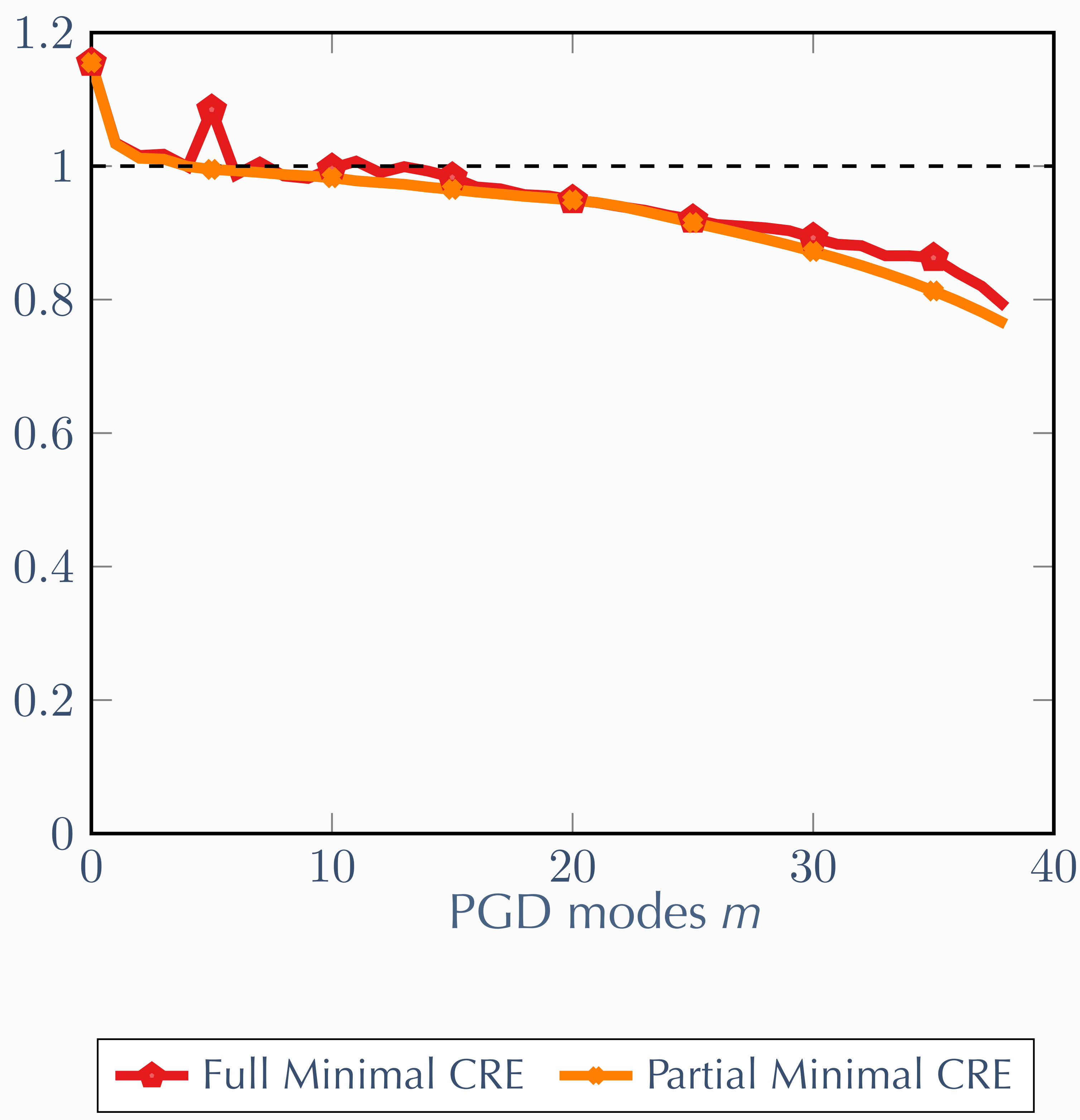
$$\overline{e_{CRE}} = \frac{\|\tau_m - \mu \frac{\partial u_m}{\partial x}\|_E}{\|\tau_m + \mu \frac{\partial u_m}{\partial x}\|_E}$$

Minimisation of CRE

Update of time fonctions (LMT method)



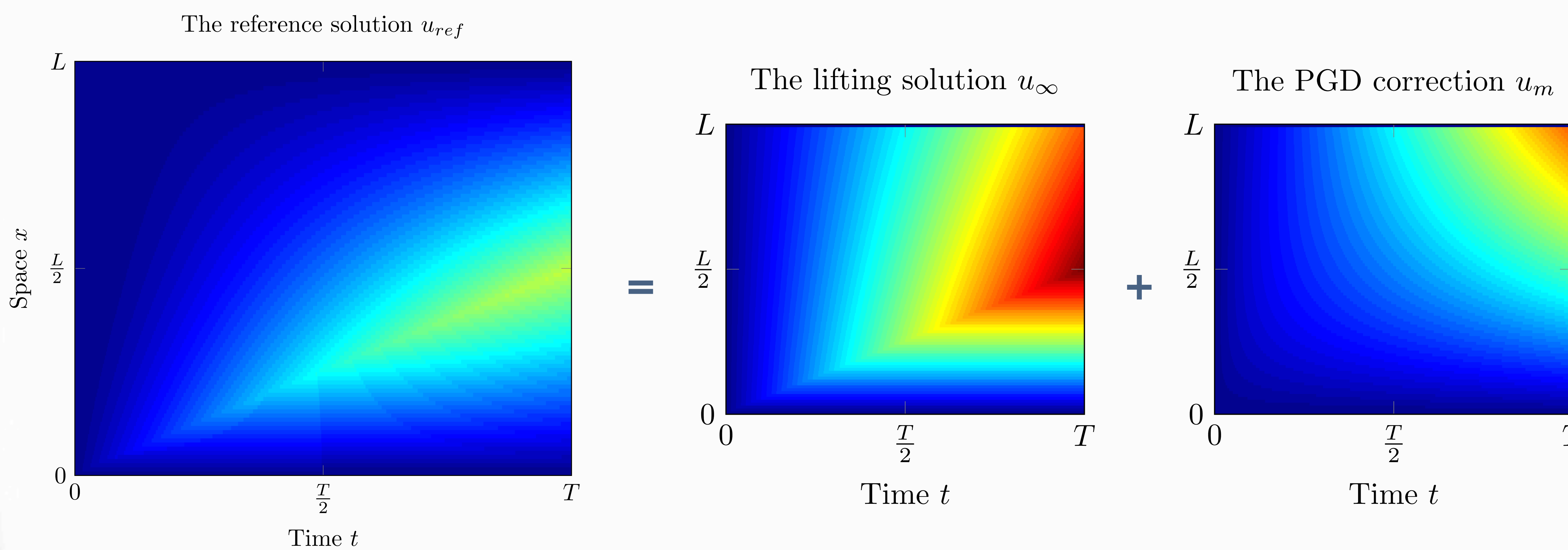
Effectivity of CRE indicator



A lifting technique

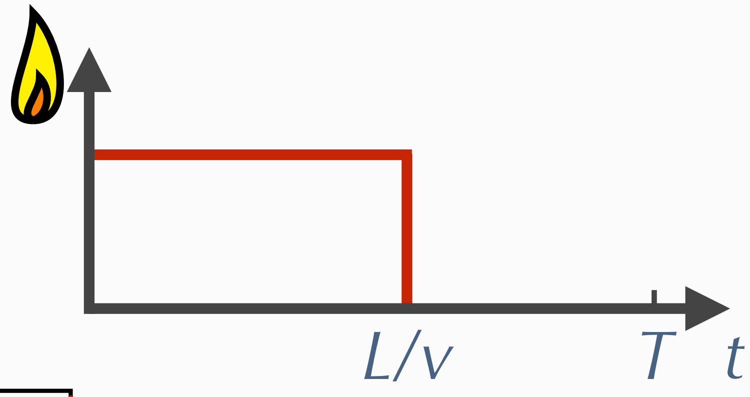
- **Lifting**
  - with the solution of infinity domain: $u_\infty(x,t) = \frac{\theta(x-vt)}{cv}\left(e^{-\frac{cv}{k}(x-vt)} - 1\right) + \frac{\theta(x)}{cv}\left(1 - e^{-\frac{cv}{k}x}\right)$
  - with space limit conditions: $\overline{u_\infty}(x,t) = u_\infty(x,t) \times \delta(0) \times \delta(L)$

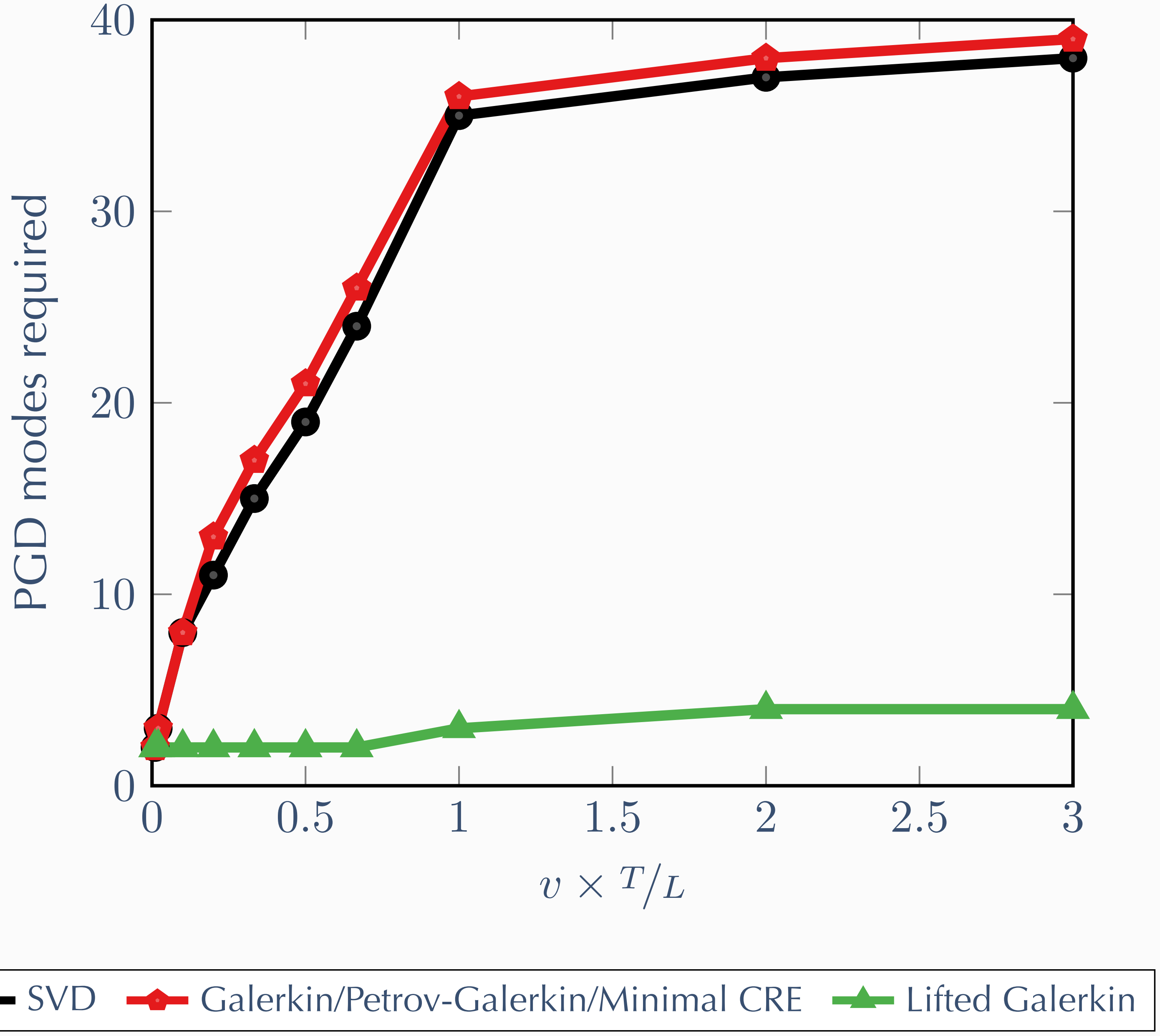
- **Galerkin PGD method for correction** $u_m(x,t) = \overline{u_\infty}(x,t) + \sum_{i=1}^{m} \lambda_i(t)\psi_i(x)$



Is the exact solution separable ?

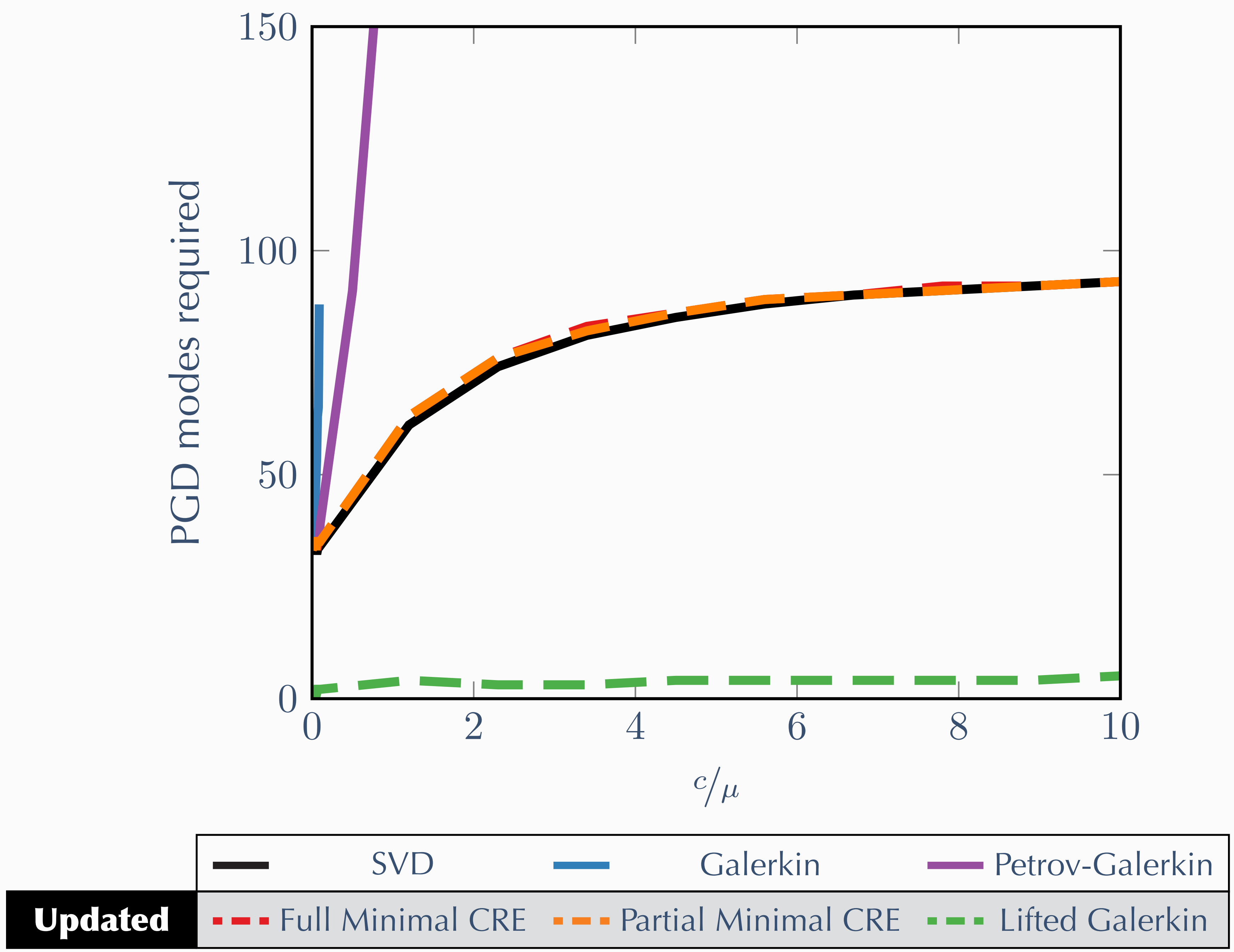
- **Influence of the instationnary term**
  - targeted error: 10^{-2}





Is the exact solution separable ?

- **Influence of the instationnary term (v=L/T)**
  - targeted error: 10^{-2}



Conclusions and prospects

- **PGD model reduction**
  - a priori construction of modes
  - explicit solution with respect to parameters
  - offline/online strategy
  - variable separation should be driven by the physics of the problem
- **Error estimation for PGD reduced models**
  - separates the sources of the error
  - allows adaptative PGD procedure
  - guaranteed bounds (robust virtual charts)
- **In progress**
  - extension to space separation: $u \simeq \sum_{i=1}^{m} \psi_i(x)\gamma_i(y)\lambda_i(z)$
  - error estimation in the non-linear case (through LATIN method)

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