Can we trust results from numerical simulations?

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informatiques mathématiques Inria

European Research Council

École des Ponts ParisTech

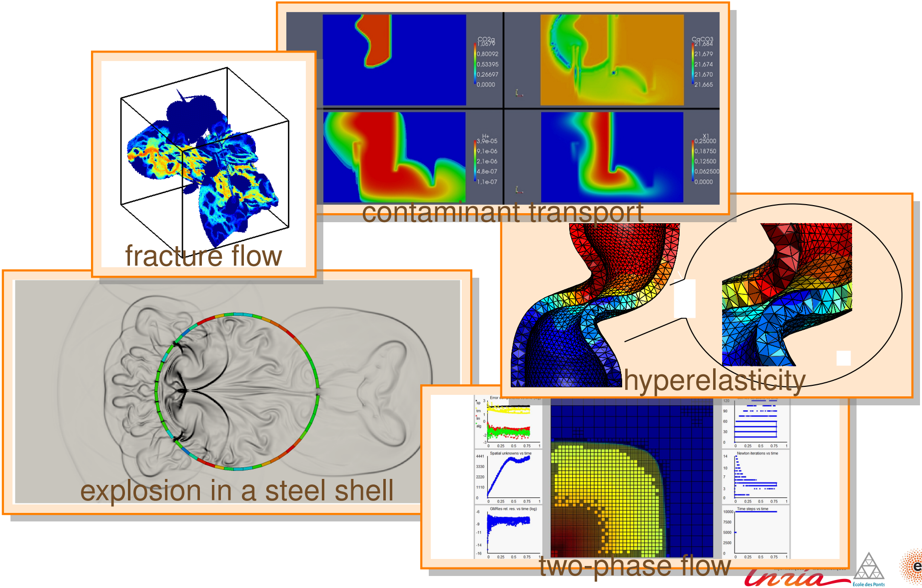
Outline

1 Introduction

2 A posteriori error estimates and adaptivity

3 Application to underground fluid flows

Examples: numerical simulations of PDEs in SERENA



Partial differential equations (PDEs)

- **describe** numerous **physical phenomena**
  - fluid flow and transport in the underground, air, oceans, rivers (weather forecast, modeling pollution, . . .)
  - solid structure and its deformations (construction of buildings/cars/planes. . .)
  - population dynamics, behavior of financial markets (demography, economy . . .)
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- include (partial) derivatives of the solution
- it is almost **never possible** to **find** analytical, **exact solutions**

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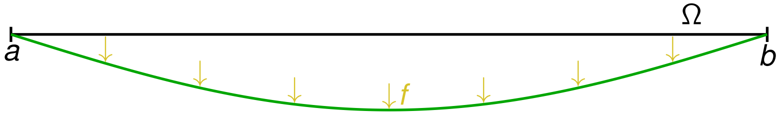
- it is almost **never possible** to **find** analytical, **exact solutions** (not even Einstein could solve PDEs with paper and pen, except in model cases . . .)

Example: elastic rod



Elastic rod subject to force f:

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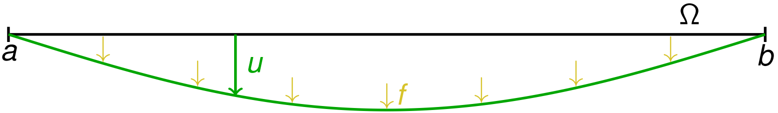

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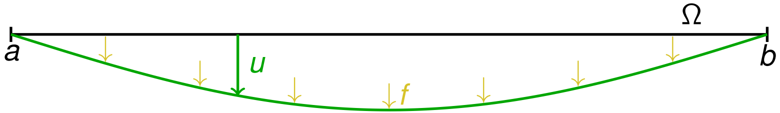

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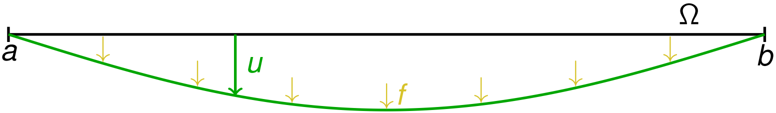

Elastic rod subject to force f: displacement u

Let Ω be an interval, $\Omega =]a, b[$, a, b two real numbers, $a < b$.
Let $f :]a, b[\to \mathbb{R}$ be a given function. Find $u :]a, b[\to \mathbb{R}$ such that

$$-(u')' = f,$$
$$u(a) = u(b) = 0.$$

Numerical approximations of PDEs

Numerical methods

- mathematically-based algorithms
- evaluated with the aid of **computers**
- deliver **approximate solutions**
- conception: more and more computational resources $\Rightarrow$ **closer and closer** to the unknown solution

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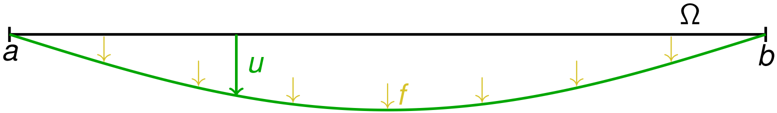

Numerical approximation u_h and its convergence to u

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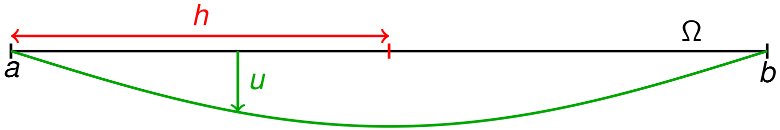

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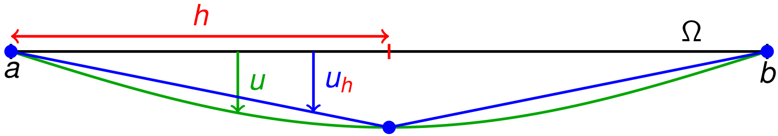

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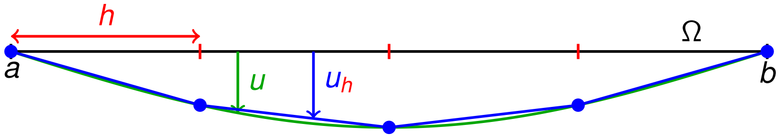

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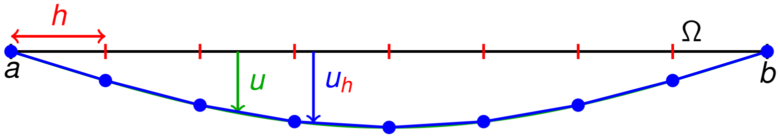

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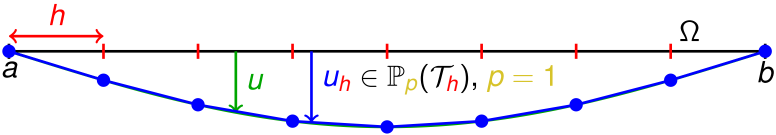

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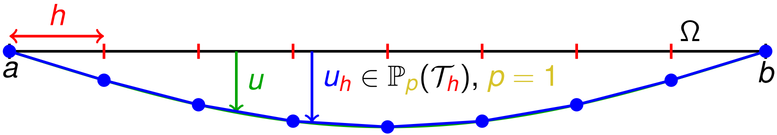

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Error

$$\|\nabla(u-u_h)\| = \left\{\int_a^b |(u-u_h)'|^2\right\}^{\frac{1}{2}}$$

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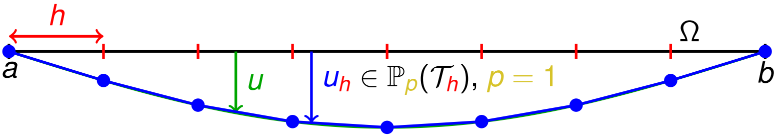

Numerical approximation u_h and its convergence to u

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Need to solve

$$\mathbb{A}_h \mathrm{U}_h = \mathrm{F}_h$$

3 crucial questions

Crucial questions

1. How **large** is the overall **error**?
2. **Where** (space, time, solver) is the error **localized**?
3. Can we **decrease** the error **efficiently**?

Assumptions

- The physical model is correct.
- We know the data.
- The computer implementation and execution of our certification methodology is safe and correct.

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Case Studies in Engineering Failure Analysis 3 (2015) 88–95

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Reliability study and simulation of the progressive collapse of Roissy Charles de Gaulle Airport

Y. El Kamari [a], W. Raphael [a,*], A. Chateauneuf [b,c]

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A posteriori error control: the principle

Elastic membrane equation

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\begin{aligned}
-\Delta u &= f \quad \text{in} \quad \Omega,\\
u &= 0 \quad \text{on} \quad \partial\Omega
\end{aligned}
$$

Guaranteed error upper bound (reliability)

$$\underbrace{\|\nabla(u-u_h)\|}_{\text{unknown error}} \le \underbrace{\eta(u_h)}_{\text{computable estimator}}$$

Error lower bound (efficiency)

$$\eta(u_h) \le C_{\text{eff}} \|\nabla(u-u_h)\|$$

- C_{eff} independent of Ω, u, u_h, h, p
- computable bound on C_{eff} available, $C_{\text{eff}} \approx 5$

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How large is the overall error? (model pb, known sol.)

h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\lVert\nabla u_h\rVert}$	$\lVert\nabla(u-u_h)\rVert$	rel. error $\frac{\lVert\nabla(u-u_h)\rVert}{\lVert\nabla u_h\rVert}$	$I^{\mathrm{eff}} = \frac{\eta(u_h)}{\lVert\nabla(u-u_h)\rVert}$
h_0	1	1.25	28%	1.07	24%	1.17
$\approx h_0/2$		[illegible]				
$\approx h_0/4$		[illegible]				
$\approx h_0/8$		[illegible]				
$\approx h_0/2$	2	[illegible]				
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$\approx h_0/2$		6.07×10^{-1}	14%	5.56×10^{-1}	13%	**1.09**
$\approx h_0/4$		3.10×10^{-1}	7.0%	2.92×10^{-1}	6.6%	**1.06**
$\approx h_0/8$		1.45×10^{-1}	3.3%	1.39×10^{-1}	3.1%	**1.04**
$\approx h_0/2$	2	4.23×10^{-2}	9.5×10^{-1}%	4.07×10^{-2}	9.2×10^{-1}%	**1.04**
$\approx h_0/4$	3	2.62×10^{-4}	5.9×10^{-3}%	2.60×10^{-4}	5.9×10^{-3}%	**1.01**
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A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

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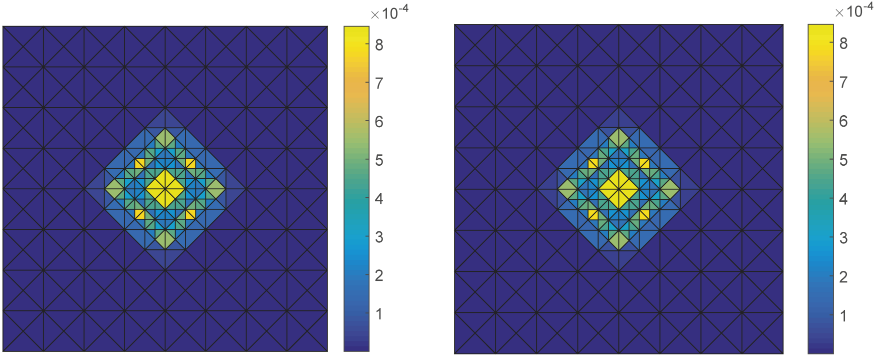
A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

Where (in space) is the error localized?

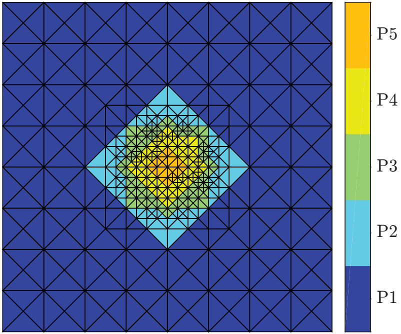


Estimated error distribution $\eta_K(u_h)$

Exact error distribution $\|\nabla(u - u_h)\|_K$

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

Can we decrease the error efficiently? (smooth solution)



Mesh $\mathcal{T}_h$ and pol. degrees p_K

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

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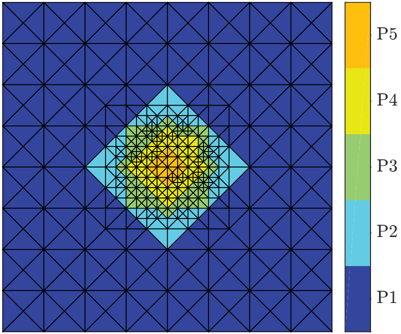

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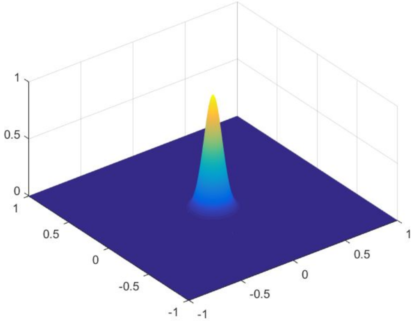

Exact solution

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

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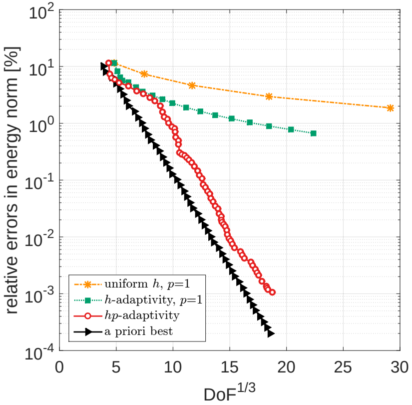

Relative error as a function of no. of unknowns

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

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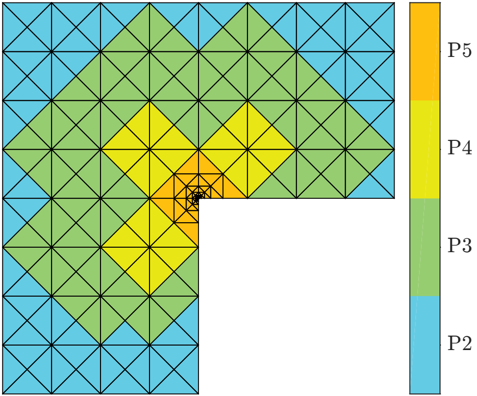
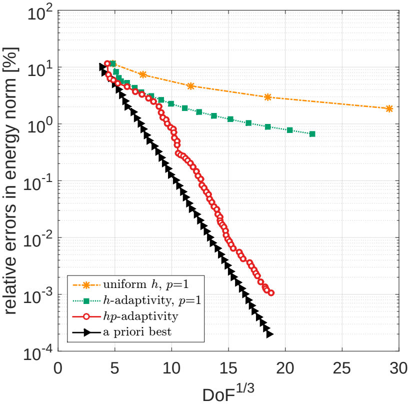


Mesh $\mathcal{T}_h$ and polynomial degrees p_K



Relative error as a function of no. of unknowns

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

Including **algebraic** error: $\mathbb{A}_h \mathrm{U}_h^i \neq \mathrm{F}_h$

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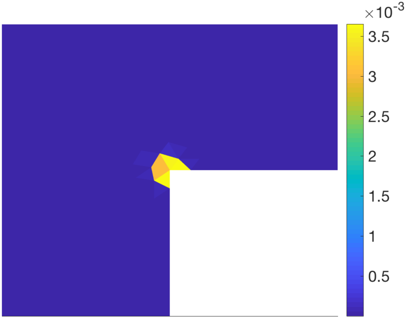
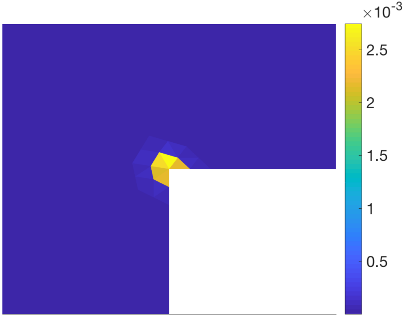


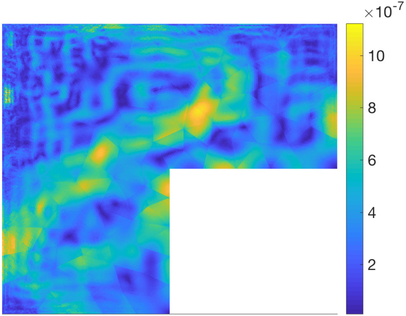
Estimated total error distribution $\eta_K(u_h^i)$



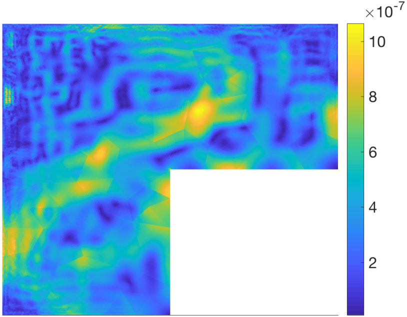
Exact total error distribution $\|\nabla(u - u_h^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, preprint (2017)

Including **algebraic** error: $\mathbb{A}_h \mathsf{U}_h^i \neq \mathsf{F}_h$



Estimated algebraic error distribution $\eta_{\mathrm{alg},K}(u_h^i)$



Exact algebraic error distribution $\|\nabla(u_h - u_h^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, preprint (2017)

Nonlinear pb $-\nabla\cdot\sigma(\nabla u) = f$: including **linearization** and **algebraic** error: $\mathcal{A}_h(\mathrm{U}_h^{k,i}) \neq \mathrm{F}_h$, $\mathbb{A}_h^{k-1}\mathrm{U}_h^{k,i} \neq \mathrm{F}_h^{k-1}$

classical

error est.	4.6%

adaptive

error est.	1.1%

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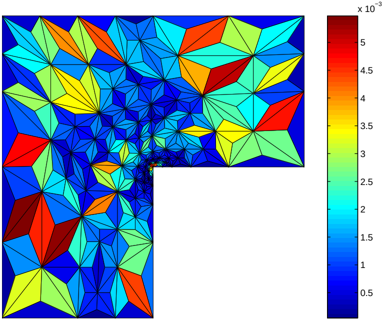

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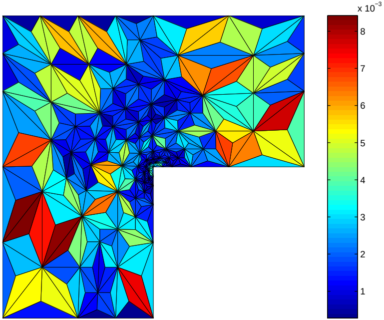

Exact error distribution
$\|\boldsymbol{\sigma}(\nabla u) - \boldsymbol{\sigma}(\nabla u_h^{k,i})\|_K$

classical

tot. alg. it.	10890
error est.	4.6%

adaptive

tot. alg. it.	242
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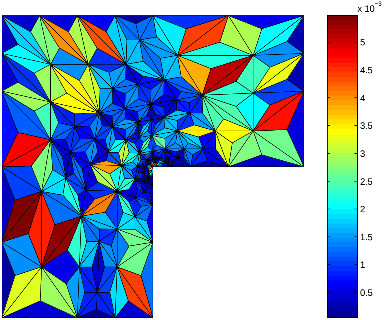

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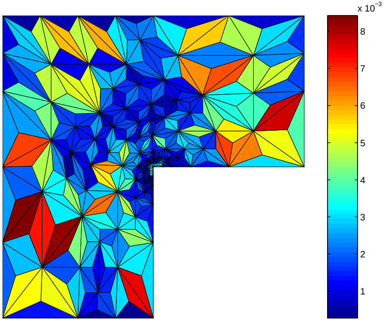

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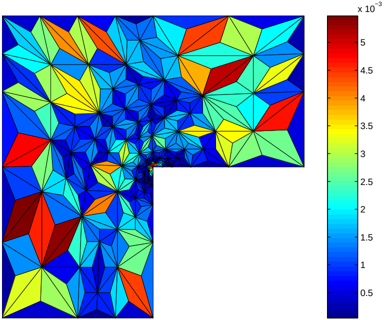

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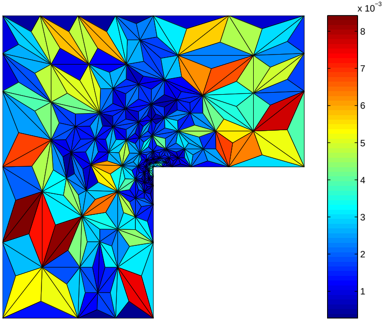

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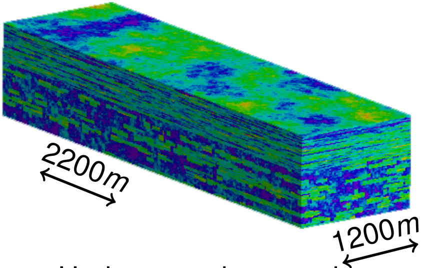
Outline

1. Introduction
2. A posteriori error estimates and adaptivity
3. Application to underground fluid flows

Can we certify error in a practical case $-\nabla\cdot(\boldsymbol{K}\nabla u) = f$: outflow error $\left|\int_{y=2200} \boldsymbol{K}\nabla(u-u_h)\cdot\mathbf{n}\right|$

no of unknowns	825	3300	13200
rel. error est.	46%	34%	24%



Underground reservoir,
10th SPE test case

G. Mallik, M. Vohralík, S. Yousef, in preparation (2018)

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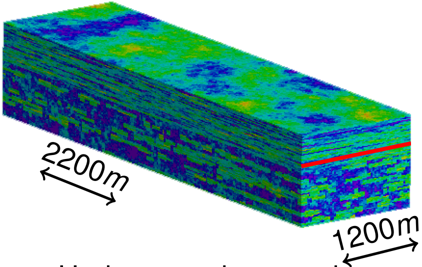

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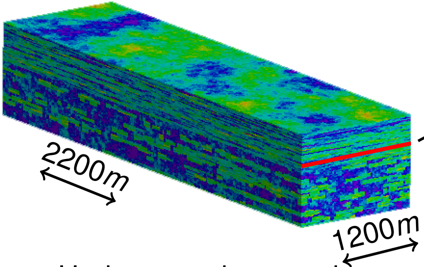
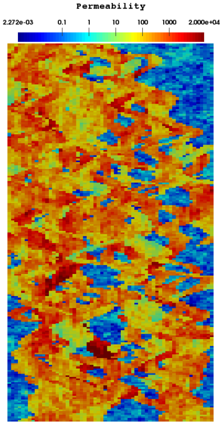


Underground reservoir, 10th SPE test case

G. Mallik, M. Vohralík, S. Yousef, in preparation (2018)



Layer permeability

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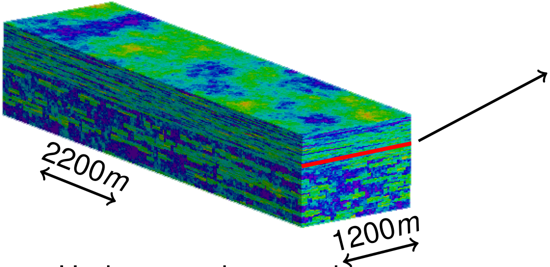

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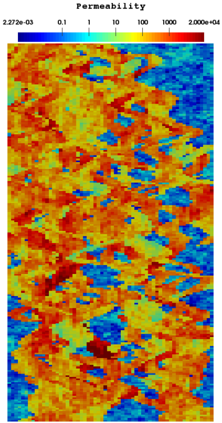

Layer permeability

Realistic environmental problem

Incompressible two-phase flow in porous media

Find *saturations* s_α and *pressures* p_α, $\alpha \in \{\mathrm{g}, \mathrm{w}\}$, such that

$$\begin{aligned} \partial_t(\phi s_\alpha) - \nabla\cdot\left(\frac{k_{\mathrm{r},\alpha}(s_\mathrm{w})}{\mu_\alpha}\boldsymbol{K}(\nabla p_\alpha + \rho_\alpha g \nabla z)\right) &= q_\alpha, \qquad \alpha \in \{\mathrm{g}, \mathrm{w}\}, \\ s_\mathrm{g} + s_\mathrm{w} &= 1, \\ p_\mathrm{g} - p_\mathrm{w} &= p_\mathrm{c}(s_\mathrm{w}) \end{aligned}$$

- unsteady, nonlinear, and degenerate problem
- coupled system of PDEs & algebraic constraints

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$$p_\mathrm{g} - p_\mathrm{w} = p_\mathrm{c}(s_\mathrm{w})$$

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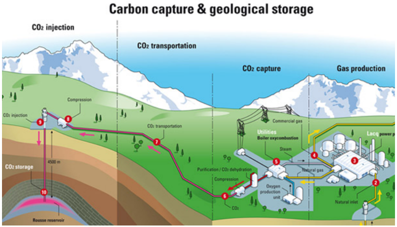
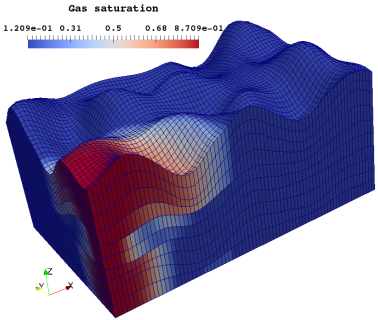


Space/time/nonlinear solver/linear solver adaptivity

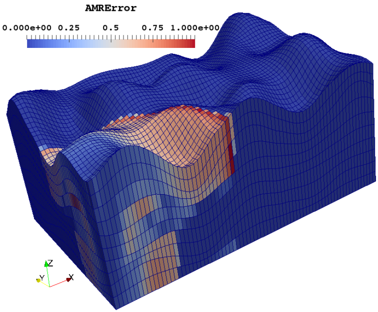
movie

M. Vohralík, M.-F. Wheeler, Computational Geosciences (2013)

Three-phase, three-components (black-oil) problem (collaboration IFPEN)



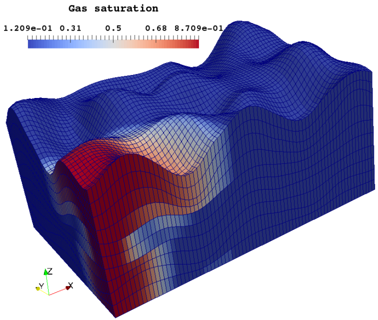
Gas saturation



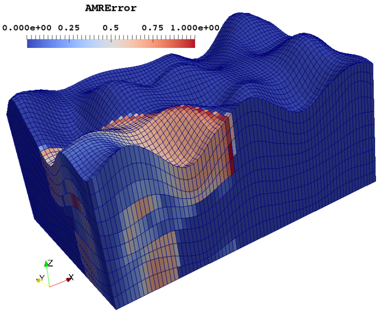
A posteriori error estimate

M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering (2018)

Three-phase, three-components (black-oil) problem (collaboration IFPEN)



Gas saturation



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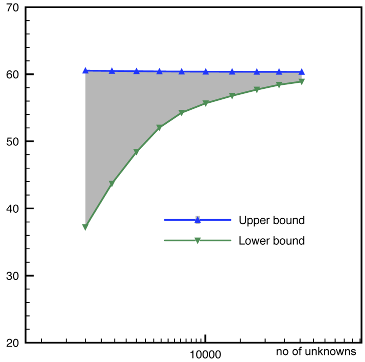
A posteriori estimates

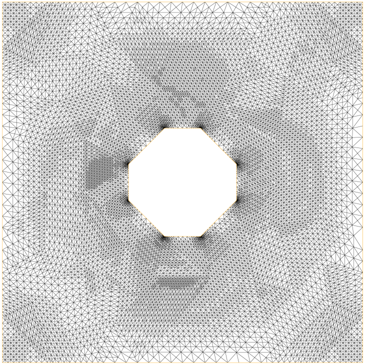
1. **certify the error**
2. **localize it**
3. **decrease it efficiently** via **adaptivity**

Laplace eigenvalue problem $-\Delta u = \lambda u$: inclusion bounds on eigenvalues and adaptivity

no of unknowns	2494	3390	4508	7602	13640	18163	23494	30533
rel. error est.	48%	32%	22%	11%	6.1%	4.5%	3.2%	2.4%



First eigenvalue inclusion



Adaptively refined mesh

E. Cancès, G. Dusson, Y. Maday, B. Stamm, M. Vohralík, SIAM Journal on Numerical Analysis (2018)

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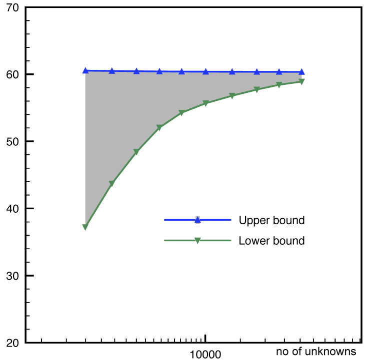

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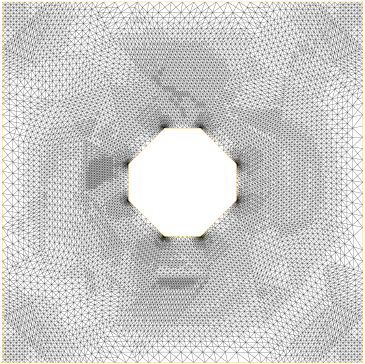

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