Mathematical modeling, numerical simulation, and a posteriori error estimates

Martin Vohralík

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Outline

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Research in France: CNRS

National Centre for Scientific Research

- Institutes of Chemistry, Ecology and Environment, Physics, Nuclear and Particle Physics, Biological Sciences, Humanities and Social Sciences, Computer Sciences, Engineering and Systems Sciences, Mathematical Sciences, Earth Sciences and Astronomy
- 26.000 permanent employees
  - research scientists (chargés de recherche)
  - research directors (directeurs de recherche)
  - engineers, technicians
  - administrative staff
- 6.000 temporary workers
- `www.cnrs.fr`

Research in France: INRIA

INRIA, Institute for Research in Computer Science and Control

- theoretical and applied research in computer science
- 1.300 research scientists & research directors
- 1000 Ph.D. students, 500 post-docs
- 8 research centers
- organization by project-teams
- `www.inria.fr`

Higher education in France

Public universities

- 81 universities
- no entrance examination

Grandes écoles

- highly selective admission based on national ranking in competitive written and oral exams
- two years of dedicated preparatory classes
- small number of students

Private universities

- a few smaller institutions

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Exchange opportunities

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- ERASMUS
- european programs
- Institut Français Prague
- Research in Paris, research scholarships
- ...

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Partial differential equations

Example of a partial differential equation (PDE)

Let $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$. Find $u : \Omega \to \mathbb{R}$ such that

$$-\nabla\cdot(\underline{\mathbf{K}}\nabla u) = f \qquad \text{in } \Omega,$$
$$u = 0 \qquad \text{on } \partial\Omega,$$

where

- $\underline{\mathbf{K}} : \Omega \to \mathbb{R}^{d\times d}$ is a diffusion tensor,
- $f : \Omega \to \mathbb{R}$ is a source term.

Form in 1D

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

$$-(ku')' = f,$$
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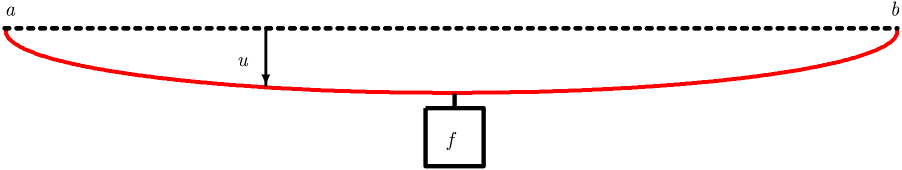
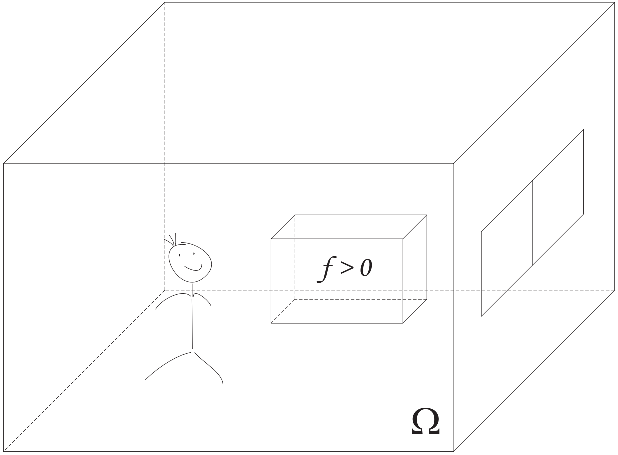
Example: elastic string



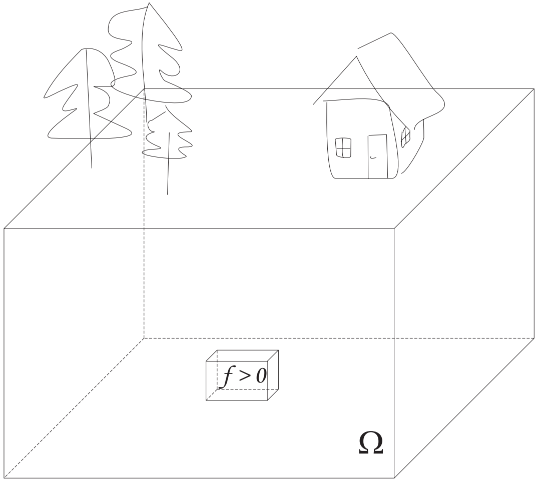
Elastic string with displacement *u* and weight *f*

Example: heat flow



A room with a heater of $f > 0$ and temperature u

Example: underground water flow



Underground with a water well of $f > 0$ and pressure head u

Comments on partial differential equations

Comments

- PDEs describe a huge number of environmental and physical phenomena
- it is almost never possible to find analytical, *exact solutions* (not even Einstein could solve PDEs . . .)
- still we need to approximate their solutions as precisely as possible so as to build bridges and dams, construct cars and planes, forecast the weather, drill oil and natural gas, depollute soils and oceans, concept medications, devise advanced health care techniques, predict population dynamics, steer economic and financial markets . . .

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Numerical approximations of PDEs

Numerical methods

- mathematically-based algorithms
- evaluated with the aid of computers
- deliver *approximate solutions*

Crucial questions

- How large is the overall error between the exact and approximate solutions?
- Where in space and in time is the error localized?

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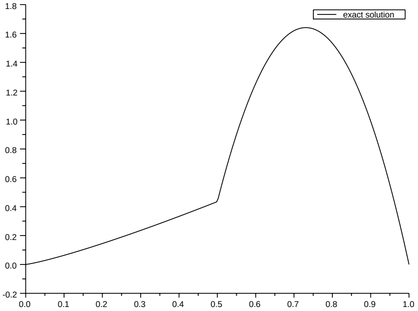
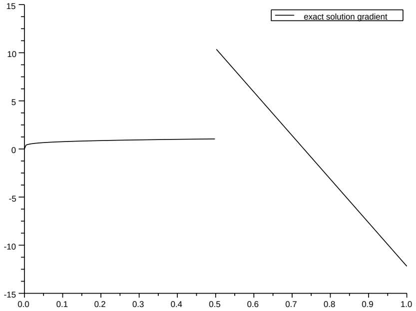
Properties of the exact solution

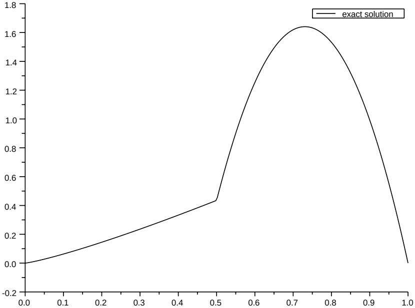


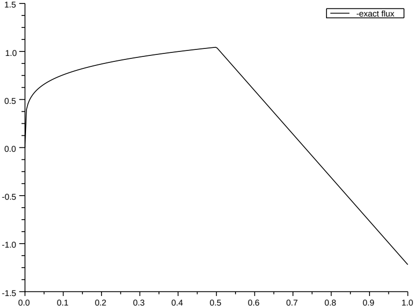
Solution u (displacement, temperature, pressure . . .) is continuous



Solution gradient ∇u (derivative u' in 1D) is not necessarily continuous

Properties of the exact solution

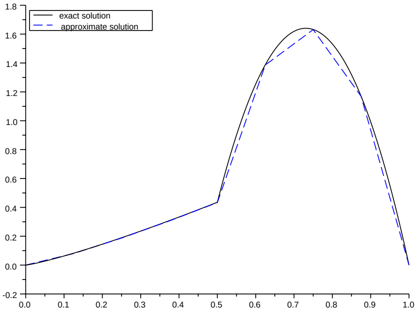


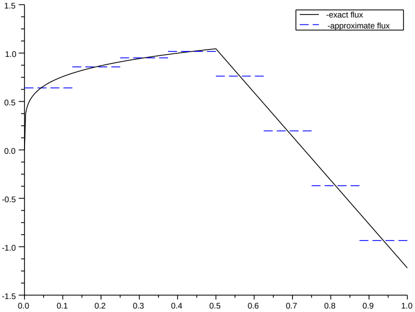


Solution u is continuous

Flux $\boldsymbol{\sigma} := -\underline{\mathbf{K}}\nabla u$ (or $-ku'$ in 1D) is continuous

Approximate solution and approximate flux





Approximate solution u_h is continuous

Approximate flux $-\underline{\mathbf{K}}\nabla u_h$ $(-ku_h')$ is not in continuous

Outline

A posteriori error estimates

A posteriori error estimate

An a posteriori error estimate is an inequality of the form

$$|||u - u_h||| \leq \left\{ \sum_{K \in \mathcal{T}_h} \eta_K^2 \right\}^{1/2},$$

where

- u is the unknown exact solution;
- u_h is the known numerical approximation;
- $|||\cdot|||$ is some suitable norm;
- $\mathcal{T}_h$ is the computational mesh of the numerical method;
- $\eta_K = \eta_K(u_h)$ is a quantity linked to the mesh element K, computable from u_h, called an *element estimator*.

Magic

We do not know u but we can estimate the error between u and u_h!!!

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A posteriori error estimates

Construction of $\eta_K(u_h)$

- recall that the exact flux $\boldsymbol{\sigma} = -\underline{\mathbf{K}}\nabla u$ is continuous
- recall that the approximate flux $-\underline{\mathbf{K}}\nabla u_h$ is not continuous
- main idea: build a discrete, approximate flux reconstruction $\boldsymbol{\sigma}_h$ which would be continuous as the exact flux $\boldsymbol{\sigma}$ is
- use $\boldsymbol{\sigma}_h$ in order to devise $\eta_K(u_h)$

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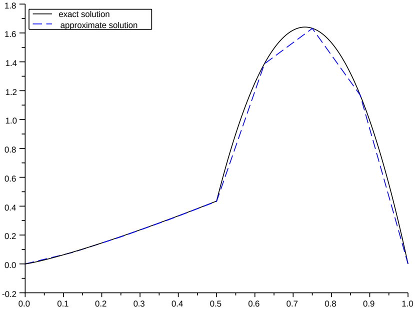
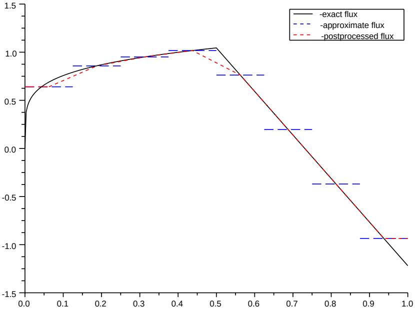
Approximate solution and postprocessed flux





Approximate solution u_h is continuous

A flux reconstruction σ_h which is continuous

Numerical experiment in 1D

Model problem

$$
\begin{aligned}
-u'' &= \pi^2 sin(\pi x) \quad \text{in }]0,1[, \\
u &= 0 \quad \text{in } 0,1
\end{aligned}
$$

Exact solution

$$u(x) = sin(\pi x)$$

Discretization by the finite element method

N given, $h = 1/(N+1)$, $x_k = kh$, $k = 0, \ldots, N+1 \Rightarrow$ piecewise affine u_h

Choice of σ_h

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\begin{aligned}
\sigma_h(x_{k+\frac{1}{2}}) &= -u_h'(x_{k+\frac{1}{2}}) \qquad k = 0, \ldots, N, \\
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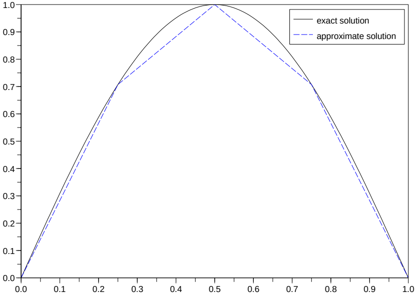
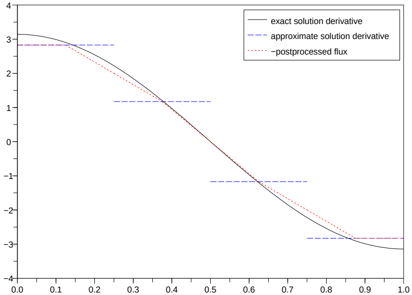
Exact and approximate solution and fluxes

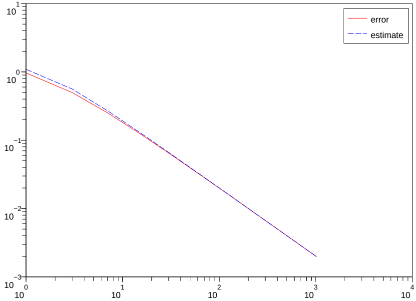


Plot of u and u_h

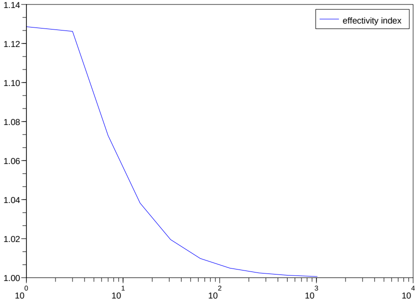


Plot of u', u_h', and $-\sigma_h$

Estimate and its efficiency



Estimated and actual error



Ratio estimate/error

Numerical experiment in 2D

Model nonlinear problem

- p-Laplacian

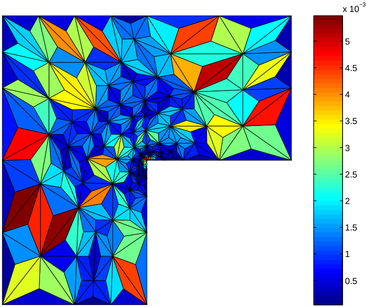
$$\begin{aligned} \nabla\cdot(|\nabla u|^{p-2}\nabla u) &= f \qquad \text{in } \Omega, \\ u &= u_0 \qquad \text{on } \partial\Omega \end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

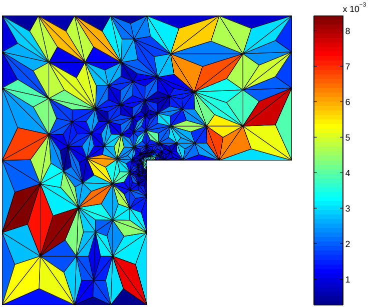
$$u(r,\theta) = r^{\frac{7}{8}} \sin(\theta \tfrac{7}{8})$$

- $p = 4$, L-shape domain, singularity at the origin
- the nonconforming finite element method used

Error distribution on an adaptively refined mesh

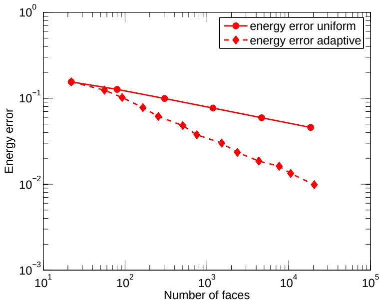


Estimated error distribution

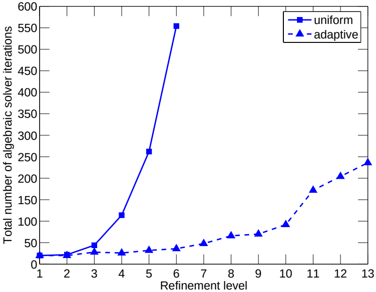


Exact error distribution

Adaptive versus uniform performance



Error for adaptive and uniform mesh refinement



Overall cost for fully adaptive and classical nonadaptive approaches

Adaptive mesh refinement–steady case

movie

Adaptive mesh refinement–unsteady case

movie

Outline

Conclusions

Smart algorithms in numerical simulations

- control of the error between the unknown exact solution and know numerical approximation: a given precision can be attained at the end of the simulation
- efficiency: as small as possible amount of computational work is needed
- achieved via a posteriori error estimates and adaptivity

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