Mathematical modeling, numerical simulation, and a posteriori error estimates

Martin Vohralík

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Outline

1. Research and education in France, INRIA
2. Introduction
3. Some properties of PDEs and of numerical methods
4. A posteriori error estimates
5. Outlook
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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
INRIA, Institute for Research in Computer Science and Control

- theoretical and applied research in computer science
- 1,300 research scientists & research directors
- 1,000 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

- ERASMUS
- European programs
- Institut Français Prague
- Research in Paris, research scholarships
- …
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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

$$-\nabla \cdot (K \nabla u) = f \quad \text{in} \; \Omega,$$

$$u = 0 \quad \text{on} \; \partial \Omega,$$

where

- $K : \Omega \to \mathbb{R}^{d \times d}$ is a diffusion tensor,
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Form in 1D

Let $\Omega$ 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

- 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?
Numerical approximations of PDEs

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Properties of the exact solution

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

**Solution gradient** $\nabla u$ (derivative $u'$ in 1D) is not necessarily continuous
Properties of the exact solution

Solution $u$ is continuous

Flux $\sigma := -K\nabla u$ (or $-ku'$ in 1D) is continuous
Approximate solution and approximate flux

Approximate solution \( u_h \) is continuous

Approximate flux \(-K \nabla u_h\) is not in continuous
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A posteriori error estimates

A posteriori error estimate

An **a posteriori error estimate** is an inequality of the form

\[ ||| u - u_h ||| \leq \left\{ \sum_{K \in T_h} \eta_K^2 \right\}^{1/2}, \]

where

- \( u \) is the **unknown exact solution**;
- \( u_h \) is the **known numerical approximation**;
- \( ||| \cdot ||| \) is some suitable norm;
- \( T_h \) 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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**Magic**

We do not know \( u \) but we can estimate the error between \( u \) and \( u_h \)!!!!
Construction of $\eta_K(u_h)$

- recall that the exact flux $\sigma = -K \nabla u$ is continuous
- recall that the approximate flux $-K \nabla u_h$ is not continuous
- main idea: build a discrete, approximate flux reconstruction $\sigma_h$ which would be continuous as the exact flux $\sigma$ is
- use $\sigma_h$ 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 $\sigma_h$ which is continuous

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Modeling, simulation, and a posteriori estimates
Numerical experiment in 1D

Model problem

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

Exact solution

\[u(x) = \sin(\pi x)\]

Discretization by the finite element method

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

Choice of \(\sigma_h\)

\[\sigma_h(x_{k+\frac{1}{2}}) = -u_h'(x_{k+\frac{1}{2}}) \quad k = 0, \ldots, N,\]
\[\sigma_h(x_k) = -(u_h'|_{x_{k-1},x_k} + u_h'|_{x_k,x_{k+1}})/2 \quad k = 1, \ldots, N,\]
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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

\[
\nabla \cdot (|\nabla u|^{p-2} \nabla u) = f \quad \text{in } \Omega,
\]
\[
u = u_0 \quad \text{on } \partial \Omega
\]

- weak solution (used to impose the Dirichlet BC)

\[
u(r, \theta) = r^{\frac{7}{8}} \sin(\theta^{\frac{7}{8}})
\]

- $p = 4$, 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

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Modeling, simulation, and a posteriori estimates
Adaptive versus uniform performance

Error for adaptive and uniform mesh refinement

Overall cost for fully adaptive and classical nonadaptive approaches

Energy error for adaptive and uniform mesh refinement.

Total number of algebraic solver iterations for uniform and adaptive approaches.

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Modeling, simulation, and a posteriori estimates
Adaptive mesh refinement—steady case
Adaptive mesh refinement—unsteady case
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Smart algorithms in numerical simulations

- **control of the error** between the unknown exact solution and known 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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