Adaptive numerical approximation of model partial differential equations

Martin Vohralík

*Inria & Ecole des Ponts, Paris, France*

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Outline

1 Introduction
2 Laplace equation: mesh adaptivity
3 Nonlinear Laplace equation: adaptive stopping criteria
4 Laplace eigenvalues and eigenvectors: guaranteed bounds
5 Two-phase flow in porous media: industrial application
6 Conclusions and outlook
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- institute for research in informatics & applied mathematics
- theoretical and applied research
- 1.300 research scientists
- 1000 Ph.D. students, 500 post-docs
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- highly selective admission based on national ranking in competitive written and oral exams
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Simulation for the Environment: Reliable and Efficient Numerical Algorithms

- conception and analysis of models based on partial differential equations (PDEs)
- **numerical** approximation methods (algorithms) (finite element method)
- algebraic solvers (domain decomposition, multigrid, Newton–Krylov)
- implementation issues (correctness of programs)
- **reliability** of the overall simulation
- **efficiency** with respect to computational resources
- current **environmental** problems
Example of a partial differential equation

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,
- $f : \Omega \to \mathbb{R}$ is a source term.

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

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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
- how 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, predict economic and financial markets behavior . . .
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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?
- Can we build adaptive methods that focus the work where the error is large?
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Estimated error distribution  

Exact error distribution
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A posteriori error control: the principle

Laplace equation

$$-\Delta u = f \text{ in } \Omega,$$
$$u = 0 \text{ on } \partial\Omega$$

Guaranteed error bound (reliability)

$$\|\nabla (u - u_h)\| \leq \eta := \left\{ \sum_{K \in T_h} \eta_K(u_h)^2 \right\}^{1/2}$$

Local efficiency (error localization)

$$\eta_K(u_h) \leq \frac{C_{st}C_{PP}}{\|\nabla (u - u_h)\|_{\omega_K}} \forall K \in T_h$$

- delicate theoretical issues of numerical analysis
- magic: do not know \(u\) but can estimate \(u - u_h\)
- future generation algorithms
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Adaptive numerical approximation of model PDEs 12 / 43
A posteriori error control: the principle

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Adaptive numerical approximation of model PDEs 12 / 43
Numerics: smooth case

Model problem

$$-\Delta u = f \quad \text{in} \; \Omega := (0, 1)^2,$$
$$u = 0 \quad \text{on} \; \partial \Omega$$

Exact solution

$$u(x, y) = \sin(2\pi x) \sin(2\pi y)$$

Discretization

- symmetric interior penalty discontinuous Galerkin method
- unstructured triangular grids
- uniform $h$ refinement
Numerics: smooth case

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Uniform refinement: \textbf{asymptotic exactness}

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<th>$| \nabla_d u_h + \sigma h |$</th>
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$\approx h_0/2$, $\approx h_0/4$, $\approx h_0/8$
Adaptive mesh refinement—steady case
Model problem

\[-\Delta u = 0 \quad \text{in} \quad \Omega := (-1, 1)^2 \setminus [0, 1]^2,\]

\[u = u_D \quad \text{on} \quad \partial \Omega\]

Exact solution

\[u(r, \phi) = r^{2/3} \sin(2\phi/3)\]

Discretization

- incomplete interior penalty discontinuous Galerkin method
- unstructured non-nested triangular grids
- $hp$-adaptive refinement
Numerics: singular case

Model problem

\[-\Delta u = 0 \quad \text{in} \; \Omega := (-1, 1)^2 \setminus [0, 1]^2,\]
\[u = u_D \quad \text{on} \; \partial \Omega\]

Exact solution

\[u(r, \phi) = r^{2/3} \sin(2\phi/3)\]

Discretization

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\[-\Delta u = 0 \quad \text{in} \quad \Omega := (-1, 1)^2 \setminus [0, 1]^2,\]
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Exact solution

\[u(r, \phi) = r^{2/3} \sin(2\phi/3)\]

Discretization

- incomplete interior penalty discontinuous Galerkin method
- unstructured non-nested triangular grids
- \(hp\)-adaptive refinement
hp-adaptive refinement: **exponential convergence**

- Error in energy norm vs. DoF^{1/3}
- Effectivity index vs. DoF^{1/3}

- Ideal and parameterized solutions
- γ = 0.30 and γ = 0.60
- Prior and hp decay
- h-adapt
hp-refinement grids

level 1

level 5

level 12

zoom 10x
Adaptive mesh refinement–unsteady case
Figure 5 – Solution post-traitée (`à gauche) et solution conforme (`à droite)

Remarque 3.2. On observe que ...

Potential reconstruction

Potential $u_h$
Potential reconstruction

Potential $u_h$

Potential reconstruction $s_h$
Equilibrated flux reconstruction
Equilibrated flux reconstruction

Flux $-\nabla u_h$
Equilibrated flux reconstruction
Outline

1. Introduction
2. Laplace equation: mesh adaptivity
3. Nonlinear Laplace equation: adaptive stopping criteria
4. Laplace eigenvalues and eigenvectors: guaranteed bounds
5. Two-phase flow in porous media: industrial application
6. Conclusions and outlook
Inexact iterative linearization

System of nonlinear algebraic equations

Nonlinear operator $A : \mathbb{R}^N \to \mathbb{R}^N$, vector $F \in \mathbb{R}^N$: find $U \in \mathbb{R}^N$ s.t.

$A(U) = F$

Algorithm (Inexact iterative linearization)

1. Choose initial vector $U^0$. Set $k := 1$.
2. $U^{k-1}$ ⇒ matrix $A^{k-1}$ and vector $F^{k-1}$: find $U^k$ s.t.
   
   $A^{k-1}U^k \approx F^{k-1}$.
3. Set $U^{k,0} := U^{k-1}$ and $i := 1$.
   1. Do an algebraic solver step ⇒ $U^{k,i}$ s.t. ($R^{k,i}$ algebraic res.)
      
      $A^{k-1}U^{k,i} = F^{k-1} - R^{k,i}$.
   2. Convergence? OK ⇒ $U^k := U^{k,i}$. KO ⇒ $i := i + 1$, back to 3.2.
Inexact iterative linearization

System of nonlinear algebraic equations

Nonlinear operator \( A : \mathbb{R}^N \rightarrow \mathbb{R}^N \), vector \( F \in \mathbb{R}^N \): find \( U \in \mathbb{R}^N \) s.t.

\[ A(U) = F \]

Algorithm (Inexact iterative linearization)

1. **Choose initial vector** \( U^0 \). **Set** \( k := 1 \).

2. \( U^{k-1} \Rightarrow \text{matrix } A^{k-1} \text{ and vector } F^{k-1} : \text{find } U^k \text{ s.t.} \)

\[ A^{k-1} U^k \approx F^{k-1} \]

3. **Set** \( U^{k,0} := U^{k-1} \text{ and } i := 1 \).

4. **Do an algebraic solver step** \( \Rightarrow U^{k,i} \text{ s.t. (} R^{k,i} \text{ algebraic res.)} \)

\[ A^{k-1} U^{k,i} = F^{k-1} - R^{k,i} \]

5. **Convergence?** OK \( \Rightarrow U^k := U^{k,i} \). KO \( \Rightarrow i := i + 1 \), back to 3.2.

6. **Convergence?** OK \( \Rightarrow \text{finish} \). KO \( \Rightarrow k := k + 1 \), back to 2.
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   \[
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   \]
3. \( \begin{align*}
   &1 \quad \text{Set } U^{k,0} := U^{k-1} \text{ and } i := 1. \\
   &2 \quad \text{Do an algebraic solver step } \Rightarrow U^{k,i} \text{ s.t. } (R^{k,i} \text{ algebraic res.}) \\
   &\quad \quad \quad \quad \quad \quad \quad \quad \quad A^{k-1} U^{k,i} = F^{k-1} - R^{k,i}.
   &3 \quad \text{Convergence? } OK \Rightarrow U^k := U^{k,i}. \, \text{KO } \Rightarrow i := i + 1, \text{ back to 3.2.}
   \end{align*} \)
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Context and questions

Approximate solution
- approximate solution $U^{k,i}$ does not solve $A(U^{k,i}) = F$

Numerical method
- underlying numerical method: the vector $U^{k,i}$ is associated with a (piecewise polynomial) approximation $u_h^{k,i}$

Partial differential equation
- underlying PDE, $u$ its weak solution: $A(u) = f$

- What is a good stopping criterion for the linear solver?
- What is a good stopping criterion for the nonlinear solver?

- How big is the error $\|u - u_h^{k,i}\|_{?,\Omega}$ on Newton step $k$ and algebraic solver step $i$, how is it distributed?
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Question (Stopping criteria)

  - What is a good stopping criterion for the linear solver?
  - What is a good stopping criterion for the nonlinear solver?

Question (Error)

  - How big is the error $\|u - u^{k,i}_h\|_{\Omega}$ on Newton step $k$ and algebraic solver step $i$, how is it distributed?
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- approximate solution $U^{k,i}$ does not solve $A(U^{k,i}) = F$

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Error distribution on an adaptively refined mesh

Estimated error distribution

Exact error distribution
Energy error and overall performance

Energy error

Overall performance
1. Introduction
2. Laplace equation: mesh adaptivity
3. Nonlinear Laplace equation: adaptive stopping criteria
4. Laplace eigenvalues and eigenvectors: guaranteed bounds
5. Two-phase flow in porous media: industrial application
6. Conclusions and outlook
Laplace eigenvalue problem

**Problem**
Find eigenvector & eigenvalue pair \((u, \lambda)\) such that

\[-\Delta u = \lambda u \quad \text{in} \ \Omega,\]

\[u = 0 \quad \text{on} \ \partial\Omega.\]

**Weak formulation**
Find \((u_i, \lambda_i) \in V \times \mathbb{R}^+, \ i \geq 1, \ \text{with} \ ||u_i|| = 1, \ \text{such that} \)

\[(\nabla u_i, \nabla v) = \lambda_i (u_i, v) \quad \forall v \in V.\]
Problem
Find eigenvector & eigenvalue pair \((u, \lambda)\) such that

\[-\Delta u = \lambda u \quad \text{in } \Omega,\]
\[u = 0 \quad \text{on } \partial \Omega.\]

Weak formulation
Find \((u_i, \lambda_i) \in V \times \mathbb{R}^+, \ i \geq 1\), with \(\|u_i\| = 1\), such that

\[(\nabla u_i, \nabla v) = \lambda_i (u_i, v) \quad \forall v \in V.\]
Main results (conforming setting)

Assumption (Conforming variational solution)

\[ (u_{ih}, \lambda_{ih}) \in V \times \mathbb{R}^+ \]
\[ \|u_{ih}\| = 1 \]
\[ \|\nabla u_{ih}\|^2 = \lambda_{ih} \]

We bound

\[ i\text{-th eigenvector energy error} \]
\[ \|\nabla (u_i - u_{ih})\| \leq \eta_i(u_{ih}, \lambda_{ih}) \]
Main results (conforming setting)

Assumption (Conforming variational solution)

- \((u_{ih}, \lambda_{ih}) \in V \times \mathbb{R}^+\)
- \(\|u_{ih}\| = 1\)
- \(\|\nabla u_{ih}\|^2 = \lambda_{ih}\)

(\(\Rightarrow \lambda_{1h} \geq \lambda_1\))

We bound

\[-\text{i-th eigenvector energy error} \leq \eta_i(u_{ih}, \lambda_{ih})\]
Main results (conforming setting)

Assumption (Conforming variational solution)
- \((u_{ih}, \lambda_{ih}) \in V \times \mathbb{R}^+\)
- \(\|u_{ih}\| = 1\)
- \(\|\nabla u_{ih}\|^2 = \lambda_{ih}\)

We bound

1. \textit{i-th eigenvalue error}

\[\lambda_{ih} - \lambda_i \leq \eta_i(u_{ih}, \lambda_{ih})^2\]

2. \textit{i-th eigenvector energy error}

\[\|\nabla (u_i - u_{ih})\| \leq \eta_i(u_{ih}, \lambda_{ih})\]
Main results (conforming setting)

Assumption (Conforming variational solution)

- \((u_{ih}, \lambda_{ih}) \in V \times \mathbb{R}^+\)
- \(\|u_{ih}\| = 1\)
- \(\|\nabla u_{ih}\|^2 = \lambda_{ih}\)

We bound

1. **i-th eigenvalue error**

   \[
   \lambda_{ih} - \lambda_i \leq \eta_i(u_{ih}, \lambda_{ih})^2
   \]

2. **i-th eigenvector energy error**

   \[
   \|\nabla (u_i - u_{ih})\| \leq \eta_i(u_{ih}, \lambda_{ih})
   \]

\(\Rightarrow \lambda_{1h} \geq \lambda_1\)
Main results (conforming setting)

Assumption (Conforming variational solution)

- \((u_{ih}, \lambda_{ih}) \in V \times \mathbb{R}^+\)
- \(\|u_{ih}\| = 1\)
- \(\|\nabla u_{ih}\|^2 = \lambda_{ih}\)

\(\Rightarrow \lambda_{1h} \geq \lambda_1\)

We bound

1. **i-th eigenvalue error**
   
   \[\lambda_{ih} - \lambda_i \leq \eta_i(u_{ih}, \lambda_{ih})^2\]

2. **i-th eigenvector energy error**
   
   \[\|\nabla (u_i - u_{ih})\| \leq \eta_i(u_{ih}, \lambda_{ih}) \leq C_{eff,i}\|\nabla (u_i - u_{ih})\|\]
Main results (conforming setting)

Assumption (Conforming variational solution)

- \((u_{ih}, \lambda_{ih}) \in V \times \mathbb{R}^+\)
- \(\|u_{ih}\| = 1\)
- \(\|\nabla u_{ih}\|^2 = \lambda_{ih}\)

We bound

1. \(i\)-th eigenvalue error

\[\lambda_{ih} - \lambda_i \leq \eta_i(u_{ih}, \lambda_{ih})^2\]

2. \(i\)-th eigenvector energy error

\[\|\nabla (u_i - u_{ih})\| \leq \eta_i(u_{ih}, \lambda_{ih}) \leq C_{\text{eff},i}\|\nabla (u_i - u_{ih})\|\]

- \(C_{\text{eff},i}\) only depends on mesh shape regularity and on \(\lambda_i, \lambda_{i-1}, \lambda_{i+1}\)
- we give computable upper bounds on \(C_{\text{eff},i}\)
Main results (conforming setting)

Assumption (Conforming variational solution)
- \((u_{ih}, \lambda_{ih}) \in V \times \mathbb{R}^+\)
- \(\|u_{ih}\| = 1\)
- \(\|\nabla u_{ih}\|^2 = \lambda_{ih}\)

(\(\Rightarrow \lambda_{1h} \geq \lambda_1\))

We bound

**i-th eigenvalue upper and lower bounds**

\[
\lambda_{ih} - \eta_i(u_{ih}, \lambda_{ih})^2 \leq \lambda_i \leq \lambda_{ih} - \tilde{\eta}_i(u_{ih}, \lambda_{ih})^2
\]

**2 i-th eigenvector energy error**

\[
\|\nabla (u_i - u_{ih})\| \leq \eta_i(u_{ih}, \lambda_{ih})
\]
Numerical results: unit square

Setting

- $\Omega = (0, 1)^2$
- $\lambda_1 = 2\pi^2, \lambda_2 = 5\pi^2$ known explicitly
- $u_1(x, y) = \sin(\pi x) \sin(\pi y)$ known explicitly

Effectivity indices

- recall $\tilde{\eta}_i^2 \leq \lambda_{ih} - \lambda_i \leq \eta_i^2$

\[
I_{\lambda,\text{eff}}^{\text{lb}} := \frac{\lambda_{ih} - \lambda_i}{\tilde{\eta}_i^2}, \quad I_{\lambda,\text{eff}}^{\text{ub}} := \frac{\eta_i^2}{\lambda_{ih} - \lambda_i}
\]

- recall $\|\nabla(u_i - u_{ih})\| \leq \eta_i$

\[
I_{u,\text{eff}}^{\text{ub}} := \frac{\eta_i}{\|\nabla(u_i - u_{ih})\|}
\]
Structured meshes

Unstructured meshes

GUARANTEED BOUNDS FOR EIGENVALUES AND EIGENVECTORS

Adaptive numerical approximation of model PDEs
## Conforming finite elements

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### Structured meshes

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### Unstructured meshes

M. Vohralík

Adaptive numerical approximation of model PDEs
## Conforming finite elements

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Unstructured meshes
Domain with a hole

Adaptively refined mesh

First eigenvalue inclusion

Upper bound
Lower bound
Outline

1. Introduction
2. Laplace equation: mesh adaptivity
3. Nonlinear Laplace equation: adaptive stopping criteria
4. Laplace eigenvalues and eigenvectors: guaranteed bounds
5. Two-phase flow in porous media: industrial application
6. Conclusions and outlook
Oil production

- oil – one of the major energy supply of today’s world
- need for efficient production
- high prices – question of rentability

SAGD Process

Reservoir
Two-phase immiscible incompressible flow

\[
\partial_t (\phi s_\alpha) + \nabla \cdot u_\alpha = q_\alpha, \quad \alpha \in \{o, w\},
\]

\[-\lambda_\alpha (s_w) K (\nabla p_\alpha + \rho_\alpha g \nabla z) = u_\alpha, \quad \alpha \in \{o, w\},
\]

\[s_o + s_w = 1,
\]

\[p_o - p_w = p_c (s_w)
\]

+ boundary & initial conditions
Geometry and meshes example
Numerical difficulties

- **highly nonlinear** (degenerate) system of partial differential equations
- coupled with nonlinear algebraic equations
- involves phase transitions
- different time and space scales (orders of magnitude difference)
- highly contrasted, discontinuous coefficients
- complicated 3D geometries
- unstructured and nonmatching grids
- presence of evolving sharp fronts
- combination of diffusive, advective, and reactive effects
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Distinguishing the error components

Theorem (Distinguishing the error components)

Let
- \( n \) be the \textit{time} step,
- \( k \) be the \textit{linearization} step,
- \( i \) be the \textit{algebraic solver} step,

with the approximations \((s_{w,h_T}^{n,k,i}, p_{w,h_T}^{n,k,i})\). Then

\[
\mathcal{J}_{s_w,p_w}^{n,k,i}(s_{w,h_T}^{n,k,i}, p_{w,h_T}^{n,k,i}) \leq \eta_{sp}^{n,k,i} + \eta_{tm}^{n,k,i} + \eta_{lin}^{n,k,i} + \eta_{alg}^{n,k,i}.
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Error components
- \( \eta_{sp}^{n,k,i} \): spatial discretization
- \( \eta_{tm}^{n,k,i} \): temporal discretization
- \( \eta_{lin}^{n,k,i} \): linearization
- \( \eta_{alg}^{n,k,i} \): algebraic solver

Full adaptivity
- only a \textbf{necessary number} of all solver iterations
- “\textit{online decisions}”: algebraic step / linearization step / space mesh refinement / time step modification

M. Vohralík

Adaptive numerical approximation of model PDEs
Distinguishing the error components

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**Full adaptivity**
- only a necessary number of all solver iterations
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Water saturation evolution
Front propagation & error estimates
Estimators and stopping criteria

Estimators in function of GMRes iterations

Estimators in function of iterative coupling iterations
GMRes iterations

Per time and iterative coupling step

Cumulated

Number of GMRes iterations

Time/iterative coupling step

Cumulative number of GMRes iterations

Time

M. Vohralík

Adaptive numerical approximation of model PDEs
Space/time/nonlinear solver/linear solver adaptivity
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- **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

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- achieved via *a posteriori error estimates* and adaptivity

- rather complicated . . .
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Bibliography

**Laplace and \( hp \) adaptivity**


**Adaptive inexact Newton**


**Eigenvalues**


**Two-phase flow**


Thank you for your attention!