

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

Inria & Ecole des Ponts

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- institute for research in informatics & applied mathematics
- theoretical and applied research
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- 1000 Ph.D. students, 500 post-docs
- 8 research centers
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Project-team SERENA

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

Partial differential equations

Example of a partial differential equation

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

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

where

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

Form in 1D

Let Ω be an interval, $\Omega =]a, b[$, a, b two real numbers, $a < b$.

Let $k :]a, b[\rightarrow \mathbb{R}$ and $f :]a, b[\rightarrow \mathbb{R}$ be two given functions. Find

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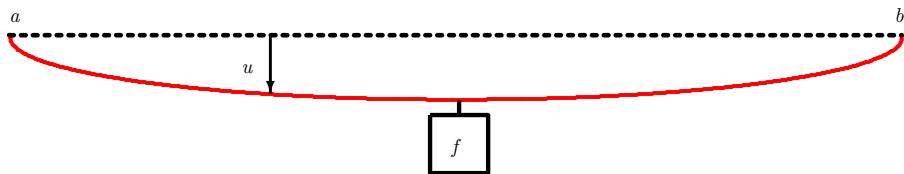
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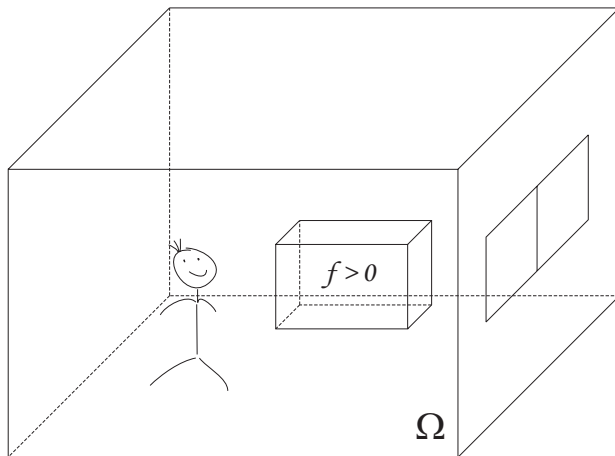


Example: elastic string



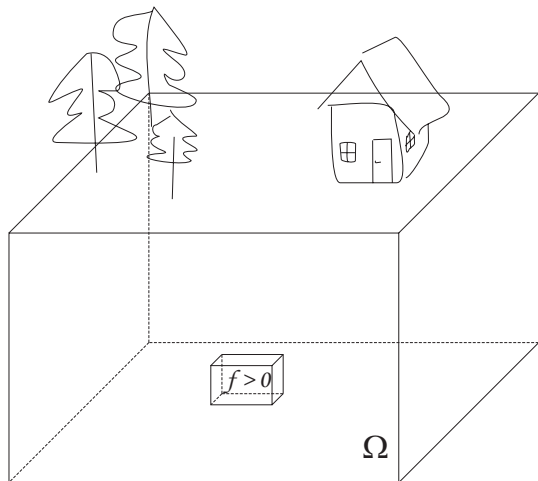
Elastic string with displacement u and weight f

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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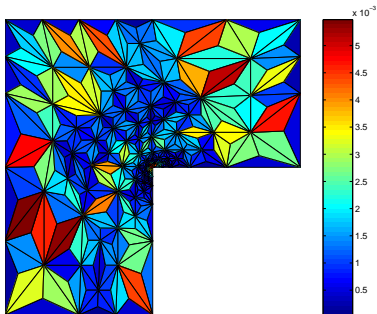
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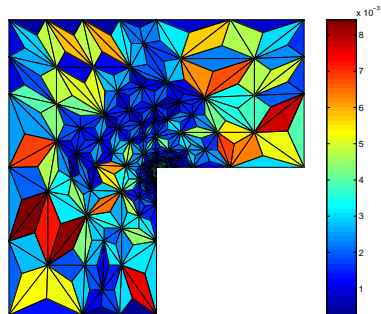
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Appetizer



Estimated error distribution



Exact error distribution

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A posteriori error control: the principle

Laplace equation

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

Guaranteed error bound (reliability)

$$\underbrace{\|\nabla(u - u_h)\|}_{\text{unknown error}} \leq \underbrace{\eta}_{\text{estimator}} := \left\{ \sum_{K \in \mathcal{T}_h} \underbrace{\eta_K(u_h)^2}_{\text{elemental contributions}} \right\}^{1/2}$$

Local efficiency (error localization)

$$\eta_K(u_h) \leq \underbrace{C_M C_{\text{ov}}}_{\substack{\text{theoretical bound,} \\ \text{depending on mesh reg.}}} \|\nabla(u - u_h)\|_{0,K} \quad \forall K \in \mathcal{T}_h$$

- delicate theoretical issues of numerical analysis
- **magic**: do not know u but can estimate $u - u_h$
- future generation algorithms

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Numerics: smooth case

Model problem

$$\begin{aligned} -\Delta u &= f & \text{in } \Omega &:= (0, 1)^2, \\ u &= 0 & \text{on } \partial\Omega \end{aligned}$$

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

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Uniform refinement: asymptotic exactness

h	p	$\ \nabla_d(u - u_h)\ $	$\ \nabla_d u_h + \sigma_h\ $	η_{osc}	$\ \nabla_d(u_h - S_h)\ $	η	ρ^{eff}
h_0	1	1.07E-00	1.12E-00	5.55E-02	4.16E-01	1.25E-00	1.17
$\approx h_0/2$		5.56E-01	5.71E-01	7.42E-03	1.82E-01	6.07E-01	1.09
$\approx h_0/4$		2.92E-01	2.96E-01	1.04E-03	8.77E-02	3.10E-01	1.06
$\approx h_0/8$		1.39E-01	1.40E-01	1.10E-04	3.85E-02	1.45E-01	1.04
h_0	2	1.54E-01	1.55E-01	5.10E-03	3.05E-02	1.63E-01	1.06
$\approx h_0/2$		4.07E-02	4.13E-02	3.53E-04	7.55E-03	4.23E-02	1.04
$\approx h_0/4$		1.10E-02	1.12E-02	2.51E-05	1.97E-03	1.14E-02	1.03
$\approx h_0/8$		2.50E-03	2.54E-03	1.30E-06	4.21E-04	2.57E-03	1.03
h_0	3	1.37E-02	1.37E-02	3.58E-04	1.74E-03	1.41E-02	1.03
$\approx h_0/2$		1.85E-03	1.85E-03	1.26E-05	2.10E-04	1.88E-03	1.01
$\approx h_0/4$		2.60E-04	2.60E-04	4.73E-07	2.54E-05	2.62E-04	1.01
$\approx h_0/8$		2.75E-05	2.75E-05	1.15E-08	2.55E-06	2.76E-05	1.01
h_0	4	9.87E-04	9.84E-04	2.12E-05	1.11E-04	1.01E-03	1.02
$\approx h_0/2$		6.92E-05	6.92E-05	3.96E-07	7.44E-06	7.00E-05	1.01
$\approx h_0/4$		5.04E-06	5.04E-06	7.58E-09	4.98E-07	5.07E-06	1.01
$\approx h_0/8$		2.58E-07	2.58E-07	8.96E-11	2.47E-08	2.60E-07	1.01
h_0	5	5.64E-05	5.63E-05	1.06E-06	4.50E-06	5.75E-05	1.02
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$\approx h_0/8$		1.86E-09	1.86E-09	1.70E-12	1.00E-10	1.86E-09	1.00
h_0	6	2.85E-06	2.85E-06	4.70E-08	2.18E-07	2.90E-06	1.02
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h	p	$\ \nabla_d(u-u_h)\ $	$\ \nabla_d u_h + \sigma_h\ $	η_{osc}	$\ \nabla_d(u_h - S_h)\ $	η	ρ^{eff}
h_0	1	1.07E-00	1.12E-00	5.55E-02	4.16E-01	1.25E-00	1.17
$\approx h_0/2$		5.56E-01	5.71E-01	7.42E-03	1.82E-01	6.07E-01	1.09
$\approx h_0/4$		2.92E-01	2.96E-01	1.04E-03	8.77E-02	3.10E-01	1.06
$\approx h_0/8$		1.39E-01	1.40E-01	1.10E-04	3.85E-02	1.45E-01	1.04
h_0	2	1.54E-01	1.55E-01	5.10E-03	3.05E-02	1.63E-01	1.06
$\approx h_0/2$		4.07E-02	4.13E-02	3.53E-04	7.55E-03	4.23E-02	1.04
$\approx h_0/4$		1.10E-02	1.12E-02	2.51E-05	1.97E-03	1.14E-02	1.03
$\approx h_0/8$		2.50E-03	2.54E-03	1.30E-06	4.21E-04	2.57E-03	1.03
h_0	3	1.37E-02	1.37E-02	3.58E-04	1.74E-03	1.41E-02	1.03
$\approx h_0/2$		1.85E-03	1.85E-03	1.26E-05	2.10E-04	1.88E-03	1.01
$\approx h_0/4$		2.60E-04	2.60E-04	4.73E-07	2.54E-05	2.62E-04	1.01
$\approx h_0/8$		2.75E-05	2.75E-05	1.15E-08	2.55E-06	2.76E-05	1.01
h_0	4	9.87E-04	9.84E-04	2.12E-05	1.11E-04	1.01E-03	1.02
$\approx h_0/2$		6.92E-05	6.92E-05	3.96E-07	7.44E-06	7.00E-05	1.01
$\approx h_0/4$		5.04E-06	5.04E-06	7.58E-09	4.98E-07	5.07E-06	1.01
$\approx h_0/8$		2.58E-07	2.58E-07	8.96E-11	2.47E-08	2.60E-07	1.01
h_0	5	5.64E-05	5.63E-05	1.06E-06	4.50E-06	5.75E-05	1.02
$\approx h_0/2$		2.01E-06	2.01E-06	9.88E-09	1.46E-07	2.03E-06	1.01
$\approx h_0/4$		7.74E-08	7.73E-08	1.01E-10	4.35E-09	7.76E-08	1.00
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h	p	$\ \nabla_d(u-u_h)\ $	$\ \nabla_d u_h + \sigma_h\ $	η_{osc}	$\ \nabla_d(u_h - S_h)\ $	η	ρ^{eff}
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Uniform refinement: asymptotic exactness

h	p	$\ \nabla_d(u-u_h)\ $	$\ u-u_h\ _{DG}$	$\ \nabla_d u_h + \sigma_h\ $	η_{osc}	$\ \nabla_d(u_h - S_h)\ $	η	η_{DG}	ρ_{DG}^{eff}	ρ_{DG}^{eff}
h_0	1	1.07E-00	1.09E-00	1.12E-00	5.55E-02	4.16E-01	1.25E-00	1.26E-00	1.17	1.16
$\approx h_0/2$		5.56E-01	5.61E-01	5.71E-01	7.42E-03	1.82E-01	6.07E-01	6.11E-01	1.09	1.09
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h_0	3	1.37E-02	1.37E-02	1.37E-02	3.58E-04	1.74E-03	1.41E-02	1.41E-02	1.03	1.03
$\approx h_0/2$		1.85E-03	1.85E-03	1.85E-03	1.26E-05	2.10E-04	1.88E-03	1.88E-03	1.01	1.01
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$\approx h_0/8$		2.58E-07	2.59E-07	2.58E-07	8.96E-11	2.47E-08	2.60E-07	2.60E-07	1.01	1.01
h_0	5	5.64E-05	5.64E-05	5.63E-05	1.06E-06	4.50E-06	5.75E-05	5.75E-05	1.02	1.02
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$\approx h_0/2$		5.42E-08	5.42E-08	5.42E-08	2.40E-10	4.02E-09	5.46E-08	5.46E-08	1.01	1.01
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Adaptive mesh refinement—steady case

movie

Numerics: singular case

Model problem

$$\begin{aligned} -\Delta u &= 0 & \text{in } \Omega &:= (-1, 1)^2 \setminus [0, 1]^2, \\ u &= u_D & \text{on } \partial\Omega \end{aligned}$$

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

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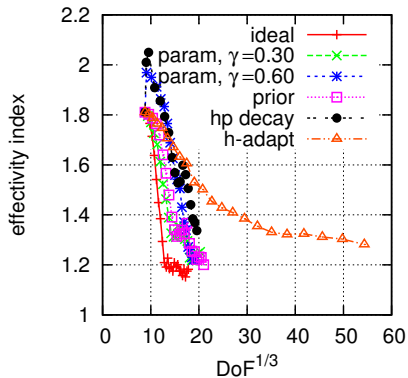
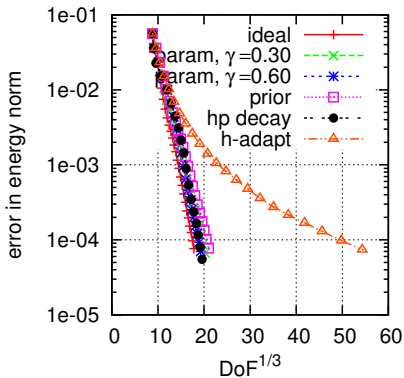
Exact solution

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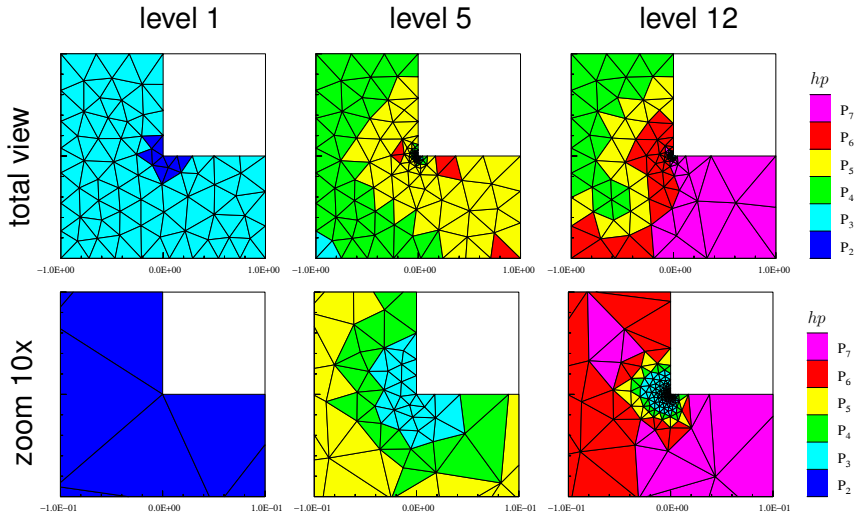
Discretization

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hp-adaptive refinement: exponential convergence



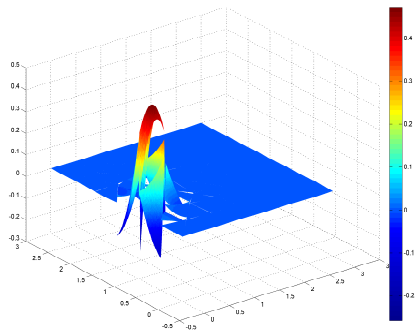
hp-refinement grids



Adaptive mesh refinement—unsteady case

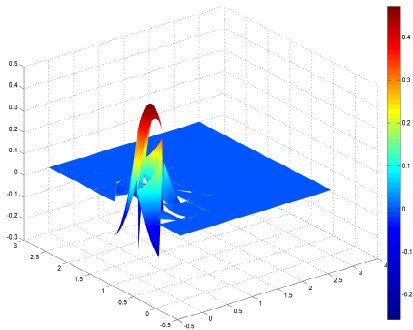
movie

Potential reconstruction

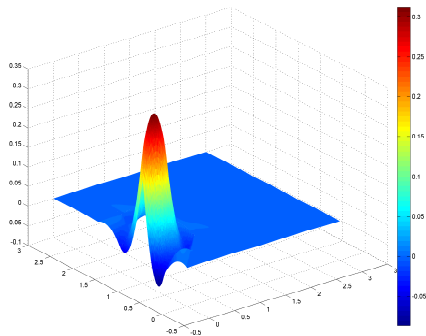


Potential u_h

Potential reconstruction

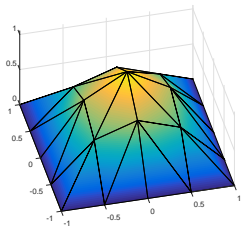


Potential u_h

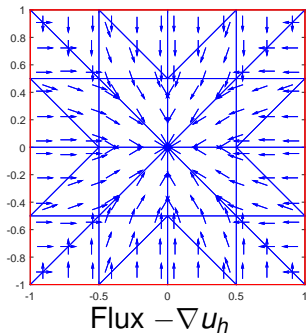
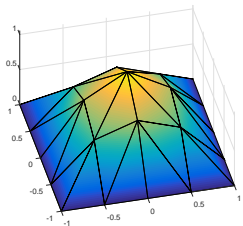


Potential reconstruction s_h

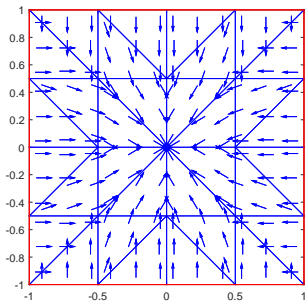
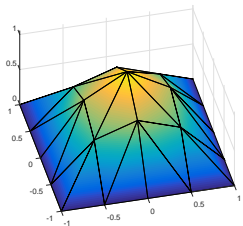
Equilibrated flux reconstruction



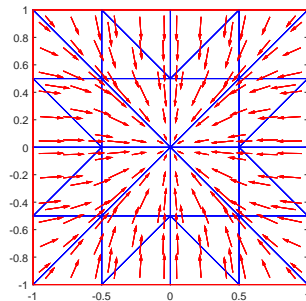
Equilibrated flux reconstruction



Equilibrated flux reconstruction



Flux $-\nabla u_h$



Flux reconstruction σ_h

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 $\mathcal{A}: \mathbb{R}^N \rightarrow \mathbb{R}^N$, vector $F \in \mathbb{R}^N$: find $U \in \mathbb{R}^N$ s.t.

$$\mathcal{A}(U) = F$$

Algorithm (Inexact iterative linearization)

- 1 Choose initial vector U^0 . Set $k := 1$.
- 2 $U^{k-1} \Rightarrow$ matrix \mathbb{A}^{k-1} and vector F^{k-1} : find U^k s.t.

$$\mathbb{A}^{k-1} U^k \approx F^{k-1}.$$
- 3
 - 1 Set $U^{k,0} := U^{k-1}$ and $i := 1$.
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Context and questions

Approximate solution

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

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**: $A(u) = f$

Question (Stopping criteria Eisenstat and Walker (1990's), Becker, Johnson, and Rannacher (1995), Deuffhard (2004 book), Arioli (2000's))

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

Question (Error Verfürth (1994), Carstensen and Klose (2003), Chaillou and Suri (2006), Kim (2007))

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

Context and questions

Approximate solution

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

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**: $A(u) = f$

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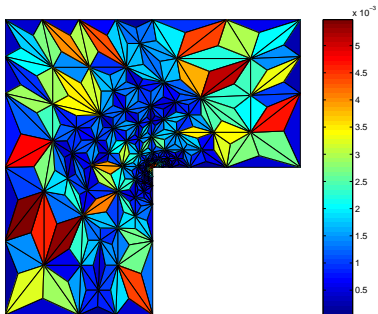
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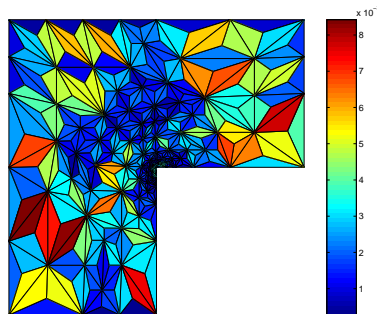
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Error distribution on an adaptively refined mesh

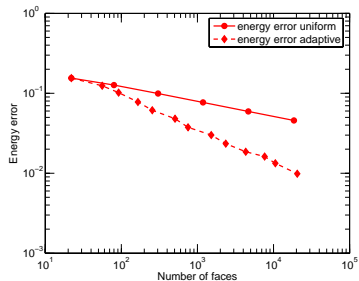


Estimated error distribution

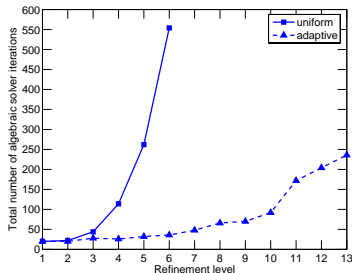


Exact error distribution

Energy error and overall performance



Energy error



Overall performance

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

Laplace eigenvalue problem

Problem

Find **eigenvector & eigenvalue pair** (u, λ) such that

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

Weak formulation

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

$$(\nabla u_i, \nabla v) = \lambda_i (u_i, v) \quad \forall v \in V.$$

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Main results (conforming setting)

Assumption (Conforming variational solution)

- $(u_{ih}, \lambda_{ih}) \in V \times \mathbb{R}^+$
- $\|u_{ih}\| = 1$
- $\|\nabla u_{ih}\|^2 = \lambda_{ih} \quad (\Rightarrow \lambda_{1h} \geq \lambda_1)$

We bound

- i -th eigenvector energy error

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

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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

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- ✓ $C_{\text{eff},i}$ only depends on mesh shape regularity and on $\lambda_i, \lambda_{i-1}, \lambda_{i+1}$
- ✓ we give computable upper bounds on $C_{\text{eff},i}$

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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

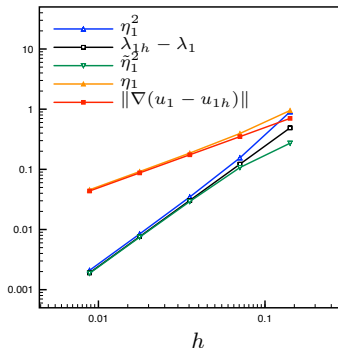
- recall $\tilde{\eta}_i^2 \leq \lambda_{ih} - \lambda_i \leq \eta_i^2$

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

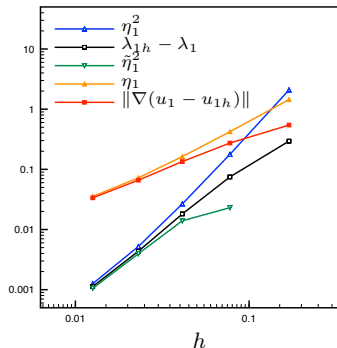
- recall $\|\nabla(u_i - u_{ih})\| \leq \eta_i$

$$l_{u, \text{eff}}^{\text{ub}} := \frac{\eta_i}{\|\nabla(u_i - u_{ih})\|}$$

Conforming finite elements



Structured meshes



Unstructured meshes

Conforming finite elements

N	h	ndof	λ_1	λ_{1h}	$\lambda_{1h} - \eta_1^2$	$\lambda_{1h} - \tilde{\eta}_1^2$	$I_{\lambda,\text{eff}}^{\text{lb}}$	$I_{\lambda,\text{eff}}^{\text{ub}}$	$E_{\lambda,\text{rel}}$	$I_{u,\text{eff}}^{\text{ub}}$
10	0.1414	121	19.7392	20.2284	19.5054	19.8667	1.35	1.48	1.84E-02	1.21
20	0.0707	441	19.7392	19.8611	19.7164	19.7486	1.08	1.19	1.63E-03	1.09
40	0.0354	1,681	19.7392	19.7696	19.7356	19.7401	1.03	1.12	2.28E-04	1.06
80	0.0177	6,561	19.7392	19.7468	19.7384	19.7393	1.02	1.10	4.56E-05	1.05
160	0.0088	25,921	19.7392	19.7411	19.7390	19.7392	1.02	1.10	1.01E-05	1.05

Structured meshes

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10	0.1698	143	19.7392	20.0336	18.8265	—	—	4.10	—	2.02
20	0.0776	523	19.7392	19.8139	19.6820	19.7682	1.63	1.77	4.37E-03	1.33
40	0.0413	1,975	19.7392	19.7573	19.7342	19.7416	1.15	1.28	3.75E-04	1.13
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Unstructured meshes

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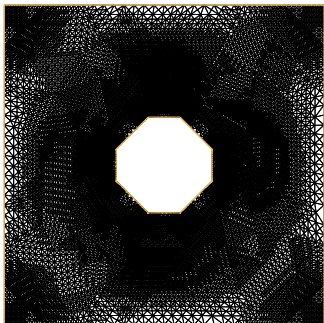
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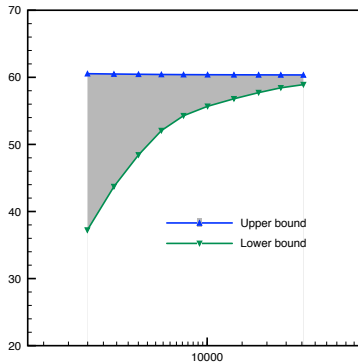
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Unstructured meshes

Domain with a hole



Adaptively refined mesh



First eigenvalue inclusion

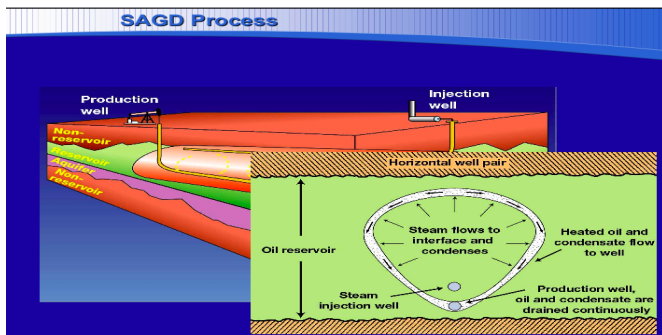
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- 2 Laplace equation: mesh adaptivity
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Oil production

Oil production

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



Reservoir

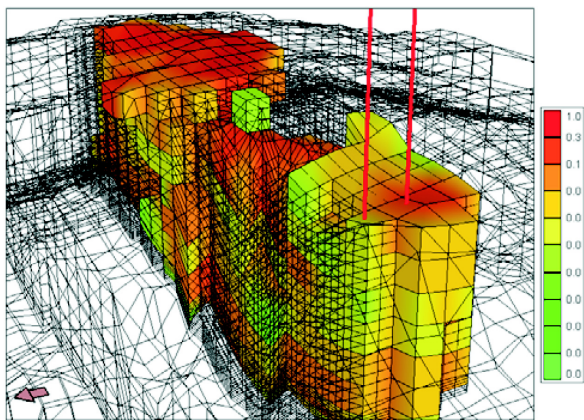
Multiphase, multi-compositional flows

Two-phase immiscible incompressible flow

$$\begin{aligned} \partial_t(\phi \mathbf{s}_\alpha) + \nabla \cdot \mathbf{u}_\alpha &= \mathbf{q}_\alpha, & \alpha \in \{\text{o}, \text{w}\}, \\ -\lambda_\alpha(\mathbf{s}_\text{w}) \underline{\mathbf{K}}(\nabla p_\alpha + \rho_\alpha \mathbf{g} \nabla z) &= \mathbf{u}_\alpha, & \alpha \in \{\text{o}, \text{w}\}, \\ \mathbf{s}_\text{o} + \mathbf{s}_\text{w} &= \mathbf{1}, \\ p_\text{o} - p_\text{w} &= p_\text{c}(\mathbf{s}_\text{w}) \end{aligned}$$

+ boundary & initial conditions

Geometry and meshes



Geometry and meshes example

Numerical difficulties

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 *time* step,
- k be the *linearization* step,
- i be the *algebraic solver* step,

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

$$\mathcal{J}_{S_w, p_w}^n(s_{w,h_T}^{n,k,i}, p_{w,h_T}^{n,k,i}) \leq \eta_{sp}^{n,k,i} + \eta_{tm}^{n,k,i} + \eta_{lin}^{n,k,i} + \eta_{alg}^{n,k,i}.$$

Error components

- $\eta_{sp}^{n,k,i}$: spatial discretization
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- only a **necessary number** of all **solver iterations**
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- only a **necessary number** of all **solver iterations**
- **“online decisions”**:
algebraic step / linearization step / space mesh refinement / time step modification

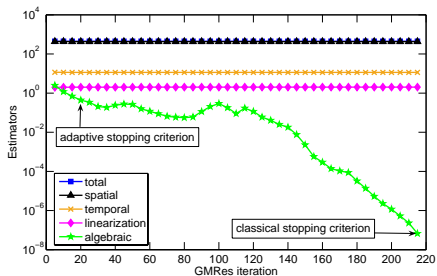
Water saturation evolution

movie

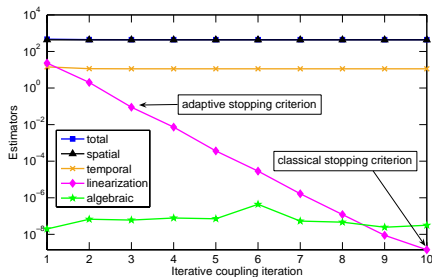
Front propagation & error estimates

movie

Estimators and stopping criteria

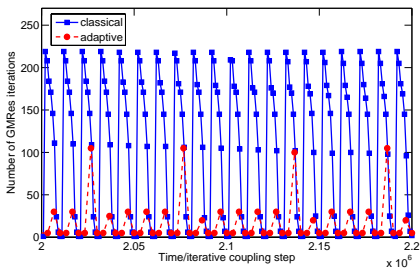


Estimators in function of GMRes iterations

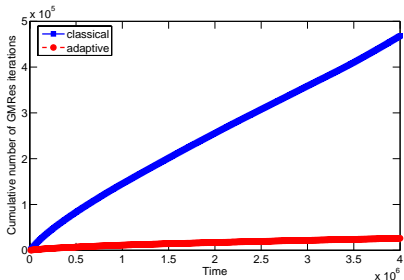


Estimators in function of iterative coupling iterations

GMRes iterations



Per time and iterative coupling step



Cumulated

Space/time/nonlinear solver/linear solver adaptivity

movie

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

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**
- rather complicated . . .

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Thank you for your attention!