Estimation d'erreur a posteriori : principe et applications

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Outline

- 1
- Introduction: a posteriori error control and adaptivity
- Laplace equation: discretization error control and mesh adaptivity
 - A posteriori error control (discretization)
 - Potential reconstruction
 - Flux reconstruction
 - Balancing error components: mesh adaptivity
- 3 Nonlinear Laplace equation: overall error control and solver adaptivity
 - A posteriori error control (overall and components)
 - Balancing error components: solver adaptivity
- 4 Reaction–diffusion equation: robustness wrt parameters
- 5 Heat equation: robustness wrt final time and space-time localization
- Helmholtz equation: asymptotic robustness
 - Conclusions

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Control the error and act adaptively: real life

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Control the error and act adaptively: real life

wandering Paris–Santiago de Compostela



Control the error and act adaptively: real life



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Control the error and act adaptively: real life



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Control the error and act adaptively: numerical simulations

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Control the error and act adaptively: numerical simulations

numerical simulation



Control the error and act adaptively: numerical simulations



numerical simulation



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Control the error and act adaptively: numerical simulations



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Numerical approximations of PDEs:

Setting

- *u*: unknown exact PDE solution
- u_h : known numerical approximation on mesh \mathcal{T}_h

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Numerical approximations of PDEs: 3 crucial questions

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- *u*: unknown exact PDE solution
- $u_h^{n,k,i}$: known numerical approximation on mesh \mathcal{T}_h , time step *n*, linearization step *k*, and linear solver step *i*

Crucial questions

• How large is the overall error between u and $u_h^{n,k,i}$?



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Numerical approximations of PDEs: **3 crucial questions &** suggested answers

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Suggested answers

 Computable a posteriori error estimates.



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Suggested answers

- Computable a posteriori error estimates.
- Identification of error components.



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Suggested answers

- Computable a posteriori error estimates.
- Identification of error components.
- Balancing error components, adaptivity (working where needed).



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A posteriori error estimates: error control

Guaranteed error upper bound (reliability) $(u_h \in \mathcal{P}_p(\mathcal{T}_h) \cap H^1_0(\Omega), p \ge 1, FEs)$



error lower bound (efficiency, $f \in \mathcal{P}_{\rho-1}(\mathcal{T}_h)$)

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

 C_{eff} a generic constant only dependent on shape regularity of T_h and thus independent of Ω, u, u_h, h, p

Laplace Nonlinear Laplace Reaction-diffusion Heat Helmholtz C Error control Potential reconstruction Flux reconstruction Mesh adaptivity A posteriori error estimates: error control Laplace equation in $\Omega \subset \mathbb{R}^d$, $d = 2, 3, f \in L^2(\Omega)$ $-\Delta \mu = f$ in Ω . $\mu = 0$ on $\partial \Omega$ Guaranteed error upper bound (reliability) $(u_h \in \mathcal{P}_p(\mathcal{T}_h) \cap H^1_0(\Omega), p \ge 1, FEs)$ $\|\nabla(u-u_h)\| \leq \eta(u_h)$ unknown error computable estimator

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Laplace Nonlinear Laplace Reaction-diffusion Heat Helmholtz C Error control Potential reconstruction Flux reconstruction Mesh adaptivity A posteriori error estimates: error control **Laplace equation** in $\Omega \subset \mathbb{R}^d$, $d = 2, 3, f \in L^2(\Omega)$ $-\Delta u = f$ in Ω . $\mu = 0$ on $\partial \Omega$ **Guaranteed error upper bound** (reliability) $(u_h \in \mathcal{P}_p(\mathcal{T}_h) \cap H_0^1(\Omega), p \ge 1, \text{FEs})$ $\underbrace{\|\nabla(u-u_h)\|}{\leq} \qquad \underbrace{\eta(u_h)}{}$ unknown error computable estimator Local error lower bound (efficiency, $f \in \mathcal{P}_{p-1}(\mathcal{T}_h)$) $\eta_{\mathsf{K}}(u_h) < C_{\mathrm{eff}} \| \nabla (u - u_h) \|_{\omega_{\mathsf{K}}} \quad \forall \mathsf{K} \in \mathcal{T}_h$ • $C_{\rm eff}$ a generic constant only dependent on shape regularity of T_h and thus independent of Ω , u, u_h , h, p• computable bound on $C_{\rm eff}$ available. $C_{\rm eff} \approx 5$

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- C_{eff} a generic constant only dependent on shape regularity of *T_h* and thus independent of Ω, *u*, *u_h*, *h*, *p*
- $\bullet\,$ computable bound on ${\it C}_{eff}$ available, ${\it C}_{eff}\approx 5$

 Prager and Synge (1947), Ladevèze (1975), Babuška & Rheinboldt (1987), Verfürth (1989), Ainsworth & Oden (1993), Destuynder & Métivet (1999), Vejchodský (2006), Braess, Pillwein, & Schöberl (2009), Ern & Vohralík (2015) **A posteriori error estimates:** error control Laplace equation in $\Omega \subset \mathbb{R}^d$, $d = 2, 3, f \in L^2(\Omega)$ $-\Delta u = f$ in Ω , u = 0 on $\partial \Omega$ **Guaranteed error upper bound** (reliability) $(u_h \in \mathcal{P}_p(\mathcal{T}_h) \cap H_0^1(\Omega), p \ge 1, FEs)$

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

Local error lower bound (efficiency, $f \in \mathcal{P}_{p-1}(\mathcal{T}_h)$)

 $\eta_{\mathbf{K}}(u_h) \leq C_{\text{eff}} \| \nabla (u - u_h) \|_{\omega_{\mathbf{K}}} \qquad \forall \mathbf{K} \in \mathcal{T}_h$

- C_{eff} a generic constant only dependent on shape regularity of *T_h* and thus independent of Ω, *u*, *u_h*, *h*, *p*
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How large is the overall error?

h	р	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\ \nabla u_h\ }$	$\ \nabla(u-u_h)\ $	rel. error $\frac{ \nabla(v-v_h) }{ \nabla v_h }$	$I^{\text{eff}} = \frac{\eta(u_h)}{\ \nabla(u-u_h)\ }$
h_0	1	1.25	28%	1.07	24%	1.17
$pprox h_0/2$	2	4.23×10^{-3}				
$\approx h_0/4$	3	2.62×10^{-1}				
$\approx h_0/8$	-4	2.60×10^{-1}				

A. Em, M. Vohralik, SIAM Journal on Numerical Analysis (2015) Dolejší, A. Em, M. Vohralik, SIAM Journal on Scientific Computing (2016)

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How large is the overall error?

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h_0	1	1.25	28%	1.07	24%	1.17
$\approx h_0/2$	2	4.23×10^{-2}	9.8 × 10 ⁻¹ 96	4.07×10^{-2}		
$\approx h_0/8$	4	2.60×10^{-7}	5.9 × 10 ⁻¹ %	2.58×10^{-7}		

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Error control Potential reconstruction Flux reconstruction Mesh adaptivity

How large is the overall error? (model pb, known smooth solution)

h	р	$\eta({m u_h})$	rel. error estimate $\frac{\eta(u_h)}{\ \nabla u_h\ }$	$\ \nabla(u-u_h)\ $	rel. error $\frac{\ \nabla(u-u_h)\ }{\ \nabla u_h\ }$	$I^{\text{eff}} = \frac{\eta(u_h)}{\ \nabla(u-u_h)\ }$
h_0	1	1.25	28%	1.07	24%	1.17
$\approx h_0/8$		1.45×10^{-1}	3.3%	1.39×10^{-1}	3.1%	
$\approx h_0/2$	2	4.23×10^{-2}	9.5×10^{-1} %	4.07×10^{-2}	9.2×10^{-1} %	
$\approx h_0/8$	-4	2.60×10^{-7}	$5.9 imes 10^{-6}$ %	2.58×10^{-4}	5.8×10^{-9}	

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$\approx h_0/4$	3	2.62×10^{-4}	5.9×10^{-3} %	2.60×10^{-4}	5.9 × 10 ⁻² %	
$pprox h_0/8$	4	2.60×10^{-7}	$5.9 imes 10^{-6}$ %	2.58×10^{-7}	5.8×10^{-9} %	

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$\approx h_0/2$	2	4.23×10^{-2}	$9.5 imes 10^{-1}$ %	4.07×10^{-2}	$9.2 imes 10^{-1}$ %	1.04
$\approx h_0/4$	3	2.62×10^{-4}	5.9×10^{-3} %	2.60×10^{-4}	$5.9 imes 10^{-3}\%$	1.01
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$\approx h_0/4$		$3.10 imes10^{-1}$	7.0%	$2.92 imes 10^{-1}$	6.6%	1.06
$\approx h_0/8$		$1.45 imes10^{-1}$	3.3%	$1.39 imes 10^{-1}$	3.1%	1.04
$\approx h_0/2$	2	$4.23 imes10^{-2}$	$9.5 imes 10^{-1}$ %	$4.07 imes 10^{-2}$	$9.2 imes10^{-1}\%$	1.04
$\approx h_0/4$	3	$2.62 imes 10^{-4}$	$5.9 imes10^{-3}\%$	$2.60 imes 10^{-4}$	$5.9 imes10^{-3}\%$	1.01
$\approx h_0/8$	4	2.60×10^{-7}	$5.9 imes 10^{-6} \%$	2.58×10^{-7}	$5.8 imes 10^{-6}\%$	1.01

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



h	<mark>ν</mark> η(υ _h)	rel. error estimate $\frac{\eta(u_h)}{\ \nabla u_h\ }$	$\ \nabla(u-u_h)\ $	rel. error $\frac{\ \nabla(u-u_h)\ }{\ \nabla u_h\ }$	$I^{\text{eff}} = \frac{\eta(u_h)}{\ \nabla(u-u_h)\ }$
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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)

Ímaia



Estimated error distribution $\eta_{\mathcal{K}}(u_h)$

Exact error distribution $\|\nabla(u - u_h)\|_{\kappa}$

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

M. Vohralík

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Theorem (Error characterization)

Let $u \in H_0^1(\Omega)$ be the weak solution and let $u_h \in H^1(\mathcal{T}_h)$ be arbitrary. Then

$$\|\nabla(u - u_h)\|^2 = \min_{\substack{\sigma \in \mathcal{H}(\operatorname{div},\Omega) \\ \nabla \cdot \sigma = f}} \|\nabla u_h + \sigma\|^2 + \min_{\substack{s \in \mathcal{H}_0^1(\Omega) \\ ||\nabla \varphi|| = 1 \\ dual norm of the residual}} + \min_{\substack{s \in \mathcal{H}_0^1(\Omega) \\ distance to \ \mathcal{H}_0^1(\Omega)}} \|\nabla(u_h - s)\|^2.$$

Comments

It is enough to choose suitable (discrete, piecewise polynomial)

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Potential reconstruction







I Laplace Nonlinear Laplace Reaction-diffusion Heat Helmholtz C Error control Potential reconstruction Flux reconstruction Mesh adaptivity



I Laplace Nonlinear Laplace Reaction-diffusion Heat Helmholtz C Error control Potential reconstruction Flux reconstruction Mesh adaptivity



Laplace Nonlinear Laplace Beaction-diffusion Heat Helmholtz C Error control Potential reconstruction Flux reconstruction Mesh adaptivity Potential reconstruction: datum $u_h \in \mathcal{P}_p(\mathcal{T}_h), p \geq 1$ For each vertex $a \in \mathcal{V}_h$, solve the local minimization problem

- cut-off by hat basis functions ψ_a
- projection of the discontinuous $\psi_a u_h$ to a conforming space
- homogeneous Dirichlet BC on $\partial \omega_{a}$: $s_{h} \in \mathcal{P}_{p+1}(\mathcal{T}_{h}) \cap H_{0}^{1}(\Omega)$

Laplace Nonlinear Laplace Beaction-diffusion Heat Helmholtz C Error control Potential reconstruction Flux reconstruction Mesh adaptivity Potential reconstruction: datum $u_h \in \mathcal{P}_p(\mathcal{T}_h), p \geq 1$ Definition (Construction of S_h Ern & V. (2015), \approx Carstensen and Merdon (2013)) For each vertex $\boldsymbol{a} \in \mathcal{V}_h$, solve the local minimization problem $s_h^{\boldsymbol{a}} := \arg \min_{\boldsymbol{v}_h \in V_h^{\boldsymbol{a}} := \mathcal{P}_{o+1}(\mathcal{T}^{\boldsymbol{a}}) \cap H_0^{\uparrow}(\omega_{\boldsymbol{a}})} \| \nabla (\psi_{\boldsymbol{a}} u_h - v_h) \|_{\omega_{\boldsymbol{a}}}$

$$(\nabla s_h^a, \nabla v_h)_{\omega_a} = (\nabla (\psi_a u_h), \nabla v_h)_{\omega_a} \qquad \forall v_h \in V_h^a.$$

Key points

- localization to patches T^a
- cut-off by hat basis functions ψ_a
- projection of the discontinuous \u03c6_au_h to a conforming space
- homogeneous Dirichlet BC on $\partial \omega_{m{a}}$: $s_h \in \mathcal{P}_{
 ho+1}(\mathcal{T}_h) \cap H^1_0(\Omega)$



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• homogeneous Dirichlet BC on $\partial \omega_{\pmb{a}}$: $\pmb{s}_h \in \mathcal{P}_{p+1}(\mathcal{T}_h) \cap H^1_0(\Omega)$

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Potential reconstruction



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Equilibrated flux reconstruction



Equilibrated flux reconstruction



Laplace Nonlinear Laplace Reaction-diffusion Heat Helmholtz C Error control Potential reconstruction Flux reconstruction Mesh adaptivity Equilibrated flux reconstruction: $-\nabla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h), p \ge 1, f \in L^2(\Omega)$ $\forall \boldsymbol{a} \in \mathcal{V}_{\boldsymbol{b}}^{\text{int}}.$

Laplace Nonlinear Laplace Beaction-diffusion Heat Helmholtz C Error control Potential reconstruction Flux reconstruction Mesh adaptivity Equilibrated flux reconstruction: $-\nabla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h), p \ge 1, f \in L^2(\Omega)$ Assumption (Orthogonality wrt hat functions) There holds $(f, \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} - (\nabla u_{\boldsymbol{h}}, \nabla \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = 0$ $\forall \boldsymbol{a} \in \mathcal{V}_{\boldsymbol{b}}^{\text{int}}.$ For each $a \in \mathcal{V}_h$, solve the local constrained minimization pb $\sigma_h^{\boldsymbol{a}} := \arg \min_{\boldsymbol{v}_h \in \boldsymbol{V}_h^{\boldsymbol{a}} = \mathcal{RT}_b(\mathcal{T}^{\boldsymbol{a}}) \cap \mathcal{H}_h(\mathrm{div},\omega_{\boldsymbol{a}})} \| \psi_{\boldsymbol{a}} \nabla u_h + \boldsymbol{v}_h \|_{\omega_{\boldsymbol{a}}}$










Error control Potential reconstruction Flux reconstruction Mesh adaptivity

Equilibrated flux reconstruction:

 $-\nabla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h), p \geq 1, f \in L^2(\Omega)$



Error control Potential reconstruction Flux reconstruction Mesh adaptivity

Equilibrated flux reconstruction: -

 $abla u_h \in \mathcal{RT}_{p-1}(\mathcal{T}_h), \, p \geq 1, \, f \in L^2(\Omega)$









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Can we decrease the error efficiently? (adaptive mesh refinement)



M. Vohralík, SIAM Journal on Numerical Analysis (2007

Singular solutions



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Estimated and actual error against the number of elements in uniformly/adaptively refined meshes (singular solutions)



Adaptive mesh refinement



Adaptive mesh refinement

$$\sum_{K\in\mathcal{T}_\ell}\eta_K(u_\ell)^2=-\eta(u_\ell)^2$$

Adaptive mesh refinement

• Dörfler marking: subset \mathcal{M}_{ℓ} containing θ -fraction of the estimates

$$\sum_{K\in \mathcal{M}_{\ell}}\eta_{K}(u_{\ell})^{2}\geq \theta^{2}\sum_{K\in \mathcal{T}_{\ell}}\eta_{K}(u_{\ell})^{2}=\theta^{2}\eta(u_{\ell})^{2}$$

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Convergence on a sequence of adaptively refined meshes

•
$$\|
abla(u-u_\ell)\| o 0$$

- some mesh elements may not be refined at all: $h \searrow 0$
- Babuška & Miller (1987), Dörfler (1996)



Adaptive mesh refinement

• Dörfler marking: subset \mathcal{M}_{ℓ} containing θ -fraction of the estimates

$$\sum_{K\in \mathcal{M}_{\ell}}\eta_K(u_{\ell})^2\geq \theta^2\sum_{K\in \mathcal{T}_{\ell}}\eta_K(u_{\ell})^2=\theta^2\eta(u_{\ell})^2$$

Optimal error decay rate wrt degrees of freedom

- $\|\nabla(u u_{\ell})\| \lesssim |\mathsf{DoF}_{\ell}|^{-p/d}$ (replaces h^p)
- same for smooth & singular solutions: higher-order only pay-off for sm. sol.
- decays to zero as fast as on a best-possible sequence of meshes
- Morin, Nochetto, Siebert (2000), Stevenson (2005, 2007), Cascón, Kreuzer, Nochetto, Siebert (2008), Canuto, Nochetto, Stevenson, Verani (2017)



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Error control Solver adaptivity

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Including algebraic error: $\mathbb{A}_{\ell} \mathbf{U}_{\ell}^{i} \neq \mathbf{F}_{\ell}$



Laplace Nonlinear Laplace Reaction-diffusion Heat Helmholtz C Error control Solver adaptivity

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I Laplace Nonlinear Laplace Reaction-diffusion Heat Helmholtz C Error control Solver adaptivity

Including algebraic error: $\mathbb{A}_{\ell} U_{\ell}^{\dagger} \neq F_{\ell}$



J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

Nonlinear pb $-\nabla \cdot \sigma(\nabla u) = f$: including linearization and algebraic error: $\mathcal{A}_{\ell}(\mathbf{U}_{\ell}^{K,i}) \neq \mathbf{F}_{\ell}, \mathbf{A}_{\ell}^{K-1}\mathbf{U}_{\ell}^{K,i} \neq \mathbf{I}_{\ell}^{K,i}$

Nonlinear pb $-\nabla \cdot \boldsymbol{\sigma}(\nabla u) = f$: including **linearization** and **algebraic** error: $\mathcal{A}_{\ell}(\mathbf{U}_{\ell}^{k,i}) \neq \mathbf{F}_{\ell}, \mathbb{A}_{\ell}^{k-1}\mathbf{U}_{\ell}^{k,i} \neq \mathbf{F}_{\ell}^{k-1}$ Nonlinear pb $-\nabla \cdot \boldsymbol{\sigma}(\nabla u) = f$: including **linearization** and **algebraic** error: $\mathcal{A}_{\ell}(\mathbf{U}_{\ell}^{k,i}) \neq \mathbf{F}_{\ell}, \mathbb{A}_{\ell}^{k-1}\mathbf{U}_{\ell}^{k,i} \neq \mathbf{F}_{\ell}^{k-1}$ I Laplace Nonlinear Laplace Reaction-diffusion Heat Helmholtz C Error control Solver adaptivity

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A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2013) Estimation d'erreur a posteriori : principe et applications 22 / 39

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Nonlinear Laplace **Beaction-diffusion Heat Helmholtz** Error control Solver adaptivity Laplace

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



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



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Solver adaptivity (nonlinear problem, inexact solvers)

Fully adaptive algorithm

• total error estimate on mesh T_{ℓ} , linearization step k, algebraic solver step i

total error discretization estimate linearization estimate



link – inexact Newton method: Bank & Rose (1982), Hackbusch & Reusken (1989), Deuflhard (1991), Eisenstat & Walker (1994)
 Convergence, optimal error decay rate wrt DoFs
 Gantner, Haberl, Praetorius, & Stiftner (2018), Heid & Wihler (2019)
 Optimal error decay rate wrt overall computational cost
 Haberl, Praetorius, Schimanko, & Vohralik (2021)

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Haberl, Praetorius, Schimanko, & Vohralík (2021)





• Gantner, Haberl, Praetorius, & Stiftner (2018), Heid & Winier (2 Optimal error decay rate wrt overall computational cost

Haberl, Praetorius, Schimanko, & Vohralík (2021)




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The reaction–diffusion equation: $f \in L^2(\Omega)$, $\varepsilon > 0$, $\kappa \ge 0$ parameters

Find $u : \Omega \to \mathbb{R}$ such that ($\varepsilon \ll \kappa$ singular perturbation)

$$-\varepsilon^2 \Delta u + \kappa^2 u = f \quad \text{in } \Omega,$$
$$u = 0 \quad \text{on } \partial \Omega$$

Guaranteed error upper bound (reliability) ($u_h \in \mathcal{P}_p(\mathcal{T}_h) \cap H_0^1(\Omega), p \ge 1$, FEs)



• $C_{\rm eff}$ a generic constant independent of Ω , u, u_h , h,



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error lower bound (efficiency, $f \in \mathcal{P}_{p-1}(\mathcal{T}_h)$)

 $\eta (u_h) \leq C_{\text{eff}} |||u - u_h||| \qquad \forall M \in \mathbb{T}$

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 $\eta_{\mathcal{A}}(u_h) \leq C_{\text{eff}} |||u - u_h||_{\text{opt}} \qquad \forall K \in \mathcal{T}_h$

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Robust local error lower bound (efficiency, $f \in \mathcal{P}_{p-1}(\mathcal{T}_h)$)

 $\eta_{K}(\boldsymbol{u}_{h}) \leq \boldsymbol{C}_{\text{eff}} \| \|\boldsymbol{u} - \boldsymbol{u}_{h} \| \|_{\omega_{K}} \qquad \forall K \in \mathcal{T}_{h}$

- C_{eff} a generic constant independent of Ω , u, u_h , h,

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 $|||u-u_h||| \leq \eta(u_h)$



Robust local error lower bound (efficiency, $f \in \mathcal{P}_{p-1}(\mathcal{T}_h)$)

 $\eta_{\mathsf{K}}(\boldsymbol{u}_h) \leq \boldsymbol{C}_{\mathsf{eff}} \| \|\boldsymbol{u} - \boldsymbol{u}_h \| \|_{\omega_{\mathsf{K}}} \qquad \forall \mathsf{K} \in \mathcal{T}_h$

• $C_{\rm eff}$ a generic constant independent of Ω , u, u_h , h, κ , ε

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The reaction–diffusion equation: $f \in L^2(\Omega)$, $\varepsilon > 0$, $\kappa \ge 0$ parameters

Find $u : \Omega \to \mathbb{R}$ such that ($\varepsilon \ll \kappa$ singular perturbation)

$$-\varepsilon^2 \Delta u + \kappa^2 u = f \quad \text{in } \Omega,$$
$$u = 0 \quad \text{on } \partial \Omega$$

Guaranteed error upper bound (reliability) $(u_h \in \mathcal{P}_p(\mathcal{T}_h) \cap H_0^1(\Omega), p \ge 1, \text{FEs})$

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Equilibrated flux and potential reconstructions

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For each vertex $\boldsymbol{a} \in \mathcal{V}$, let

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- $J^{\boldsymbol{a}}_{\boldsymbol{u}_h}(\boldsymbol{v}_h, q_h) := \boldsymbol{w}^2_{\boldsymbol{a}} \| \varepsilon \psi_{\boldsymbol{a}} \nabla u_h + \varepsilon^{-1} \boldsymbol{v}_h \|^2_{\boldsymbol{\omega}_{\boldsymbol{a}}} + \| \kappa \left[\Pi_h(\psi_{\boldsymbol{a}} u_h) q_h \right] \|^2_{\boldsymbol{\omega}_{\boldsymbol{a}}}$

Comments

- local discrete constrained minimization problems
- choose the locally best-possible estimators
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Ínría Este de Prets

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Boundary layer, solution $u(x, y) = e^{-\frac{\kappa}{\varepsilon}x} + e^{-\frac{\kappa}{\varepsilon}y}$, p = 2



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Outline

- Introduction: a posteriori error control and adaptivity
- 2 Laplace equation: discretization error control and mesh adaptivity
 - A posteriori error control (discretization)
 - Potential reconstruction
 - Flux reconstruction
 - Balancing error components: mesh adaptivity
- 3 Nonlinear Laplace equation: overall error control and solver adaptivity
 - A posteriori error control (overall and components)
 - Balancing error components: solver adaptivity
- 4 Reaction–diffusion equation: robustness wrt parameters
- 5 Heat equation: robustness wrt final time and space-time localization
- 6 Helmholtz equation: asymptotic robustness
 - Conclusions

The heat equation $(f \in L^2(0, T; L^2(\Omega)), u_0 \in L^2(\Omega))$

The heat equation

$$\partial_t u - \Delta u = f$$
 in $\Omega \times (0, T)$,
 $u = 0$ on $\partial \Omega \times (0, T)$,
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Spaces

$$\begin{split} & \mathcal{X} \coloneqq L^2(0, T; H^1_0(\Omega)), \|v\|_X^2 \coloneqq \int_0^T \|\nabla v\|^2 \, \mathrm{d}t, \\ & \mathcal{Y} \coloneqq L^2(0, T; H^1_0(\Omega)) \cap H^1(0, T; H^{-1}(\Omega)), \|v\|_Y^2 \coloneqq \int_0^T \|\partial_t v\|_{H^{-1}(\Omega)}^2 + \|\nabla v\|^2 \, \mathrm{d}t + \|v(T)\|^2 \, \mathrm{d}t \end{split}$$

Y norm error is the dual X norm of the residual + initial condition error

$$\|u - u_{h\tau}\|_{Y}^{2} = \sup_{v \in X, \, \|v\|_{X} = 1} \left[\int_{0}^{T} (f, v) - \langle \partial_{t} u_{h\tau}, v \rangle - (\nabla u_{h\tau}, \nabla v) \, \mathrm{d}t \right]^{2} + \|u_{0} - u_{h\tau}(0)\|^{2}$$

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 $\partial_t u - \Delta u = f$ in $\Omega \times (0, T)$, u = 0 on $\partial \Omega \times (0, T)$, $u(0) = u_0$ in Ω

Guaranteed error upper bound (reliability) ($u_{h\tau}$ FE in space, DG in time approx.)

 $\underbrace{\||\boldsymbol{u} - \boldsymbol{u}_{h\tau}||}_{\text{unknown error}} \leq \underbrace{\eta(\boldsymbol{u}_{h\tau})}_{\text{computable estimator}}$

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Robust local in space and in time error lower bound (efficiency)

 $\eta_{\mathcal{K}, l_n}(u_{h\tau}) \leq \frac{C_{\text{eff}}}{\|u - u_{h\tau}\|}_{\omega_{\mathcal{K}} \times l_n}$

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 Verfürth (2003), Bergam, Bernardi, and Mghazli (2005), Makridakis and Nochetto (2005), Em and Vohralik (2010), Em, Smears, and Vohralik (2017)

The heat equation $(f \in L^2(0, T; L^2(\Omega)), u_0 \in L^2(\Omega))$

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 $\partial_t u - \Delta u = f$ in $\Omega \times (0, T)$, u = 0 on $\partial \Omega \times (0, T)$, $u(0) = u_0$ in Ω

Guaranteed error upper bound (reliability) ($u_{h\tau}$ FE in space, DG in time approx.)

 $\underbrace{\||u - u_{h\tau}||}_{\text{unknown error}} \leq \underbrace{\eta(u_{h\tau})}_{\text{computable estimator}}$

Robust local in space and in time error lower bound (efficiency)

 $\eta_{\mathcal{K},l_n}(\boldsymbol{u}_{\boldsymbol{h}\tau}) \leq \boldsymbol{C}_{\text{eff}} \| \boldsymbol{u} - \boldsymbol{u}_{\boldsymbol{h}\tau} \|_{\omega_{\mathcal{K}} \times l_n}$

• C_{eff} a generic constant independent of Ω , u, $u_{h\tau}$, h, p, τ , q, T

 Verfürth (2003), Bergam, Bernardi, and Mghazli (2005), Makridakis and Nochetto (2006), Ern and Vohralík (2010), Ern, Smears, and Vohralík (2017)

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The heat equation $(f \in L^2(0, T; L^2(\Omega)), u_0 \in L^2(\Omega))$

The heat equation

 $\begin{aligned} \partial_t u - \Delta u &= f \quad \text{in } \Omega \times (0, T), \\ u &= 0 \quad \text{on } \partial \Omega \times (0, T), \\ u(0) &= u_0 \quad \text{in } \Omega \end{aligned}$

Guaranteed error upper bound (reliability) ($u_{h\tau}$ FE in space, DG in time approx.)

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Robust local in space and in time error lower bound (efficiency)

 $\eta_{\mathbf{K},\mathbf{I}_{n}}(u_{h\tau}) \leq \mathbf{C}_{\text{eff}} \| || u - u_{h\tau} |||_{\omega_{\mathbf{K}} \times \mathbf{I}_{n}}$

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Equilibrated flux reconstruction

Definition (Equilibrated flux reconstruction)

For each time-step interval I_n and for each vertex $\mathbf{a} \in \mathcal{V}^n$, let

$$\sigma_{h_{\mathcal{T}}}^{\boldsymbol{a},n} \coloneqq \arg \min_{\substack{\boldsymbol{v}_h \in \boldsymbol{V}_{h_{\mathcal{T}}}^{\boldsymbol{a},n} \\ \nabla \cdot \boldsymbol{v}_h = \psi_{\boldsymbol{a}}(f - \partial_t \mathcal{I} \boldsymbol{u}_{h_{\mathcal{T}}}) - \nabla \psi_{\boldsymbol{a}} \cdot \nabla u_{h_{\mathcal{T}}}} \int_{I_n} \|\boldsymbol{v}_h + \psi_{\boldsymbol{a}} \nabla u_{h_{\mathcal{T}}}\|_{\omega_{\boldsymbol{a}}}^2 \, \mathrm{d}t.$$

Then set

$${\pmb\sigma}_{h au}\coloneqq \sum_{n=1}^N\sum_{{\pmb a}\in {\mathcal V}^n}{\pmb\sigma}_{h au}^{{\pmb a},n}.$$

Comments

- satisfies $\sigma_{h au} \in L^2(0, T; H(\operatorname{div}, \Omega))$ with $abla \cdot \sigma_{h au} = f \partial_t \mathcal{I} u_{h au}$
- a priori a local space-time problem, $V_{h\tau}^{a,n} \coloneqq Q_q(I_n; V_h^{a,n})$
- uncouples to q elliptic problems posed in V^a_b



M. Vohralík

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$$\boldsymbol{\sigma}_{h\tau} \coloneqq \sum_{n=1}^{N} \sum_{\boldsymbol{a} \in \mathcal{V}^n} \boldsymbol{\sigma}_{h\tau}^{\boldsymbol{a},n}.$$

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- uncouples to q elliptic problems posed in $V_h^{a,n}$
Geological sequestration of CO₂, CO₂ saturation



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

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Geological sequestration of CO₂, overall a posteriori estimate



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

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Geological sequestration of CO₂, full adaptivity



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

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Outline

- Introduction: a posteriori error control and adaptivity
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- 6 Heat equation: robustness wrt final time and space-time localization
- 6 Helmholtz equation: asymptotic robustness





The Helmholtz equation: $f \in L^2(\Omega)$, $\varepsilon > 0$, $\kappa \ge 0$ parameters

Find $u: \Omega \to \mathbb{C}$ such that $(\varepsilon \leq \kappa)$

$$-\varepsilon^2 \Delta u - \kappa^2 u = f \quad \text{in } \Omega,$$
$$u = 0 \quad \text{on } \partial \Omega$$

Guaranteed error upper bound (reliability) ($u_h \in \mathcal{P}_p(\mathcal{T}_h) \cap H^1_0(\Omega), p \ge 1$, FEs)

error lower bound (efficiency, $f \in \mathcal{P}_{p-1}(\mathcal{T}_h))$

 $\eta (U_h) \leq C_{\text{eff}} ||| U - U_h |||$

• C_{eff} a generic constant independent of Ω , u, u_h , h,

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The Helmholtz equation: $f \in L^2(\Omega)$, $\varepsilon > 0$, $\kappa \ge 0$ parameters

Find $u : \Omega \to \mathbb{C}$ such that $(\varepsilon \leq \kappa)$

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Guaranteed error upper bound (reliability) ($u_h \in \mathcal{P}_p(\mathcal{T}_h) \cap H_0^1(\Omega), p \ge 1$, FEs)

 $\underbrace{\||\boldsymbol{u} - \boldsymbol{u}_h||}_{\text{unknown error}} \leq \underbrace{\eta(\boldsymbol{u}_h)}_{\text{computable estimator}}$

error lower bound (efficiency, $f \in \mathcal{P}_{p-1}(\mathcal{T}_h)$)

 $\eta (u_h) \leq C_{\text{eff}} ||| u - u_h ||| \qquad \forall M \in \mathbb{T}_h$

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Guaranteed error upper bound (reliability) $(u_h \in \mathcal{P}_p(\mathcal{T}_h) \cap H_0^1(\Omega), p \ge 1, \text{FEs})$

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

local error lower bound (efficiency, $f\in\mathcal{P}_{p-1}(\mathcal{T}_h)$)

 $\eta_{\mathbb{K}}(u_h) \leq C_{ ext{eff}} \| u - u_h \|_{ ext{order}} \quad orall K \in \mathcal{T}_h$

• C_{eff} a generic constant independent of Ω , u, u_h , h,

Babulka, Manburg, & Strouboulla (1997), Dörlar & Sautar (2013), Sautar & Zach (2015), Chaumont-Freiat, Ern, & Vohralik (2021)

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

Asymptotically robust local error lower bound (efficiency, $f \in \mathcal{P}_{p-1}(\mathcal{T}_h)$)

 $\eta_{\mathsf{K}}(u_h) \leq \frac{\mathcal{O}_{\mathrm{eff}}}{\|u - u_h\|}_{\omega_{\mathsf{K}}} \qquad \forall \mathsf{K} \in \mathcal{T}_h$

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 $\eta_{\mathsf{K}}(u_h) \leq C_{\mathrm{eff}} ||| u - u_h |||_{\omega_{\mathsf{K}}} \qquad \forall \mathsf{K} \in \mathcal{T}_h$

• C_{eff} a generic constant independent of Ω , u, u_h , h, κ , ε if $\frac{\kappa h}{\epsilon_0} \leq 1$

 Babuška, Ihlenburg, & Strouboulis (1997), Dörfler & Sauter (2013), Sauter & Zech (2015), Chaumont-Frelet, Ern, & Vohralik (2021)

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Plane wave, p = 1 and $\kappa = \pi$



$$\begin{split} \boldsymbol{\mathcal{E}}_{\text{fem}} &:= \| \| \boldsymbol{e}_h \| \|_{\kappa,\Omega} \\ \boldsymbol{\mathcal{E}}_{\text{est}} &:= \eta \\ \widetilde{\boldsymbol{\mathcal{E}}}_{\text{est}} &:= (1 + C_{\text{ap}})\eta \end{split}$$

Plane wave, p = 1 and $\kappa = 10\pi$



$$egin{aligned} & \mathcal{E}_{ ext{fem}} := \|\|oldsymbol{ heta}_{\hbar}\|\|_{\kappa,\Omega} \ & \mathcal{E}_{ ext{est}} := \eta \ & \widetilde{\mathcal{E}}_{ ext{est}} := (1+C_{ ext{ap}})\eta \end{aligned}$$

Plane wave, p = 4 and $\kappa = 10\pi$



$$egin{aligned} & \mathcal{E}_{ ext{fem}} := \| |oldsymbol{e}_{\hbar} \| |_{\kappa,\Omega} \ & \mathcal{E}_{ ext{est}} := \eta \ & \widetilde{\mathcal{E}}_{ ext{est}} := (1+C_{ ext{ap}})\eta \end{aligned}$$

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Plane wave, p = 4 and $\kappa = 60\pi$



 $egin{aligned} & m{E}_{ ext{fem}} := \|\|m{e}_{\hbar}\|\|_{\kappa,\Omega} \ & m{E}_{ ext{est}} := \eta \ & \widetilde{E}_{ ext{est}} := (1+C_{ ext{ap}})\eta \end{aligned}$

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Estimation d'erreur a posteriori : principe et applications 37 / 39

Scattering by an non-trapping obstacle



Estimator $\eta_{\mathcal{K}}$ (left) and elementwise error $\||\boldsymbol{e}_h||_{\kappa,\mathcal{K}}$ (right)



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• a posteriori error control



M. Vohralík

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 a posteriori error control adaptivity: space mesh, time step,



 a posteriori overall error control adaptivity: space mesh, time step,



- a posteriori overall error control
- full adaptivity: space mesh, time step, linear solver, nonlinear solver, regularization, model,



- a posteriori overall error control
- full adaptivity: space mesh, time step, linear solver, nonlinear solver, regularization, model, polynomial degree



- a posteriori overall error control
- full adaptivity: space mesh, time step, linear solver, nonlinear solver, regularization, model, polynomial degree
- recovering mass balance in any situation

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Thank you for your attention!



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Outline

Motivation

• Polynomial-degree (p) adaptivity



CDG Terminal 2E collapse in 2004 (opened in 2003)



no earthquake, flooding, tsunami, heavy rain, extreme temperature
deterministic, steady problem, PDE known, data known, implementation OK



CDG Terminal 2E collapse in 2004 (opened in 2003)



- no earthquake, flooding, tsunami, heavy rain, extreme temperature
- deterministic, steady problem, PDE known, data known, implementation OK



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probably numerical simulations done with insufficient precision,

Case Studies in Engineering Failure Analysis 3 (2015) 88-92



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

Y. El Kamari^a, W. Raphael^{a,*}, A. Chateauneur^{El,c} *Coli Softward Righters de Reynouth (CER), Université Sater Joseph, CET Mar Rooker, PO Roc 11-514, Rood II Sath Beine 11672820, Johann Ínría Lestos Preta

M. Vohralík

Estimation d'erreur a posteriori : principe et applications 40 / 39

CDG Terminal 2E collapse in 2004 (opened in 2003)



no earthquake, flooding, tsunami, heavy rain, extreme temperature

• deterministic, steady problem, PDE known, data known, implementation OK

probably numerical simulations done with insufficient precision, I believe without error control

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M. Vohralík

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Outline

Motivation

• Polynomial-degree (p) adaptivity



Best-possible error decrease: hp adaptivity, (smooth solution)



Mesh \mathcal{T}_{ℓ} and pol. degrees p_{K}

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Ap

Best-possible error decrease: *hp* adaptivity, (smooth solution)





Exact solution

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Mesh \mathcal{T}_{ℓ} and pol. degrees $p_{\mathcal{K}}$

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Best-possible error decrease: *hp* adaptivity, (singular solution)



Mesh \mathcal{T}_{ℓ} and polynomial degrees p_K

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Appl



M. Vohralík

Best-possible error decrease: hp adaptivity, (singular solution)



M. Vohralík

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Parti Pe