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Adaptive BEM with inexact PCG solver yields almost optimal computational costs

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joint work with

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Introduction

Overall aim

- compute $\phi_h \approx \phi^\star$ with $|||\, \phi^\star - \phi_h \,||| \le$ tolerance
- subject to minimal computational costs

- out of reach at the moment
- but clearly requires
  - adaptivity — to resolve singularities
  - effective solver — to avoid unnecessary costs
  - matrix compression — in particular for dense BEM matrices

Tasks / Questions / Outline

- design adaptive algorithm which also steers (iterative) solver?
- convergence of adaptive strategy?
- optimal convergence rate w.r.t. degrees of freedom?
- new: optimal convergence rate w.r.t. computational work / time?
  - at least for standard FEM / BEM

Dahmen, Harbrecht, Schneider: Math. Comp. 76 (2007)
Gantner, Haberl, Praetorius, Stiftner: IMA J. Numer. Anal. 38 (2018) [open access]
Führer, Haberl, Praetorius, Schimanko: Numer. Math. 141 (2019) [open access]

Optimal computational costs?

$$\|\phi^\star\|_{\mathbb{A}_s} := \sup_{N>0} \Big(N^s \min_{\mathcal{T}_{\rm opt}\in\mathbb{T}_N} \big[\, |\!|\!| \, \phi^\star - \phi^\star_{\rm opt} \, |\!|\!| + \eta_{\rm opt}(\phi^\star_{\rm opt}) \, \big] \Big)$$

$$\simeq \sup_{\ell\in\mathbb{N}_0} (\#\mathcal{T}_\ell)^s \big[\, |\!|\!| \, \phi^\star - \phi^\star_\ell \, |\!|\!| + \eta_\ell(\phi^\star_\ell) \, \big]$$

$$\simeq \sup_{(\ell,n)\in\mathcal{Q}} (\#\mathcal{T}_\ell)^s \big[\, |\!|\!| \, \phi^\star - \phi^n_\ell \, |\!|\!| + \eta_\ell(\phi^n_\ell) \, \big]$$

$$\simeq \sup_{(\ell,n)\in\mathcal{Q}} \Big(\sum_{\substack{(\ell',n')\in\mathcal{Q} \\ (\ell',n')\le(\ell,n)}} \#\mathcal{T}_{\ell'} \Big)^s \big[\, |\!|\!| \, \phi^\star - \phi^n_\ell \, |\!|\!| + \eta_\ell(\phi^n_\ell) \, \big]$$

- goal: thorough proof of these equivalences for adaptive algorithm!
- but: out of reach for standard BEM with dense matrices

Almost optimal computational costs!

optimal

$$\|\phi^\star\|_{\mathbb{A}_s} := \sup_{N>0} \Big(N^s \min_{\mathcal{T}_{\rm opt}\in\mathbb{T}_N} \big[\,|\!|\!|\, \phi^\star - \phi^\star_{\rm opt} \,|\!|\!|\, + \eta_{\rm opt}(\phi^\star_{\rm opt}) \big] \Big)$$

$$\simeq \sup_{(\ell,n)\in\mathcal{Q}} \Big(\sum_{\substack{(\ell',n')\in\mathcal{Q}\\(\ell',n')\le(\ell,n)}} \#\mathcal{T}_{\ell'} \Big)^s \big[\,|\!|\!|\, \phi^\star - \phi^n_\ell \,|\!|\!|\, + \eta_\ell(\phi^n_\ell) \big]$$

almost optimal

$$\|\phi^\star\|_{\mathbb{A}_s} := \sup_{N>0} \Big(N^s \min_{\mathcal{T}_{\rm opt}\in\mathbb{T}_N} \big[\,|\!|\!|\, \phi^\star - \phi^\star_{\rm opt} \,|\!|\!|\, + \eta_{\rm opt}(\phi^\star_{\rm opt}) \big] \Big) < \infty$$

$$\Longrightarrow \sup_{(\ell,n)\in\mathcal{Q}} \Big(\sum_{\substack{(\ell',n')\in\mathcal{Q}\\(\ell',n')\le(\ell,n)}} \#\mathcal{T}_{\ell'} \Big)^{s-\varepsilon} \big[\,|\!|\!|\, \phi^\star - \phi^n_\ell \,|\!|\!|\, + \eta_\ell(\phi^n_\ell) \big] < \infty \qquad \forall \varepsilon > 0$$

Gantner, Haberl, Praetorius, Stiftner: IMA J. Numer. Anal. 38 (2018) [open access]

BEM Model Problem

Weakly-singular integral equation

- $\Omega \subset \mathbb{R}^d, \quad d = 2, 3$
- $\Gamma := \partial\Omega$
- $[V\phi](x) = \int_\Gamma G(x-y)\phi(y)\,\mathrm{d}\Gamma(y),$ e.g., $G(z) = -\frac{1}{2\pi}\log|z|$

Given $f \in H^{1/2}(\Gamma)$, find $\phi^\star \in H^{-1/2}(\Gamma)$ s.t.

- $\langle V\phi^\star\,,\,\psi\rangle = \langle f\,,\,\psi\rangle$ for all $\psi \in H^{-1/2}(\Gamma)$

- Lax–Milgram $\Longrightarrow$ existence & uniqueness

Find $\phi_h^\star \in \mathcal{P}^0(\mathcal{T}_h)$ s.t.

- $\langle V\phi_h^\star \, , \, \psi_h \rangle = \langle f \, , \, \psi_h \rangle$ for all $\psi_h \in \mathcal{P}^0(\mathcal{T}_h)$

- $f - V\phi_h^\star = V(\phi^\star - \phi_h^\star) \in H^{1/2}(\Gamma)$
- $V(\phi^\star - \phi_h^\star) \perp \mathcal{P}^0(\mathcal{T}_h)$

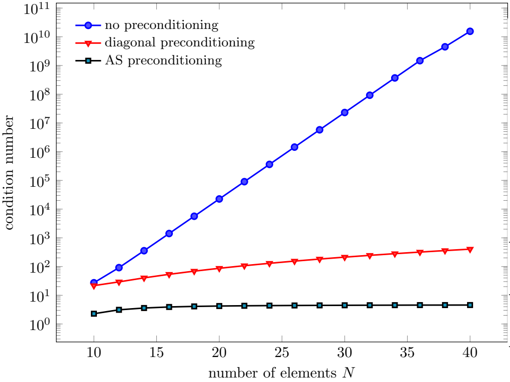
$$\Longrightarrow \quad |\!|\!| \, \phi^\star - \phi_h^\star \, |\!|\!| \simeq \|f - V\phi_h^\star\|_{H^{1/2}} \lesssim \|h^{1/2}\nabla(f - V\phi_h^\star)\|_{L^2} =: \eta_h(\phi_h^\star)$$

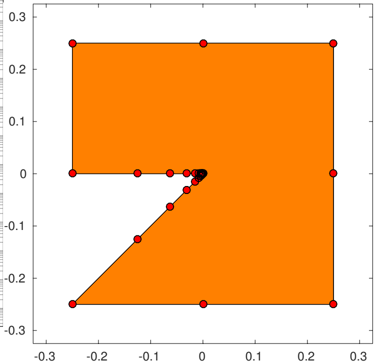
- $\eta_h(T, \psi_h) := \mathrm{diam}(T)^{1/2} \, \|\nabla(f - V\psi_h)\|_{L^2(T)}$

Carstensen, Maischak, Stephan: Numer. Math. 90 (2001)

PCG solver

Preconditioning?!





- no-preconditiong $\implies$ $\mathrm{cond}(\boldsymbol{A}) \simeq (h_{\max}/h_{\min})^d \, N^{1/(d-1)}$
- diagonal preconditioning $\implies$ $\mathrm{cond}(\boldsymbol{D}^{-1}\boldsymbol{A}) \simeq N^{1/(d-1)}$
- local multilevel additive Schwarz $\implies$ $\mathrm{cond}(\boldsymbol{P}^{-1}\boldsymbol{A}) \simeq 1$

Graham, McLean: SIAM J. Numer. Anal. 44 (2006)
Führer, Haberl, Praetorius, Schimanko: Numer. Math. 141 (2019) [open access]

PCG solver

book]Golub, Van Loan: John Hopkins University Press, 2013 (fourth edition)

- applies for $\boldsymbol{A}$ being SPD with SPD preconditioner $\boldsymbol{P}$

- PCG is an energy method!
  - implicitly standard CG for SPD matrix $\boldsymbol{P}^{-1/2}\boldsymbol{A}\boldsymbol{P}^{-1/2}$

- suppose: $\mathrm{cond}(\boldsymbol{P}^{-1}\boldsymbol{A}) \le C$

$\Longrightarrow$ classical: $\|\!|\, \phi_\ell^\star - \phi_\ell^n \,|\!\|\le 2\left[\frac{\sqrt{C}-1}{\sqrt{C}+1}\right]^n \|\!|\, \phi_\ell^\star - \phi_\ell^0 \,|\!\|$ a-priori

$\Longrightarrow$ less known: $\|\!|\, \phi_\ell^\star - \phi_\ell^n \,|\!\| \le \frac{C-1}{C} \|\!|\, \phi_\ell^\star - \phi_\ell^{n-1} \,|\!\|$

$\Longrightarrow$ $\|\!|\, \phi_\ell^\star - \phi_\ell^n \,|\!\| \lesssim \|\!|\, \phi_\ell^n - \phi_\ell^{n-1} \,|\!\|$ a-posteriori

Adaptive Algorithm

A-posteriori error control

- $\| \phi^\star - \phi_\ell^n \| \le \| \phi^\star - \phi_\ell^\star \| + \| \phi_\ell^\star - \phi_\ell^n \|$
- estimator: $\| \phi^\star - \phi_\ell^\star \| \lesssim \eta_\ell(\phi_\ell^\star) \lesssim \eta_\ell(\phi_\ell^n) + \| \phi_\ell^\star - \phi_\ell^n \|$
- PCG: $\| \phi_\ell^\star - \phi_\ell^n \| \lesssim \| \phi_\ell^n - \phi_\ell^{n-1} \|$

$$\Longrightarrow \quad \big[\| \phi^\star - \phi_\ell^n \| + \eta_\ell(\phi_\ell^n) \big] \lesssim \eta_\ell(\phi_\ell^n) + \| \phi_\ell^n - \phi_\ell^{n-1} \|$$

- adaptive algorithm should equilibrate RHS

Aurada, Feischl, Führer, Karkulik, Melenk, Praetorius: Math. Comp. 86 (2017)

Adaptive algorithm

- initial mesh $\mathcal{T}_0$ with initial guess $\phi_0^0 := 0$
- adaptivity parameters $0 < \theta \le 1$ and $\lambda > 0$

For all $\ell = 0, 1, 2, \dots$, iterate:

1. REPEAT for $n = 1, 2, 3, \dots$
   - do one PCG step to obtain ϕ_ℓ^n from ϕ_ℓ^{n-1}
   - compute $\eta_\ell(T, \phi_\ell^n) = \mathrm{diam}(T)^{1/2} \, \|\nabla(f - V\phi_\ell^n)\|_{L^2(T)}$ for all $T \in \mathcal{T}_\ell$

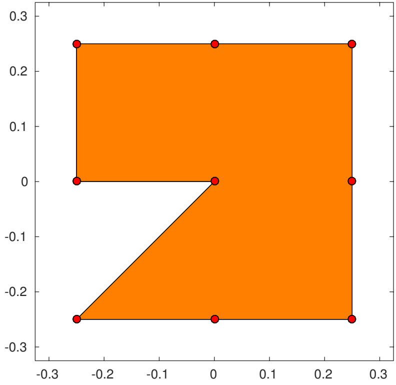
   UNTIL $\|\!| \phi_\ell^n - \phi_\ell^{n-1} |\!\| \le \lambda \, \eta_\ell(\phi_\ell^n)$
2. find (essentially minimal) set $\mathcal{M}_\ell \subseteq \mathcal{T}_\ell$ s.t.

$$\theta \sum_{T \in \mathcal{T}_\ell} \eta_\ell(T, \phi_\ell^n)^2 \le \sum_{T \in \mathcal{M}_\ell} \eta_\ell(T, \phi_\ell^n)^2$$

3. refine (at least) all $T \in \mathcal{M}_\ell$ to obtain $\mathcal{T}_{\ell+1} = \mathrm{refine}(\mathcal{T}_\ell, \mathcal{M}_\ell)$
4. define $\underline{n} := \underline{n}(\ell)$ and $\phi_{\ell+1}^0 := \phi_\ell^{\underline{n}}$ (nested iteration)

2D Experiment

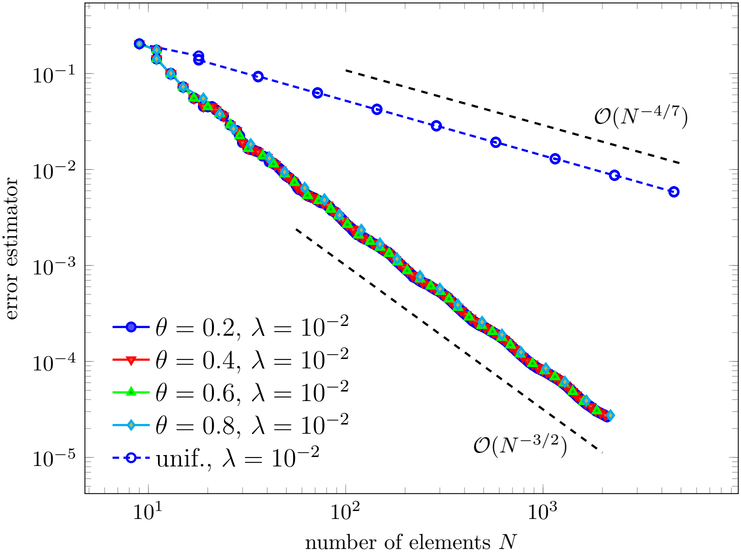
Dirichlet problem on Z-shaped domain



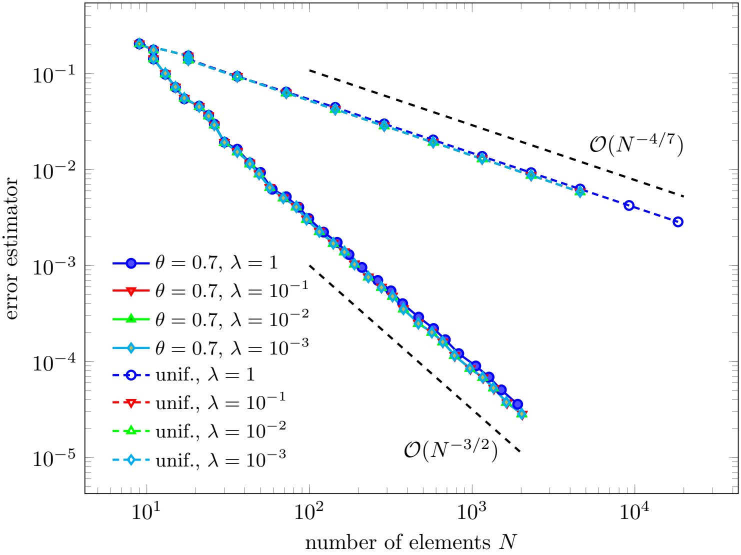
$$\begin{aligned} -\Delta u &= 0 \quad \text{in } \Omega \\ u &= g \quad \text{on } \Gamma \end{aligned} \quad \Longleftrightarrow \quad V\phi = (K + 1/2)g \quad \text{on } \Gamma$$

- prescribed singular solution $u(x) = r^{4/7}\cos(4\xi/7)$ in polar coordinates

Dependence on θ for $\lambda = 10^{-2}$



Dependence on λ for $\theta = 0.7$



Number of PCG iterations

- question: How many PCG iterations necessary?

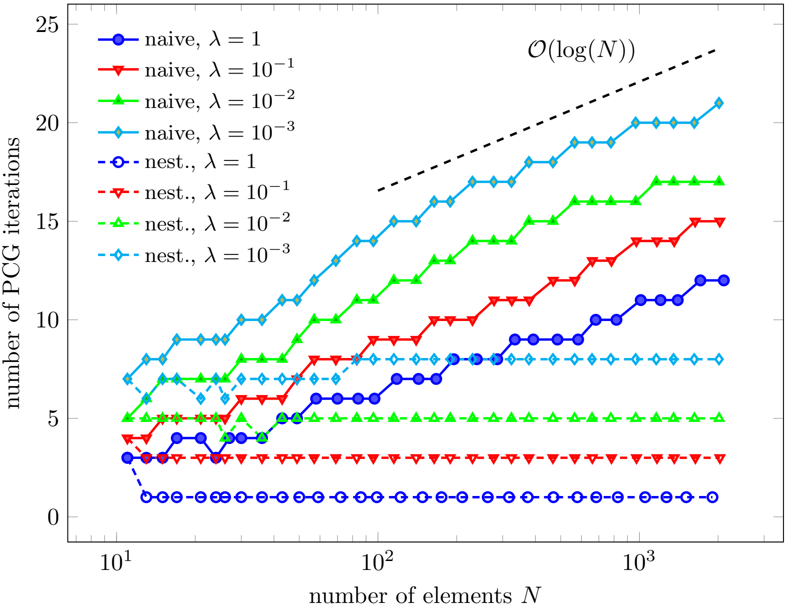
Proposition (Gantner, Haberl, P., Stiftner '18)

- given $0 < \theta \leq 1, \quad \lambda > 0$
- $\underline{n}(\ell) \leq C + C' \log\Big(\max\Big\{1, \frac{\eta_{\ell-1}(\phi_{\ell-1}^{\underline{n}})}{\eta_\ell(\phi_\ell^{\underline{n}})}\Big\}\Big)$

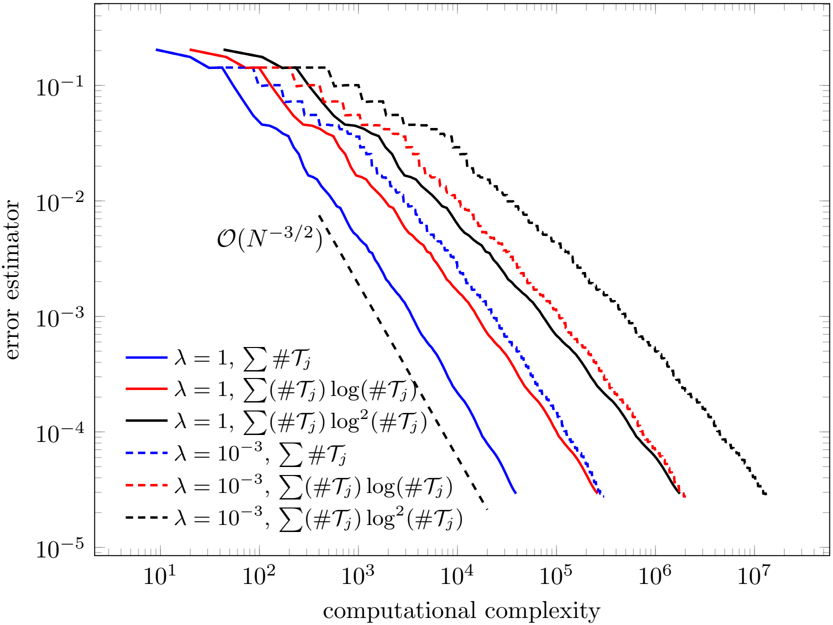
- follows from elementary calculations and nested iteration
- generically: constant number of PCG iterations!

Gantner, Haberl, Praetorius, Stiftner: IMA J. Numer. Anal. 38 (2018) [open access]

Number of PCG iterations ($\theta = 0.4$)



Computational costs



Axioms of Adaptivity

(A1) stability on non-refined elements

- $\exists C_{\rm stb} > 0 \quad \forall \mathcal{T}_H \quad \forall \mathcal{T}_h \in \mathrm{refine}(\mathcal{T}_H) \quad \forall \psi_H \in \mathcal{P}^0(\mathcal{T}_H) \quad \forall \psi_h \in \mathcal{P}^0(\mathcal{T}_h)$

$$\Big| \Big(\sum_{T \in \mathcal{T}_H \cap \mathcal{T}_h} \eta_h(T, \psi_h)^2 \Big)^{1/2} - \Big(\sum_{T \in \mathcal{T}_H \cap \mathcal{T}_h} \eta_H(T, \psi_H)^2 \Big)^{1/2} \Big| \le C_{\rm stb} \, \| \psi_h - \psi_H \|$$

(A2) reduction on refined elements

- $\exists 0 < q_{\rm red} < 1 \quad \forall \mathcal{T}_H \quad \forall \mathcal{T}_h \in \mathrm{refine}(\mathcal{T}_H) \quad \forall \psi_H \in \mathcal{P}^0(\mathcal{T}_H) \subseteq \mathcal{P}^0(\mathcal{T}_h)$

$$\Big(\sum_{T \in \mathcal{T}_h \setminus \mathcal{T}_H} \eta_h(T, \psi_H)^2 \Big)^{1/2} \le q_{\rm red} \Big(\sum_{T \in \mathcal{T}_H \setminus \mathcal{T}_h} \eta_H(T, \psi_H)^2 \Big)^{1/2}$$

Cascon, Kreuzer, Nochetto, Siebert: SIAM J. Numer. Anal. 46 (2008)

Feischl, Karkulik, Melenk, Praetorius: SIAM J. Numer. Anal. 51 (2013)

Aurada, Feischl, Führer, Karkulik, Melenk, Praetorius: Math. Comp. 86 (2017)

(A3) discrete reliability

- $\exists C_{\rm rel} > 0 \quad \forall \mathcal{T}_H \quad \forall \mathcal{T}_h \in \mathrm{refine}(\mathcal{T}_H)$

$$\|\!| \phi_h^\star - \phi_H^\star |\!\| \le C_{\rm rel} \Big(\sum_{T \in \mathrm{patch}(\mathcal{T}_H \setminus \mathcal{T}_h)} \eta_H(T, \phi_H^\star)^2 \Big)^{1/2}$$

- discrete reliability for (non-computable) discrete solution $\phi_H^\star$
- discrete reliability $\implies$ reliability
- (A1) + reliability (A3) + contraction

$\implies \|\!| \phi^\star - \phi_\ell^n |\!\| + \eta_\ell(\phi_\ell^n) \lesssim \eta_\ell(\phi_\ell^n) + \|\!| \phi_\ell^n - \phi_\ell^{n-1} |\!\|.$

Stevenson: Found. Comput. Math. 7 (2007)
Feischl, Karkulik, Melenk, Praetorius: SIAM J. Numer. Anal. 51 (2013)

Main results

Key observation: Full linear convergence

- $\mathcal{Q} := \big\{(\ell,n) \in \mathbb{N}_0 \times \mathbb{N}_0 \,:\, (\ell,n)$ used in algorithm$\big\}$
- $|(\ell,n)| \quad \rightsquigarrow \quad$ number of overall PCG iterations until ϕ_ℓ^n

Theorem (Führer, Haberl, P., Schimanko '19)

- ABEM with residual error estimator on shape-regular meshes
- $0 < \theta \le 1$ arbitrary
- $\lambda > 0$ arbitrary
- quasi-error $\quad \Lambda_\ell^n := \big[\, |\!|\!| \, \phi - \phi_\ell^n \, |\!|\!| + \eta_\ell(\phi_\ell^n) \,\big]$

$\Longrightarrow \quad \exists\, C \ge 1 \;\exists\, 0 < q < 1 \;\forall\, (\ell',n') > (\ell,n) \quad \Lambda_{\ell'}^{n'} \le C\, q^{|(\ell',n')|-|(\ell,n)|}\, \Lambda_\ell^n$

- algorithm yields linear improvement in each step (PCG or refinement)
- follows from (A1)–(A3) & Galerkin orthogonality & contractive solver

Führer, Haberl, Praetorius, Schimanko: Numer. Math. 141 (2019) [open access]

Optimal convergence rates

Theorem (Führer, Haberl, P., Schimanko '19)

- ABEM with residual error estimator on NVB meshes
- $s > 0$ arbitrary
- $0 < \theta \ll 1$ sufficiently small
- $0 < \lambda \ll 1$ sufficiently small
- $\mathcal{M}_\ell$ has (essentially) minimal cardinality

$$\Longrightarrow \quad \sup_{(\ell,n)\in\mathcal{Q}} (\#\mathcal{T}_\ell)^s \Lambda_\ell^n \simeq \sup_{(\ell,0)\in\mathcal{Q}} (\#\mathcal{T}_\ell)^s \Lambda_\ell^\star \overset{\checkmark}{\simeq} \underbrace{\sup_{N>0} \Big(N^s \min_{\mathcal{T}_{\mathrm{opt}}\in\mathbb{T}_N} \Lambda_{\mathrm{opt}}^\star \Big)}_{=:\, \|\phi^\star\|_{\mathbb{A}_s}}$$

$\Longrightarrow$ optimal decay of Λ_ℓ^n w.r.t. degrees of freedom

- observe: $\Lambda_\ell^n := \big[\, |\!|\!| \, \phi - \phi_\ell^n \, |\!|\!| + \eta_\ell(\phi_\ell^n) \big] \lesssim \Lambda_\ell^0 \simeq \Lambda_{\ell-1}^n \simeq \Lambda_{\ell-1}^\star$

Feischl, Karkulik, Melenk, Praetorius: SIAM J. Numer. Anal. 51 (2013)

Führer, Haberl, Praetorius, Schimanko: Numer. Math. 141 (2019) [open access]

Almost optimal computational cost

- costs for one step: $\mathcal{O}\big((\#\mathcal{T}_\ell)\log^2(1+\#\mathcal{T}_\ell)\big)$ ($\mathcal{H}^2$-matrices)
- costs for $(\ell', n') \in \mathcal{Q}$: $\mathcal{O}\Big(\sum_{\substack{(\ell,n)\in\mathcal{Q}\\(\ell,n)\le(\ell',n')}} (\#\mathcal{T}_\ell)\log^2(1+\#\mathcal{T}_\ell)\Big)$

Corollary (Führer, Haberl, P., Schimanko '19)

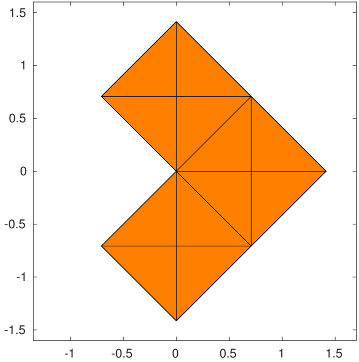
- same assumptions as for optimal rates!
- $s > 0$ with $\|\phi^\star\|_{\mathbb{A}_s} < \infty$
- $\varepsilon > 0$ arbitrary

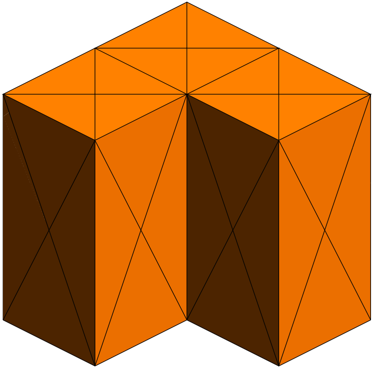
$$\Longrightarrow \sup_{(\ell',n')\in\mathcal{Q}} \Big(\sum_{\substack{(\ell,n)\in\mathcal{Q}\\(\ell,n)\le(\ell',n')}} (\#\mathcal{T}_\ell)\log^2(1+\#\mathcal{T}_\ell)\Big)^{s-\varepsilon} \Lambda_{\ell'}^{n'} < \infty$$

- not only: convergence with rate s w.r.t. degrees of freedom
- but also: convergence with rate $s-\varepsilon$ w.r.t. costs

Führer, Haberl, Praetorius, Schimanko: Numer. Math. 141 (2019) [open access]

3D Experiment





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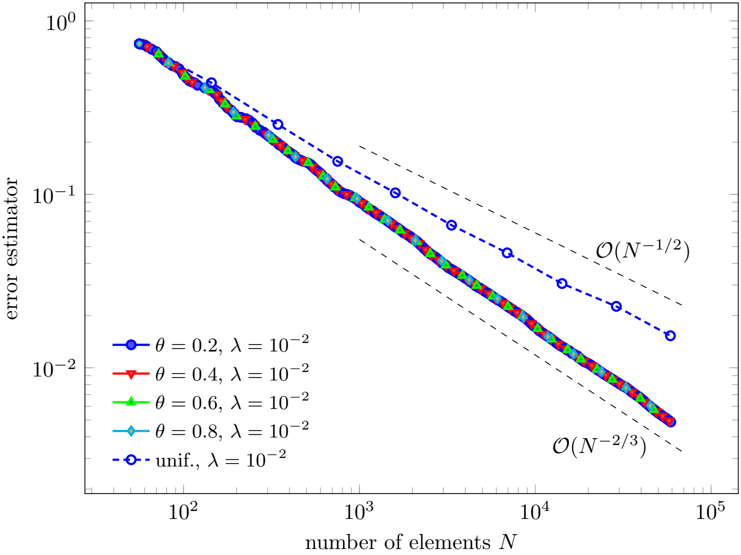
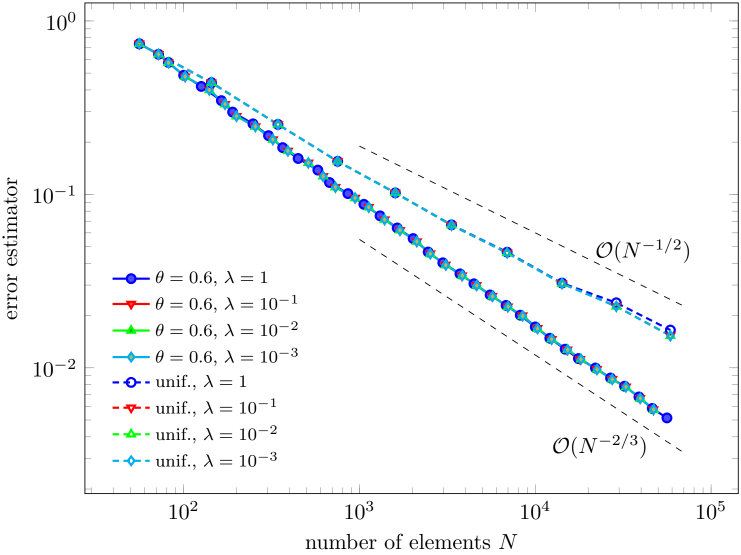
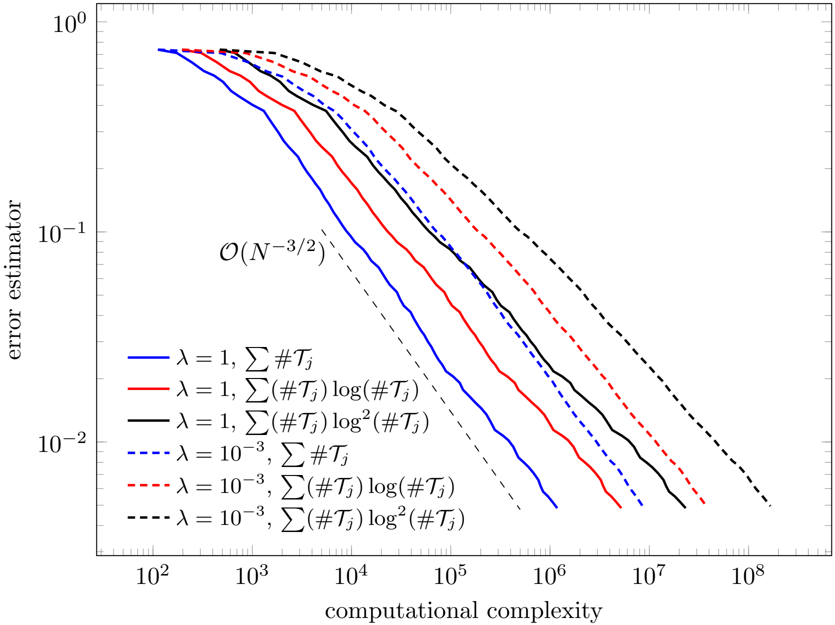
Dependence on θ for $\lambda = 10^{-2}$



Dependence on λ for $\theta = 0.6$



Computational costs



Conclusion

Conclusion

- adaptivity should care about the solver to minimize costs

- full linear convergence $+$ optimal rates w.r.t. dofs

$\Longrightarrow$ (almost) optimal rates w.r.t. computational costs

- for BEM: almost optimal costs (due to $\log$-terms form $\mathcal{H}^2$-matrices)

- for FEM: analysis even yields optimal costs

- done: analysis can be extended from PCG to contractive solver

- to do: compression of dense BEM matrices should be included

- open: analysis restricted to isotropic refinement

Thanks for Listening!

Führer, Haberl, Praetorius, Schimanko:

Adaptive BEM with inexact PCG solver
yields almost optimal computational costs

Numerische Mathematik 141 (2019)
[open access]

CMAM 2020

July 13–17, 2020 – TU Wien – CMAM-9
Computational Methods in Applied Mathematics
https://www.asc.tuwien.ac.at/cmam2020/

The conference is organized under the aegis of the journal Computational Methods in Applied Mathematics (CMAM) and is focused on theoretical numerical analysis and applications to modeling, simulation, and scientific computing. The scientific program will include invited plenary lectures, minisymposia, parallel sessions with contributed talks, and a poster session.

Confirmed plenary speakers
Daniele Boffi (University of Pavia)
Thomas Führer (Pontifical Catholic University of Chile)
Philipp Grohs (University of Vienna)
Jun Hu (Peking University)
Barbara Kaltenbacher (University of Klagenfurt)
Dalibor Lukas (Technical University of Ostrava)
Svetozar Margenov (Bulgarian Academy of Sciences)
Neela Nataraj (IIT Bombay)
Christoph Ortner (University of Warwick)
Amiya Kumar Pani (IIT Bombay)
Sergei Pereverzyev (Austrian Academy of Sciences)
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Venue
Building: TU Wien, Neues EI
Address: Gußhausstraße 27–29, 1040 Vienna

Der Wissenschaftsfonds.

- define Haar functions $\varphi_{\bullet,E}|_{T^\pm} := \pm\frac{|E|}{|T^\pm|}$ with $T^+ \cap T^- = E$
- define $\mathcal{E}_\ell$ as set of all edges, where $\varphi_{\ell,E}|_{T^\pm}$ has changed / is new
- define $\mathcal{X}_H := \mathcal{P}^0(\mathcal{T}_H)$ and $\mathcal{X}_{H,E} := \mathrm{span}\{\varphi_{H,E}\}$

$$\Longrightarrow \quad \mathcal{X}_L = \mathcal{X}_0 + \sum_{\ell=1}^{L} \sum_{E\in\mathcal{E}_\ell} \mathcal{X}_{\ell,E} \quad \text{for all } L \in \mathbb{N}_0$$

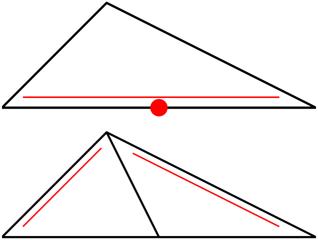
- decomposition yields local multilevel preconditioner
- matrix representation

$$\boldsymbol{P}_L^{-1} := \boldsymbol{I}_{0,L}\boldsymbol{A}_0^{-1}\boldsymbol{I}_{0,L}^T + \sum_{\ell=1}^{L} \boldsymbol{I}_{\ell,L}\boldsymbol{H}_\ell\boldsymbol{D}_\ell\boldsymbol{H}_\ell^T\boldsymbol{I}_{\ell,L}^T.$$

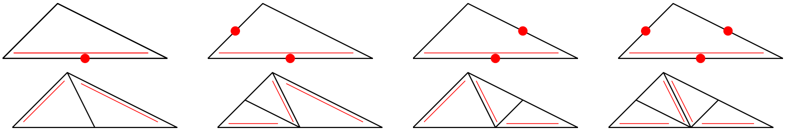
  - $\boldsymbol{I}_{k,\ell}$ $\rightsquigarrow$ embedding $\mathcal{P}^0(\mathcal{T}_k) \hookrightarrow \mathcal{P}^0(\mathcal{T}_\ell)$ for $k < \ell$
  - $\boldsymbol{H}_\ell$ $\rightsquigarrow$ represents Haar functions
  - $\boldsymbol{D}_\ell$ $\rightsquigarrow$ certain diagonal matrix

Newest Vertex Bisection (NVB)

- each element has reference edge
- refinement by bisection
  - T' son of T $\implies$ $|T'| = |T|/2$
- new reference edges are opposite to newest vertex
- for $T \in \mathcal{T}$, obtain unique binary tree with possible successors T' with $T' \subsetneq T$



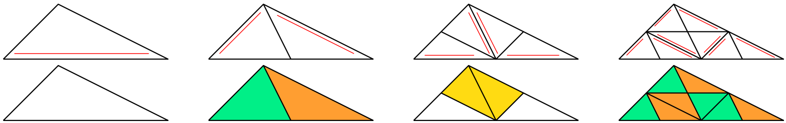
- initialization
  - for all marked elements $T \in \mathcal{T} \cap \mathcal{M}$, mark its reference edge
- recursion
  - if element's edge is marked, mark at least its reference edge
  - terminates, since each triangulation has only finitely many edges
- refinement according to scheme



- note that each case is iterated NVB
- each refined element has 2, 3, or 4 sons

NVB guarantees finitely many shapes

- NVB leads to only finitely many similarity classes of triangles
  - depends only on T and its reference edge



- in particular, uniform shape regularity
  - $\dfrac{\mathrm{diam}(T')^2}{|T'|} \le \gamma(T) < \infty$ for all NVB successors T' of T