Adaptive Multiscale Methods for the Numerical Treatment of Systems of PDEs

Angela Kunoth

Universität zu Köln, Germany

Sketch of Contents

- Elliptic and parabolic partial differential equations (PDEs) in weak form; regularity of solutions
- Control problems constrained by elliptic and parabolic PDEs
- Numerical approximations of solutions on uniform and non-uniform/adaptive grids
- Concepts of multiscale methods and adaptivity; convergence proofs and complexity estimates
- Realization of these concepts by B-spline-wavelets
- Fast solvers: multilevel preconditioning; implementation issues

Literature: see References in notes_kunoth.pdf

Part I: Multilevel Preconditioning for Isogeometric Analysis

(joint work with Annalisa Buffa, Helmut Harbrecht & Giancarlo Sangalli)

[BHKS] Comput. Methods Appl. Mech. Engrg. 265, 2013

Setup

- Elliptic PDE on physical domain $\Omega \subset \mathbb{R}^d$, $d \geq 2$
- Isogeometric analysis $\mathbf{F} : \hat{\Omega} \to \Omega$ for parametric domain $\hat{\Omega} \subset [0,1]^d$ with regular mapping $\mathbf{F}$

Goal: High order approximate solution with fast iterative method

Essential Ingredients

- Isogeometric discretization by tensor product B-splines of degree p
- Iterative solution with multilevel preconditioner and nested iteration

$\rightsquigarrow$ Result: Solution in optimal linear complexity

Problem Setup

Elliptic PDE of order $2r$ on physical domain Ω

$$\begin{array}{llll} r = 1: & -\Delta u = f & \text{in } \Omega, & u|_{\partial\Omega} = 0 \\ r = 2: & \Delta^2 u = f & \text{in } \Omega, & u|_{\partial\Omega} = \mathbf{n} \cdot \nabla u|_{\partial\Omega} = 0 \end{array}$$

Weak operator form: for given $f \in H^{-r}(\Omega)$, find $u \in H_0^r(\Omega)$ such that

$$\boxed{Au = f \quad \text{in} \quad H^{-r}(\Omega)}$$

Elliptic operator A defined by $\langle Av, w \rangle := a(v, w)$ symmetric, continuous

and coercive on $H_0^r(\Omega)$: $\quad \|Av\|_{H^{-r}(\Omega)} \sim \|v\|_{H^r(\Omega)}$

Mapping $\mathbf{F} : \hat{\Omega} \to \Omega$ from parametric domain $\hat{\Omega} \subset [0,1]^d$ to physical domain Ω

$\mathbf{F}$ regular: $\quad \|D\mathbf{F}(\mathbf{x})\| \sim 1$ for all $\mathbf{x} \in \hat{\Omega}$

Numerical Solution on Physical Space

Discretization on uniform grid: $V_h \subset H_0^r(\Omega)$ $\quad \dim V_h < \infty \quad \rightsquigarrow \quad \boxed{A_h\, u_h = f_h \qquad (*)}$

$0 < h < 1$ grid size

Goal: Realize discretization error accuracy ε

with minimal amount of work $\mathcal{O}(N(\varepsilon))$ in amount of unknowns $N(\varepsilon)$

Obstructions for fast numerical solution:

- Large sparse linear system of equations $(*)$ $\rightsquigarrow$ iterative solver
- Convergence speed of iterative solver depends on $\mathrm{cond}_2(A_h)$
- Standard discretizations with finite differences or finite elements $\rightsquigarrow$ $\mathrm{cond}_2(A_h) \sim h^{-2r}$

  $0 < h < 1$ grid size
- High desired accuracy, resolution of singularities in data and/or geometry $\rightsquigarrow$ small h

  $\rightsquigarrow$ larger problem $\rightsquigarrow$ worse condition number

Ingredients for reaching goal:

(i) Multilevel preconditioner C_h
multigrid methods, BPX preconditioner, wavelet discretizations $\rightsquigarrow$ $\mathrm{cond}_2(C_h A_h) \sim 1$

(ii) Nested iteration

A-priori Estimates for Finite Elements

Quality measure: Approximation in norm $\|u - u_h\|_{L_2(\Omega)} \leq \varepsilon$

A–priori error estimates: $\Omega \subset \mathbb{R}^d$ $\quad \dim V_h = N \sim h^{-d}$ $\quad$ uniform grid

$$\|u - u_h\|_{L_2(\Omega)} \lesssim h^s \, \|u\|_{H^s(\Omega)} \qquad u_h \in V_h \qquad 0 \leq s \leq p+1$$

$$\Longleftrightarrow \qquad \|u - u_N\|_{L_2(\Omega)} \lesssim N^{-s/d} \, \|u\|_{H^s(\Omega)}$$

N degrees of freedom $\longleftrightarrow$ accuracy $\mathcal{O}(N^{-(p+1)/d})$

Approximation rate determined by

(i) (piecewise polynomials of degree $p \rightsquigarrow$) approximation order $p+1$ of V_h

(ii) space dimension d

(iii) amount of smoothness of u in L_2

Target:

Realize discretization error accuracy $\varepsilon \sim h^{p+1} \sim 2^{-(p+1)J}$ for grid with spacing $h \sim 2^{-J}$

Problem complexity: For $h \sim 2^{-J}$ a total of $N \sim 2^{Jd}$ unknowns

Optimal complexity for iterative solver: Minimal amount of work is $\mathcal{O}(N)$

Isogeometric Elements of Degree p

Mesh on $[0,1]$: $\Xi := \{\xi_1, \dots, \xi_{n+p+1}\}$ a p-open knot vector such that

$$0 = \xi_1 = \ldots = \xi_{p+1} < \xi_{p+2} \le \ldots \le \xi_n < \xi_{n+1} = \ldots = \xi_{n+p+1} = 1$$

(allowing internal repeated knots having multiplicity $m_i \le p - r + 1$)

B-splines of degree p on Ξ defined recursively by

$$p = 0: \qquad N_{i,0}(\zeta) = \begin{cases} 1 & \text{if } \xi_i \le \zeta < \xi_{i+1}, \\ 0 & \text{otherwise,} \end{cases}$$

$$p \ge 1: \qquad N_{i,p}(\zeta) = \frac{\zeta - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\zeta) + \frac{\xi_{i+p+1} - \zeta}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\zeta)$$

$\rightsquigarrow$ n B-splines spanning spline space of piecewise polynomials of degree p

with $p - m_i$ continuous derivatives at inner nodes

$$S_h(\hat{\Omega}) := \text{span}\left\{ B_i(\mathbf{x}) := \prod_{\ell=1}^{d} N_{i_\ell,p}(x_\ell), \; i = 1, \dots, N := nd \right\}$$

Mapping $\mathbf{F} = (F_1, \dots, F_d)^T \qquad F_i \in S_{\tilde{h}}(\hat{\Omega})$ for some $\tilde{h} \gg h$

$$\rightsquigarrow V_h := \{ v_h \in H_0^r(\Omega) : \; v_h \circ \mathbf{F} \in S_h(\hat{\Omega}) \}$$

$$\|v\|^2_{L_2(\Omega)} := \int_{\hat{\Omega}} |v(\mathbf{F}(\mathbf{x}))|^2 \|D\mathbf{F}(\mathbf{x})\| d\mathbf{x}$$

Theorem

(S) Uniform stability of basis with respect to $L_2(\Omega)$

$$\| \sum_{i=1}^{N} c_i \, B_i \circ \mathbf{F}^{-1} \|^2_{L_2(\Omega)} \sim \sum_{i=1}^{N} |c_i|^2 =: \|\mathbf{c}\|^2_{\ell_2} \qquad \text{for any } \mathbf{c} \in \ell_2 \quad \text{constants} = c(p,d) \neq c(h)$$

(J) Direct or Jackson estimates

$$\inf_{v_h \in V_h} \|v - v_h\|_{L_2(\Omega)} \lesssim h^s \, |v|_{H^s(\Omega)} \qquad \text{for any } v \in H^s(\Omega) \quad 0 \leq s \leq p+1$$

(B) Inverse or Bernstein estimates

$$\|v_h\|_{H^s(\Omega)} \lesssim h^{-s} \|v_h\|_{L_2(\Omega)} \qquad \text{for any } v_h \in V_h \text{ and } 0 \leq s \leq p$$

Multilevel Preconditioner

Asymptotically optimal preconditioner: C_h such that

$$\mathrm{cond}_2(C_h A_h) \sim 1 \quad \text{independent of } h$$

and setup and application of C_h in optimal linear complexity $\mathcal{O}(N)$

Schwarz iterative schemes based on subspace corrections

$\rightsquigarrow$ Multilevel schemes yielding optimal preconditioners:

- Multiplicative schemes $\rightsquigarrow$ multigrid methods — Brandt, Braess, Bramble, Hackbusch, Zulehner ...
  IgA: Gahalaut, Kraus, Tomar ...
- Additive schemes $\rightsquigarrow$ BPX preconditioner; wavelet discretization
  Bramble, Pasciak, Xu, Yserentant, Oswald, Dahmen, Kunoth ...

Relevant idea from Approximation Theory: Multilevel characterization of function spaces and norm equivalences

Not optimal are preconditioners based on domain decomposition, overlapping Schwarz, hierarchical basis preconditioners... Beirao da Veiga, Cho, Pavarino. Scacci, Kleiss, Pechstein, Jüttler, Langer ...

Multilevel Characterization of Function Spaces

$V_h \longleftrightarrow V_j \qquad h \sim 2^{-j} \qquad j$ resolution level

Multiresolution $V_{j_0} \subset V_{j_0+1} \subset \ldots \subset V_j \subset V_{j+1} \subset \ldots H_0^r(\Omega)$

$$\mathrm{clos}_{H^r(\Omega)} \left(\bigcup_{j=j_0}^{\infty} V_j \right) = H_0^r(\Omega)$$

Linear orthogonal projectors $Q_j : H_0^r(\Omega) \to V_j$ s.th. $Q_j Q_\ell = Q_j$ for $j \leq \ell \rightsquigarrow Q_j - Q_{j-1}$ projector

Corollary

(S) Φ_j uniformly stable basis for V_j: $\qquad \|\mathbf{c}\|_{\ell_2} \sim \|\mathbf{c}^T \Phi_j\|_{L_2(\Omega)}$

(J) Jackson estimate

$$\inf_{v_j \in V_j} \|v - v_j\|_{L_2(\Omega)} \lesssim 2^{-sj} \|v\|_{H^s(\Omega)} \qquad v \in H^s(\Omega) \qquad 0 < s \leq \delta$$

(B) Bernstein inequality $\qquad \|v_j\|_{H^s(\Omega)} \lesssim 2^{sj} \|v_j\|_{L_2(\Omega)} \qquad v_j \in V_j \qquad s < \tau$

$\Longrightarrow$ Norm equivalence

$$\|v\|_{H^r(\Omega)}^2 \sim \sum_{j=j_0}^{J} 2^{2rj} \|(Q_j - Q_{j-1})v\|_{L_2(\Omega)}^2 \qquad v \in V_J$$

Proof: Norm equivalence on $\hat{\Omega}$ [Dahmen, Kunoth '92] [Oswald '92]
(J) and discrete Hardy inequality $\rightsquigarrow$ upper estimate for $\|\cdot\|_{H^s(\Omega)}$
(B), $\|Q_j\|_{L_2(\Omega)} \lesssim 1$ and Whitney estimate $\rightsquigarrow$ lower estimate
F regular mapping

Norm Equivalence for Optimal Preconditioning

Corollary: For $H_0^r(\Omega)$ $\qquad C_J^{-1} := A_{j_0} Q_{j_0} \circ \mathbf{F}^{-1} + \sum_{j=j_0}^{J} 2^{2rj} (Q_j - Q_{j-1}) \circ \mathbf{F}^{-1}$

is optimal preconditioner for $A_J : V_J \to V_J$: $\qquad \mathrm{cond}_2(C_J^{1/2} A_J C_J^{1/2}) \sim 1 \quad$ as $J \to \infty$

Proof: [Jaffard '92], [Dahmen, Kunoth '92], [Oswald '92]

Isomorphism $\|Av\|_{H^{-r}(\Omega)} \sim \|v\|_{H^r(\Omega)}$ combined with norm equivalence for $H_0^r(\Omega)$ and $\mathbf{F}$ regular mapping

BPX realization of C_J^{-1}: replace $C_J = A_{j_0} Q_{j_0} \circ \mathbf{F}^{-1} + \sum_{j=j_0}^{J} 2^{-2rj} (Q_j - Q_{j-1}) \circ \mathbf{F}^{-1}$

by spectrally equivalent preconditioner

$$\hat{C}_J := A_{j_0} Q_{j_0} \circ \mathbf{F}^{-1} + \sum_{j=j_0}^{J} 2^{-2rj} Q_j \circ \mathbf{F}^{-1} \qquad \text{is optimal}$$

developed by [Bramble, Pasciak, Xu '90], optimality proved by [Dahmen, Kunoth '92], [Oswald '92]

Hierarchical basis preconditioner by [Yserentant '89] not optimal

$$\hat{C}_J := A_{j_0} Q_{j_0} \circ \mathbf{F}^{-1} + \sum_{j=j_0}^{J} 2^{-2rj} Q_j \circ \mathbf{F}^{-1} \text{ using } Q_j = \sum_{i \in I_j} (\,\cdot\,, B_{i,j} \circ \mathbf{F}^{-1})_{L_2(\Omega)}\, B_{i,j} \circ \mathbf{F}^{-1}$$

$\rightsquigarrow$

$$G_J = A_{j_0}^{-1} \sum_{i \in I_0} (\,\cdot\,, B_{i,j_0} \circ \mathbf{F}^{-1})_{L_2(\Omega)}\, B_{i,j_0} \circ \mathbf{F}^{-1}$$

$$+ \sum_{j=j_0+1}^{J} 2^{-2jr} \sum_{i \in I_j} (\,\cdot\,, B_{i,j} \circ \mathbf{F}^{-1})_{L_2(\Omega)}\, B_{i,j} \circ \mathbf{F}^{-1}$$

Implementation: refinement relation for B-splines

$\rightsquigarrow$ prolongation $\mathbf{I}_j^{j+1} : V_j \to V_{j+1}$ restriction $\mathbf{I}_{j+1}^{j} = (\mathbf{I}_j^{j+1})^T$

For $p = 2$, restriction is $\mathbf{I}_{j+1}^{j} = 2^{-1/2} \begin{bmatrix} \frac{1}{2} & \frac{9}{8} & \frac{3}{8} & & & & & & & \\ & \frac{1}{4} & \frac{3}{4} & \frac{3}{4} & \frac{1}{4} & & & & & \\ & & & \frac{1}{4} & \frac{3}{4} & \frac{3}{4} & \frac{1}{4} & & & \\ & & & & & \ddots & \ddots & & & \\ & & & & & \frac{1}{4} & \frac{3}{4} & \frac{3}{4} & \frac{1}{4} & \\ & & & & & & & \frac{3}{8} & \frac{9}{8} & \frac{1}{2} \end{bmatrix} \in \mathbb{R}^{2^j \times 2^{j+1}}$

$\rightsquigarrow$ $\mathbf{I}_j^J := \mathbf{I}_{J-1}^{J} \mathbf{I}_{J-2}^{J-1} \cdots \mathbf{I}_j^{j+1}$ and $\mathbf{I}_J^j := \mathbf{I}_{j+1}^{j} \mathbf{I}_{j+2}^{j+1} \cdots \mathbf{I}_J^{J-1}$

$$\rightsquigarrow \quad \tilde{\mathbf{G}}_J = \sum_{j=j_0}^{J} \mathbf{I}_j^J (\operatorname{diag} \mathbf{A}_j)^{-1} \mathbf{I}_J^j \circ \mathbf{F}^{-1}$$

First Numerical Results

Condition numbers $\mathrm{cond}_2(\tilde{\mathbf{G}}_J \mathbf{A}_J)$ for Laplacian on $\Omega = (0,1)^d$ for $d = 1, 2, 3$
with above BPX preconditioning

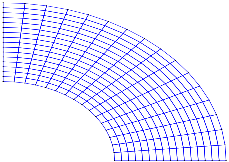
level j	interval				square				cube			
	$p=1$	$p=2$	$p=3$	$p=4$	$p=1$	$p=2$	$p=3$	$p=4$	$p=1$	$p=2$	$p=3$	$p=4$
3	7.43	3.81	7.03	5.93	5.93	7.31	22.8	133	3.49	39.5	356	5957
4	8.87	4.40	9.47	7.81	5.00	9.03	40.2	225	4.85	50.8	624	9478
5	10.2	4.67	11.0	9.36	5.70	9.72	51.8	293	5.75	56.6	795	11887
6	11.3	4.87	12.1	10.7	6.27	10.1	58.7	340	6.40	59.7	895	13185
7	12.2	5.00	12.7	11.5	6.74	10.4	63.1	371	6.91	61.3	961	13211
8	13.0	5.10	13.0	11.9	7.14	10.5	66.0	391	7.34	62.2	990	13234
9	13.7	5.17	13.2	12.1	7.48	10.6	68.0	403	7.70	62.6	1016	13255
10	14.2	5.22	13.4	12.2	7.77	10.6	69.3	411	7.99	62.9	1040	

$d = 1$: no dependence on p

Numerical Results: Dependence on Parametric Mapping **F**

Condition numbers of the BPX-preconditioned Laplacian on an analytic arc

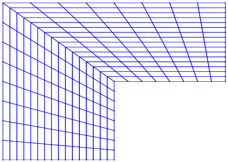
level	$p = 1$	$p = 2$	$p = 3$	$p = 4$
3	5.04 (21.8)	12.4 (8.64)	31.8 (31.8)	184 (184)
4	11.1 (90.2)	16.3 (34.3)	54.7 (32.9)	291 (173)
5	25.3 (368)	19.0 (139)	70.1 (98.9)	376 (171)
6	31.9 (1492)	21.4 (560)	79.2 (401)	436 (322)
7	37.4 (6015)	23.1 (2255)	84.4 (1620)	471 (1297)
8	42.1 (241721)	24.3 (9062)	87.3 (6506)	490 (5217)
9	45.7 (969301)	25.2 (36353)	89.0 (26121)	500 (20945)
10	48.8 (388690)	25.9 (145774)	90.1 (104745)	505 (83975)



(numbers in brackets: no preconditioning)

... relative to a $\mathcal{C}^0$-parametrization of an L-shaped domain

level	$p = 1$	$p = 2$	$p = 3$	$p = 4$
3	14.0	13.4	33.5	194
	(25.8)	(10.2)	(33.5)	(194)
4	25.2	20.6	56.7	301
	(108)	(41.1)	(34.7)	(182)
5	36.9	26.8	72.1	383
	(452)	(168)	(123)	(180)
6	47.9	31.8	80.5	442
	(1845)	(689)	(500)	(400)
7	57.4	35.4	85.5	477
	(7465)	(2790)	(2025)	(1620)
8	65.3	38.0	88.3	496
	(30047)	(11244)	(8157)	(6533)
9	71.8	40.0	90.0	505
	(120603)	(45172)	(32773)	(26264)
10	77.0	41.2	91.0	511
	(483618)	(181140)	(131418)	(105381)

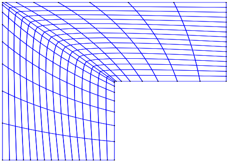


(numbers in brackets: no preconditioning)

Numerical Results: Dependence on Parametric Mapping **F**

Condition numbers of the BPX-preconditioned Laplacian relative to a singular $\mathcal{C}^1$-parametrization of an L-shaped domain

level	$p = 1$	$p = 2$	$p = 3$	$p = 4$
3	15.0	14.7	32.8	185
	(28.8)	(13.2)	(32.8)	(185)
4	44.1	36.2	56.7	303
	(133)	(53.7)	(38.5)	(189)
5	91.1	70.9	95.7	388
	(568)	(225)	(158)	(196)
6	167	147	155	463
	(2341)	(931)	(639)	(557)
7	443	385	385	887
	(9502)	(3804)	(2587)	(2350)
8	1136	960	1021	2417
	(38544)	(15353)	(10491)	(9604)
9	2797	2301	2588	6251
	(155276)	(61619)	(42355)	(38695)
10	6664	5362	6318	15505
	(622565)	(247091)	(169844)	(155143)



Further Improvement: BPX with SSOR

Split $\mathbf{A}_j = \mathbf{L}_j + \mathbf{D}_j + \mathbf{L}_j^T$ and replace $(\operatorname{diag} \mathbf{A}_j)^{-1}$ by SSOR preconditioner

$$\tilde{\mathbf{G}}_J = \sum_{j=j_0}^{J} \mathbf{I}_j^J (\mathbf{D}_j + \mathbf{L}_j)^{-T} \mathbf{D}_j (\mathbf{D}_j + \mathbf{L}_j)^{-1} \mathbf{I}_J^j \circ \mathbf{F}^{-1}$$

(application in optimal $\mathcal{O}(N)$ complexity)

Spectral condition numbers of BPX-preconditioned Laplacian for cubic B-splines ($p = 3$) on different geometries and using a SSOR preconditioning on each level

level	square, simple BPX	square	analytic arc	$\mathcal{C}^0$-map of L-shaped domain	singular $\mathcal{C}^1$-map of L-shaped domain
3	22.8	3.61	3.65	3.67	3.80
4	40.2	6.58	6.97	7.01	7.05
5	51.8	8.47	10.2	10.2	14.8
6	58.7	9.73	13.1	13.2	32.2
7	63.1	10.5	14.9	15.2	77.7
8	66.0	11.0	15.9	16.3	180
9	68.0	11.2	16.5	17.0	411
10	69.3	11.4	16.9	17.7	933

Ingredients for Efficient Numerical Solution: Nested Iteration

Recall goal: realize discretization error accuracy $\varepsilon_J \sim h^2 \sim 2^{-2J}$ for grid with spacing $h \sim 2^{-J}$ with minimal amount of work $\mathcal{O}(N)$ $N \sim 2^{Jd}$ unknowns

Naive strategy:

- Iterate only on highest level J and iterate until discretization error accuracy needs $\mathcal{O}(J) = \mathcal{O}(-\log \varepsilon_J)$ iterations to achieve prescribed discretization error accuracy $\varepsilon_J \sim 2^{-2J}$
- Each application of optimally conditioned $\mathbf{A}_J$ requires $\mathcal{O}(N_J)$ arithmetic operations
  $\rightsquigarrow$ a total of $\mathcal{O}(J\, N_J)$ arithmetic operations iterating on finest level only

Theorem:
Starting with coarsest level j_0, solve $\mathbf{A}_j \mathbf{y}_j = \mathbf{f}_j$ on each level j up to discretization error accuracy ε_j and prolongate result from level j to next level $j+1$ as initial guess

$\rightsquigarrow$ Optimal preconditioner + nested iteration yields method of optimal complexity $\mathcal{O}(N_J)$

to reach discretization error accuracy on finest level J

Proof: For multiplicative Schwarz schemes: known as full multigrid
For additive preconditioners: optimal condition of $\mathbf{A}_j \rightsquigarrow$ fixed amount of iterations on each level to reach discretization error accuracy on that level;
spaces nested and $N_j \sim 2^{dj}$ and geometric series argument [Dahmen, Kunoth, Schneider '99]

Summary

- Proof for optimal multilevel preconditioner such that $\text{cond}_2(\tilde{\mathbf{G}}_J \mathbf{A}_J) = \mathcal{O}(1)$ based on generating system from hierarchical B-splines
  ($\neq$ (suboptimal) hierarchical basis preconditioner)
- Optimal complexity of the solver: optimal preconditioner + nested iteration
- Use of SSOR within BPX strongly reduces effect of isomorphism constants, parametric mappings. . .

Remarks and Outlook

- Multigrid preconditioners for high order FE based on low order functions [Sundar, Stadler, Biros '14]
- Extensions for nurbs, generalized splines
- Dependence of condition numbers on p ? [Manni et al '14], [Gahalaut, Tomar, Douglas '14], [Zulehner et al '14]
- A-posteriori error estimates $\rightsquigarrow$ local refinement Gianellli, Jüttler, Simeon, Vazquez . . .
  $\rightsquigarrow$ BPX preconditioner possible

(Further) Literature

BPX for C^0, C^1 elements	[Dahmen, Kunoth '92] [Kunoth '94] [Oswald '92, '94]
BPX for C^0, C^1 elements on sphere	[Maes, Kunoth, Bultheel '07]
(Monotone) multigrid for higher order B-splines (for pricing American options)	[Holtz, Kunoth '07]

Iteration history for basis functions of degree $p = 2$ and $p = 3$