Shape uncertainty quantification with compactly supported basis functions

Wouter van Harten

w.vanharten@math.ru.nl

Joint work with L. Scarabosio

Institute for Mathematics, Astrophysics, and Particle Physics (IMAPP)
Radboud University Nijmegen

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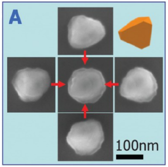
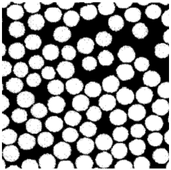
Geometric uncertainties

In applications, one encounters geometric uncertainties:

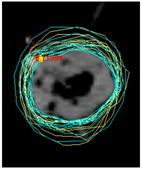


Sannomiya, Diss. ETHZ 18747



Babuška et al. (1999)

serc.carleton.edu



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Effects?

Quantifying the effects

- Evaluate model repeatedly
  - Pick realizations $\boldsymbol{y} \in Y$
  - Expensive solves
- Polynomial approximation
  - Expensive *Off-line* setup
  - Cheap *On-line* evaluations

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{[-1,1]^{\mathbb{N}} = Y} \arrow[r, "\text{Model}"'] \arrow[r, bend left, "\text{Polynomial approx.}"] & V
\end{tikzcd}
$$

How can we efficiently find a polynomial approximation for $\boldsymbol{y} \mapsto u(\boldsymbol{y})$*?*

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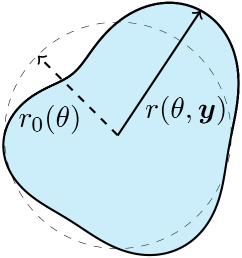
Model Problem

We consider the Laplacian on a parametrized domain:

$$\begin{cases} -\nabla \cdot (a \nabla u) = f & \text{in } D(\boldsymbol{y}), \\ u = 0 & \text{on } \partial D(\boldsymbol{y}), \\ \text{for every } \boldsymbol{y} \in Y, \end{cases} \tag{1}$$

for $f \in L^2(D_H), a \in L^\infty(D_H)$,



where

$D(\boldsymbol{y}) := \{\boldsymbol{x} \in \mathbb{R}^2 : |\boldsymbol{x}| \leq r(\theta(\boldsymbol{x}); \boldsymbol{y})\} \subset D_H,$
and affine radius expansion

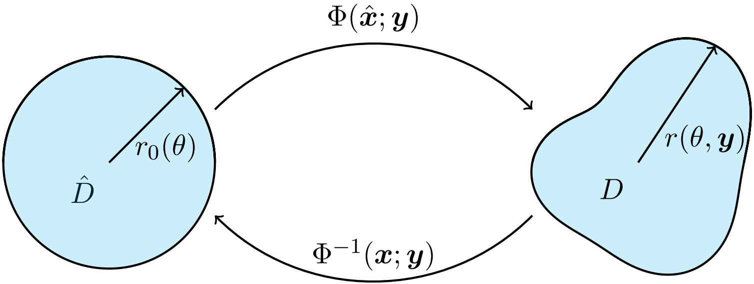
$$r(\theta; \boldsymbol{y}) = r_0(\theta) + \sum_{j>0} \psi_j(\theta) y_j,$$

with

$$\boldsymbol{y} = (y_1, y_2, \cdots) \in [-1, 1]^{\mathbb{N}}.$$

Mapping approach

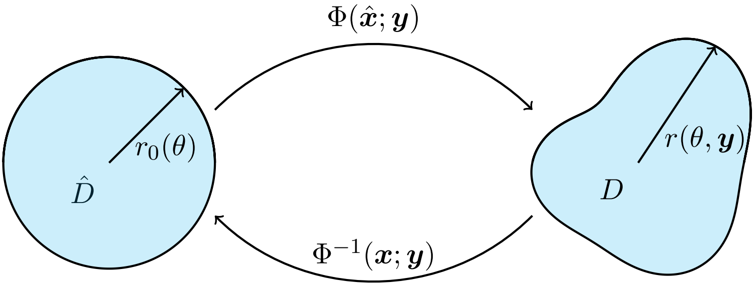
Simple PDE on difficult domain $\rightsquigarrow$ Difficult PDE on simple domain



Mapping Φ can, for example, be a *radial rescaling*

$$\Phi(\hat{\boldsymbol{x}};\boldsymbol{y}) = \begin{bmatrix}\cos(\theta(\hat{\boldsymbol{x}}))\\ \sin(\theta(\hat{\boldsymbol{x}}))\end{bmatrix} r(\theta(\hat{\boldsymbol{x}}),\boldsymbol{y})\frac{|\hat{\boldsymbol{x}}|}{r_0(\theta(\hat{\boldsymbol{x}}))}$$

Mapping approach



$$\int_{D(\boldsymbol{y})} a\nabla u(\boldsymbol{y})\cdot\nabla v\,\mathrm{d}\boldsymbol{x} = \int_{D(\boldsymbol{y})} f\cdot v\,\mathrm{d}\boldsymbol{x}$$

Transforms to the parametrized elliptic variational formulation

$$\int_{\hat{D}} \underbrace{\mathrm{D}_x\Phi^{-1}\,\mathrm{D}_x\Phi^{-T}\det(\mathrm{D}_x\Phi)a\circ\Psi}_{\hat{A}(\boldsymbol{y})}\hat{\nabla}\hat{u}(\boldsymbol{y})\cdot\hat{\nabla}\hat{v}\,\mathrm{d}\hat{\boldsymbol{x}} = \int_{\hat{D}} \underbrace{\det(\mathrm{D}_x\Phi)f\circ\Psi}_{\hat{f}(\boldsymbol{y})}\cdot\hat{v}\,\mathrm{d}\hat{\boldsymbol{x}}$$

Polynomial approximation

We have

$$\int_{\hat{D}} \hat{A}(\boldsymbol{y})\hat{\nabla}\hat{u}(\boldsymbol{y}) \cdot \hat{\nabla}\hat{v}\,\mathrm{d}\hat{\boldsymbol{x}} = \int_{\hat{D}} \hat{f}(\boldsymbol{y}) \cdot \hat{v}\,\mathrm{d}\hat{\boldsymbol{x}}.$$

Now, we write a polynomial (Taylor) expansion

$$\hat{u}(\boldsymbol{y}) = \sum_{\mu \in \mathcal{F}} t_\mu \boldsymbol{y}^\mu$$

with

$$\mathcal{F} = \{\mu =\in \mathbb{N}_0^{\mathbb{N}}, \mathsf{supp}(\mu) < \infty\}$$
$$\boldsymbol{y}^\mu = \Pi_{j=1}^{\mathsf{supp}(\mu)} y_j^{\mu_j}$$

with t_μ given by

$$t_\mu = \frac{1}{\mu!} \frac{\partial^{|\mu|}}{\partial \boldsymbol{y}^\mu} \hat{u}(\boldsymbol{y}).$$

Polynomial approximation

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$$t_\mu = \frac{1}{\mu!} \frac{\partial^{|\mu|}}{\partial \boldsymbol{y}^\mu} u(\boldsymbol{y}).$$

The variational formulation for t_μ is

$$\int_{\hat{D}} \hat{\nabla} t_\mu \cdot \hat{\nabla} \hat{v} \, \mathrm{d}\hat{\boldsymbol{x}} = -\sum_{\nu < \mu} \frac{1}{(\mu - \nu)!} \int_{\hat{D}} \partial^{\mu-\nu} \hat{A}(0) \hat{\nabla} t_\nu \cdot \hat{\nabla} \hat{v} \, \mathrm{d}\hat{\boldsymbol{x}} + \int_{\hat{D}} \partial^\mu \hat{f}(0) v \, \mathrm{d}\hat{\boldsymbol{x}}.$$

How fast can a polynomial approximation for $\boldsymbol{y} \mapsto \hat{u}(\boldsymbol{y})$ converge?

Previous results

Theorem (Hiptmair et al., 2018) ($p < 1/2$)

If $(\|\psi_j'\|_\infty)_{j\in\mathbb{N}} \in \ell^p(\mathbb{N})$, *we have that* $\|t_\nu\|_{H_0^1}$ *decays with rate* $s = \frac{1}{p} - 1$

Note: Similar results in **[Castrillón-Candás et al., Harbrecht et al.]**

Example (Sinusoidal basis)

If we take a sinusoidal basis $\psi_j(\theta) \sim j^{-\alpha}\sin(j\theta)$, we would expect a decay rate of $\alpha - 1$.

Example (Wavelet basis)

Layered wavelets $\psi_j(\theta)$; scaled such that $\|\psi_j\|_\infty \sim 2^{-\alpha l(j)}$.
Decay rate $\alpha - 1$ as well.

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Localized supports

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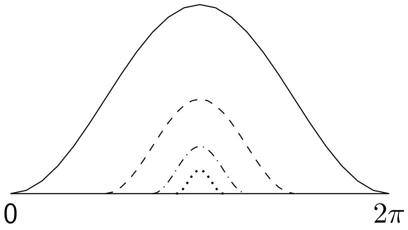

$\|\cdot\|_\infty$ does not represent the 'size' accurately.

$$\Downarrow$$

Intuitively, the $\|\cdot\|_\infty$-bound is a restrictive convergence result.

Wavelets

Example (Wavelet basis)

We take a basis with layered wavelets $\psi_j(\theta)$; each layer consisting of double the number of wavelets with half the support.
Decay rate $\alpha - 1$ as well.

$\|\cdot\|_\infty$ does not represent the 'size' accurately.

$$\Downarrow$$

Intuitively, the $\|\cdot\|_\infty$-bound is a restrictive convergence result.

Motivated by [**Bachmayr et al., 2017**] we close this gap:

- Finding a pointwise bound instead of $\|\cdot\|_\infty$ bound
- Supported by numerical evidence

Note: For generic mapping, closely related to **[Diss. ETHZ Zech, 2018]**

General result

Assumption

The transformation $\Phi(\hat{\boldsymbol{x}};\boldsymbol{y})$ is such that, for an affine boundary expansion we have an affine mapping expansion:

$$\Phi(\hat{\boldsymbol{x}};\boldsymbol{y}) = \hat{\boldsymbol{x}} + \sum_{j\geq 1} y_j \Phi_j(\hat{\boldsymbol{x}}).$$

Theorem – informal (van Harten, Scarabosio '23)

If there exists $(\rho_j)_{j\in\mathbb{N}}$, $\rho_j > 1$, $(\rho_j^{-1})_{j\in\mathbb{N}} \in \ell^q(\mathcal{F})$ and the series $\sum_{j\geq 1} \rho_j \left[\|\Phi_j\|(\hat{\boldsymbol{x}}) + \|\mathrm{D}_x \Phi_j\|_{2,2}(\hat{\boldsymbol{x}})\right] < K_T$ for all $\hat{\boldsymbol{x}} \in \hat{D}$,

then the Taylor coefficients $\|t_\mu\|_{H_0^1(\hat{D})}$ converge with rate $\frac{1}{p} = \frac{1}{q} - \frac{1}{2}$.

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Example (Wavelet basis)

Layered wavelets $\psi_j(\theta)$; scaled such that $\|\phi_j\|_\infty \sim 2^{-\alpha l(j)}$.

Bounding $\|\phi_j\|(\hat{\boldsymbol{x}}) + \|\mathrm{D}_x\Phi_j\|_{2,2}(\hat{\boldsymbol{x}})$ *pointwise* $\rightsquigarrow$ Decay rate $\alpha - \frac{1}{2}$
.

Mollfier mapping

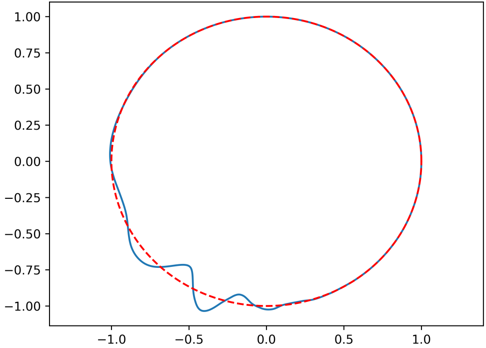
Mapping Φ can, for example, be a *linear mollifier*

$$\Phi(\hat{\boldsymbol{x}};\boldsymbol{y}) = \hat{\boldsymbol{x}} + \chi(\hat{\boldsymbol{x}})\left(r(\theta_{\hat{\boldsymbol{x}}},\boldsymbol{y}) - r_0(\theta_{\hat{\boldsymbol{x}}})\right)\frac{\hat{\boldsymbol{x}}}{\|\hat{\boldsymbol{x}}\|}$$

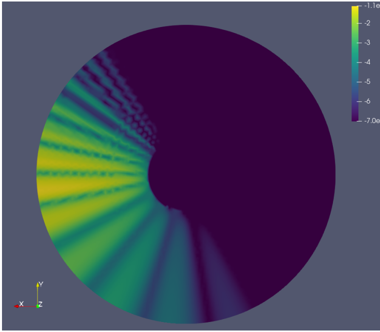
- explicit transformation
- radial dependence on boundary values
- only as smooth as the wavelet $\psi_j(\theta)$

Hence, we can estimate the convergence of $(\| \mathrm{D}_x \Phi_j \|_{2,2}(\hat{\boldsymbol{x}}))_{j\geq 1}$.

Single-wavelet domain – Mollifier mapping



Exaggerated single-wavelet effect on domain.



Logarithm of $\| \mathrm{D}_x \Phi_j \|_{2,2}(\hat{\boldsymbol{x}})$

Clear locality properties of Φ_j

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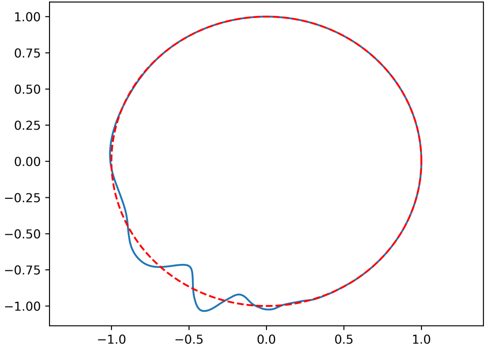

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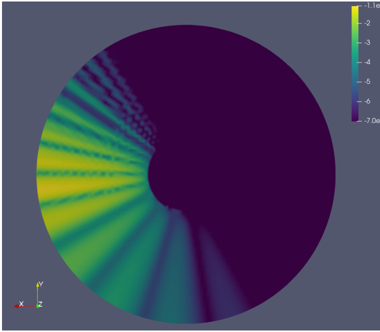

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Conclusion – Mollifier mapping

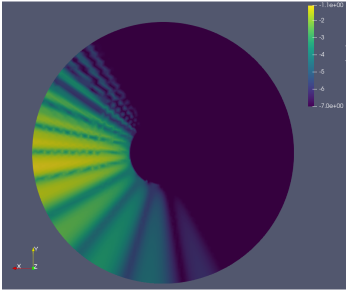
Then, we have, on the boundary

$$\sum_{j\geq 1} \| \mathrm{D}_x \Phi_j \|_{2,2}(\hat{\boldsymbol{x}})$$

$$= \sum_{\text{all layers}} \underbrace{\sum_{\text{single layer}} \| \mathrm{D}_x \Phi_j \|_{2,2}(\hat{\boldsymbol{x}})}_{\text{Locality properties of Wavelets}}$$

$$\leq \sum_{\text{all layers}} C_1 2^{-\alpha l}.$$

$\Longrightarrow$ provable convergence properties.



- Academic example

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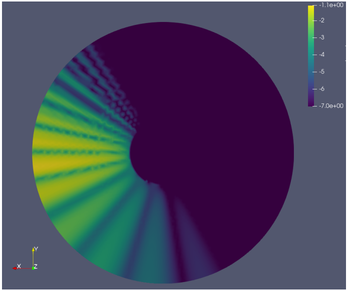


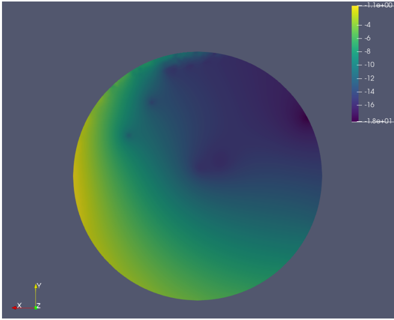
PDE based mapping

- Define mapping through Laplace equation

$$\begin{cases} \Delta\Phi = 0 & \text{in } D \\ \Phi = r_0 + \sum_{j\geq 1} \psi_j y_j & \text{on } \partial D \end{cases}$$

with partial transformations

$$\begin{cases} \Delta\Phi_j = 0 & \text{in } D \\ \Phi_j = \psi_j & \text{on } \partial D \end{cases}$$



Logarithm of $\|\mathrm{D}_x\Phi_j\|_{2,2}(\hat{\boldsymbol{x}})$ for Harmonic mapping.

- Smoother transformation $\implies$ better convergence properties
- Difficult to bound $\|\mathrm{D}_x\Phi_j\|_{2,2}(\hat{x})$ $\implies$ difficult to prove rigorously

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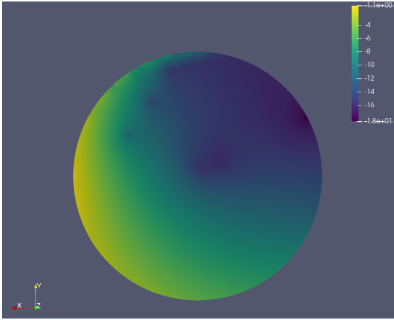

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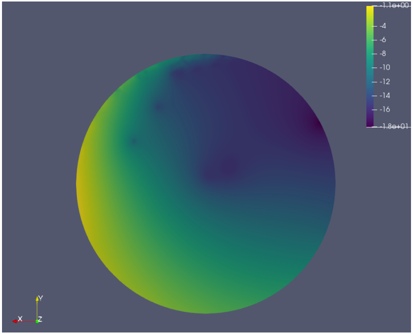
No radial dependence (log scale)

$\log(\| \mathrm{D}_x \Phi_j \|_{2,2}(\hat{\boldsymbol{x}}))$
Harmonic mapping mapping



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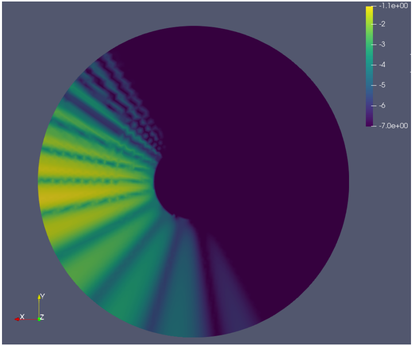
Mollifier mapping



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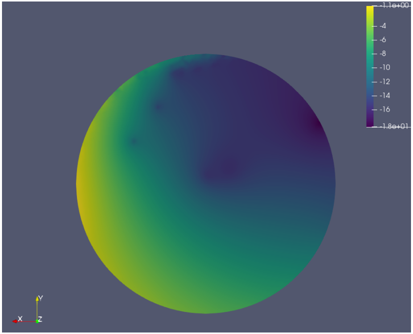

- 'By eye' similar summability properites hold
- No locality of $\| \mathrm{D}_x \Phi_j \|_{2,2}(\hat{\boldsymbol{x}})$
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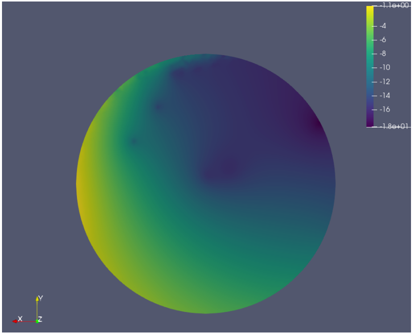

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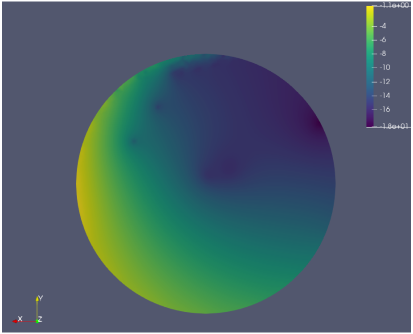

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Summability Harmonic mapping

Alternative approach for Harmonic mapping:

Use the **maximum principle** for weakly subharmonic functions to move to the boundary on the unit disk D, we solve

$$\begin{cases} \Delta\Phi_j = 0 & \text{in } D \\ \Phi_j = \psi_j & \text{on } \partial D \end{cases}$$

by separation of variables to obtain, at the boundary of D,

$$\| \mathrm{D}_x \Phi_j \|_{2,2}^2 = (\psi_j'^2 + \mathcal{H}(\psi_j')^2)^{\frac{1}{2}} = |\psi_j' + \mathcal{H}(\psi_j')i| = A(\psi_j')$$

where $\mathcal{H}$ is the *Hilbert transform* (DtN), such that $A(\psi_j')$ denotes the *Analytic envelope* of ψ_j'.

Conclusion – Harmonic mapping

Then, we have, at the boundary

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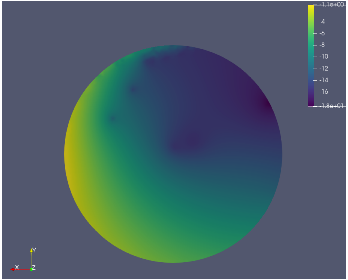
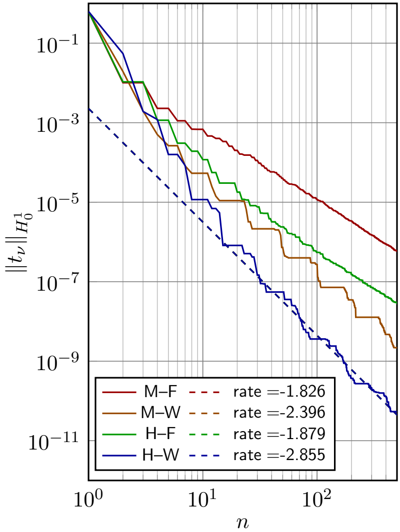


Numerical results ($\alpha = 3$)

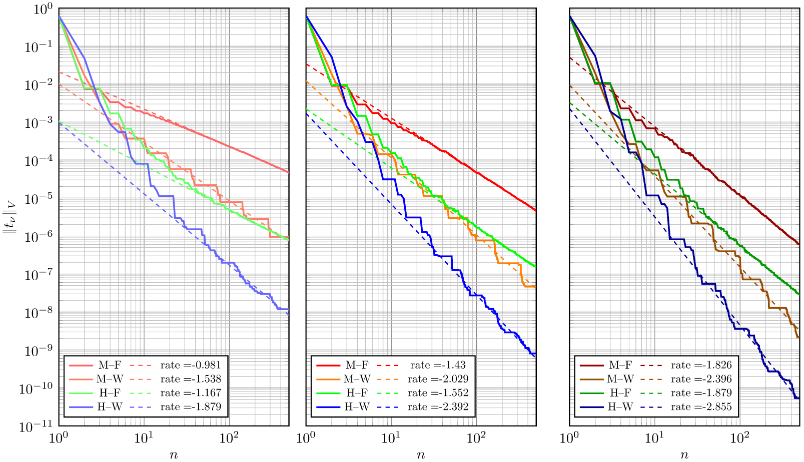


Coefficients calculated using Alternating Greedy Algorithm in Python, with Dolfinx, Gmsh, and PETSc.

$\vartheta = 5\%$ Max shape variation
mesh size to resolve Φ

Mollifier (M)
Harmonic (H)
Fourier (F)
Wavelet (W)

Effect persists for different α



(a) $\alpha = 2$ (b) $\alpha = 2.5$ (c) $\alpha = 3$

Spatial convergence, Wavelet expansion

	$h = 4$		$h = 2$		$h = 1$		$h = 1/2$
ϑ	M	H	M	H	M	H	H
4%	2.512	2.376	2.457	2.629	2.409	2.867	2.944
8%	2.341	2.496	2.320	2.729	2.408	2.858	2.877
16%	2.431	2.491	2.421	2.629	2.376	2.700	2.720
32%	2.200	2.369	2.194	2.489	2.193	2.507	2.507

Rate degenerates for larger shape variations.
For fine meshes, harmonic extension outperforms theoretical rate.
Rates for harmonic mapping more sensitive to mesh size.

Remarks and conclusion

- Main result is more general than shape; extension to 'nice' $A(\boldsymbol{y})$, $f(\boldsymbol{y})$.
- Compactness of supports not required, *localization* is enough.
- Different surrogates potentially benefit.

Take home message:

- *L*ocalized supports improve convergence rate of polynomial expansion.

Thank you for your attention!

W. van Harten, L. Scarabosio, *Exploiting locality in sparse polynomial approximation of parametric elliptic PDEs and application to parameterized domains.* arXiv:2308.06188.