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Innovative Approaches to the Numerical Approximation of PDEs

Organized by
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Abstract. This workshop was about the numerical solution of PDEs for which classical approaches, such as the finite element method, are not well suited or need further (theoretical) underpinnings. A prominent example of PDEs for which classical methods are not well suited are PDEs posed in high space dimensions. New results on low rank tensor approximation for those problems were presented. Other presentations dealt with regularity of PDEs, the numerical solution of PDEs on surfaces, PDEs of fractional order, numerical solvers for PDEs that converge with exponential rates, and the application of deep neural networks for solving PDEs.

Mathematics Subject Classification (2010): 65Mxx, 65Nxx, 35Jxx, 35Kxx, 46E35, 65Dxx.

Introduction by the Organizers

The workshop *Innovative Approaches to the Numerical Approximation of PDEs* was organised by Stephan Dahlke (Marburg), Gitta Kutyniok (Berlin), Ricardo Nochetto (Maryland), and Rob Stevenson (Amsterdam). The meeting was attended by 47 participants from 9 countries. Unfortunately, it turns out that Ricardo Nochetto was not able to attend the meeting.

Numerical approximation of PDEs is one of the central areas of computational mathematics, stimulated by the multitude of applications of PDEs in mathematical models in the sciences, engineering and economics. There is a rich arsenal of numerical techniques for PDEs, including finite difference methods, finite element methods, finite volume methods, spectral methods, and wavelet methods, to name

just a few. The finite element method (FEM), in particular, has been successfully applied to linear and nonlinear PDEs in, typically, conservative form, that arise in continuum mechanics, such as the fundamental partial differential equations of solid and fluid mechanics. Some of the noteworthy features of finite element methods include their applicability to a wide class of problems, their convenience in terms of the use of locally refined computational grids and local variation of the polynomial degree in the finite element space, their flexibility in representing computational domains possessing complicated geometries, and their solid theoretical foundation.

There are, however, areas where the finite element theory needs further developments, or where the finite element approach is less suited or even not applicable at all. Exactly those topics were the focus of the workshop.

Examples where the theory needs further developments include (adaptive) hp finite element methods, or other numerical methods that can provide exponential convergence rates, and the convergence theory of (h-)adaptive finite element methods for non-elliptic PDEs.

Ultimately the convergence of any numerical solution method hinges on a certain type of regularity of the exact solution of the PDE. This is a very well studied question for elliptic PDEs, but less is known for e.g. nonlinear PDEs and parabolic PDEs, whereas for low rank tensor approximation methods it is even less clear what kind of regularity is required to guarantee favourable rates.

Other examples where numerical solution techniques are currently under development include PDEs on possibly moving interfaces, and PDEs of fractional order. A currently emerging field is that of the simultaneous space-time discretisation methods of evolutionary PDEs, as an alternative for the classical time marching schemes. Advantages of the space-time methods include the possibility of a massively parallel implementation, and the potential for space-time adaptive refinements that provide optimal convergence rates.

A nowadays very important area where classical numerical methods as the finite element method are not applicable are PDEs in very high space dimensions, as they arise in e.g. quantum chemistry or as reformulations of stochastic PDEs as deterministic PDEs with many or even infinitely many parameters. For those problems low rank tensor approximation methods and model order reduction methods are in the center of interest.

Finally, deep neural networks are rapidly emerging in many fields of science and technology. Restricting to solving PDEs they seem to have the largest potential for 'difficult' problems where classical methods are known to fail, in particular PDEs in high space dimensions.

The workshop features 27 talks. Highlights of the presentations include:

- **Reduced modeling for state estimation:** Wolfgang Dahmen discussed approximating the solution of a parametric PDE where the parameters are unknown, but where instead information on the solution is available in the form of values of m linear functionals. He demonstrated that a quasi-optimal approximation of the solution is possible from a reduced

basis space V_n when the angle between V_n and the span of the Riesz representers of the measurement functionals is under control.

- **Numerical solution of surface Stokes equations:** Arnold Reusken presented a surface analogy of the Taylor-Hood mixed finite element method for solving the Stokes equations. Main issues are the enforcement of the tangential flow constraint, which is realised by replacing the surface PDE by a PDE on the ambient space while penalising normal components of the velocity, and a sufficiently accurate approximation of the surface. The latter is realized by defining the trial spaces as traces of finite element spaces in the ambient space while adding an appropriate stabilisation term to control instabilities caused by exceptionally small cuts of the finite element with the surface.
- ***hp*-fem for the fractional Laplacian:** Since the work of Caffarelli and Silvestre it is known that the solution of the (spectral) fractional Laplace equation on a two-dimensional polygon Ω can be obtained as a boundary trace of the solution of a degenerate elliptic second order PDE on the cylinder $\Omega \times (0, \infty)$. Markus Melenk presented a very carefully designed hp-fem discretisation w.r.t. geometrically refined tensor meshes with which the solution can be approximated at an exponential rate.
- **Empirical risk minimization over deep neural networks overcomes the curse of dimensionality in the numerical approximation of Kolmogorov equations:** In this talk, Julius Berner explained how ideas from deep learning can be applied to the numerical treatment of high-dimensional PDEs. The approach applies to PDEs that admit a statistical interpretation in the sense of Kolmogorow equations. Then, one can reformulate the numerical solution of the Kolmogorow equation as a classical statistical learning problem. It seems that by proceeding this way one can overcome the curse of dimensionality to some extent, at least it is possible to go up to dimensions where even modern tensor approximation schemes fail.
- **Higher regularity of the p-Poisson equation in the plane:** In this talk, Lars Diening presented new regularity results of the solutions to nonlinear elliptic PDEs, i.e., the p-Poisson equations, in specific Besov and Triebel-Lizorkin spaces. This kind of regularity determines the approximability of solutions by means of adaptive finite elements. The proofs are based on the fact that it is possible to transfer the local Besov and Triebel-Lizorkin regularity up to first order derivatives from the force to the flux.

The gained scientific knowledge can be summarized as follows. For high-dimensional problems, low rank tensor approximations schemes demonstrated their very high potential. The theory is still not completely developed and will be the topic of further researches. Fractional PDEs will probably be one of the hot topics in the future. Some important progress has been achieved, but there seems to be

an urgent need for alternative discretization schemes beyond, e.g., the Caffarelli-Sylvestre approach. A quite positive surprise was the fact that even in the well-established field of adaptive finite element methods new and important challenges showed up, in particular concerning adaptive *hp*- finite element and their possibly exponential convergence. For the numerical solution of geometric PDEs such as equations on possibly moving surfaces several competing approaches have been presented that differ in the way the surface is approximated, and whether the PDE posed on the surface is extended to a (small) neighbourhood in the ambient space or not. A new aspect that came into play was the application of deep learning for the numerical approximation of PDEs. This will probably also one of the hot topics in the future. Current numerical experiments are quite impressive, but the theoretical foundation of this approach is still in its infancy.

During this workshop there have been many lively discussions in a good atmosphere. The organisers would like to take the opportunity to thank MFO for providing support and a very inspiring environment for the workshop.

Acknowledgement: The MFO and the workshop organizers would like to thank the National Science Foundation for supporting the participation of junior researchers in the workshop by the grant DMS-1641185, "US Junior Oberwolfach Fellows".

Workshop: Innovative Approaches to the Numerical Approximation of PDEs

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Abstracts

Analysis of tensor approximation schemes for continuous functions

Helmut Harbrecht
(joint work with Michael Griebel)

1. Introduction

We analyze tensor approximation schemes for continuous functions. We assume that the function to be approximated lies in an isotropic Sobolev space and discuss the cost when approximating this function in the continuous analogue of the Tucker tensor format or of the tensor train format. We especially show that the cost of both approximations are dimension-robust when the Sobolev space under consideration provides appropriate dimension weights.

2. Tucker tensor format

2.1. **Continuous Tucker decomposition.** We consider a product domain which consists of m different domains $\Omega_j \subset \mathbb{R}^{n_j}$, $j = 1, \ldots, m$. For given $f \in L^2(\Omega_1 \times \cdots \times \Omega_m)$ and $j \in \{1, 2, \ldots, m\}$, we apply the singular value decomposition to separate the variables $\boldsymbol{x}_j \in \Omega_j$ and

$$(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{j-1}, \boldsymbol{x}_{j+1}, \ldots, \boldsymbol{x}_m) \in \Omega_1 \times \cdots \times \Omega_{j-1} \times \Omega_{j+1} \times \cdots \times \Omega_m.$$

We hence get

$$f(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{j-1}, \boldsymbol{x}_j, \boldsymbol{x}_{j+1}, \ldots, \boldsymbol{x}_m) = \sum_{\alpha_j=1}^{\infty} \sqrt{\lambda_j(\alpha_j)}\varphi_j(\boldsymbol{x}_j, \alpha_j)\psi_j(\alpha_j, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{j-1}, \boldsymbol{x}_{j+1}, \ldots, \boldsymbol{x}_m),$$

where the left eigenfunctions $\{\varphi_j(\alpha_j)\}_{\alpha_j \in \mathbb{N}}$ form an orthonormal basis in $L^2(\Omega_j)$. Consequently, if we iterate over all $j \in \{1, 2, \ldots, m\}$, this yields an orthonormal basis $\{\varphi_1(\alpha_1) \otimes \cdots \otimes \varphi_m(\alpha_m)\}_{\boldsymbol{\alpha} \in \mathbb{N}^m}$ of $L^2(\Omega_1 \times \cdots \times \Omega_m)$, and we arrive at the representation

$$f(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m) = \sum_{|\boldsymbol{\alpha}|=1}^{\infty} \omega(\boldsymbol{\alpha})\varphi_1(\alpha_1, \boldsymbol{x}_1) \cdots \varphi_m(\alpha_m, \boldsymbol{x}_m).$$

The tensor $\big[\omega(\boldsymbol{\alpha})\big]_{\boldsymbol{\alpha} \in \mathbb{N}^m}$ is the *core tensor*, where a single coefficient is given by

$$\omega(\alpha_1, \ldots, \alpha_m) = \int_{\Omega_1 \times \cdots \times \Omega_m} f(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m)\varphi_1(\alpha_1, \boldsymbol{x}_1) \cdots \varphi_m(\alpha_m, \boldsymbol{x}_m)\, \mathrm{d}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m).$$

Theorem 1. *Let $f \in H^k(\Omega_1 \times \cdots \times \Omega_m)$ and choose the ranks according to $r_j = \varepsilon^{-n_j/k}$ for all $j = 1, \ldots, m$. Then, the truncation error of the truncated Tucker decomposition is*

$$\left\| f - f^{TF}_{r_1,\ldots,r_m} \right\|_{L^2(\Omega_1 \times \cdots \times \Omega_m)} \lesssim \sqrt{m}\varepsilon,$$

while the cost of the core tensor are $\prod_{j=1}^m r_j = \varepsilon^{-(n_1+\cdots+n_m)/k}$.

2.2. **Sobolev spaces with dimension weights.** The cost of the core tensor of the Tucker decomposition exhibit the curse of dimension as the number m of subdomains increases. Nonetheless, in case of Sobolev spaces with dimension weights, the curse of dimension can be beaten.

For sake of simplicity, we assume that all subdomains are identical to a single domain $\Omega \subset \mathbb{R}^n$ of dimension n. Moreover, we assume Sobolev spaces with dimension weights by means of the property

$$\left\| \frac{\partial^k f}{\partial \boldsymbol{x}_j^{\boldsymbol{\beta}}} \right\|_{L^2(\Omega^m)} \lesssim \gamma_j^k \|f\|_{H^k(\Omega^m)} \text{ for all } |\boldsymbol{\beta}| = k \text{ and } j = 1, 2, \ldots, m. \tag{1}$$

It turns out that algebraically decaying weights (2) are sufficient to beat the curse of dimension in case of the Tucker tensor decomposition.

Theorem 2. *Let $f \in H^{k+n}(\Omega^m)$. Choose $\delta > 0$ and assume that the weights in (1) decay like*

$$\gamma_j \lesssim j^{-(1+\delta')/k} \text{ for some } \delta' > \delta + \frac{k}{n}, \tag{2}$$

and choose the ranks in accordance with

$$r_j = \left\lceil \gamma_j^n j^{(1+\delta)n/k} \varepsilon^{-n/k} \right\rceil.$$

Then, the error of the continuous Tucker decomposition is of order ε while the complexity of the core tensor stays bounded independent of the dimension m.

3. Tensor train format

3.1. **Continuous tensor train decomposition.** For the discussion of the continuous tensor train decomposition, we should assume that the domains $\Omega_j \subset \mathbb{R}^{n_j}$, $j = 1, \ldots, m$, are arranged in such a way that it holds $n_1 \leq \cdots \leq n_m$.

Now, consider $f \in H^k(\Omega_1 \times \cdots \times \Omega_m)$ and separate the variables $\boldsymbol{x}_1 \in \Omega_1$ and $(\boldsymbol{x}_2, \ldots, \boldsymbol{x}_m) \in \Omega_2 \times \cdots \times \Omega_m$ by the singular value decomposition

$$f(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n) = \sum_{\alpha_1=1}^{\infty} \sqrt{\lambda_1(\alpha_1)} \varphi_1(\boldsymbol{x}_1, \alpha_1) \psi_1(\alpha_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_m).$$

Since

$$\left[\sqrt{\lambda_1(\alpha_1)} \psi_1(\alpha_1) \right]_{\alpha_1=1}^{\infty} \in \ell^2(\mathbb{N}) \otimes L^2(\Omega_2 \times \cdots \times \Omega_m),$$

we can separate $(\alpha_1, \boldsymbol{x}_2) \in \mathbb{N} \times \Omega_2$ from $(\boldsymbol{x}_3, \dots, \boldsymbol{x}_m) \in \Omega_3 \times \cdots \times \Omega_m$ by means of a second singular value decomposition and arrive at

$$\begin{aligned}\Big[\sqrt{\lambda_1(\alpha_1)}\psi_1(\alpha_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_m)\Big]_{\alpha_1=1}^{\infty} \\ = \sum_{\alpha_2=1}^{\infty} \sqrt{\lambda_2(\alpha_2)}\Big[\varphi_2(\alpha_1, \boldsymbol{x}_2, \alpha_2)\Big]_{\alpha_1=1}^{\infty} \psi_2(\alpha_2, \boldsymbol{x}_3, \dots, \boldsymbol{x}_m).\end{aligned}$$

By repeating the last step and successively separating $(\alpha_{j-1}, \boldsymbol{x}_j) \in \mathbb{N} \times \Omega_j$ from $(\boldsymbol{x}_{j+1}, \dots, \boldsymbol{x}_m) \in \Omega_{j+1} \times \cdots \times \Omega_m$ for $j = 3, \dots, m-1$, we finally arrive at the representation

$$\begin{aligned}f(\boldsymbol{x}_1, \dots, \boldsymbol{x}_m) = \sum_{\alpha_1=1}^{\infty} \cdots \sum_{\alpha_{m-1}=1}^{\infty} \varphi_1(\alpha_1, \boldsymbol{x}_1)\varphi_2(\alpha_1, \boldsymbol{x}_2, \alpha_2) \\ \cdots \varphi_{m-1}(\alpha_{m-2}, \boldsymbol{x}_{m-1}, \alpha_{m-1})\varphi_m(\alpha_{m-1}, \boldsymbol{x}_m),\end{aligned}$$

where

$$\varphi_m(\alpha_{m-1}, \boldsymbol{x}_m) = \sqrt{\lambda_{m-1}(\alpha_{m-1})}\psi_{m-1}(\alpha_{m-1}, \boldsymbol{x}_m).$$

In contrast to the Tucker format, we do not obtain a huge core tensor since each of the $m-1$ singular value decompositions of the tensor train decomposition removes the actual first spatial domain from the approximant. We just obtain a product of *matrix*-valued functions (except for the first and last factor which are vector-valued functions), each of which is related with a specific domain Ω_j. This especially results in only $m-1$ sums in contrast to the m sums for the Tucker format.

Theorem 3. *Let $f \in H^{k+\max\{n_1,\dots,n_m\}}(\Omega_1 \times \cdots \times \Omega_m)$. Then, the over-all truncation error of the tensor train decomposition with truncation ranks* (4) *is*

$$\|f - f^{TT}_{r_1,\dots,r_{m-1}}\|_{L^2(\Omega_1\times\cdots\times\Omega_m)} \lesssim \sqrt{m}\varepsilon.$$

The cost of the tensor train format are given by

$$r_1 + \sum_{j=2}^{m-1} r_{j-1}r_j = \varepsilon^{-n_1/k} + \varepsilon^{-(2n_1+n_2)/k} + \cdots + \varepsilon^{-(2n_1+\cdots+2n_{m-2}+n_{m-1})/k} \tag{3}$$

and hence are bounded by $\mathcal{O}(\varepsilon^{-(2m-1)\max\{n_1,\dots,n_{m-1}\}/k})$.

3.2. **Sobolev spaces with dimension weights.** Like for the Tucker decomposition, the cost of the tensor train decomposition suffer from the curse of dimension as the number m of subdomains increases. We therefore consider again appropriately Sobelev spaces with dimension weights, where we assume that all subdomains are identical to a single domain $\Omega \subset \mathbb{R}^n$ of dimension n.

Theorem 4. *Let $f \in H^{k+n}(\Omega^m)$. Choose $\delta > 0$ and assume that the weights in* (1) *decay like* (2) *and choose the ranks successively in accordance with*

$$r_j = \lceil r_{j-1}\gamma_j^n j^{(1+\delta)n/k}\varepsilon^{-n/k}\rceil \tag{4}$$

if $j \leq M$ and $r_j = 0$ if $j > M$, where $M = \varepsilon^{-1/(1+\delta')}$. Then, the error of the continuous tensor train decomposition is of order ε while the complexity of the core tensor stays bounded independent of the dimension m.

References

[1] H. Harbrecht and M. Griebel, *Analysis of tensor approximation schemes for continuous functions*, arXiv e-prints (2019), arXiv:1903.04234.

New notions of numerical conditioning for multilevel tensor representations of differential operators

Markus Bachmayr
(joint work with Vladimir Kazeev)

By folding vectors of size 2^L into Lth-order tensors of mode sizes $2 \times \cdots \times 2$ and applying low-rank decomposition in the tensor train format to these tensors, one can obtain nonlinearly parametrized compressed representations or approximations. For instance, provided that the corresponding rank parameters remain bounded independently of L, the number of required coefficients in the tensor decomposition scales linearly in L and thus logarithmically with respect to the original number of degrees of freedom. This multilevel decomposition technique, also termed *quantized tensor trains* or *tensorization* in the literature, has been shown to result in highly efficient approximations when applied to grid vectors obtained for various classes of functions, including solutions of elliptic PDEs on nonsmooth domains [4] or with oscillatory data [3]. Such a tensor-structured approach is attractive because it leads to highly efficient, adaptive approximations based on simple uniform discretizations.

Standard choices of the underlying bases, such as piecewise multilinear finite elements on uniform tensor product grids, entail the well-known *matrix ill-conditioning* of discrete operators. In [1] we demonstrate that, for low-rank representations, the use of multilevel tensor structure for discretized differential operators itself additionally introduces *representation ill-conditioning*, a new effect specific to computations in tensor networks. The main difficulty here is that the action of such multilevel tensor decompositions of stiffness matrices on corresponding vector representations leads to higly redundant representations of result vectors that contain substantial cancellations; any further numerical manipulation of these result representations can then introduce extremely large deviations in the represented vectors. To quantify this effect, we introduce on the one hand notions of amplification factors and condition numbers of vector representations in tensor train form, and on the other hand a representation condition number of corresponding matrix representations. This latter representation condition number gives the smallest upper bound for the factor by which the application of the matrix representation can deteriorate the condition number of a vector representation. For the considered discretizations, we find this representation condition number to scale exactly as the usual matrix condition number, that is, as $\mathcal{O}(4^L)$.

These two condition numbers, however, are independent of each other: in particular, well-conditioned matrices can be given in ill-conditioned multilevel tensor representations.

As the main result of [1], we show how a careful construction of tensor decompositions of preconditioned matrices can be used to mitigate these issues. We first analyze the tensor structure of a BPX preconditioner for second-order linear elliptic operators and construct an explicit tensor-structured representation of the preconditioner, with ranks independent of the number L of discretization levels. The straightforward application of the preconditioner yields discrete operators whose matrix conditioning is uniform with respect to the discretization parameter, but in decompositions that suffer from unchanged representation ill-conditioning. By explicitly eliminating redundancies in the representations of the preconditioned discrete operators, we obtain reduced-rank decompositions that are free of both matrix and representation ill-conditioning. For an iterative solver based on soft thresholding of low-rank tensors analyzed in [2], we obtain convergence and complexity estimates and demonstrate its reliability and efficiency for discretizations with up to 2^{50} nodes in each dimension.

References

[1] M. Bachmayr and V. Kazeev, *Stability of low-rank tensor representations and structured multilevel preconditioning for elliptic PDEs*, arXiv Preprint arXiv:1802.09062 (2018).
[2] M. Bachmayr and R. Schneider, *Iterative methods based on soft thresholding of hierarchical tensors*, Found. Comput. Math. **17** (2017), 1037–1083.
[3] V. Kazeev, I. Oseledets, M. Rakhuba, and C. Schwab, *QTT-finite-element approximation for multiscale problems I: model problems in one dimension*, Adv. Comput. Math. **43** (2017), 411–442.
[4] V. Kazeev and C. Schwab, *Quantized tensor-structured finite elements for second-order elliptic PDEs in two dimensions*, Numerische Mathematik **138** (2018), 133–190.

Dynamical low rank approximation of random time dependent PDEs

Fabio Nobile

In this talk we consider time dependent PDEs with few random parameters and seek for an approximate solution in separable form that can be written, at each time instance, as a linear combination of a fixed number of linearly independent spatial functions multiplied by linearly independent random variables (low rank approximation). Since the optimal deterministic and stochastic modes can significantly change over time, we consider a dynamical approach where those modes are computed on the fly as solutions of suitable evolution equations. We discuss the construction of the method, present an existence result for the low rank approximate solution of a random semi-linear evolutionary equation of dissipative type, and introduce a possible unnumerical discretization of the low rank equations for which we can prove conditional stability.

Higher Regularity of the p-Poisson Equation in the Plane

Lars Diening
(joint work with Anna Kh. Balci, Markus Weimar)

In this work we are concerned with the regularity of solutions of the p-Laplace equation

$$-\operatorname{div}(A(\nabla u)) := -\operatorname{div}(|\nabla u|^{p-2}\nabla u) = -\operatorname{div} F$$

on a planar domain Ω. We focus in this work on the super-linear case $2 \le p < \infty$. We show that it is possible to transfer the local Besov and Triebel-Lizorkin regularity up to first order derivatives from the force F to the flux $A(\nabla u)$.

In particular, we show that if $s \in (0,1)$ and $\rho, q \in (0,\infty]$ are such that

$$2\left(\frac{1}{\rho} - \frac{1}{p'}\right)_+ < s < 1, \tag{1}$$

i.e., $\mathbf{B}^s_{\rho,q}(B) \hookrightarrow\hookrightarrow L^{p'}(B)$. Then for any ball B with $2B \subset \Omega$ there holds

$$|A(\nabla u)|_{\mathbf{B}^s_{\rho,q}(B)} \le c\,|F|_{\mathbf{B}^s_{\rho,q}(2B)} + \left(\frac{1}{|2B|}\int_{2B} |A(\nabla u) - \langle A(\nabla u)\rangle_{2B}|^{p'}\,dx\right)^{\frac{1}{p'}}. \tag{2}$$

If additionally $\rho < \infty$ and

$$d\left(\frac{1}{q} - \frac{1}{p'}\right)_+ < s < 1, \tag{3}$$

then the same estimate (2) holds true when $\mathbf{B}^s_{\rho,q}$ is replaced by $\mathbf{F}^s_{\rho,q}$.

This kind of regularity determines the approximability of solutions my means of the adaptive finite element method. The higher the differentiability s, the better it is possible to approximate a function by means of adaptivity.

The proof of the regularity transfer is based on the characterization of regularity by means of oscillation estimates. As a crucial ingredient we derive new almost linear decay estimates of the flux of a p-harmonic function. Such estimates are only possible in the super-linear case due to the limited regularity of p-harmonic functions. Our estimates rely on complex analysis and are therefore restricted to the plane.

The optimal regularity for p-harmonic functions for dimensions $d \ge 3$ is still a well known open problem. Based on the Kacanov iteration proposed in [1] we explain how to solve this problems numerically. So far we were able to recover the exponents of the planar case up to a relative error of 10^{-4} for $p \in [1.1, 10]$. The results for the 3D case will be presented in a future work.

References

[1] L. Diening, M. Fornasier, R. Tomasi, M. Wank, *A Relaxed Ka??anov Iteration for the p-Poisson Problem*, Numerische Mathematik (2019), accepted.

[2] A. Kh-Balci, L. Diening, M. Weimar, *Higher Order Calderón-Zygmund Estimates for the p-Laplace Equation*, Journal of Differential Equations (2019), accepted.

Sobolev and Besov regularity of parabolic PDEs

Cornelia Schneider
(joint work with Stephan Dahlke)

The talk is concerned with the regularity of solutions to linear and nonlinear evolution equations on nonsmooth domains. In particular, we study the smoothness in a specific scale of Besov spaces. It is known that in many cases the order of convergence of adaptive wavelet schemes depends on the regularity of the solution in these Besov spaces. On the other hand it is the fractional Sobolev regularity which determines the rate of convergence of non-adaptive (uniform) algorithms. Therefore, in order to justify the use of adaptive schemes for solving parabolic PDEs, an analysis of the regularity of the solution in the scale of Besov spaces and a comparison with its Sobolev regularity is needed.

We show that for all cases under consideration the Besov regularity is high enough to justify the use of adaptive algorithms. The talk is based on the papers [2] and [1].

References

[1] S. Dahlke and C. Schneider, *Besov regularity of parabolic and hyperbolic PDEs*, Anal. and Appl. **17** (2019), 235–291.
[2] S. Dahlke and C. Schneider, *Describing the singular behaviour of parabolic equations on cones in fractional Sobolev spaces*, GEM **9** (2018), 817–841.

Regularity and rate of approximation for obstacle problems for a class of integro-differential operators

Abner J. Salgado
(joint work with A. Bonito, J.P. Borthagaray, W. Lei, R.H. Nochetto)

We consider the finite element approximation of a nonlocal obstacle problem. Let $\Omega \subset \mathbb{R}^n$ be a bounded, Lipschitz domain. We seek for $u : \mathbb{R}^n \to \mathbb{R}$ that satisfies

$$\min\{-b\Delta u + \beta \cdot \nabla u + (-\Delta)^s u - f, u - \chi\} = 0, \quad \text{in } \Omega, \qquad u = 0, \quad \text{in } \Omega^c. \tag{1}$$

Here $b \in \mathbb{Z}_2$, β is a sufficiently smooth and solenoidal vector field, f is a given and sufficiently smooth source term, and χ is an obstacle which we assume satisfies the condition $\chi < 0$ on $\partial\Omega$. By $(-\Delta)^s$ we mean the *integral fractional Laplacian* of order $s \in (0, 1)$, which is given by

$$(-\Delta)^s w(x) = c_{n,s} v.p. \int_{\mathbb{R}^d} \frac{w(x) - w(y)}{|x - y|^{n+2s}} dy, \qquad c_{n,s} = \frac{2^{2s}\Gamma\left(s + \frac{n}{2}\right)}{\pi^{n/2}\Gamma(1 - s)}$$

The study of (1) is motivated by optimal stopping time problems [PS06] for stochastic processes with Lévy jumps; a model for American options [CT04].

Case $b = 0$, $\beta = 0$. In [BNS18] we consider the obstacle problem for the integral fractional Laplacian. One of the main difficulties in the numerical approximation of problems involving the integral fractional Laplacian is its lack of regularity. As [VÈ65, Gru15] shows, if Ω is C^∞, and $g \in L^2(\Omega)$, then Φ_g, solution of

$$(-\Delta)^s \Phi_g = g, \quad \text{in } \Omega, \qquad \Phi_g = 0, \quad \text{in } \Omega^c, \tag{2}$$

satisfies $\Phi_g \in H^{\min\{2s, s+1/2-\epsilon\}}(\Omega)$. This is result is sharp [Get61].

We extend the regularity results on weighted Sobolev spaces for the linear case of [AB17], which in turn rely on the Hölder estimates of [ROS14], to the obstacle problem. Define, for $\theta \in (0,1)$ and $\alpha \geq 0$ the weighted Sobolev norm

$$\|w\|_{\tilde{H}^{1+\theta}_\alpha(\Omega)} = \|w\|^2_{H^1_\alpha(\Omega))} + \iint_{\mathbb{R}^n \times \mathbb{R}^n} \frac{|\nabla w(x) - \nabla w(y)|^2}{|x-y|^{n+2\theta}} \delta(x,y)^{2\theta} dxdy,$$
$$\text{with } \delta(x,y) = \min\{dist(x, \partial\Omega), dist(y, \partial\Omega)),$$
$$\text{and } \|w\|_{H^1_\alpha(\Omega))} = \|(w + \nabla w) dist(\cdot, \partial\Omega)^\alpha\|_{L^2(\Omega)}.$$

Theorem 1 (regularity)**.** *Let $u \in \tilde{H}^s(\Omega)$ solve (1) with $b = 0$ and $\beta = 0$. Then*

$$\|u\|_{\tilde{H}^{1+s-2\epsilon}_{1/2-\epsilon}(\Omega)} \leq \frac{c}{\epsilon}.$$

In addition, the so-called Lagrange multiplier $\Lambda := (-\Delta)^s u - f \in C^{0,1-s}(\bar{\Omega})$.

The proof is by a nonstandard localization. Because of nonlocality, if η is a smooth cutoff function that equals one in a neighborhood of a point $z \in \Omega$ then $(-\Delta)^s(\eta w)(z) \neq (-\Delta)^s w(z)$. A correction term appears and must be dealt with.

This theorem lays the foundation for the numerical approximation of (1) with $b = 0$ and $\beta = 0$. In particular, in two dimensions, one can consider a finite element space V_h of piecewise linears over a shape regular simplicial mesh $\tau_h = \{T\}$ that is graded according to the rule

$$h_T \approx \begin{cases} h^2, & T \cap \partial\Omega \neq \emptyset, \\ h \cdot dist(T, \partial\Omega)^{1/2}, & T \cap \partial\Omega = \emptyset. \end{cases} \tag{3}$$

Here $h > 0$ is a parameter. Note that $\#\tau_h \approx h^{-2} |\log h|$.

Theorem 2 (error estimate)**.** *Let $u \in \tilde{H}^s(\Omega)$ solve (1) with $b = 0$ and $\beta = 0$. Let $u_h \in V_h$ be its finite element approximation where V_h is constructed over a mesh that is graded and satisfies (3). Then we have the following error estimate.*

$$\|u - u_h\|_{\tilde{H}^s(\Omega)} \leq ch |\log h|.$$

We comment that the proof of this result contains two key steps. First, the properties of the positivity preserving interpolation operator of [CN00] need to be extended to fractional Sobolev spaces using the localization results of [Fae00, Fae02]. Second, a subtle interplay between the complementarity conditions and growth conditions on the solution and Lagrange multiplier must be used.

We conclude by mentioning that our regularity results, and thus the finite element error estimates, apply to more general integral operators of convolution type, provided that they satisfy suitable ellipticity conditions.

Case $b = 0$, $\beta \neq 0$. In [BLS19] we analyze the remaining cases. For $s \geq \frac{1}{2}$ we studied the fractional Laplacian with drift. Note that the fractional Laplacian is an operator of order $2s$, so that for $s > \frac{1}{2}$ the drift is a compact perturbation of it. This is enough to conclude well posedness. In the case $s = \frac{1}{2}$ the operators are of the same order, so a smallness condition must be imposed on the drift.

A bootstrapping argument allows us to show that, if Ω is C^∞ the linear problem: Given g find $\Phi_g \in \tilde{H}^s(\Omega)$ that solves

$$(-\Delta)^s \Phi_g + \beta \cdot \nabla \Phi_g = g, \quad \text{in } \Omega, \qquad \Phi_g = 0, \quad \text{in } \Omega^c$$

has the same regularity as the solution to (2). This will be used when studying the regularity of the solution to (1) in this case.

Case $b \neq 0$. To study the full problem we must consider first the regularity of the linear problem. In [BLS19] we showed the following result.

Theorem 3 (regularity)**.** *Let $g \in L^2(\Omega)$ and $\Phi_g \in H^1_0(\Omega)$ solve*

$$-\Delta \Phi_g + (-\Delta)^s \Phi_g + \beta \cdot \nabla \Phi_g = g, \quad \textit{in } \Omega, \qquad \Phi_g = 0, \quad \textit{in } \Omega^c.$$

Then $\Phi_g \in H^\mu(\Omega)$ with $\mu = 2$ if $s < \frac{3}{4}$ and $\mu = \frac{7}{2} - 2s - \epsilon$ otherwise.

We do not know if this result is sharp for $s \geq \frac{3}{4}$.

A penalization argument, that follows the techniques of [KS00] allows us to carry these results to the obstacle problem. Thus, we can show.

Theorem 4 (error estimate)**.** *Let $u \in \tilde{H}^s(\Omega)$ solve (1) with $s \geq \frac{1}{2}$ if $b = 0$. Assume that $u_h \in V_h$ is its finite element approximation over a space V_h of piecewise linears constructed on a quasiuniform mesh. In the setting of Theorem 3 we have*

$$\|u - u_h\|_{\tilde{H}^s(\Omega)} + b\|u - u_h\|_{H^1_0(\Omega)} \leq c h^{\min\{\sigma, 3/2 - s - \epsilon\}} |\log h|,$$

where

$$\sigma = \begin{cases} \frac{1}{2} - \epsilon, & b = 0, \\ \min\left\{1, \frac{5}{2} - 2s - \epsilon\right\}, & b = 1. \end{cases}$$

In computations, the bilinear form of the fractional Laplacian can be treated as in [BLP19].

References

[AB17] G. Acosta and J.P. Borthagaray. A fractional Laplace equation: Regularity of solutions and finite element approximations. *SIAM J. Numer. Anal.*, 55(2):472–495, 2017.

[BLP19] A. Bonito, W. Lei, and J.E. Pasciak. Numerical approximation of the integral fractional Laplacian. *Numer. Math.*, 142(2):235–278, 2019.

[BLS19] A. Bonit, W. Lei, and A. J. Salgado. Finite element approximation of an obstacle problem for a class of integro-differential operators. ESAIM:M2AN (accepted), 2019.

[BNS18] J. P. Borthagaray, R. H. Nochetto, and A. J. Salgado. Weighted sobolev regularity and rate of approximation of the obstacle problem for the integral fractional Laplacian. arXiv:1806.08048, 2018.

[CN00] Z. Chen and R.H. Nochetto. Residual type a posteriori error estimates for elliptic obstacle problems. *Numer. Math.*, 84(4):527–548, 2000.

[CT04] R. Cont and P. Tankov. *Financial modelling with jump processes*. Chapman & Hall/CRC Financial Mathematics Series. Chapman & Hall/CRC, Boca Raton, FL, 2004.

[Fae00] B. Faermann. Localization of the Aronszajn-Slobodeckij norm and application to adaptive boundary element methods. I. The two-dimensional case. *IMA J. Numer. Anal.*, 20(2):203–234, 2000.

[Fae02] B. Faermann. Localization of the Aronszajn-Slobodeckij norm and application to adaptive boundary element methods. II. The three-dimensional case. *Numer. Math.*, 92(3):467–499, 2002.

[Get61] R. K. Getoor. First passage times for symmetric stable processes in space. *Trans. Amer. Math. Soc.*, 101:75–90, 1961.

[Gru15] G. Grubb. Fractional Laplacians on domains, a development of Hörmander's theory of μ-transmission pseudodifferential operators. *Adv. Math.*, 268:478–528, 2015.

[KS00] David Kinderlehrer and Guido Stampacchia. *An introduction to variational inequalities and their applications*, volume 31 of *Classics in Applied Mathematics*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2000. Reprint of the 1980 original.

[PS06] G. Peskir and A. Shiryaev. *Optimal stopping and free-boundary problems*. Lectures in Mathematics ETH Zürich. Birkhäuser Verlag, Basel, 2006.

[ROS14] X. Ros-Oton and J. Serra. The Dirichlet problem for the fractional Laplacian: regularity up to the boundary. *J. Math. Pures Appl.*, 101(3):275 – 302, 2014.

[VÈ65] M. I. Višik and G. I. Èskin. Convolution equations in a bounded region. *Uspehi Mat. Nauk*, 20(3 (123)):89–152, 1965. English translation in *Russian Math. Surveys*, 20:86-151, 1965.

Stochastic subspace correction and fault tolerance

Peter Oswald

(joint work with Michael Griebel)

With the recent advent of petascale compute systems and exascale computers to arrive in the near future, there is tremendous parallel compute power available for huge parallel simulations. However, it is predicted that large parallel applications may suffer from faults as frequently as once every 30 minutes on future exascale platforms. Thus, for growing parallel computers there is the need to develop not just scalable and fast parallel algorithms but to make them fault-tolerant as well.

One particular idea to achieve fault-tolerance is to adapt and to apply results on stochastic subspace correction methods which have recently gained a lot of attention for large-scale convex optimization, see [1, 6, 7]. The attractive feature of stochastic subspace correction schemes in this respect is the fact that hard faults such as compute node failure or communication losses (as long as they are detectable) can be modeled as a random process of selecting the set of acceptable subproblem solves in each iteration step. Depending on the communication structure of the compute network, the randomness and independence assumptions of the convergence theory developed in [2, 5] are fulfilled either ideally or approximately which ultimately leads to convergence guarantees also in a faulty setting. As illustration, and to test the theory in numerical simulations, in [5] we have used a standard overlapping domain decomposition (DD) method for the Poisson problem

as prototypical example of scalable and asymptotically optimal subspace correction methods for solving second-order elliptic PDE problems. In particular, our tests show that a larger amount of local storage and communication redundancy in a typical distributed DD implementation potentially improves the performance of the algorithm and makes it more robust in a faulty compute network.

In the talk, we have surveyed some of our work on stochastic subspace correction methods for solving symmetric and coercive variational problems in a separable Hilbert space V equipped with $a(\cdot,\cdot)$ as scalar product: For given $F \in V'$, find $u \in V$ such that

$$a(u,v) = F(v) \quad \forall v \in V. \tag{1}$$

The underlying *space splitting* is given by a collection of separable Hilbert spaces V_i with scalar products $a_i(\cdot,\cdot)$ (not necessarily subspaces of V), and bounded linear operators $R_i : V_i \to V$ such that their ranges span V, where i belongs to a certain index set I. Their adjoints $T_i = R_i^* : V \to V_i$ are given by solving subproblems in V_i:

$$a_i(T_i v, v_i) = a(v, R_i v_i) \qquad \forall\, v_i \in V_i. \tag{2}$$

In the m-th step of a prototypical stochastic subspace correction method for solving (1), for each $i \in I_m$ from a certain random finite index subset $I_m \subset I$ the corresponding subproblem (2) is solved with $v = e_u^{(m)} := u - u^{(m)}$, and an update of the form

$$u^{(m+1)} = \alpha_m u^{(m)} + \xi_m d_u^{(m)}, \qquad d_u^{(m)} := \sum_{i \in I_m} \omega_i R_i T_i e_u^{(m)}, \qquad m = 0, 1, \ldots, \tag{3}$$

is performed, where the relaxation parameters α_m, ξ_m are at our disposal, and ω_i are given scaling parameters. The recursion (3) basically represents a one-step method, we also considered two-step methods inspired by [6] for acceleration.

The convergence theory of such methods is usually cast in terms of the expectation $\mathbb{E}(\|e_u^{(m)}\|^2)$ of the squared error which controls both expectation and variance of the random error trajectory $\{e_u^{(m)}\}$. The results depend on the spectral properties of the positive operator $P := \sum_{i \in I} \omega_i R_i T_i : V \to V$, on assumptions on the distribution and independence of the index subsets I_m, and are qualitively different for finite and infinite I. For the case of infinite I which appears in applications to incremental approximation processes in infinite-dimensional V and online learning with kernels, the one-step method (3) was considered in [3, 4] under the assumption that I_m is a singleton randomly and independently chosen according to a fixed probability distribution on I. Convergence $\mathbb{E}(\|e_u^{(m)}\|^2) \to 0$ can be established for arbitrary $u \in V$, rates of the form $\mathbb{E}(\|e_u^{(m)}\|^2) = \mathrm{O}(m^{-s})$, $0 < s \leq 1$, are proved for u belonging to compact subsets of V determined in terms of spectral classes induced by the operator P. For infinite I, the theory of accelerated methods is still incomplete.

For the case of finite $I := \{0, 1, \ldots, n\}$ which is typical for applications to large-scale numerical discretization methods, in [2] we considered singleton I_m, and in [5] a more general case of I_m using the following assumptions:

A I_m is a uniformly at random chosen subset of size p_m in $I = \{0, 1, \ldots, n\}$, i.e., $|I_m| = p_m$ and $\mathbb{P}(i \in I_m) = \mathbb{P}(i' \in I_m)$ for all $i, i' \in \{0, 1, \ldots, n\}$.

B The choice of I_m is independent for different m.

While **A** suffices to prove expected error reduction rates per iteration step, assumption **B** is needed to obtain asymptotic convergence results. Let $\lambda_{\min}(P)$ and $\lambda_{\max}(P)$ denote (tight) lower and upper spectral bounds for P, respectively, and set $\kappa(P) = \lambda_{\max}(P)/\lambda_{\min}(P)$.

Theorem 1 ([5])**.** *Let the relaxation parameters in (3) be given by $\alpha_m = 1$ and $0 < \xi_m := \xi < 2/\lambda_{\max}(P)$. If* **A** *holds then in each step the algorithm (3) reduces the squared error in expectation according to*

(4)
$$\mathbb{E}(\|e_u^{(m+1)}\|^2 \,|\, u^{(m)}) \le \left(1 - \frac{\lambda_{\max}\xi(2 - \lambda_{\max}\xi)p_m}{\kappa(P)(n+1)}\right) \|e_u^{(m)}\|^2, \qquad m = 0, 1, \ldots.$$

If in addition **B** *holds then the algorithm (3) converges in expectation for any $u \in V$ and*

$$\mathbb{E}(\|e_u^{(m)}\|^2) \le \prod_{s=0}^{m-1} \left(1 - \frac{\lambda_{\max}\xi(2 - \lambda_{\max}\xi)p_s}{\kappa(n+1)}\right) \|u\|^2, \qquad m = 1, 2, \ldots. \tag{5}$$

In order to apply this result, an upper bound for $\lambda_{\max}(P)$ is needed. If ξ_m is determined for given $u^{(m)}$ and $d_u^{(m)}$ by the steepest descent rule, such knowledge is not necessary, and the theorem holds with $\xi\lambda_{\max}(P)$ replaced by 1.

The dependence on $\kappa(P)$ can be reduced to a dependence on $\sqrt{\kappa(P)}$ by running a two-step iteration method. In the deterministic case, there are several slightly different proposals to achieve this kind of acceleration. It turns out that so far only versions of Nesterov acceleration can be extended to the stochastic setting with convergence guarantees while generalizations of the heavy ball and conjugate gradient methods seem to fail. Following in spirit [6], we consider a two-step iteration written in vector form: With $u^{(0)} = v^{(0)} = 0$ at start, for $m = 0, 1, \ldots$ execute

$$\begin{aligned} u^{(m+1)} &= u^{(m)} + \xi_m d_v^{(m)}, \\ v^{(m+1)} &= u^{(m+1)} + \theta_m(u^{(m+1)} - u^{(m)}) + \eta_m d_v^{(m)}, \end{aligned} \qquad m \ge 0. \tag{6}$$

As for the iteration (3), in each step p_m subproblems have to be solved but storage and update work slightly increase. The following result was proved in [5] using a equivalent form of (6):

Theorem 2. *Under the assumptions* **A, B** *and with parameters $\xi_m = \lambda_{\max}(P)^{-1}$, and η_m, θ_m depending on $\kappa(P)$ and $\{p_m\}$, the vector iteration (6) admits the estimate*

$$\mathbb{E}(\|e_u^{(m)}\|^2) \le 2 \prod_{s=0}^{m-1} \left(1 - \frac{p_s}{(n+1)\sqrt{\bar{\kappa}}}\right) \|u\|^2, \qquad m = 1, 2, \ldots. \tag{7}$$

Note that the dependence of the convergence on the quotient $p_m/(n+1)$ (the portion of subproblems solved in the m-th step) is to be expected and in some sense the best one can hope for. Work on making the parameter choice in accelerated methods less dependent on a priori knowledge about the spectral properties of the underlying operator P is in progress.

References

[1] O. Fercoq, P. Richtárik, *Optimization in high dimensions via accelerated, parallel and proximal coordinate descent* SIAM Review **58** (2016), 739–771.

[2] M. Griebel, P. Oswald, *Greedy and randomized versions of the multiplicative Schwarz method*, Lin. Alg. Appl. **437** (2012), 1596–1610.

[3] M. Griebel, P. Oswald, *Schwarz iterative methods: Infinite space splittings*, Constr. Approx. **44** (2016), 121–139.

[4] M. Griebel, P. Oswald, *Stochastic subspace correction method in Hilbert spaces*, Constr. Approx. **48** (2018), 501–521.

[5] M. Griebel, P. Oswald, *Stochastic subspace correction methods and fault tolerance*, Math. Comp. **89** (2020), 279–312; arXiv:1807.11315; Univ. Bonn, INS Preprint No. 1809.

[6] Y. Nesterov, *Efficiency of coordinate descent methods on huge-scale optimization problems*, SIAM J. Optim. **22** (2012), 341–362.

[7] P. Richtárik, M. Takáč, *Stochastic reformulations of linear systems: Algorithms and convergence theory*, arxiv:1706.01109v2 (6 Jun 2017).

Optimal Adaptivity and Infinite Matrices

Michael Feischl

The theory of rate optimal adaptive algorithms for finite element methods originated in the seminal paper [23] by Stevenson and was further improved in [8] by Cascon, Kreuzer, Nochetto, and Siebert. (Note that the notion of rate optimality differs from that of instance optimality for adaptive finite element methods introduced in the seminal papers [4, 11].) These papers prove essentially, that a standard adaptive algorithm of the form

$$\boxed{\text{Solve}} \longrightarrow \boxed{\text{Estimate}} \longrightarrow \boxed{\text{Mark}} \longrightarrow \boxed{\text{Refine}}$$

generates asymptotically optimal meshes for the approximation of the solution of a Poisson problem. The new ideas sparked a multitude of papers applying and extending the techniques to different problems, see e.g., [20, 9] for conforming methods, [22, 2, 3, 6, 21] for nonconforming methods, [10, 7, 19] for mixed formulations, and [17, 18, 1, 15, 14] for boundary element methods (the list is not exhausted, see also [5] and the references therein). All the mentioned results, however, focus on symmetric and definite problems in the sense that the underlying equation induces a symmetric and definite operator. The missing link required to extend the theory to non-symmetric and indefinite problems is the quasi-orthogonality and consequently the linear convergence of the error. The first is usually an estimate of the form

$$\|u_{\ell+1} - u_\ell\|^2 \le c\|u - u_\ell\|^2 - C\|u - u_{\ell+1}\|^2 + \text{terms of higher order} \tag{1}$$

with $c \approx C \approx 1$. However, for indefinite and non-symmetric problems such an estimate does not seem to hold. The first proof of rate optimality for a non-symmetric problem which does not rely on additional assumptions on the initial mesh is given in [16] for a general second order elliptic operator with non-vanishing diffusion coefficient of the form

$$-\mathrm{div}(A\nabla u) + b \cdot \nabla u + cu = f.$$

This approach, however, relies heavily on the fact that the non-symmetric part of the operator $(b \cdot \nabla u + cu)$ is only a compact perturbation (one differentiation instead of two for the diffusion part). The first optimality proof of a strongly non-symmetric problem was given in the recent work [12] for a finite-element/boundary-element discretization of a transmission problem. The proof relies on a novel form of quasi-orthogonality introduced in [5, 16] called *general quasi-orthogonality*

$$\sum_{k=\ell}^{\infty} \|u_{k+1} - u_k\|^2 \lesssim \|u - u_\ell\|^2. \tag{2}$$

This notion of quasi-orthogonality is the last missing building block to apply the theory developed in [23, 8] and culminating in [5] to prove linear convergence and ultimately rate optimal convergence for strongly non-symmetric problems

The first idea to prove (2) and hence optimality of strongly non-symmetric problems was as follows: Find an $\mathcal{X}$-orthogonal basis $\boldsymbol{v}_1, \boldsymbol{v}_2, \dots$ of $\mathcal{X}$ such that all the adaptive spaces generated by the adaptive algorithm are spanned by it, i.e., $\mathcal{X}_\ell = \mathrm{span}\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_{N_\ell}\}$ for all $\ell \in \mathbb{N}$ and numbers $N_\ell \in \mathbb{N}$. Then, consider the infinite stiffness matrix $A \in \mathbb{R}^{\mathbb{N}\times\mathbb{N}}$, $A_{ij} := a(\boldsymbol{v}_j, \boldsymbol{v}_i)$ (where $a(\cdot,\cdot)$ is the bilinear form corresponding to the problem at hand) and rewrite the original problem as an infinite matrix problem. Then, we show that a (block)-LU-factorization $A = LU$ with bounded factors implies general quasi-orthogonality (2). A bound on the factors L and U would hence conclude the proof.

The main problem here is that the available LU-factorization results are not strong enough to show that the matrix A has a bounded LU-factorization. Hence, we require more structure (bandedness, exponential decay) of the infinite stiffness matrix and therefore have to replace the orthogonal basis $\boldsymbol{v}_1, \boldsymbol{v}_2, \dots$ by a hierarchical (wavelet-type) Riesz basis which is local in a certain sense. Unfortunately, this introduces some technical difficulties as well as the need for mildly graded meshes. It seems that the topic of the stability of the LU-factorization is very complex and not well-understood in the literature. Advances in this direction could significantly reduce the length of this work.

The benefit of this undertaking is that the abstract theory allows us to ask questions about matrices instead of asking questions about Galerkin approximations. This allows us to prove optimality of a standard adaptive algorithm for the stationary Stokes problem with standard Taylor-Hood discretization in [13] as well as optimality of a standard adaptive algorithm for a Poisson transmission problem discretized via finite-element/boundary-element coupling in [12].

References

[1] M. Aurada, M. Feischl, T. Führer, M. Karkulik, and D. Praetorius, *Efficiency and optimality of some weighted-residual error estimator for adaptive 2D boundary element methods*, J. Comput. Appl. Math., 255 (2014), pp. 481–501.

[2] R. Becker and S. Mao, *Quasi-optimality of adaptive nonconforming finite element methods for the Stokes equations*, SIAM J. Numer. Anal., 49 (2011), pp. 970–991.

[3] R. Becker, S. Mao, and Z. Shi, *A convergent nonconforming adaptive finite element method with quasi-optimal complexity*, SIAM J. Numer. Anal., 47 (2010), pp. 4639–4659.

[4] P. Binev, W. Dahmen, and R. DeVore, *Adaptive finite element methods with convergence rates*, Numer. Math., 97 (2004), pp. 219–268.

[5] C. Carstensen, M. Feischl, M. Page, and D. Praetorius, *Axioms of adaptivity*, Comput. Math. Appl., 67 (2014), pp. 1195–1253, https://doi.org/10.1016/j.camwa.2013.12.003, http://dx.doi.org/10.1016/j.camwa.2013.12.003.

[6] C. Carstensen, D. Peterseim, and H. Rabus, *Optimal adaptive nonconforming FEM for the Stokes problem*, Numer. Math., 123 (2013), pp. 291–308.

[7] C. Carstensen and H. Rabus, *The adaptive nonconforming FEM for the pure displacement problem in linear elasticity is optimal and robust*, SIAM J. Numer. Anal., 50 (2012), pp. 1264–1283.

[8] J. M. Cascon, C. Kreuzer, R. H. Nochetto, and K. G. Siebert, *Quasi-optimal convergence rate for an adaptive finite element method*, SIAM J. Numer. Anal., 46 (2008), pp. 2524–2550.

[9] J. M. Cascon and R. H. Nochetto, *Quasioptimal cardinality of AFEM driven by nonresidual estimators*, IMA J. Numer. Anal., 32 (2012), pp. 1–29.

[10] L. Chen, M. Holst, and J. Xu, *Convergence and optimality of adaptive mixed finite element methods*, Math. Comp., 78 (2009), pp. 35–53.

[11] L. Diening, C. Kreuzer, and R. Stevenson, *Instance optimality of the adaptive maximum strategy*, Found. Comput. Math., 16 (2016), pp. 33–68, https://doi.org/10.1007/s10208-014-9236-6, https://doi.org/10.1007/s10208-014-9236-6.

[12] M. Feischl, *Optimal adaptivity for non-symmetric fem/bem coupling*, arXiv-preprint 2019+.

[13] Michael Feischl. Optimal adaptivity for a standard finite element method for the stokes problem. *to appear SIAM. J. Numer. Anal.*, 2019.

[14] M. Feischl, T. Führer, M. Karkulik, J. Melenk, and D. Praetorius, *Quasi-optimal convergence rates for adaptive boundary element methods with data approximation, part II: Hypersingular integral equation*, Electron. Trans. Numer. Anal., 44 (2015), pp. 153–176.

[15] M. Feischl, T. Führer, M. Karkulik, J. M. Melenk, and D. Praetorius, *Quasi-optimal convergence rates for adaptive boundary element methods with data approximation, part I: weakly-singular integral equation*, Calcolo, 51 (2014), pp. 531–562, https://doi.org/10.1007/s10092-013-0100-x, http://dx.doi.org/10.1007/s10092-013-0100-x.

[16] M. Feischl, T. Führer, and D. Praetorius, *Adaptive FEM with optimal convergence rates for a certain class of nonsymmetric and possibly nonlinear problems*, SIAM J. Numer. Anal., 52 (2014), pp. 601–625, https://doi.org/10.1137/120897225, http://dx.doi.org/10.1137/120897225.

[17] M. Feischl, M. Karkulik, J. Melenk, and D. Praetorius, *Quasi-optimal convergence rate for an adaptive boundary element method*, SIAM J. Numer. Anal., 51 (2013), pp. 1327–1348.

[18] T. Gantumur, *Adaptive boundary element methods with convergence rates*, Numerische Mathematik, 124 (2013), pp. 471–516.

[19] H. Jian Guo and X. Yi Feng, *Convergence and complexity of arbitrary order adaptive mixed element methods for the Poisson equation*, Sci China Math, 55 (2012), pp. 1083–1098.

[20] C. Kreuzer and K. G. Siebert, *Decay rates of adaptive finite elements with Dörfler marking*, Numer. Math., 117 (2011), pp. 679–716.
[21] S. Mao, X. Zhao, and Z. Shi, *Convergence of a standard adaptive nonconforming finite element method with optimal complexity*, Appl. Numer. Math., 60 (2010), pp. 673–688.
[22] H. Rabus, *A natural adaptive nonconforming FEM of quasi-optimal complexity*, Comput. Methods Appl. Math., 10 (2010), pp. 315–325.
[23] R. Stevenson, *Optimality of a standard adaptive finite element method*, Found. Comput. Math., 7 (2007), pp. 245–269.

Adaptive quarkonial domain decomposition methods for elliptic partial differential equations

Alexander Sieber
(joint work with Stephan Dahlke, Ulrich Friedrich, Philipp Keding, Thorsten Raasch)

This talk is concerned with new discretization methods for the numerical treatment of elliptic partial differential equations. We derive an adaptive frame scheme that is based on quarkonial decompositions. These new frames are constructed from a finite set of functions by translation, dilation and multiplication by monomials. By means of nonoverlapping domain decompositions, we establish quarkonial frames on domains that can be decomposed into the union of parametric images of unit cubes. We also show that these new representation systems constitute stable frames in scales of Sobolev spaces. The construction is performed in such a way that, similar to the wavelet setting, the frame elements, the so-called quarklets, possess a certain amount of vanishing moments. This enables us to generalize the basic building blocks of adaptive wavelet algorithms to the quarklet case. The applicability of the new approach is demonstrated by numerical experiments for the Poisson equation on L-shaped domains.

References

[1] S. Dahlke, U. Friedrich, P. Keding, T. Raasch, A. Sieber, *Adaptive quarkonial domain decomposition methods for elliptic partial differential equations*, Bericht Mathematik Nr. 2018-01 des Fachbereichs Mathematik und Informatik, Universität Marburg (2018).

Adaptive *hp* discontinuous Galerkin methods for the Helmholtz equation

Ilaria Perugia
(joint work with Scott Congreve, Joscha Gedicke)

Consider the Helmholtz problem with impedance boundary condition

$$\begin{aligned} -\Delta u - k^2 u &= f \quad \text{in } \Omega, \\ \nabla u \cdot \mathbf{n} - iku &= g \quad \text{on } \partial\Omega, \end{aligned} \tag{1}$$

where $\Omega \subset \mathbb{R}^2$ is a bounded, Lipschitz domain, $\mathbf{n}$ the outer unit normal to $\partial\Omega$, $f \in L^2(\Omega)$, $g \in L^2(\partial\Omega)$, and $k > 0$ is the (constant) wavenumber.

Following [1], I have presented an *hp a posteriori* error estimator for a polynomial-based discontinuous Galerkin (DG) approximation of problem (1), which is based on the technique of equilibrated fluxes.

On a triangulation $\mathcal{T}$ of Ω with sets of interior and boundary edges denoted by $\mathcal{E}(\Omega)$ and $\mathcal{E}(\partial\Omega)$, respectively, the considered DG formulation reads as follows: Find $u_{hp} \in V_{hp}$ such that

$$a_{hp}(u_{hp}, v_{hp}) = F_{hp}(v_{hp}) \quad \text{for all } v_{hp} \in V_{hp}, \tag{2}$$

with the DG space V_{hp} defined by

$$V_{hp} := \{v_{hp} \in L^2(\Omega) \,:\, v_{hp}|_T \in \mathbb{P}_{p_T}(T) \text{ for all } T \in \mathcal{T}\},$$

$\mathbb{P}_{p_T}(T)$ being the space of polynomials of degree at most $p_T \geq 1$ on T,

$$\begin{aligned} a_{hp}(u,v) := {} & (\nabla_h u, \nabla_h v) - k^2(u,v) \\ & - \sum_{E\in\mathcal{E}(\Omega)} (\llbracket u \rrbracket_N, \{\!\{\nabla_h v\}\!\})_E - \sum_{E\in\mathcal{E}(\Omega)} (\{\!\{\nabla_h u\}\!\}, \llbracket v \rrbracket_N)_E \\ & - \left(\gamma k \frac{\mathsf{h}}{\mathsf{p}} u, \nabla_h v \cdot \mathbf{n}\right)_{\partial\Omega} - \left(\gamma k \frac{\mathsf{h}}{\mathsf{p}} \nabla_h u \cdot \mathbf{n}, v\right)_{\partial\Omega} \\ & - i \sum_{E\in\mathcal{E}(\Omega)} \left(\beta \frac{\mathsf{h}}{\mathsf{p}} \llbracket \nabla_h u \rrbracket_N, \llbracket \nabla_h v \rrbracket_N\right)_E - i \sum_{E\in\mathcal{E}(\Omega)} \left(\alpha \frac{\mathsf{p}^2}{\mathsf{h}} \llbracket u \rrbracket_N, \llbracket v \rrbracket_N\right)_E \\ & - i \left(\gamma \frac{\mathsf{h}}{\mathsf{p}} \nabla_h u \cdot \mathbf{n}, \nabla_h v \cdot \mathbf{n}\right)_{\partial\Omega} - i \left(k(1 - \gamma k \frac{\mathsf{h}}{\mathsf{p}}) u, v\right)_{\partial\Omega}, \end{aligned}$$

and

$$F_{hp}(v) := (f, v) - i \left(\frac{\gamma \mathsf{h}}{\mathsf{p}} g, \nabla_h v \cdot \mathbf{n}\right)_{\partial\Omega} + \left((1 - \gamma k \frac{\mathsf{h}}{\mathsf{p}}) g, v\right)_{\partial\Omega}.$$

Here, with standard DG notation, ∇_h denotes the elementwise application of ∇, $\{\!\{\cdot\}\!\}$ and $\llbracket \cdot \rrbracket_N$ denote the interelement averages and (normal) jumps, respectively, and h and p are the piecewise constant mesh size function and polynomial degree function, respectively, defined on the mesh faces as follows: $\mathsf{h}|_E = \min(h_{T_+}, h_{T_-})$ and $\mathsf{p}|_E = \max(p_{T_+}, p_{T_-})$, if $E = \partial T_+ \cap \partial T_-$, or $\mathsf{h}|_E = h_T$ and $\mathsf{p}|_E = p_T$, if $E = \partial T \cap \partial\Omega$. Finally, $\alpha > 0$, $\beta > 0$, and $0 < \gamma < 1/3$ are constant penalty parameters. The discrete problem (2) is unconditionally well-posed, and its *a priori* error analysis was carried out in [4].

The presented *a posteriori* estimator for (2) is defined in terms of an equilibrated flux reconstruction for the shifted Neumann-Poisson problem

$$\begin{aligned} -\Delta w &= f + k^2 u_{hp} && \text{in } \Omega, \\ \nabla w \cdot \mathbf{n} &= g + iku_{hp} - \gamma k \frac{\mathsf{h}}{\mathsf{p}} (g - \nabla_h u_{hp} \cdot \mathbf{n} + iku_{hp}) && \text{on } \partial\Omega; \end{aligned}$$

the error due to the nonconformity of the discretization is controlled by a potential reconstruction [2, 3]. The estimator is defined by

(3)
$$\eta_{hp}^2 := \sum_{T\in\mathcal{T}} \Bigg(\|\mathcal{G}(u_{hp}) + \boldsymbol{\sigma}_{hp}\|_{0,T} + \frac{\operatorname{diam}(T)}{j_{1,1}} \|f + k^2 u_{hp} - \operatorname{div} \boldsymbol{\sigma}_{hp}\|_{0,T} + C_{tr} \sum_{E\in\mathcal{E}(T)\cap\mathcal{E}(\partial\Omega)} |E|^{1/2} \|\boldsymbol{\sigma}_{hp}\cdot\mathbf{n} + g + iku_{hp} - \gamma k \frac{\mathsf{h}}{\mathsf{p}} (g - \nabla_h u_{hp}\cdot\mathbf{n} + iku_{hp})\|_{0,E} \Bigg)^2 + \sum_{T\in\mathcal{T}} \|\mathcal{G}(u_{hp}) - \nabla s_{hp}\|_{0,T}^2.$$

Here, $\mathcal{G}$ denotes the *DG gradient* defined in terms of local gradients and jump liftings by

$$\mathcal{G}(u_{hp}) := \nabla_h u_{hp} - \sum_{E\in\mathcal{E}(\Omega)} \mathcal{L}_E^0([\![u_{hp}]\!]_N) - \sum_{E\in\mathcal{E}(\Omega)} \mathcal{L}_E^1([\![\nabla u_{hp}]\!]_N),$$

$\boldsymbol{\sigma}_{hp}$ and s_{hp} are equilibrated flux and potential reconstructions, respectively, C_{tr} is a trace inequality constant, and $j_{1,1}$ is the first positive root of the Bessel function of the first kind of index 1.

For any $\boldsymbol{\sigma}_{hp} \in H(\operatorname{div};\Omega)$ satisfying the equilibration conditions

$$\int_T \operatorname{div} \boldsymbol{\sigma}_{hp}\, dx = \int_T f + k^2 u_{hp}\, dx \qquad \forall T\in\mathcal{T},$$
$$\int_E \boldsymbol{\sigma}_{hp}\cdot\mathbf{n}\, ds = \int_E -(g + iku_{hp}) + \gamma k \frac{\mathsf{h}}{\mathsf{p}} (g - \nabla_h u_{hp}\cdot\mathbf{n} - iku_{hp})\, ds \quad \forall E\in\mathcal{E}(\partial\Omega),$$

and any $s_{hp} \in H^1_*(\Omega) := \{v \in H^1(\Omega) : (v,1) = 0\}$, η_{hp} defined in (3) is proven to be a *reliable* estimator for the error $\|\nabla u - \mathcal{G}(u_{hp})\|_{0,\Omega}$, up to an additional L^2 error term, which resembles the pollution error, similarly to the residual a posteriori error estimator for the DG method in [5]. A specific local construction of $\boldsymbol{\sigma}_{hp}$ and s_{hp} on vertex patched is devised, for which η_{hp} is also p-uniformly efficient.

References

[1] S. Congreve, J. Gedicke, and I. Perugia, *Robust adaptive hp discontinuous Galerkin finite element methods for the Helmholtz equation*, SIAM J. Sci. Comp., 41 (2019), pp. A1121–A1147.

[2] V. Dolejší, A. Ern, and M. Vohralík, *hp-adaptation driven by polynomial-degree-robust a posteriori error estimates for elliptic problems*, SIAM J. Sci. Comput., 38 (2016), pp. A3220–A3246.

[3] A. Ern and M. Vohralík, *Polynomial-degree-robust a posteriori estimates in a unified setting for conforming, nonconforming, discontinuous Galerkin, and mixed discretizations*, SIAM J. Numer. Anal., 53 (2015), pp. 1058–1081.

[4] J. M. Melenk, A. Parsania, and S. Sauter, *General DG-methods for highly indefinite Helmholtz problems*, J. Sci. Comput., 57 (2013), pp. 536–581.

[5] S. Sauter and J. Zech, *A posteriori error estimation of hp-dG finite element methods for highly indefinite Helmholtz problems*, SIAM J. Numer. Anal., 53 (2015), pp. 2414–2440.

Adaptive energy minimization for *hp*–finite element methods

Thomas P. Wihler
(joint work with Paul Houston)

This presentation is concerned with an energy-driven adaptive mesh refinement approach for the purpose of solving numerically convex, possibly nonlinear variational problems. More precisely, we develop an iterative minimization technique which allows for the successive enrichment of an underlying discrete approximation space in an adaptive manner. Specifically, we outline a new methodology in the context of *hp*-adaptive FEM employed for the efficient numerical solution of linear and nonlinear second-order boundary value problems. Numerical experiments are presented which highlight the practical performance of this new *hp*-refinement technique for both one- and two-dimensional problems.

References

[1] P. Houston and T. P. Wihler, *Adaptive energy minimisation for hp-finite element methods*, Computers and Mathematics with Applications **71** (2016), 977–990.

Gradient Flow Finite Element Discretizations with Energy-Based Adaptivity for the Gross-Pitaevskii Equation

Benjamin Stamm
(joint work with Pascal Heid, Thomas Wihler)

In this talk, we considered the results presented in [1] for the numerical discretization of the Gross-Pitaevskii Equation (GPE), which is a *nonlinear eigenvalue problem* that represents the Euler-Lagrange equation of the Gross–Pitaevskii energy functional, given by

$$\mathsf{E}(v) := \int_\Omega \left(\frac{1}{2}|\nabla v|^2 + V(\boldsymbol{x})|v|^2 + \frac{\beta}{2}|v|^4 \right) \mathsf{d}\boldsymbol{x}, \tag{1}$$

under the following normalization constraint for the single particle functions v:

$$v \in S_{\mathbb{H}} := \{ v \in \mathbb{H} : \|v\|_{\mathrm{L}^2(\Omega)} = 1 \}. \tag{2}$$

Here, $\Omega \subset \mathbb{R}^d$, $d = \{1, 2, 3\}$, is a bounded, connected, and open set with Lipschitz boundary, $V \in L^\infty(\Omega)$ is a potential function with $V \geq 0$ almost everywhere, and $\beta \geq 0$ is a constant. We note that the fourth-order term in E (causing the associated eigenvalue to be nonlinear if $\beta > 0$) results from the interaction of particles. The global minimizer of E under the constraint (2) is called the *(normalized) ground state* of (1).

The Fréchet derivative of the energy functional E on the Sobolev space $\mathbb{H} := \mathrm{H}_0^1(\Omega)$ is given by

$$\langle \mathsf{E}'(v), w \rangle = \int_\Omega \left(\nabla v \cdot \nabla w + 2V(\boldsymbol{x}) vw + 2\beta |v|^2 vw \right) \mathsf{d}\boldsymbol{x}, \qquad v, w \in \mathbb{H}, \tag{3}$$

where $\langle \cdot, \cdot \rangle$ signifies the dual product in $\mathbb{H}^\star \times \mathbb{H}$. The Euler-Lagrange formulation of the constrained minimization problem

$$\arg\min_{v \in S_{\mathbb{H}}} \mathsf{E}(v),$$

is given by

$$v \in \mathbb{H}: \qquad \langle \mathsf{E}'(v), w \rangle = \lambda (v, w)_{\mathrm{L}^2(\Omega)} \qquad \forall w \in \mathbb{H}. \tag{4}$$

Here, the scalar λ takes the role of a Lagrange multiplier corresponding to the norm constraint (2). The *nonlinear* eigenvalue problem (4) is called the *Gross–Pitaevskii equation (GPE)*. Given that $V \geq 0$ (almost everywhere in Ω) and $\beta \geq 0$, the Gross–Pitaevskii eigenvalue problem (4) has a unique ($\mathrm{L}^2(\Omega)$-normalized) positive eigenfunction $u_{\mathrm{GS}} > 0$ which is the ground state of the Bose–Einstein condensate (1), see [2, Lem. 5.4]; in particular, u_{GS} is an eigenfunction to the minimal (and simple) eigenvalue, signified by λ_{GS} of (4), see [3].

The ground state u_{GS} will be determined iteratively. To this end, we employ the *projected gradient flow* approach proposed in [2]. One of the key ideas is to introduce a weighted energy inner product on $\mathbb{H} \times \mathbb{H}$, which, for fixed $z \in \mathbb{H}$, is given by

$$a_z(v, w) := \int_\Omega \left(\nabla v \cdot \nabla w + 2V(\boldsymbol{x}) v w + 2\beta |z|^2 v w \right) \mathrm{d}\boldsymbol{x}, \qquad v, w \in \mathbb{H}. \tag{5}$$

We now introduce the tangent space

$$\mathbb{T}_z := \{ w \in \mathbb{H} : (z, w)_{\mathrm{L}^2(\Omega)} = 0 \}.$$

Owing to the Riesz representation theorem, for any $v \in \mathbb{H}$, there exists a unique $\mathsf{G}_z(v) \in \mathbb{H}$ such that

$$a_z(\mathsf{G}_z(v), w) = (v, w)_{\mathrm{L}^2(\Omega)} \qquad \forall w \in \mathbb{H}. \tag{6}$$

Then, we can give an explicit expression for the orthogonal projection $\mathsf{P}_z : \mathbb{H} \to \mathbb{T}_z$, defined by

$$a_z(v - \mathsf{P}_z(v), w) = 0 \qquad \forall v \in \mathbb{H}, \, \forall w \in \mathbb{T}_z, \tag{7}$$

by

$$\mathsf{P}_z(v) = v - \frac{(z, v)_{\mathrm{L}^2(\Omega)}}{a_z(\mathsf{G}_z(z), \mathsf{G}_z(z))} \mathsf{G}_z(z). \tag{8}$$

We now consider a trajectory $u : [0, \infty) \to \mathbb{H}$ which, for a given initial value $u(0) = u_0 \in S_{\mathbb{H}}$, follows the dynamical system

$$\dot{u}(t) = -\mathsf{P}_{u(t)}(u(t)), \qquad t > 0, \tag{9}$$

which is the continuous gradient flow with respect to the inner product (5). The existence of a solution u has been discussed in [2, Sec. 3.1 & 3.2].

For the purpose of computing an approximation of the continuous gradient flow trajectory from (9), we use the forward Euler discretization method. For a given initial value $u^0 \in S_{\mathbb{H}}$ this yields a sequence of functions $\{u^n\}_{n\geq 0} \subset S_{\mathbb{H}}$ which, for $n \geq 0$, is defined by

$$u^{n+1} = \frac{\widehat{u}^{n+1}}{\|\widehat{u}^{n+1}\|_{\mathrm{L}^2(\Omega)}} \qquad \text{where} \qquad \widehat{u}^{n+1} = u^n - \tau_n \mathsf{P}_{u_n}(u_n), \tag{10}$$

where $\{\tau_n\}_{n\geq 0}$ is a sequence of positive (discrete) time steps. The scheme (10) is called *discrete gradient flow iteration (GFI)*.

Consider a sequence of conforming and shape-regular partitions $\{\mathcal{T}_N\}_{N\in\mathbb{N}}$ of the domain Ω into simplicial elements $\mathcal{T}_N = \{\kappa\}_{\kappa\in\mathcal{T}_N}$ (i.e. triangles for $d = 2$ and tetrahedra for $d = 3$). Moreover, for a (fixed) polynomial degree $p \in \mathbb{N}$ and any subset $\omega \subset \mathcal{T}_N$, we introduce the finite element space

$$\mathbb{V}(\omega) = \left\{ v \in \mathbb{H} : \, v|_\kappa \in \mathbb{P}_p(\kappa), \kappa \in \omega, \, v|_{\Omega\setminus\omega} = 0 \right\},$$

with $\mathbb{P}_p(\kappa)$ signifying the (local) space of all polynomials of maximal total degree p on κ, $\kappa \in \mathcal{T}_N$. Furthermore, similarly as before, we denote by

$$S_{\mathbb{V}(\omega)} = \left\{ v \in \mathbb{V}(\omega) : \, \|v\|_{\mathrm{L}^2(\Omega)} = 1 \right\}$$

the $\mathrm{L}^2(\Omega)$-unit sphere in $\mathbb{V}(\omega)$. In the sequel, we apply the notations $\mathbb{X}_N := \mathbb{V}(\mathcal{T}_N)$ and $S_N := S_{\mathbb{V}(\mathcal{T}_N)}$. Due to the compactness of S_N, it exists a minimizer $u_N \in \mathbb{X}_N$ of E_N, i.e. $\mathsf{E}(u_N) = \min_{v\in S_N} \mathsf{E}(v)$.

From a practical viewpoint, once the discrete GFI approximation $u_N^n \in \mathbb{X}_N$ from (10) is close to the solution $u_N \in \mathbb{X}_N$, we expect that any further GFI steps will no longer contribute an essential decay to the energy in (11). In this case, in order to further reduce the energy, we need to enrich the finite element space appropriately. More specifically, for $N \geq 1$, suppose that we have performed a reasonable number $n \geq 1$ (possibly depending on N) of GFI-iterations (10) in $\mathbb{X}_{N-1}$. Consider now a (hierarchically) refined mesh $\mathcal{T}_N$ of $\mathcal{T}_{N-1}$. Then we may embed the final guess $u_{N-1}^n \in \mathbb{X}_{N-1}$ on the previous space into the enriched finite element space $\mathbb{X}_N$ in order to obtain an initial guess on the refined mesh $\mathcal{T}_N$:

$$u_N^0 := u_{N-1}^n \in \mathbb{X}_N.$$

For each GFI-iteration n we monitor two quantities. Firstly, we introduce the increment on each iteration given by

$$\mathrm{inc}_N^n := \mathsf{E}(u_N^{n-1}) - \mathsf{E}(u_N^n), \qquad n \geq 1.$$

Secondly, we compare inc_N^n to the energy loss as compared to the previous mesh refinement, i.e.

$$\Delta\mathsf{E}_N^n := \mathsf{E}(u_N^0) - \mathsf{E}(u_N^n), \qquad n \geq 1. \tag{11}$$

We stop the iteration for $n \geq 1$ as soon as inc_N^n becomes small compared to $\Delta\mathsf{E}_N^n$, i.e. once there is no notable benefit (relatively speaking) in performing any more discrete GFI steps on the current space $\mathbb{X}_N$. Specifically, for $n \geq 1$, this is expressed by the bound

$$\mathrm{inc}_N^n \leq \gamma \Delta\mathsf{E}_N^n, \tag{12}$$

for some parameter $0 < \gamma < 1$.
In the sequel, we will outline the mesh refinement procedure. Assume that an approximation $u_N^n \in \mathbb{X}_N$, after $n \geq 0$ gradient flow iterations in $\mathbb{X}_N$, is given and that the criteria (12) indicates a mesh-refinement. Then, for any element $\kappa \in \mathcal{T}_N$ we consider the open patch ω_κ comprising of κ and its immediate face-wise neighbours. Moreover, given $\kappa \in \mathcal{T}_N$, we define the modified patch $\widetilde{\omega}_\kappa$ by uniformly (red) refining the element κ into a (fixed) number of subelements and by removing hanging nodes in ω_κ by doing (e.g. green) refinements of the adjacent elements. We consider basis functions $\{\xi_\kappa^1, \dots, \xi_\kappa^{m_\kappa}\}$ of the locally supported space $\mathbb{V}(\widetilde{\omega}_\kappa)$. Furthermore, we introduce the extended space

$$\widehat{\mathbb{V}}(\widetilde{\omega}_\kappa; u_N^n) := span\{\xi_\kappa^1, \dots, \xi_\kappa^{m_\kappa}, u_N^n\}.$$

Then, by performing one local discrete GFI-step in $\widehat{\mathbb{V}}(\widetilde{\omega}_\kappa; u_N^n) \subset \mathbb{H}$ we obtain a new local approximation, denoted by $\widetilde{u}_{N,\kappa}^n \in \widehat{\mathbb{V}}(\widetilde{\omega}_\kappa; u_N^n)$, with $\widetilde{u}_{N,\kappa}^n \in S_{\mathbb{H}}$.

By modus operandi, the above construction leads to the (local) energy decay

$$-\Delta\mathsf{E}_N^n(\kappa) := \mathsf{E}(\widetilde{u}_{N,\kappa}^n) - \mathsf{E}(u_N^n) \leq 0,$$

for all $\kappa \in \mathcal{T}_N$. The value $\Delta\mathsf{E}_N^k(\kappa)$ indicates the potential energy reduction due to a refinement of the element κ. These local energy-decays are then used within a Dörfler marking strategy to select elements for the next mesh-refinement

We finish with a numerical test. We choose $\Omega = (-6, 6)^2$ and $\beta = 1000$, with an oscillating potential function V. More precisely, the energy functional is given by

$$\mathsf{E}(u) = \frac{1}{2} \int_\Omega \left(|\nabla u|^2 + 2 \left(\frac{|\boldsymbol{x}|^2}{2} + 20 + 20 \sin(2\pi x) \sin(2\pi y) \right) |u|^2 + 1000 |u|^4 \right) \mathrm{d}\boldsymbol{x}.$$

This experiment was also considered in [2] with an asserted approximation $\mathsf{E}(u_{\mathrm{GS}}) \approx 30.40965$ of the ground state energy. Based on the adaptive Algorithm presented in this work, a smaller value for the ground state energy has been computed; we suppose that this (improved) approximation results from the adaptive (and thereby more effective) refinement of the meshes. In Figure 1 (left) we have depicted the error for the approximations of the ground state energy with respect to our reference value. This plot indicates an asymptotically optimal rate of convergence of the adaptive algorithm for the given problem. The suboptimal behaviour in the pre-asymptotic phase is due to the fact that the mesh is not fine enough to resolve the oscillations of the potential V sufficiently well.

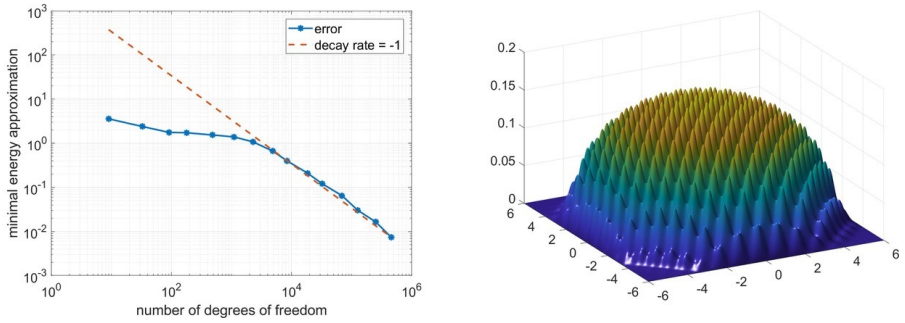

FIGURE 1. Left: Convergence plot for the ground state energy. Right: Approximated ground state.

REFERENCES

[1] P. Heid, B Stamm and Th. Wihler, *Gradient Flow Finite Element Discretizations with Energy-Based Adaptivity for the Gross-Pitaevskii Equation*, Tech. Report 1906.06954, arxiv.org, 2019.

[2] P. Henning and D. Peterseim, *Sobolev gradient flow for the Gross-Pitaevskii eigenvalue problem: global convergence and computational efficiency*, Tech. Report 1812.00835, arxiv.org, 2018.

[3] E. Cancès, R. Chakir, and Y. Maday, *Numerical analysis of nonlinear eigenvalue problems*, J. Sci. Comput. **45** (2010), 90–117.

[4] A. Zhou, *An analysis of finite-dimensional approximations for the ground state solution of Bose-Einstein condensates*, Nonlinearity **17** (2004), no. 2, 541–550.

Low-Rank Approximability and Entropy Area Laws for PDEs

MAZEN ALI

1. CURSE OF DIMENSIONALITY AND TENSOR PRODUCT APPROXIMATION

Let $u \in L^2(\mathbb{R}^d)$ represent the solution of a partial differential equation (PDE). The computational complexity of accurate approximations to u is a central question of numerics of PDEs. Suppose we approximate u as

$$u \approx u_N := \sum_{k=1}^{N} c_k v_k,$$

where the coefficients c_k are determined by a numerical procedure and v_k is chosen from some a priori fixed set of basis functions. The statement is very roughly as follows [4]: the function u has Besov/Sobolev smoothness s if and only if

$$\|u - u_N\|_{L^2} \leq CN^{-s/d},$$

for come constant $C > 0$. The estimate can be improved if we consider product domains and sparse grid or adaptive approximations [6, 5]. However, in all cases, for a given approximation accuracy, the required number of degrees of freedom N

in general grows exponentially with d. This is an expression of the so-called *curse of dimensionality*.

Tensor methods are a common and effective tool to combat this curse. Suppose we approximate u by a sum of tensor products as

$$u \approx u_r := \sum_{k=1}^{r} v_k^1 \otimes \cdots \otimes v_k^d.$$

If we require $\mathcal{O}(n)$ degrees of freedom for each v_k^j, then overall we require $\mathcal{O}(ndr)$ degrees of freedom to represent u_r. In order for this ansatz to truly break the curse of dimensionality, both n and r have to scale at most polynomially in d for a fixed approximation accuracy. If we assume as before Sobolev regularity for u and consider a more sophisticated tensor format, we obtain the general statement [12]

$$\|u - u_r\|_{L^2} \leq C r^{-s/d},$$

for some constant $C > 0$. It seems we have not gained anything by considering tensor formats. Yet, experience shows such formats perform quite well [3, 11]. Hence, we require different structural assumptions on u than classical Sobolev/Besov smoothness.

2. Operator Structure

We consider Hamiltonians of the following nearest neighbor interaction (NNI) structure

$$H = \sum_{j=1}^{d-1} H_{j,j+1}, \quad H_{j,j+1} = H_j + H_{j+1} + \Phi_{j,j+1}, \tag{1}$$

acting on a tensor product Hilbert space $\mathcal{X} = \mathcal{X}_1 \otimes \cdots \otimes \mathcal{X}_d$, where H_j, H_{j+1} are unbounded one-site operators and $\Phi_{j,j+1}$ is a two-site bounded interaction. A typical example to keep in mind is the following.

Let $\mathcal{X} = \bigotimes_{j=1}^{d} \mathcal{X}_j = \bigotimes_{j=1}^{d} L^2(\mathbb{R}^n)$, where in practice $n \in \{1, 2, 3\}$. Let the PDE operator be given as

$$H = -\Delta + V.$$

The Laplacian Δ is the one-site unbounded operator where $H_j = -\frac{\partial^2}{\partial x_j^2}$. The potential V contains the bounded interaction operators. E.g., $V = \sum_{j=1}^{d-1} \Phi_{j,j+1}$, where $\Phi_{j,j+1} : \mathcal{X} \to \mathcal{X}$ is a bounded operator such as

$$(\Phi_{j,j+1} u)(x) = c(x_j, x_{j+1}) u(x), \quad \text{or}$$

$$(\Phi_{j,j+1} u)(x) = \int_{\mathbb{R}^{2n}} \kappa(x_j, x_{j+1}, y_j, y_{j+1}) u(x_1, \ldots, y_j, y_{j+1}, \ldots, x_d) \, \mathrm{d}(y_j, y_{j+1}),$$

where $c(\cdot)$ is a bounded coefficient function and $\kappa(\cdot)$ is an integral kernel.

3. Results and Key Techniques

Our result [1] states the following: given a Hamiltonian of the form as in (1) and the corresponding ground state

$$\rho_0 = \langle \cdot,\, u_0 \rangle_{\mathcal{X}}, \quad H u_0 = 0, \quad \|u_0\|_{\mathcal{X}} = 1,$$

for any $1 \leq j \leq d-1$ and any $0 \leq l \leq \min\{j-1,\, d-1-j\}$, there exist bounded, self-adjoint operators O_L, O_R and O_B supported (roughly) on $[1,\, j]$, $[j+1,\, d]$ and $[j-l,\, j+1+l]$, respectively, such that

$$\|\rho_0 - O_B O_L O_R\|_{\mathcal{L}} \leq C \exp(-cl), \tag{2}$$

for some constants $C,\, c > 0$. Under additional assumptions on the operator O_B, this implies an area law for the ground state. The constants $C,\, c$ depend on the physical properties of the system such as spectral gap and interaction strength, not on $j,\, l$ or the order of the tensor product d. This result is based on the work for 1D entropy area laws for NNI spin systems from [7]. We single out two key techniques to establish the bound in (2).

First, *quasi-adiabatic continuation* by Hastings [8]. The idea is roughly based on two ground states belonging to the same *phase* [2]. Two gapped ground states $u_0^{\tau=0}$ and $u_0^{\tau=1}$ are said to belong to the same phase, if there exists a curve of Hamiltonians $H(\tau)$ for a parameter $\tau \in [0,1]$, differentiable (in the strong sense) in τ, such that $u_0^{\tau=0}$ is the ground state for $H(0)$ and $u_0^{\tau=1}$ the ground state for $H(1)$. In this case, there exists a family of unitary operators $U(\tau)$ such that we have the evolution

$$\rho_0^{\tau} = U(\tau) \rho_0^{\tau=0} U(\tau)^*, \quad \tau \in [0,\, 1]. \tag{3}$$

Applying this to (2), we set $\rho_0^{\tau=1} := \rho_0$, i.e., the ground state of $H =: H(1)$, and find a corresponding *local* $H(0)$ with a local ground state $\rho_0^{\tau=0}$ that we evolve as in (3) to $\rho_0^{\tau=1} = \rho_0$.

The next step is to show that this $\rho_0^{\tau=1}$, obtained by a quasi-adiabatic evolution from a local $\rho_0^{\tau=0}$, is at least *approximately* local. To this end, we use the second key technique of this work: *Lieb-Robinson bounds* [9, 10]. Such estimates bound the velocity of information propagation in a system governed by a Hamiltonian satisfying certain properties. Put in terms of equations: if A and B are two bounded operators on $\mathcal{X}$ with disjoint support such that $[A,\, B] = 0$, then, if we evolve A according to our system Hamiltonian

$$A(t) := \exp(\mathrm{i}Ht) A \exp(-\mathrm{i}Ht), \quad t \in \mathbb{R},$$

the operator $A(t)$ remains approximately local in the sense

$$[A(t),\, B] \approx 0,$$

for "small" $|t|$.

References

[1] M. Ali, *Low-rank approximability and entropy area laws for pdes*, arXiv e-prints (2019).
[2] S. Bachmann, S. Michalakis, B. Nachtergaele and R. Sims, *Automorphic equivalence with gapped phases of quantum lattice systems*, Communications in Mathematical Physics **309** (2012), 835–871.
[3] M. Bachmayr, R. Schneider and A. Uschmajew, *Tensor networks and hierarchical tensors for the solution of high-dimensional partial differential equations*, Foundations of Computational Mathematics **16** (2016), 1423–1472.
[4] R. A. DeVore, *Nonlinear approximation*, Acta numerica **7** (1998), 51–150.
[5] T. J. Dijkema, C. Schwab and R. Stevenson, *An adaptive wavelet method for solving high-dimensional elliptic pdes*, Constructive Approximation **30** (2009), 423–455.
[6] M. Griebel and S. Knapek, *Optimized tensor-product approximation spaces*, Constructive Approximation **16** (2000), 525–540.
[7] M. B. Hastings, *An area law for one-dimensional quantum systems*, Journal of Statistical Mechanics: Theory and Experiment (2007), P08024.
[8] M. B. Hastings and X. Wen, *Quasi-adiabatic continuation of quantum states: the stability of topological ground state degeneracy and emergent gauge invariance*, Physical Review B **B72** (2005), 045141.
[9] E. H. Lieb and D. W. Robinson, *The finite group velocity of quantum spin systems*, Communications in Mathematical Physics **28** (1972), 251–257.
[10] B. Nachtergaele, H. Raz, B. Schlein and R. Sims, *Lieb-Robinson bounds for harmonic and anharmonic lattice systems*, Communications in Mathematical Physics **286** (2009), 1073–1098.
[11] R. Orus, *Tensor networks for complex quantum systems*, arXiv e-prints (2018).
[12] R. Schneider and A. Uschmajew, *Approximation rates for the hierarchical tensor format in periodic Sobolev spaces*, Journal of Complexity **30** (2014), 56–71.

Quantic Tensor-rank bounds for point singularities in $\mathbb{R}^3$

Christoph Schwab
(joint work with Carlo Marcati, Maksim Rakhuba)

In $Q = (0,1)^3$, we consider tensor-formatted function approximation in $W^{1,2}(Q)$ of functions u in weighted Gevrey-classes in Q with sing supp$(u) = \{0\}$; i.e.

$$u \in \kappa_\gamma^{\overline{\omega},p}(Q, C, A, \delta) := \{v \in \bigcap_{s\in\mathbb{N}} \kappa_\gamma^{s,p}(Q) : \|v\|_{\kappa_\gamma^{s,p}(Q)} \le CA^s(s!)^\delta, s \in \mathbb{N}\},$$

where, for $1 \le p < \infty$, $\kappa_\gamma^{s,p}(Q)$ is the weighted Kondrat'ev space with norm

$$\|v\|_{\kappa_\gamma^{s,p}(Q)} = \sum_{|\alpha|\le s} \|r^{|\alpha|-\gamma}\partial^\alpha v\|^p_{L^p(Q)} \quad \text{(Kondrat'ev space)}$$

We show: for $0 < \varepsilon \le 1$ ex. quantized tensor train formatted ("qTT") approximation $v^\varepsilon_{qTT} \in H^1(Q)$ s.t.

$$\|u - v^\varepsilon_{qTT}\|_{H^1(Q)} \le \varepsilon \quad \text{and} \quad N_{dof}(v^\varepsilon_{qTT}) \le C_u(1 + |\log(\varepsilon)|^R)$$

where N_{dof} denotes # of degrees of freedom in v^ε_{qTT}, $H^1 = W^{1,2}$ (i.e. $p = 2$), $C_u > 0$ depends on C, A, δ,

$R > 0$ depends on the tensor format and on the regularity parameter $\delta \geq 1$:

$$R = \begin{cases} 4\delta + 3 & \text{classic qTT,} \\ 6\delta + 1 & \text{transposed order qTT,} \\ 3\delta + 3 & \text{Tucker qTT.} \end{cases}$$

References

[1] Quantic Tensor Rank Bounds for Point Singularities in $\mathbb{R}^3$, Carlo Marcati, Maksim Rakhuba and Christoph Schwab Technical Report, SAM, ETH Zürich (2019).

Reduced Modeling for State and Parameter Estimation

Wolfgang Dahmen
(joint work with Albert Cohen, Ron DeVore, Olga Mula, James Nichols)

Physical processes are often modeled by partial differential equations (PDEs) involving coefficients that need yet to be determined in order to approximately identify partially observed states of interest. Additional information on such states, in turn, is often given in terms of data obtained through measurements or sensors. Neither the mathematical model by itself nor available data usually suffice to recover the states of interest with satisfactory accuracy. Trying to best integrate classical model based and data-driven methods is sometimes referred to as data-assimilation or state and parameter estimation which incidentally amounts to regularizing such otherwise ill-posed estimation tasks. We discuss concepts that could be viewed as alternatives to stochastic regularization through Baysian inversion.

We focus in this talk on models where coefficients in the underlying PDEs depend on parameter vectors y that range over a parameter domain $\mathcal{Y}$. We always assume though that the variational formulations of the underlying parametric family of PDEs are uniformly stable with respect to a suitable pair U, V of trial and test (Hilbert) spaces. We are particularly concerned with scenarios where the dimension of $\mathcal{Y}$ is large or even infinite. This situation arises, for instance, when a random diffusion coefficient field of a second order elliptic problem is parametrized through a Karhunen-Loève expansion.

The set $\mathcal{M} \subset U$ of states that can be obtained when the parameters y range over $\mathcal{Y}$ is often referred to as *solution manifold* and is used to provide priors for the estimation tasks. Numerical tractability in the above scenario, even for infinitely many parameters, hinges in the elliptic case on the fact that the *parameter-to-solution map* $y \mapsto u(y)$ is holomorphic. From this one can deduce, in particular, that under suitable assumptions on the parametric expansions, the Kolmogorov n-widths of the solution manifold decay rapidly independent of the parametric dimension, [5].

Specifically, this talk is concerned with estimation problems of the following type. Given data provided by a *fixed* finite number m of sensors in terms of

bounded linear functionals on the Hilbert space U, (i) recover a state that (approximately) gives rise to the observed data and is possibly close to the solution manifold $\mathcal{M}$, or (ii) find a parameter $y \in \mathcal{Y}$ so that the corresponding state $u(y)$ (approximately) gives rise to the observed data. For elliptic problems and affine parameter expansions, using well-posedness of the underlying PDEs, (ii) can be reduced to a constrained linear least squares problem once a good state estimate is at hand. Therefore, we concentrate on state estimation (i), discussing related benchmarks, intrinsic information limits, and the construction of optimal recovery schemes.

We adopt the *Adaptive Parametrized Background Data-Weak* (APBDW) framework introduced in [6] and further analyzed in [2], i.e., the measurement functionals are (Riesz-)lifted to the ambient energy space U so that their representers in U span an m-dimensional subspace $W \subset U$, referred to as *measurement space*. Considering for conceptual clarity the noise-free case, we are then interested in finding recovery maps $A : W \to U$ of the form $A(w) = w + B(w)$, where $B : W \to W^\perp$ may be any map. Defining $E(A, W) := \sup_{u\in\mathcal{M}} \|u - A(P_W u)\|_U$, where P_W is the U-orthogonal projection to W, the recovery benchmark is $E(\mathcal{M}, W) := \inf_{A:W\to U} E(A, W)$.

A central role in the construction of such maps A is played by judiciously chosen "reduced spaces" $U_n \subset U$. In fact, suppose one has at hand a space U_n satisfying $\mathrm{dist}\,(\mathcal{M}, U_n)_U := \sup_{u\in\mathcal{M}} \|u - P_{U_n} u\|_U \le \varepsilon_n$ with a computable bound ε_n. The initially ill-posed estimation problem can be regularized by exploiting the knowledge that the observations $w = P_W u$ stem from a state u that belongs to, or more realsistically, is close to $\mathcal{M}$. This can be done by replacing $\mathcal{M}$ with the ε_n-neighborhood $\mathcal{K}^n$ of the space U_n which contains $\mathcal{M}$. One can then show that the optimal lifting operator $B^* = B^*(U_n) : W \to W^\perp$ is *linear* and can be realized through a least squares problem of size n in U_n followed by a correction in W. In fact, for each slice $\mathcal{K}^n_w := \mathcal{K}^n \cap (w + W^\perp)$, this determines the Chebychev radius of the ellipsoid $\mathcal{K}^n_w$ which realizes $E(\mathcal{K}^n_w, W)$, see [2]. The sharp recovery error-bound for $A^*_{U_n}(w) = w + B^*(w)$ is then given by

$$E(A^*_{U_n}, W) \le \mu(U_n, W)\mathrm{dist}\,(\mathcal{M}, U_n)_U, \tag{1}$$

where $\mu(U_n, W) := \sup_{v\in U_n} \|v\|_U / \|P_W v\|_U$, see [2, 6]. Thus, the recovery error is finite only if $n = \dim U_n \le m = \dim W$ since otherwise $U_n \cap W^\perp$ is non-trivial. This is called in [2] the *one-space method* because there is a one-to-one relation between a given space U_n and the corresponding optimal lifting operator B^* and hence the whole recovery map $A^* = A^*_{U_n}$.

These results extend verbatim when replacing the linear space U_n by an *affine* space which one expects can have, for a given dimension, a favorable effect on the stability factor $\mu(U_n, W)$ and the approximation accuracy [4]. In view of its bearing on parameter estimation, it would be highly desirable to identify a *best* space U_n. A first natural option for determining a "good" space U_n is to employ the weak greedy algorithm used in the *Reduced Basis Method*. This generates a nested sequence of subspaces U^{wg}_n. Specifically, given U^{wg}_k, $k \le n$, it generates U^{wg}_{n+1} by including

an element u_{n+1} from $\mathcal{M}$ that satisfies $\|u_{n+1} - P_{U_n^{\mathrm{wg}}} u_{n+1}\|_U \geq \gamma \mathrm{dist}\,(\mathcal{M}, U_n^{\mathrm{wg}})_U$, where $\gamma \in (0,1]$ is a fixed *weakness parameter*. It is shown in [1] that these spaces are *rate-optimal* in the following sense: suppose that the *Kolmogorov-n-widths* $d_n(\mathcal{M})_U := \inf_{\dim V = n} \mathrm{dist}\,(\mathcal{M}, V)_U$ are bounded by $Cn^{-\alpha}$ or Ce^{-cn^β} for some positive constants $c, C, \beta \leq 1$, then the quantities $\mathrm{dist}\,(\mathcal{M}, U_n^{\mathrm{wg}})_U$ are also bounded by $\bar{C}n^{-\alpha}$ or $\bar{C}e^{-\tilde{c}n^\beta}$, where $\bar{C}$ and $\tilde{c}$ depend in an explicitly given way on c, C, α, β and γ. For elliptic problems with affine parameter dependence this is, in principle, an established strategy. Since the quantities $\mu(U_n, W)$ can be computed via a Singular Value Decomposition of the cross-Gramian of a basis for U_n and a basis for W, tight a posteriori bounds for $\mathrm{dist}\,(\mathcal{M}, U_n^{\mathrm{wg}})_U$ allow one to evaluate the quantities $\mu(U_n^{\mathrm{wg}}, W)\mathrm{dist}\,(\mathcal{M}, U_n^{\mathrm{wg}})_U$ for $n = 1, \ldots, m$. This suggest taking the space

$$U^* = U_{n^*}^{\mathrm{wg}}, \quad n^* = \mathrm{argmin}\,\{\mu(U_n^{\mathrm{wg}}, W)\mathrm{dist}\,(\mathcal{M}, U_n^{\mathrm{wg}})_U : n = 1, \ldots, m\}. \tag{2}$$

It is however, not clear whether this yields a *near-best* affine recovery map of the form $A_{\mathrm{aff}} = \mathrm{id} + z + B$, $B : W \to W^\perp$ linear, which would be given by

$$A_{\mathrm{aff}}^* \in \mathrm{argmin}\,\Big\{ \sup_{u \in \mathcal{M}} \|P_{W^\perp} u - z - B P_W u\|_U : z \in W^\perp,\, B \in \mathcal{L}(W, W^\perp)\Big\}. \tag{3}$$

It is shown in [4] that a minimizer of (3) exists. Of course, it cannot be computed exactly since this would require exploring the whole solution manifold $\mathcal{M}$ as well as minimizing over all linear mappings B with range in the infinite-dimensional space $W^\perp$. Instead in [4] a computable minimization problem is analyzed where $\mathcal{M}$ and $W^\perp$ are replaced by an η-net of $\mathcal{M}$ and a finite dimensional space $\tilde{W}^\perp$, respectively. Specifically, $\tilde{W}^\perp$ is the orthogonal complement of W in a finite-dimensional space of the form $W + U_L$. It can be shown that if η and $\mathrm{dist}\,(\mathcal{M}, U_L)_U$ are of the order of $d_{m+1}(\mathcal{M})_U$ the minimizer of the correspondingly perturbed recovery scheme $\tilde{A}_{\mathrm{aff}}^*$ realizes an estimation error that remains proportional to the one achieved by the ideal map (3). For the model problem considered in [4] the accuracy achieved by $\tilde{A}_{\mathrm{aff}}^*$ is observed to be indeed significantly better than that provided by the adapted one-space estimator (2), at the expense of a significantly higher computational cost though.

The above requirement on the space U_L shows that also in this context it is important to have rate-optimal reduced spaces. In the high-dimensional parameter regime one can expect an algebraic decay of the n-widths of $\mathcal{M}$ (perhaps of high order, depending on the parameter expansion). This suggest taking U_L^{wg} with L proportional to $m = \dim W$. However, in the high-dimensional parameter regime already the corresponding off-line cost in running the weak greedy scheme turns out to be a serious obstruction. Although each surrogate evaluation is relatively inexpensive the size of training sets $\tilde{\mathcal{Y}} \subset \mathcal{Y}$, needed to ensure the weak greedy property over all of $\mathcal{Y}$, would be subject to the *Curse of Dimensionality* and would quickly become prohibitively large when d increases, see [3]. As a possible remedy deterministic certifiability of the reduced bases can be traded against probabilistic accuracy guaranties. It is shown in [3] that running the greedy algorithm over randomly selected training sets whose size grows only algebraically with respect

to the target accuracy, gives under certain circumstances rise to reduced bases that realize this accuracy with *high probability* while their dimension grows at a quantifiable but slightly suboptimal rate.

References

[1] P. Binev, A. Cohen, W. Dahmen, R. DeVore, G. Petrova, P. Wojtaszczyk, *Convergence Rates for Greedy Algorithms in Reduced Basis Methods*, SIAM J. Math. Anal., **43** (2011), 1457–1472.

[2] P. Binev, A. Cohen, W. Dahmen, R. DeVore, G. Petrova, P. Wojtaszczyk, *Data Assimilation in Reduced Modeling*, SIAM J. Uncertainty Quantification, **5**(1) (2017), 1–29, doi 10.1137/15M1025384, http://arxiv.org/abs/1506.04770 [math.NA],

[3] A. Cohen, W. Dahmen, R. DeVore, *Reduced Basis Greedy Selection Using Random Training Sets*, Preprint Oct. 2018, http://arxiv.org/abs/1810.09344 [math.NA].

[4] A. Cohen, W. Dahmen, R. DeVore, J. Fadili, O. Mula, J. Nichols, *Optimal reduced model algorithms for data-based state estimation*, http://arxiv.org/abs/1903.07938

[5] A. Cohen and R. DeVore, *Approximation of high-dimensional PDEs*, Acta Numerica, **24** (2015), 1–159.

[6] Y. Maday, A.T. Patera, J.D. Penn and M. Yano, *A parametrized-background data-weak approach to variational data assimilation: Formulation, analysis, and application to acoustics*, Int. J. Numer. Meth. Eng., Special Issue:Model Reduction, **102** (5) (2015), 931–1292 https://doi.org/10.1002/nme.4747

Advances in Model Order Reduction for Large Scale or Multi-Scale Problems

Mario Ohlberger

(joint work with A. Buhr, D. Eikhorn, C. Engwer, S. Rave)

Model order reduction for parameterized systems has gained a lot of attention in recent years. Classical approaches such as the Reduced Basis Method, Balanced Truncation or Proper Generalized Decomposition are meanwhile well established for parameterized PDEs with a fast decay of the Kolmogorov width of the solution manifold [2, 1]. However, challenges still exist for problems with either a slow decay of the Kolmogorov width or for large scale or multi-scale problems, where the enormous computational and storage requirements of model reduction methods in the so called "offline-phase" are still prohibitive. One such example is model order reduction for degradation processes of lithium-ion batteries [8] where we employ a POD-Greedy algorithm [9] together with empirical operator interpolation [7]. As we don't have efficient and robust a posteriori error estimators at hand for such complex applications, we make use of an heuristic strategy based on hierarchical error estimation [10].

Localization, with respect to both parameter and space provide a path to solution for such problems in combining ideas from numerical multiscale methods, domain decomposition and model order reduction. Here we refer for instance to the recent review article [5], where a common framework for localized model reduction has been presented. This framework includes non-conforming approaches,

such as the localized reduced basis multiscale method [11], as well as conforming approaches. If V_h denotes an underlying high dimensional reference Hilbert space with inner product, we call the direct sum decomposition of V_h into subdomain spaces, interface spaces, edge spaces and vertex spaces a localizing domain decomposition with respect to a given macroscopic underlying grid $\mathcal{T}_H$, i.e.

$$V_h = \bigoplus_{m=1}^{M} V_h^m \oplus \bigoplus_{\gamma \in \mathcal{T}_H^\gamma} V_h^\gamma \oplus \bigoplus_{e \in \mathcal{T}_H^e} V_h^e \oplus \bigoplus_{v \in \mathcal{T}_H^v} V_h^v, \tag{1}$$

The approach is called conforming, if $V_h \subset V$, where V is the underlying infinite dimensional solution space of a variational problem. The idea of projection-based localized model order reduction is then to consider local reduced approximation spaces for each element of the localizing space decomposition (1), in order to obtain a similarly decomposed reduced space $V_N \subset V_h$:

$$V_N = \bigoplus_{m=1}^{M} V_N^m \oplus \bigoplus_{\gamma \in \mathcal{T}_H^\gamma} V_N^\gamma \oplus \bigoplus_{e \in \mathcal{T}_H^e} V_N^e \oplus \bigoplus_{v \in \mathcal{T}_H^v} V_N^v, \tag{2}$$

with reduced subdomain spaces $V_N^m \subset V_h^m$, reduced interface spaces $V_N^\gamma \subset V_h^\gamma$, reduced edge spaces $V_N^e \subset V_h^e$ and reduced vertex spaces $V_N^v \subset V_N^v$.

As a promising conforming approach to construct the local reduced approximation spaces, we present a localized method that is able to deal with parameterized problems that in addition can handle arbitrary local modifications (ArbiLoMod) of the underlying problem [3, 4]. Important ingredients of this method are randomized local training to construct the interface spaces and a local Greedy algorithm to construct the local volume spaces. Additionally, we employ an adaptive enrichment procedure to incorporate missing global information in the local reduced approximation spaces. To this end, we derive efficient localized a posteriori error estimates that are derived from localizing the dual norm of the residual of the underlying variational problem.

A rigoros framework for randomized local training has recently been presented in [6]. We apply major ideas of this approach in a new setting with localized Robin-type transfer operators for the efficient approximation of the Helmholtz equation in the context of a generalized finite element method (GFEM). Numerical experiments demonstrate the efficiency of the approach. Numerically we evaluate how to optimally choose the Robin-type boundary condition in the localization process. The results suggest, that the optimal Robin parameter depends on the wave number of the underlying Helmholtz problem in a quadratic manner.

References

[1] P. Benner, M. Ohlberger, A. T. Patera, G. Rozza, K. Urban. Model reduction of parametrized systems. Selected papers from the 3rd MoRePaS Conference held at the International School for Advanced Studies (SISSA), Trieste, October 13–16, 2015. MS&A. Modeling, Simulation and Applications, 17. Springer, Cham, 2017. xii+504 pp. doi: 10.1007/978-3-319-58786-8.

[2] P. Benner, A. Cohen, M. Ohlberger, K. Willcox. Model Reduction and Approximation: Theory and Algorithms. Computational Science & Engineering, 15. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2017. xx+412 pp. doi: 10.1137/1.9781611974829.
[3] A. Buhr, C. Engwer, M. Ohlberger, S. Rave. ArbiLoMod: Local Solution Spaces by Random Training in Electrodynamics. In Model Reduction of Parametrized Systems, edited by Benner P., Ohlberger M., Patera A., Rozza G., Urban K., 137–148. Cham: Springer International Publishing, 2017. doi: 10.1007/978-3-319-58786-8_9
[4] A. Buhr, C. Engwer, M. Ohlberger, S. Rave. ArbiLoMod, a Simulation Technique Designed for Arbitrary Local Modifications. *SIAM J. Sci. Comput.* 39(4):A1435–A1465, 2017. doi: 10.1137/15M1054213.
[5] A. Buhr, L. Iapichino, M. Ohlberger, S. Rave, F. Schindler, K. Smetana. Localized model reduction for parameterized problems. ArXiv e-prints arXiv:1902.08300 [math.NA], Preprint (Submitted to Handbook on Model Order Reduction, edited by Benner P, Grivet-Talocia S, Quarteroni A, Rozza G, Schilders W, Sileira L, 51.) - 2019.
[6] A. Buhr and K. Smetana. Randomized Local Model Order Reduction. *SIAM J. Sci. Comput.*, 40(4):A2120–A2151, 2018. doi: 10.1137/17M1138480.
[7] M. Drohmann, B. Haasdonk, and M. Ohlberger. Reduced basis approximation for nonlinear parametrized evolution equations based on empirical operator interpolation. *SIAM J. Sci. Comput.*, 34:A937-A969, 2012. doi: 10.3182/20120215-3-AT-3016.00128.
[8] J. Feinauer, S. Hein, S. Rave, S. Schmidt, D. Westhoff, J. Zausch, O. Iliev, A. Latz, M. Ohlberger, V. Schmidt. MULTIBAT: Unified workflow for fast electrochemical 3D simulations of lithium-ion cells combining virtual stochastic microstructures, electrochemical degradation models and model order reduction. *Journal of Computational Science* 31: 172–184, 2019. doi: 10.1016/j.jocs.2018.03.006.
[9] B. Haasdonk, and M. Ohlberger. Reduced basis method for finite volume approximations of parametrized evolution equations. *M2AN Math. Model. Numer. Anal.*, 42(2):277-302, 2008. doi: 10.1051/m2an:2008001.
[10] S. Hain, M. Ohlberger, M. Radic, K. Urban. A Hierarchical A-Posteriori Error Estimatorfor the Reduced Basis Method. *Advances in Computational Mathematics*, 2019. doi: 10.1007/s10444-019-09675-z. .
[11] M. Ohlberger, F. Schindler. Error control for the localized reduced basis multi-scale method with adaptive on-line enrichment. *SIAM J. Sci. Comput.* 37(6):A2865–A2895, 2015. doi: 10.1137/151003660.

hp-FEM for the spectral fractional Laplacian in polygons

Jens M. Melenk
(joint work with Lehel Banjai, Christoph Schwab)

We consider two different discretizations of problem (1) involving the spectral fractional Laplacian in a polygon. The first one is a high order discretization (*hp*-FEM) of the (degenerate) elliptic problem given by the Caffarelli-Silvestre extension. The second discretization is based on approximating the integral representation of the solution, the so-called Balakrishnan formula. Both discretizations rely on geometric meshes on the polygon Ω that are refined (anisotropically) towards the edges of Ω and also refined towards its vertices. Exponential convergence is achieved assuming analyticity of the data f.

Model problem and the Caffarelli-Silvestre extension. On a bounded polygon $\Omega \in \mathbb{R}^2$, we consider for the *spectral fractional Laplacian* $(-\Delta)^s$ with

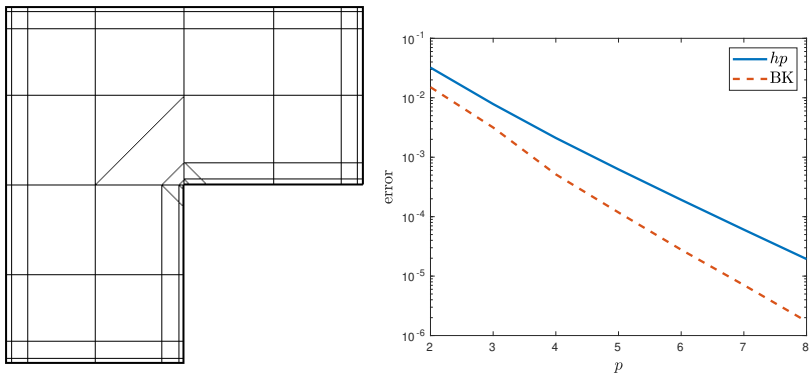

FIGURE 1. Left: geometric mesh $\mathcal{T}_x$ that is anisotropically refined towards the edges and isotropically towards the vertices. Right: error versus polynomial degree p for $s = 0.8$ for the Galerkin method (3) (solid line) and Balakrishnan formula (9) (dashed line). error $= \int_\Omega f(u - u_N)$. For (3), $q = p \sim L_x \sim L_y \sim \mathcal{Y}$; for (9) $p \sim L_x \sim M$. Ω is shown on the left, $f \equiv 1$.

$s \in (0,1)$ the following problem: Given $f \in H^{-s}(\Omega)$, find $u \in \widetilde{H}^s(\Omega)$ such that (in strong form)

$$(-\Delta)^s u = f \quad \text{in } \Omega, \quad u|_{\partial\Omega} = 0. \tag{1}$$

Here, $\widetilde{H}^s(\Omega)$ is the closure of $C_0^\infty(\Omega)$ under the $H^s(\Omega)$-norm and $H^{-s}(\Omega) = \left(\widetilde{H}^s(\Omega)\right)'$. The operator $(-\Delta)^s$ is a nonlocal operator. However, Caffarelli and Sivestre showed (for the fractional Laplacian in $\mathbb{R}^d$) [7] and then Cabré & Tan [6] and Stinga & Torrea [11] for bounded domains that this operator can be understood as a Dirichlet-to-Neumann operator for a (degenerate) elliptic problem. That is, the solution u of (1) is given by the trace $u = \operatorname{tr}_\Omega U$, where the function $U = U(x,y)$ on $\mathcal{C} = \Omega \times (0,\infty)$ satisfies

$$-\nabla \cdot (y^\alpha \nabla U) = 0 \quad \text{in } \mathcal{C}, \qquad \alpha = 1 - 2s, \tag{2a}$$

$$U(x,y) = 0, \quad (x,y) \in \partial\Omega \times (0,\infty), \tag{2b}$$

$$-\lim_{y\to 0} y^\alpha \partial_y U(\cdot,y) = d_s f, \qquad d_s = 2^{1-2s}\Gamma(1-s)/\Gamma(s). \tag{2c}$$

The pertinent norm is the *energy norm* $\|v\|_E := (\int_{\mathcal{C}} y^\alpha |\nabla v|^2)^{1/2}\, dx\, dy$ and the relevant space is $\mathring{H}^1(\mathcal{C}) = \{v \,|\, \|v\|_E < \infty, v(x,y) = 0 \text{ for } (x,y) \in \partial\Omega \times (0,\infty)\}$. One has the trace estimate $\|\operatorname{tr}_\Omega v\|_{\widetilde{H}^s(\Omega)} \le C\|v\|_E$.

***hp*-FEM based on the Caffarelli-Silvestre extension.** The solution U of (2) can be approximated by a Galerkin method, [10, 1]: Given a subspace

$V_N \subset \mathring{H}^1(\mathcal{C})$ with $\dim V_N = N$, the approximation $U_N^{Gal} \in V_N$ is determined by

$$a(U_N^{Gal}, v) := \int_{\mathcal{C}} y^\alpha \nabla U_N^{Gal} \cdot \nabla v = d_s \int_\Omega f v \qquad \forall v \in V_N. \tag{3}$$

We select $V_N = S_0^p(\mathcal{T}_x) \otimes S_{\{\mathcal{Y}\}}^q(\mathcal{T}_y)$ where $\mathcal{T}_x$, $\mathcal{T}_y$ are regular meshes on Ω and the interval $(0, \mathcal{Y})$, respectively. Here, we denote by $S^r(\mathcal{T})$ the space consisting of globally continuous, piecewise polynomials of degree r on the mesh $\mathcal{T}$; the subscript 0 indicates the incorporation of homogeneous boundary conditions, and the subscript $\{\mathcal{Y}\}$ indicates that homogeneous boundary conditions are enforced at $y = \mathcal{Y}$. The solution U is analytic in y, [1], it decays exponentially in y, and it has an algebraic singularity at $y = 0$, [10]. Thus, the mesh $\mathcal{T}_y$ is taken to be a geometric mesh on $(0, \mathcal{Y})$ with mesh points $0, \sigma^{L_x}\mathcal{Y}, \sigma^{L_x-1}\mathcal{Y}, \ldots, \sigma^0\mathcal{Y}$, where $\sigma \in (0,1)$ is the grading factor and $L_x \in \mathbb{N}_0$ is the number of layers of geometric refinement. The exponential decay of U as $y \to \infty$ and the algebraic singularity at $y = 0$ lead one to select $\mathcal{Y} \sim L_x \sim q$. To motivate the choice of the mesh $\mathcal{T}_x$, we consider the semi-discrete Galerkin approximation $U^{semi} \in H_0^1(\Omega) \otimes S_{\{\mathcal{Y}\}}^q(\mathcal{T}_y)$ to U. It can be written in the form $U^{semi} = \sum_{i=1}^{\mathcal{M}} U_i(x) v_i(y)$, where $\mathcal{M} = \dim S_{\{\mathcal{Y}\}}^q(\mathcal{T}_y)$, the $(\mu_i, v_i) \in \mathbb{R} \times S_{\{\mathcal{Y}\}}^q(\mathcal{T}_y)$ are the eigenpairs of

$$\mu_i \int_0^{\mathcal{Y}} y^\alpha v_i'(y) w'(y)\, dy = \int_0^{\mathcal{Y}} y^\alpha v w\, dy \ \forall w \in S_{\{\mathcal{Y}\}}^q(\mathcal{T}_y), \ \int_0^{\mathcal{Y}} y^\alpha |v_i'(y)|^2\, dy = 1, \tag{4}$$

and the functions U_i are given by

$$\mu_i \int_\Omega \nabla U_i \cdot \nabla v + U_i v\, dx = d_s v_i(0) \int_\Omega f v\, dx \quad \forall v \in H_0^1(\Omega). \tag{5}$$

By [1] one has $q^{-2}\mathcal{Y}^2\sigma^{2L_x} \lesssim \mu_i \lesssim \mathcal{Y}^2$ so that, for smooth f, the problems (5) are of singular perturbation type. For this problem class on polygonal domains Ω, exponential approximability can be established on geometric meshes that are refined towards the boundary as well as the vertices:

Theorem 1 ([2], [9])**.** *Let $\Omega \subset \mathbb{R}^2$ be a polygon and f be analytic on $\overline{\Omega}$. Fix $c_1 > 0$. Let $\widetilde{u}$ solve, for some $\varepsilon \in (0,1]$,*

$$-\varepsilon^2 \Delta \widetilde{u} + \widetilde{u} = f \quad \text{in } \Omega, \qquad \widetilde{u}|_{\partial\Omega} = 0.$$

Let $\mathcal{T}_x$ be a geometric mesh that is (anisotropically) refined towards the edges and (isotropically) towards the vertices with L_x layers of refinement and grading factor $\sigma \in (0,1)$. Assume that p and L_x satisfy $\sigma^{L_x}/(p\varepsilon) \le c_1$. Then:

$$\inf_{v \in S_0^p(\mathcal{T}_x)} \varepsilon \|\widetilde{u} - v\|_{H^1(\Omega)} + \|\widetilde{u} - v\|_{L^2(\Omega)} \le C \left[\exp(-bp) + \exp(-b' L_x)\right], \tag{6}$$

where C, b, b' depend only on Ω, f, and c_1.

An example of a geometric mesh $\mathcal{T}_x$ that is refined towards the edges and vertices is depicted in Fig. 1. A systematic construction of geometric meshes having the approximation properties of Theorem 1 that is based on the concept of *mesh patches* is given in [2]. Based on Theorem 1, one obtains for the Galerkin error the following exponential convergence result:

Theorem 2 ([3]). *Let $\Omega \subset \mathbb{R}^2$ be a polygon, f be analytic on $\overline{\Omega}$, and let U be the solution of (2). Let $\mathcal{T}_y$ be the geometric mesh on $(0,\mathcal{Y})$ with L_y layers and grading factor $\sigma \in (0,1)$, and let $\mathcal{T}_x$ be a geometric mesh on Ω that is refined towards the edges and vertices of Ω with L_x layers and grading factor $\sigma \in (0,1)$. Assuming $q \sim L_y \sim \mathcal{Y} \sim L_x \sim p$, the Galerkin approximation U_N^{Gal} from (3) satisfies*

$$\|\operatorname{tr}_\Omega(U - U_N^{Gal})\|_{\widetilde{H}^s(\Omega)} \le C_1 \|U - U_N^{Gal}\|_E \le C_2 \exp(-bp), \qquad N = \dim V_N \le C_3 p^6,$$

where the constants C_1, C_2, C_3, $b > 0$ are independent of p.

Balakrishnan formula. An alternative to using the extension problem is to use the Balakrishnan formula, a solution formula for (1), given by

$$u = ((-\Delta)^s)^{-1} f = c_B \int_{t=-\infty}^{\infty} e^{-st} \left(\mathrm{I} - e^{-t}\Delta\right)^{-1} f \, dt, \qquad c_B = \frac{\sin \pi s}{\pi}. \tag{7}$$

As proposed in [4], sinc-quadrature can be brought to bear by approximating the integal with the trapezoidal rule:

$$\widetilde{u}_M := c_B k \sum_{j=-M}^{M} \varepsilon_j^{2s} \left(\mathrm{I} - \varepsilon_j^2 \Delta\right)^{-1} f, \qquad \varepsilon_j := e^{-y_j/2}, \quad y_j := jk := jM^{-1/2}.$$

One has the semi-discrete error bound $\|u - \widetilde{u}_N\|_{\widetilde{H}^s(\Omega)} \le C e^{-\sqrt{M}} \|f\|_{L^2(\Omega)}$, [3]. Computing $\widetilde{u}_M$ amounts to solving $2M+1$ decoupled (singularly perturbed) elliptic problems. A fully discrete scheme is obtained by discretizing these problems: For a mesh $\mathcal{T}_x$ on Ω let $u_j \in S_0^p(\mathcal{T}_x)$ solve

$$\int_\Omega \varepsilon_j^2 \nabla u_j \cdot \nabla v + u_j v \, dx = \int_\Omega f v \, dx \qquad \forall v \in S_0^p(\mathcal{T}_x) \tag{8}$$

and set

$$u_N^{BK} := c_M k \sum_{j=-M}^{M} u_j. \tag{9}$$

The functions u_j are Galerkin approximations to the solutions $\widetilde{u}_j := (\mathrm{I} - \varepsilon_j^2 \Delta)^{-1} f$ of singularly perturbed problems (if ε_j is small); Theorem 1 shows that exponential convergence can be achieved for the errors $\widetilde{u}_j - u_j$ if the meshes are geometrically refined towards the edges and vertices of the polygon Ω. We therefore obtain:

Theorem 3 ([3]). *Let $\Omega \subset \mathbb{R}^2$ be a polygon, and let f be analytic on $\overline{\Omega}$. Let $\mathcal{T}_x$ be a geometric mesh that is refined towards the edges and vertices of Ω with L_x layers and grading factor $\sigma \in (0,1)$. If $M \sim p \sim L_x$, then*

$$\|u - u_N^{BK}\|_{\widetilde{H}^s(\Omega)} \le C \exp(-bp),$$

where C, b are independent of p. The total problem size is $O(p^6)$.

Fig. 1 illustrates for $f \equiv 1$ and the L-shaped domain Ω shown in Fig. 1 the convergence of both the Galerkin *hp*-FEM based on the extension problem and the Balakrishnan formula. The error measure is $|\int_\Omega f(u - u_N)|$ (with u_N being $\operatorname{tr}_\Omega U_N^{Gal}$ or u_N^{BK}). Exponential convergence in the polynomial degree is visible.

References

[1] Banjai, L., Melenk, J.M., Nochetto, R.H., Otárola, E., Salgado, A.J., Schwab, C.: *Tensor FEM for Spectral Fractional Diffusion*, Found. Comput. Math., **19** (2019), 901–962

[2] Banjai, L., Melenk, J.M., Schwab, C.: *hp-FEM for reaction diffusion equations II. Robust exponential convergence for multiple length scales in corner domains.* (In prep.)

[3] Banjai, L., Melenk, J.M., Schwab, C.: *Exponential convergence of hp-FEM for spectral fractional diffusion in polygons.* (In prep.)

[4] Bonito, A., Pasciak, J.: *Numerical approximation of fractional powers of elliptic operators,* Math. Comp. **84**(295), 2083–2110 (2015)

[5] Bonito, A., Borthagaray, J.P., Nochetto, R.H., Otárola, E., Salgado, A.J.: *Numerical methods for fractional diffusion,* Computing and Visualization in Science **19**, 19–46 (2018)

[6] Cabré, X., Tan, J.: *Positive solutions of nonlinear problems involving the square root of the Laplacian,* Adv. Math. **224**(5), 2052–2093 (2010)

[7] Caffarelli, L., Silvestre, L.: *An extension problem related to the fractional Laplacian.* Comm. Part. Diff. Eqs. **32**(7-9), 1245–1260 (2007)

[8] Lischke, A., Pang, G., Gulian, M., Song, M., Glusa, C., Zheng, X., Mao, Z., Cai, W, Meerschaert, M., Ainsworth, M., and Karniadakis, G.: *What Is the Fractional Laplacian?*, arXiv e-prints (2018), arXiv:1801.09767

[9] Melenk, J.M.:*hp-finite element methods for singular perturbations*, LNM 1796, Springer Verlag, 2002

[10] Nochetto, R., Otárola, E., Salgado, A.: *A PDE approach to fractional diffusion in general domains: a priori error analysis,* Found. Comput. Math. **15**(3), 733–791 (2015).

[11] Stinga, P., Torrea, J.: *Extension problem and Harnack's inequality for some fractional operators,* Comm. Partial Differential Equations **35**(11), 2092–2122 (2010)

Neural networks for the approximation of solutions of PDEs and related problems

Ivan Oseledets

Deep learning has become very popular in the recent years, yielding wonderful results. In this talk, I gave a brief overview of basic definitions in machine learning, deep learning and their possible applications, including solutions of PDEs, approximations of solution manifolds. I also discussed the connections beween ResNet and OdeNet.

Empirical risk minimization over deep neural networks overcomes the curse of dimensionality in the numerical approximation of Kolmogorov equations

Julius Berner

(joint work with Philipp Grohs, Arnulf Jentzen)

The development of new classification and regression algorithms based on empirical risk minimization (ERM) over deep neural network hypothesis classes, coined Deep Learning, revolutionized the area of artificial intelligence, machine learning, and data analysis. Moreover, these methods have been applied to the numerical

solution of high dimensional PDEs with great success. Recent simulations indicate that deep learning based algorithms are capable of overcoming the curse of dimensionality for the numerical solution of linear Kolmogorov equations

$$\begin{cases} \partial_t u(t,x) = \frac{1}{2}\mathrm{Trace}\big(\sigma(x)\sigma^T(x)\mathrm{Hess}_x u(t,x)\big) + \mu(x)\cdot\nabla_x u(t,x) \\ u(0,x) = \varphi(x), \end{cases}$$

which are widely used in models from engineering, finance, and the natural sciences [1].

We mathematically supported these empirical observations by establishing combined approximation and generalization results. We considered under which conditions ERM over a deep neural network hypothesis class approximates, with high probability, the end value $u(T,\cdot)$ of a d-dimensional Kolmogorov equation with affine drift μ and diffusion σ coefficients up to error ε. We show that such an approximation can be achieved with both the size of the hypothesis class and the number of training samples scaling only polynomially in d and ε^{-1} [4]. The proofs are based on tools from statistical learning theory [5] and the following key properties of linear Kolmogorov equations:

(1) One can reformulate the numerical solution as a classical statistical learning problem [1].
(2) Typical initial conditions φ arising from problems in computational finance are exactly representable as neural networks with ReLU activation function without incurring the curse of dimensionality [6].
(3) Efficient approximation of the initial condition φ and coefficient functions σ, μ by neural networks transfers to an efficient approximation of the end value $u(T,\cdot)$ [6].

In joint work with Dennis Elbrächter, we investigated the regularity properties of neural networks to further develop the approximation theory of neural networks in the context of PDEs. In particular, we analyzed the (weak) derivative of a neural network with ReLU activation function [3]. This can then be used to approximate a large class of functions (including multivariate polynomials, high-frequent sinusoidal functions, and Sobolev-regular functions) in the $W^{1,\infty}$-norm [7, 8]. Moreover, one can obtain global pointwise error estimates and Lipschitz constant estimates of the approximating networks, as required, for instance, in (3).

To understand the optimization of neural networks (which is not included in the analysis above) we recently considered the stability of neural network parametrization, asking if the proximity of realization functions must imply proximity of corresponding parametrizations. After discovering several pathologies which prevent this in general, we established a restricted set of parametrizations where we have stability w.r.t. to the $W^{1,\infty}$-norm [2].

Future plans include the extension of the above work to the solution map $(\varphi, \sigma, \mu, t, x) \mapsto u(t,x)$ and to more general PDEs with stochastic representation (general Kolmogorov equations, combined Dirichlet-Poisson problems, semi-linear parabolic PDEs), including numerical simulations.

References

[1] C. Beck, S. Becker, P. Grohs, N. Jaafari, and A. Jentzen, *Solving stochastic differential equations and Kolmogorov equations by means of deep learning*, arXiv:1806.00421, (2018).

[2] J. Berner, D. Elbrächter, and P. Grohs, *How degenerate is the parametrization of neural networks with the ReLU activation function?*, arXiv:1905.09803, (2019). Accepted at NeurIPS 2019.

[3] J. Berner, D. Elbrächter, P. Grohs, and A. Jentzen, *Towards a regularity theory for ReLU networks–chain rule and global error estimates*, arXiv:1905.04992, (2019). Accepted for presentation at SampTA 2019.

[4] J. Berner, P. Grohs, and A. Jentzen, *Analysis of the generalization error: Empirical risk minimization over deep artificial neural networks overcomes the curse of dimensionality in the numerical approximation of Black-Scholes partial differential equations*, arXiv:1809.03062, (2018).

[5] F. Cucker and S. Smale, *On the mathematical foundations of learning*, Bulletin of the American mathematical society, 39 (2002), pp. 1–49.

[6] P. Grohs, F. Hornung, A. Jentzen, and P. von Wurstemberger, *A proof that artificial neural networks overcome the curse of dimensionality in the numerical approximation of black-scholes partial differential equations*, arXiv:1809.02362v1, (2018).

[7] P. Grohs, D. Perekrestenko, D. Elbrächter, and H. Bölcskei, *Deep Neural Network Approximation Theory*, arXiv:1901.02220, (2019).

[8] I. Gühring, G. Kutyniok, and P. Petersen, *Error bounds for approximations with deep ReLU neural networks in $W^{s,p}$ norms*, arXiv:1902.07896, (2019).

Towards exponential convergence of adaptive quarklet methods

Thorsten Raasch

(joint work with Stephan Dahlke, Ulrich Friedrich, Philipp Keding, Alexander Sieber)

We are concerned with the design and applications of compressive quarkonial frames within the adaptive numerical solution of operator equations on a bounded computational domain [1]. Such so-called quarklet systems can be seen as a wavelet version of *hp*-finite element dictionaries, as the individual quarklet functions take the shape of polynomially enriched spline wavelets. Rescaled quarklet systems are frames in a large range of Sobolev and Besov spaces, including negative-order spaces, which enables their application in numerical solvers for differential and singular integral equations, and in anisotropic tensor product approximation.

In [2], we have shown that smooth functions with local singularities can be approximated from spline quarklet dictionaries $\Psi = \{\psi_\lambda : \lambda \in \mathcal{J}\}$ at subexponential rates. Similar results are known for *hp*-finite element dictionaries since the early 1980s [3, 4], thereby justifying the application of such super-redundant ansatz systems to the adaptive numerical solution of operator equations.

As a first step, we have proved in [2] that that the univariate singularity function $u(x) = x^\gamma$ on $(0, 1)$, $\gamma > 1/2$, can be approximated from spline quarklets of order

$m \geq 2$ with a best N-term H^1 approximation error bounded by

$$\inf_{\substack{|\Lambda| \leq N \\ v = \sum_{\lambda \in \Lambda} v_\lambda \psi_\lambda}} \|u - v\|_{H^1(0,1)} \leq C e^{-\alpha N^\beta}, \quad N \geq 0, \tag{1}$$

where $\alpha, \beta > 0$ are suitable rate parameters. A subexponential rate $\beta \geq 1/5$ can be achieved by expanding the variable-knot, variable degree spline approximand from [3] into a multiscale quarklet dictionary. In fact, a more refined analysis based on discussions during and after the workshop has revealed that β can be improved to $1/3$ in special cases, which is very close to the approximation rate $1/2$ of univariate *hp*-finite element dictionaries [3] that, however, are not stable in $L_2(0,1)$.

As a second step, we have investigated the case of anisotropic edge singularities on a two-dimensional box domain $(0,1)^2$. It is straightforward to see that the special singularity function $u(\mathbf{x}) = x_1^\gamma$ or, similarly, $u(\mathbf{x}) = x_1^\gamma r(x_2)$ with $r \in \mathbb{P}_q$, can be approximated from tensor product quarklet dictionaries at the very same one-dimensional rates $\beta = 1/5$ or $1/3$. In the case of more complicated edge singularities like $u(\mathbf{x}) = x_1^\gamma v(x_2)$ with smooth v, the rate β will most likely deteriorate slightly, which is due to the additional approximation of v via, e.g., truncated Legendre series. However, we expect that for such anisotropic edge singularities and also for corner singularities like $u(\mathbf{x}) = \|\mathbf{x}\|_2^\gamma$, the applicateion of sparse grid tensor product approximation techniques known from the wavelet setting [5] can ensure the exponential approximability of singularity functions from quarklet dictionaries with rates that only mildly depend on the spatial dimension.

Current research focuses on the design and analysis of adaptive quarklet schemes that can realize such subexponential rates also in practice, without a priori assumptions on the distribution of active quarklet expansion coefficients.

References

[1] S. Dahlke, U. Friedrich, P. Keding, T. Raasch and A. Sieber, *Adaptive quarkonial domain decomposition methods for elliptic partial differential equations*, Preprint, 2018.

[2] S. Dahlke, T. Raasch and A. Sieber, *Exponential convergence of adaptive quarklet approximation*, Preprint, 2019.

[3] W. Gui and I. Babuška, *The h, p and h-p versions of the finite element method in 1 dimension. II. The error analysis of the h- and h-p versions*, Numer. Math. **49** (1986), 613–657.

[4] B. Guo and I. Babuška, *The h-p version of the finite element method. Part 1: The basic approximation results*, Comput. Mech. **1** (1986), 21–41.

[5] P.-A. Nitsche, *Sparse approximation of singularity functions*, Constr. Approx. **21** (2005), 63-81.

Higher order trace finite element methods for surface Stokes equations

Arnold Reusken
(joint work with Thomas Jankuhn, Maxim Olshanskii)

In the past two decades many papers on numerical methods for scalar partial differential equations on surfaces have appeared, starting with the work of Dziuk-Elliott around 2000, cf. the overview paper [2]. Very few papers on numerical methods for surface (Navier-)Stokes equations have appeared. In recent work [1, 3, 4, 5] we studied numerical methods for surface Stokes equations. In particular a class of unfitted finite element methods, also called trace FEM or cut FEM, is investigated. In this presentation recent results, obtained in [5, 3], are treated.

We consider the surface analogon of the very popular Taylor-Hood pair. Not only the lowest order P_2–P_1 pair but also higher order ones are treated. Compared to Stokes equations in Euclidean domains, the surface variant leads to several additional issues that have to be addressed. The two most important issues are the following:

1. *Tangential flow constraint.* In surface flow problems the flow has to be tangential to the surface. It is not obvious how this constraint (which is trivially satisfied in Euclidean domains) can be treated numerically. A technique used in several recent papers is as follows: the surface PDE for the tangential flow field is replaced by a PDE that allows fully three-dimensional velocities, defined on the surface and a penalty approach is used to control the component of the velocity field that is normal to the surface.
2. *Sufficiently accurate geometry approximation.* This topic resembles the problem of a sufficiently accurate boundary approximation for (Navier-)Stokes equations in Euclidean domains. For the latter the isoparametric finite element technique is a standard approach. It is evident that for the case in which the domain is a surface the issue of geometry approximation becomes much more important. To say it differently, for problems in Euclidean domains with a polygonal boundary standard higher order finite elements can yield optimal higher order accuracy, whereas in a surface finite element method one always needs a "sufficiently accurate" surface approximation for optimal higher order accuracy.

As mentioned above, we restrict to trace finite element techniques. In such a setting, already for the case of scalar surface PDEs, one needs an appropriate stabilization to control instabilities caused by "small cuts".

In this setting several important questions arise that are non-existent in Stokes problems in Euclidean domains. For example, what is an appropriate scaling (in terms of the mesh size parameter h) of the penalty parameter, or, how does the error in the geometry approximation influence the discretization error.

We present a class of mixed trace finite element methods with the following key ingredients:

- We use a penalty formulation for treating the tangential constraint.
- We use the parametric trace finite element spaces, known from scalar surface PDEs and unfitted FEM for scalar interface problems, to obtain a higher order surface approximation.
- A specific stabilization, namely the so-called volume normal derivative stabilization, known from the literature, is used.
- Specific parameter choices are proposed, based on recently obtained rigorous results on P_2–P_1 surface Taylor-Hood elements and on error bounds for trace FEM applied to surface vector-Laplace equations.

In the presentation these ingredients are explained and rigorous results concerning LBB stability and error bounds are briefly addressed. Results of numerical experiments are shown that illustrate the optimal order convergence of this class of finite element methods for surface Stokes equations.

References

[1] T. Jankuhn, M. Olshanskii, A. Reusken, *Incompressible fluid problems on embedded surfaces: Modeling and variational formulations*, Interfaces and Free Boundaries **20** (2018), 353–377.

[2] G. Dziuk, C. Elliott, *Finite element methods for surface PDEs*, Acta Numerica **22** (2013), 289–396.

[3] T. Jankuhn, A. Reusken, *Higher order trace finite element methods for the surface Stokes equation*, IGPM preprint 491, RWTH Aachen University (2019).

[4] T. Jankuhn, A. Reusken, *Trace finite element methods for surface vector-Laplace equations*, arXiv preprint: 1904.12494 (2019).

[5] M. Olshanskii, A. Reusken, A.Zhiliakov *Inf-sup stability of the trace P_2-P_1 Taylor-Hood elements for surface PDEs*, arXiv preprint: 1909.02990 (2019).

Quasi-optimal and pressure robust discretizations of the Stokes equations.

Pietro Zanotti

(joint work with Christian Kreuzer, Rüdiger Verfürth)

Abstract discretization of the Stokes equations. Let $\Omega \subseteq \mathbb{R}^d$, $d \in \{2, 3\}$, be an open and bounded polytopic domain. The weak formulation of the stationary Stokes equations in Ω, with viscosity $\mu > 0$ and load $f \in H^{-1}(\Omega)$, looks for $u \in H^1_0(\Omega)^d$ and $p \in L^2_0(\Omega)$ such that

$$
\begin{aligned}
&\forall v \in H^1_0(\Omega)^d \qquad && \mu \int_\Omega \nabla u \colon \nabla v - \int_\Omega p \operatorname{div} v = \langle f, v \rangle \\
&\forall q \in L^2_0(\Omega) && \int_\Omega q \operatorname{div} u = 0.
\end{aligned} \tag{1}
$$

Here : denotes the euclidean scalar product of $d \times d$ tensors and $\langle \cdot, \cdot \rangle$ is the dual pairing of $H^{-1}(\Omega)$ and $H^1_0(\Omega)^d$. Due to the boundary condition on the analytical velocity u, the analytical pressure p belongs to $L^2_0(\Omega) := \{q \in L^2(\Omega) \mid \int_\Omega q = 0\}$.

Let V_h and Q_h be finite dimensional linear spaces. We assume $Q_h \subseteq L^2_0(\Omega)$, whereas V_h is possibly nonconforming, meaning that it is not required to be a subspace of $H^1_0(\Omega)^d$. Hence, we equip the sum $H^1_0(\Omega)^d + V_h$ with an extension $\|\cdot\|_h$ of the H^1-norm. We assume also that the pair V_h/Q_h is inf-sup stable, meaning that there is a bilinear form $b_h : V_h \times Q_h \to \mathbb{R}$ satisfying

$$\sup_{v_h \in V_h} \frac{b_h(v_h, q_h)}{\|v_h\|_h} \geq \beta \|q_h\|_{L^2(\Omega)} \tag{2}$$

for some $\beta > 0$ and for all $q_h \in Q_h$.

We consider the following abstract discretization of (1): Find $u_h \in V_h$ and $p_h \in Q_h$ such that

$$\begin{aligned} &\forall v_h \in V_h \qquad \mu a_h(u_h, v_h) + b_h(v_h, p_h) = \langle f, E_h v_h \rangle \\ &\forall q_h \in Q_h \qquad\qquad\qquad\quad b_h(u_h, q_h) = 0, \end{aligned} \tag{3}$$

where $a_h : V_h \times V_h \to \mathbb{R}$ is a coercive bilinear form and $E_h : V_h \to H^1_0(\Omega)^d$ is a linear operator. It is also worth introducing the discrete divergence $\underline{\mathrm{div}}_h : V_h \to Q_h$

$$\forall q_h \in Q_h \quad \int_\Omega q_h \underline{\mathrm{div}}_h v_h = -b_h(v_h, q_h). \tag{4}$$

Quasi-optimality and pressure robustness. We are interested in the question whether the discretization (3) enjoys the following a priori error estimates.

(i) We say that (3) is a quasi-optimal discretization of (1) when there is a constant $C_{\mathrm{qo}} \geq 1$ such that

$$\mu \|u - u_h\|_h + \|p - p_h\|_{L^2(\Omega)} \leq C_{\mathrm{qo}} \left(\mu \inf_{w_h \in V_h} \|u - w_h\|_h + \inf_{q_h \in Q_h} \|p - q_h\|_h \right)$$

for all $f \in H^{-1}(\Omega)$ and $\mu > 0$.

(ii) We say that (3) is a quasi-optimal and pressure robust discretization of (1) when there is a constant $C_{\mathrm{qopr}} \geq 1$ such that

$$\|u - u_h\|_h \leq C_{\mathrm{qopr}} \inf_{w_h \in V_h} \|u - w_h\|_h$$

for all $f \in H^{-1}(\Omega)$ and $\mu > 0$.

Property (i) entails that the pair (u_h, p_h) is a near-best approximation of (u, p) in $V_h \times Q_h$. Similarly, property (ii) entails that u_h is a near-best approximation of u in V_h. An abstract framework to verify the validity of such conditions and to identify the respective best constants can be found in [5]. Interestingly, property (ii) ensures also that u_h is pressure robust, i.e. independent of p and μ, thus reproducing a remarkable invariance property of its analytical counterpart u. The importance of pressure robustness in the context of the (Navier)-Stokes equations has been the subject of several recent research papers, see e.g. [2, 4] and the references therein.

The following results are well-established in the literature, see [1, Chapter 5].

- Property (i) holds if (3) is a standard discretization of (1) with a conforming pair, i.e. $V_h \subseteq H^1_0(\Omega)^d$ and

$$a_h(w_h, v_h) = \int_\Omega \nabla w_h \colon \nabla v_h \qquad b_h(v_h, q_h) = -\int_\Omega q_h \mathrm{div} v_h \qquad E_h = \mathrm{Id}_{V_h}.$$

  Moreover, the constant C_{qo} can be bounded in terms of the inverse of the inf-sup constant β from (2).
- Properties (i) and (ii) hold if (3) is a standard discretization of (1) with a conforming and divergence-free pair pair, meaning that $V_h \subseteq H^1_0(\Omega)^d$ with $\mathrm{div} V_h = Q_h$ and a_h, b_h and E_h as above. In this case, both C_{qo} and C_{qopr} are bounded in terms of β^{-1}.

More recently, the following result has been established for general conforming pairs V_h/Q_h of finite element spaces on a simplicial mesh $\mathcal{M}$ of Ω, see [3].

- Assume that the discrete divergence $\underline{\mathrm{div}}_h$ from (4) satisfies

$$\forall K \in \mathcal{M} \qquad \int_K \underline{\mathrm{div}}_h v_h = \int_K \mathrm{div} v_h \tag{5}$$

  for all $v_h \in V_h$. There is a linear operator $E_h : V_h \to H^1_0(\Omega)$, which can be computed element-wise, such that $\mathrm{div} E_h v_h = \underline{\mathrm{div}}_h v_h$. Then, setting

$$a_h(w_h, v_h) = \int_\Omega \nabla E_h w_h \colon \nabla E_h v_h + \int_\Omega \nabla (E_h w_h - w_h) \colon \nabla (E_h v_h - v_h)$$

  with $\eta > 0$ and letting b_h be as above, the discretization (3) enjoys properties (i) and (ii), with C_{qo} and C_{qopr} depending only on β^{-1} and the shape parameter of $\mathcal{M}$.

Variants of this result have been established for nonconforming pairs as well, see [3, 6].

Future perspectives. The following issues are still left open by the aforementioned results.

- The a priori estimates in (i) and (ii) are not fully satisfactory if the approximation of p by p_h is concerned separately from the approximation of u by u_h. Indeed, the pressure error can be guaranteed to be smaller than a prescribed tolerance only if both the best velocity error and the best pressure are sufficiently small. In other words, the *velocity robustness* of the pressure error is not guaranteed. In this respect, it would be desirable to find pairs V_h/Q_h and (computationally feasible) forms a_h, b_h and E_h such that the discretization (3) satisfies a pressure error estimate in the form $\|p - p_h\|_{L^2(\Omega)} \leq C_{\mathrm{qovr}} \inf_{q_h \in Q_h} \|p - q_h\|_{L^2(\Omega)}$ for some constant $C_{\mathrm{qovr}} \geq 1$ and for all $f \in H^{-1}(\Omega)$ and $\mu > 0$.
- In general, condition (5) fails to hold for conforming pairs with continuous pressure (i.e. $Q_h \subseteq C^0(\Omega)$), like the so-called Hood-Taylor pairs. It is shown in [3, section 4.2], that this issue can be circumvented, at the price of a significantly more involved construction of the operator E_h. A simplification of that idea could be obtained introducing a nonstandard

modification of the bilinear form b_h (or, equivalently, of the discrete divergence $\underline{\mathrm{div}}_h$). This, however, requires the proof of a new variant of the inf-sup condition (2).

References

[1] D. Boffi, F. Brezzi, and M. Fortin, *Mixed Finite Element Methods and Applications*, vol. 44 of Springer Series in Computational Mathematics, Springer, Heidelberg, 2013.

[2] N. R. Gauger, A. Linke, and P. W. Schroeder, *On high-order pressure-robust space discretisations, their advantages for incompressible high Reynolds number generalised Beltrami flows and beyond*, arXiv:1808.10711v3, 2018.

[3] C. Kreuzer and P. Zanotti, *Quasi-optimal and pressure robust discretizations of the Stokes equations by new augmented Lagrangian formulations*, to appear.

[4] A. Linke, *On the role of the Helmholtz decomposition in mixed methods for incompressible flows and a new variational crime*, Comput. Methods Appl. Mech. Engrg., **268** (2014), 782–800.

[5] A. Veeser and P. Zanotti, *Quasi-optimal nonconforming methods for symmetric elliptic problems. I—Abstract theory*, SIAM J. Numer. Anal., **56** (2018), 1621–1642.

[6] R. Verfürth and P. Zanotti, *A quasi-optimal Crouzeix–Raviart discretization of the Stokes equations*, SIAM J. Numer. Anal., **57** (2019), 1082–1099.

On a diffuse interface approach to PDEs on surfaces and networks

Björn Stinner

(joint work with Oliver Dunbar, Kei Fong (Andrew) Lam, Andreas Dedner, Charles Elliott)

Problems with free, usually moving boundaries involving lateral processes feature in numerous applications, for instance, in cell biology (biochemistry on the cell boundaries), in materials science (diffusion along grain boundaries), or in multiphase flow (surface active agents). We are particularly interested in the case of more than two phases so that the phase interfaces can form triple junctions where three phases meet. Diffuse interface models based on the phase field methodology represent the phase interfaces by thin layers so that, as the interfacial thickness converges to zero, a model with moving hypersurfaces is obtained. Interface capturing approaches such as the phase field method naturally account for topological changes and make relatively standard numerical approches such as adaptive finite element methods accessible.

Our objective has been to account for any interfacial processes in the diffuse interface approach. Assuming that these phenomena can be described by partial differential equations on the moving hypersurfaces, the question is how these equations can be consistently approximated if the hypersurfaces are replaced by thin layers, and are recovered when the thickness converges to zero.

To illustrate the problem, consider a stationary situation as in Figure 1 on the left. Three phases occupying domains $\Omega^{(i)}$ are separated by interfaces $\Gamma^{(i,j)}$ that form a triple junction $T^{(i,j,k)}$, $i, j, k \in \{0, 1, 2\}$. On the interfaces there are species

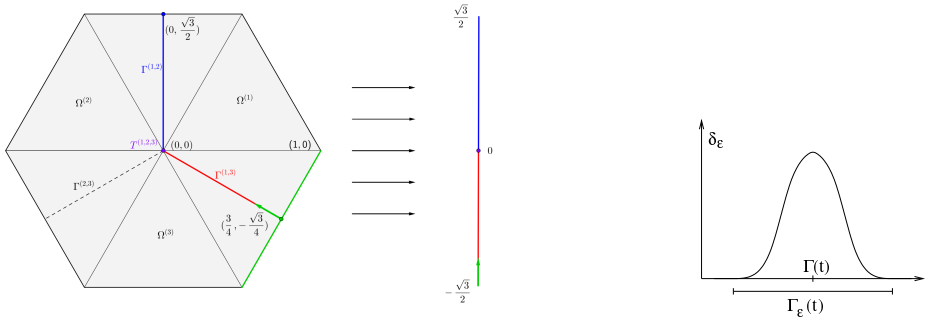

FIGURE 1. Domain separated into three phases (left) for some numerical tests and a cross profile of a function to approximate a surface distribution (right).

densities $c^{(i,j)}$ subject to diffusion equations of the form

$$\partial_t c^{(i,j)} = -\nabla_{\Gamma^{(i,j)}} \cdot \boldsymbol{J}_c^{(i,j)}, \quad \boldsymbol{J}_c^{(i,j)} = -M_c^{(i,j)} \nabla_{\Gamma^{(i,j)}} c^{(i,j)}$$

where $\nabla_{\Gamma^{(i,j)}}$ is the surface gradient on $\Gamma^{(i,j)}$ and $M_c^{(i,j)} > 0$ is a diffusion constant. In the triple junctions we assume a Robin type condition of the form

$$\boldsymbol{J}_c^{(i,j)} \cdot \boldsymbol{\mu}^{(i,j,k)} = \beta_{(i,j)\leftrightarrow(i,k)} \big(c^{(i,j)} - c^{(i,k)}\big) + \beta_{(i,j)\leftrightarrow(j,k)} \big(c^{(i,j)} - c^{(j,k)}\big)$$

where $\boldsymbol{\mu}^{(i,j,k)}$ is the external co-normal of $\Gamma^{(i,j)}$ and the $\beta_{(i,j)\leftrightarrow(i,k)} > 0$ are constants.

Following and extending the arguments in [1] we can write this problem in a distributional form:

$$\begin{aligned}\partial_t \big(\delta_{\Gamma^{(i,j)}} c^{(i,j)}\big) - \nabla \cdot \big(\delta_{\Gamma^{(i,j)}} M_c^{(i,j)} \nabla_{\Gamma^{(i,j)}} c^{(i,j)}\big) \\ = \sum_{k \neq i,j} \tau_{T^{(i,j,k)}} \big(\beta_{(i,k)\leftrightarrow(i,j)} (c^{(i,k)} - c^{(i,j)}) + \beta_{(j,k)\leftrightarrow(i,j)} (c^{(j,k)} - c^{(i,j)})\big)\end{aligned}$$

where $\delta_{\Gamma^{(i,j)}}(\phi) = \int_{\Gamma^{(i,j)}} \phi$ and $\tau_{T^{(i,j,k)}}(\phi) = \phi(T^{(i,j,k)})$ for $\phi \in C_0^\infty(\Omega)$ are interface and triple junction distributions, respectively. An idea to model these equations in a diffuse interface is to replace these distributions by smoothed distributions $\delta_{i,j} \to \delta_{\Gamma^{(i,j)}}$ and $\tau_{i,j,k} \to \tau_{T^{(i,j,k)}}$ as $\varepsilon \to 0$ where ε is a small smoothing parameter related to the interfacial thickness. A cross profile for $\delta_{i,j}$ is illustrated in Figure 1 on the right. These concepts date back to [6] and have been rigorously proved to be successful, for instance, in [4] for the case of a moving curve.

Computational approaches have to account for the degeneracy of the *profile functions* $\delta_{i,j}$ and $\tau_{i,j,k}$. Own computations are based on the method presented in [5]. The profile functions are expressed in terms of phase fields that are relaxed using the method described in [2]. In a specific example illustrated in Figure 1 on the left, species are present at the interfaces $\Gamma^{(1,2)}$ (green interval) and $\Gamma^{(0,1)}$ (blue interval) only so that the problem can be re-parameterized and formulated

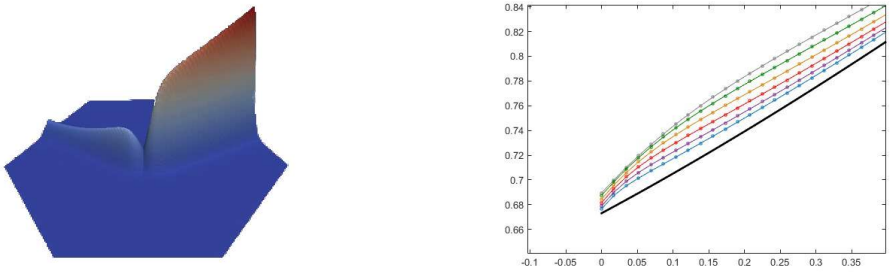

FIGURE 2. Left: Snapshot of a typical simulation, we display the fields $\delta_{i,j} c^{(i,j)}$. Right: Convergence of profiles close to the triple junction as ε decreases (from grey to blue), the solution to the limiting model is black.

over a real interval, which here is chosen so that the triple junction is in the point zero. Initially, the species densities are zero. Mass is then provided by a Dirichlet boundary condition in the point where $\Gamma^{(1,2)}$ intersects with the domain boundary (green dot in Figure 1), whilst we impose a no-flux boundary condition on the point where $\Gamma^{(0,1)}$ intersects the boundary (blue dot).

Figure 2 on the left shows a snapshot after some time, indicating that the species has been diffusing into $\Gamma^{(1,2)}$ and has been transported to the other interface $\Gamma^{(0,1)}$ through the triple junction. As $\varepsilon \to 0$ we observe convergence of the profiles along the interfaces to the solution profile of the limiting model. See Figure 2 on the right for a zoom into several profiles close to the triple junction (which is located at zero). A formal asymptotic analysis predicts convergences rates of one, EOCs for our simulations reveal slightly lower values around 0.9.

The above approach can been used to model surface active agents in multi-phase flow involving three or more fluids. We refer to [3] for a recent preprint on a thermodynamically consistent phase field model for this problem including an formal asymptotic analysis.

REFERENCES

[1] H.W. Alt, *The entropy principle for interfaces. Fluids and solids*, Adv. Math. Sci. Appl. **19** (2009), 585–663.

[2] F. Boyer, C. Lapuerta, *Study of a three component Cahn–Hilliard flow model*, ESAIM: M2AN **40** (2006), 653–687.

[3] O. Dunbar, K.F. Lam, B. Stinner, *Phase field modelling of surfactants in multi-phase flow*, arXiv preprint arXiv:1810.12274 (2018), to appear in Interfaces and Free Boundaries.

[4] C.M. Elliott, B. Stinner, *Analysis of a diffuse interface approach to an advection diffusion equation on a moving surface*, Math. Models Methods Appl. Sc. **19** (2009), 787–802.

[5] C.M. Elliott, B. Stinner, V. Styles, and R. Richard, *Numerical computation of advection and diffusion on evolving diffuse interfaces*, IMA J. Numer. Analysis **31** (2011), 786–812.

[6] A. Rätz, A. Voigt, *PDE's on surfaces—a diffuse interface approach*, Commun. Math. Sci. **4** (2006), 575–590.

A fully practical phase field method for an elliptic surface PDE

Klaus Deckelnick
(joint work with John W. Barrett, Vanessa Styles)

Let $\Gamma \subset \mathbb{R}^{n+1}\,(n = 1, 2)$ be a compact hypersurface without boundary. We consider the elliptic surface PDE

$$-\Delta_\Gamma u + u = f \qquad \text{on } \Gamma, \tag{1}$$

in which Δ_Γ denotes the Laplace–Beltrami operator and f is a given function on Γ. Let us briefly describe the various approaches in order to tackle (1) numerically. Further references can be found in the survey articles [8] and [2].

A finite element method that uses a shape regular polyhedral approximation of Γ was proposed by Dziuk in [7]. The trace finite element method, suggested by Olshanskii, Reusken and Grande in [11], employs an approximation of Γ that is in general not regular. In both approaches piecewise linear finite elements are used and optimal error estimates are obtained. Extensions of the above approaches to higher order FEM spaces have been investigated in [6] and [9] respectively.

If Γ is given implicitly, methods which avoid a direct approximation of Γ have been proposed. In [1] the authors consider a PDE which holds in an open neighbourhood of Γ and has the property that (1) is satisfied simultaneously on all neighboring level surfaces. The discretization of this problem then is amenable to bulk methods: in [1] finite differences are used, while Burger investigates a finite element scheme in [3] . An error analysis in a narrow band setting has been carried out in [4].

A difficulty for the above approach lies in the fact that the extended PDE is degenerate in normal direction. One can address this problem by considering the extension of u which is constant in normal direction as it is done in the closest point method, see e.g. [10] in the parabolic case.

In order to make this idea more precise we denote by d the signed distance function to Γ. It is well known that there exists $\delta > 0$ such that for every $x \in U_\delta := \{x \in \mathbb{R}^{n+1} \,|\, |d(x)| < \delta\}$ there exists a unique $p(x) \in \Gamma$ such that $|x - p(x)| = \min_{y\in\Gamma} |x - y|$ and

$$x = p(x) + d(x)\nu(p(x)),$$

where ν denotes the unit outer normal to Γ. The function $u^e : U_\delta \to \mathbb{R}$ given by $u^e(x) := u(p(x))$ then extends u constantly in normal direction and it can be shown that u^e satisfies the uniformly elliptic PDE

$$-\Delta u^e + u^e = f^e + d\, g(\cdot, \nabla_\Gamma u, \nabla^2_\Gamma u) \qquad \text{in } U_\delta. \tag{2}$$

The derivation of (2) and the precise form of g can be found in [5], where a finite element method based on (2) is proposed and analyzed both on an approximate surface and in a narrow band around Γ which is not fitted to a bulk mesh.

A way to aovid the calculation of an approximate surface or a narrow band is offered by a diffuse interface approach, see [12]. In this approach, the geometry is incorporated into a phase field function which enters as a weight into the weak

formulation. More precisely, let $\epsilon > 0$ and define $\varrho(x) := \sigma\big(\frac{d(x)}{\epsilon}\big)$, where the profile function σ is chosen as

$$\sigma(r) := \begin{cases} \cos^4 r & |r| \le \frac{\pi}{2}, \\ 0 & |r| > \frac{\pi}{2}. \end{cases}$$

Multiplying (2) by $\epsilon^{-1} v\, \varrho$, integrating over $U_{\frac{\epsilon\pi}{2}}$ and using integration by parts as well as the relation $\nabla u^e \cdot \nabla d = 0$ we obtain

$$(3) \quad \frac{1}{\epsilon} \int_{U_{\frac{\epsilon\pi}{2}}} \big(\nabla u^e \cdot \nabla v + u^e\, v\big)\, \varrho\, dx = \frac{1}{\epsilon} \int_{U_{\frac{\epsilon\pi}{2}}} \big(f^e + d\, g\big)\, v\, \varrho\, dx, \quad \forall v \in H^1(U_{\frac{\epsilon\pi}{2}}).$$

In view of the coarea formula, the above relation can be seen to approximate the weak form of (1) for small $\epsilon > 0$.

Let us next use (3) in order to derive a finite element scheme. To do so, we denote by $(\mathcal{T}_h)_{0<h<h_0}$ a regular family of triangulations of a neighbourhood of Γ with mesh size $h := \max_{T\in\mathcal{T}_h} \mathrm{diam} T < \epsilon$. In order to define our computational domain we set

$$\tilde{\mathcal{T}}_h := \{T \in \mathcal{T}_h \,|\, |d(a)| < \epsilon \arccos(\frac{h}{\epsilon}) \text{ for each vertex } a \in T\} \text{ and } D_h := \bigcup_{T\in\tilde{\mathcal{T}}_h} T.$$

Introducing the finite element space

$$V_h := \{v_h \in C^0(D_h) \,|\, v_{h|T} \in P_1(T) \text{ for all } T \in \tilde{\mathcal{T}}_h\}$$

we now define our fully practical scheme as follows: find $u_h \in V_h$ such that

$$(4) \quad \frac{1}{\epsilon} \int_{D_h} \Big(\nabla u_h \cdot \nabla v_h\, I_h\varrho + I_h\big(u_h v_h \varrho\big)\Big) dx = \frac{1}{\epsilon} \int_{D_h} I_h\big(f^e v_h \varrho\big)\, dx \quad \forall v_h \in V_h.$$

In the above, I_h denotes the standard Lagrange interpolation operator, so that the implementation of the method is straightforward. Our main result reads:

Theorem. *The scheme (4) has a unique solution $u_h \in V_h$ and the error $e_h := I_h u^e - u_h$ satisfies*

$$\Big(\frac{1}{\epsilon} \int_{D_h} \big(|\nabla e_h|^2 I_h\varrho + I_h(e_h^2\, \varrho)\big) dx\Big)^{\frac{1}{2}} \le C\big(h + (\frac{h}{\epsilon})^2 + \epsilon^2\big).$$

If in addition there exists a constant $\gamma > 0$ which is independent of h such that $\gamma h \le h_T$ for all $T \in \mathcal{T}_h$ with $|T \cap \Gamma| > 0$, then

$$\|u - u_h\|_{H^1(\Gamma)} \le C \sqrt{\frac{\epsilon}{h}} \Big(h + (\frac{h}{\epsilon})^2 + \epsilon^2\Big).$$

Remark. *The above result suggests to couple the width ϵ to the mesh size h in the form $\epsilon = \sqrt{h}$ yielding $u_h \to u$ in $H^1(\Gamma)$ with a rate of $O(h^{\frac{3}{4}})$ as $h \to 0$. A relation of the form $\epsilon = h^\alpha$ with $\frac{1}{2} < \alpha < 1$ will give a worse convergence rate, but leads to a smaller computational effort.*

References

[1] M. Bertalmio, L.T. Cheng, S. Osher, G. Sapiro, *Variational problems and partial differential equations on implicit surfaces: The framework and examples in image processing and pattern formation*, J. Comput. Phys. **174**, 759–780 (2001).

[2] A. Bonito, A. Demlow, R.H. Nochetto, *Finite element methods for the Laplace-Beltrami operator*, arXiv:1906.02786, to appear in the Handbook of Numerical Analysis (2019).

[3] M. Burger, *Finite element approximation of elliptic partial differential equations on implicit surfaces*, Comput. Vis. Sci. **12**, 87–100 (2009).

[4] K. Deckelnick, G. Dziuk, C.M. Elliott, C.-J. Heine, *An h-narrow band finite-element method for elliptic equations on implicit surfaces*, IMA J. Numer. Anal. **30**, 351–376 (2010).

[5] K. Deckelnick, C.M. Elliott, T. Ranner, *Unfitted finite element methods using bulk meshes fur surface partial differential equations*, SIAM J. Numer. Anal. **52**, 2137–2162 (2014).

[6] A. Demlow, *Higher-order finite element methods and pointwise error estimates for elliptic problems on surfaces*, SIAM J. Numer. Anal. **47**, no. 2, 805–827 (2009).

[7] G. Dziuk, *Finite elements for the Beltrami operator on arbitrary surfaces*, in: Partial differential equations and calculus of variations, S. Hildebrandt and R. Leis, eds., vol. 1357 of Lecture Notes in Mathematics, Springer-Verlag, Berlin, 1988, pp. 142–155.

[8] G. Dziuk, C.M. Elliott, *Finite element methods for surface PDEs*, Acta Numer. **22**, 289–396 (2013).

[9] J. Grande, C. Lehrenfeld, A. Reusken, *Analysis of a high-order trace finite element method for PDEs on level set surfaces*, SIAM J. Numer. Anal. **56**, 228–255 (2018).

[10] C.B Macdonald, S.J Ruuth, *The Implicit Closest Point Method for the Numerical Solution of Partial Differential Equations on Surfaces*, SIAM J. Sci. Comput. **31**, 4330–4350 (2009).

[11] M.A. Olshanskii, A. Reusken, J. Grande, *A finite element method for elliptic equations on surfaces*, SIAM J. Numer. Anal. **47**, no. 5, 3339–3358 (2009).

[12] A. Rätz, A. Voigt, *PDE's on surfaces - a diffuse interface approach*, Comm. Math. Sci. **4**, 575–590 (2006).

Port-Hamiltonian Partial- Differential-Algebraic Systems: A New Approach for Multiscale, Multiphysics Modelling, Simulations and Control

Volker Mehrmann

Motivated by modern energy networks, in particular those from different physical domains the modelling framework of port-Hamiltonian systems is discussed. The classical PH approach is extended to construct dynamical stems (partial-differential-algebraic equations). A new algebraically and geometric defined structure is derived which has more favourable mathematical properties. It is shown that this structure is invariant under projection, changes of basis in space and time, and a dissipation inequality holds. We show that the new representation is close to physics, robust to perturbations and many mathematical properties (like stability and positivity) follow from the structure.

Space–time finite element methods

Olaf Steinbach
(joint work with Marco Zank)

Space–time finite element methods for time–dependent partial differential equations are well suited for an adaptive resolution of the solution simultaneously in space and time, and for the space–time parallel solution of the resulting linear systems. Applications include problems in moving domains, and optimal control problems subject to time–dependent partial differential equations, where the adjoint problem is backward in time.

As a first model problem we consider the Dirichlet problem for the heat equation,

$$\begin{aligned} \alpha\partial_t u(x,t) - \Delta_x u(x,t) &= f(x,t) && \text{for } (x,t) \in Q := \Omega \times (0,T), \\ u(x,t) &= 0 && \text{for } (x,t) \in \Sigma := \partial\Omega \times (0,T), \\ u(x,0) &= 0 && \text{for } x \in \Omega, \end{aligned}$$

where $\Omega \subset \mathbb{R}^n$, $n = 2, 3$, is a bounded Lipschitz domain, $\alpha > 0$ is the heat capacity, and f is a given source term. The related variational formulation is to find $u \in X$ such that

$$\int_0^T \int_\Omega \Big[\alpha\partial_t u(x,t)v(x,t) + \nabla_x u(x,t) \cdot \nabla_x v(x,t)\Big] dx\, dt = \int_0^T \int_\Omega f(x,t)v(x,t)\, dx\, dt$$

is satisfied for all $v \in Y$, where the test and ansatz spaces Y and X have to be specified, respectively. Unique solvability of this general Galerkin–Petrov variational formulation then follows from a stability condition of the associated bilinear form,

$$c_S \, \|u\|_X \leq \sup_{0 \neq v \in Y} \frac{a(u,v)}{\|v\|_Y} \quad \text{for all } u \in X.$$

The most standard choice, see, e.g., [3, 4], is to consider the Bochner spaces $X := L^2(0,T;H^1_0(\Omega)) \cap H^1_{0,}(0,T;H^{-1}(\Omega))$ and $Y := L^2(0,T;H^1_0(\Omega))$. Moreover, for conforming finite element spaces $X_h \subset X$ and $Y_h \subset Y$ satisfying $X_h \subset Y_h$ and using a discrete norm in X_h we can prove a discrete inf–sup condition, and we can establish quasi–optimal a priori error estimates [3] for the space–time finite element solution. A different choice is to consider the anisotropic Sobolev spaces $X := H^{1,1/2}_{0;0,}(Q) = L^2(0,T;H^1_0(\Omega)) \cap H^{1/2}_{0,}(0,T;L^2(\Omega))$, and $Y := H^{1,1/2}_{0;,0}(Q)$, respectively; for the related stability condition see [5]. For $u \in H^1_{0,}(0,T)$ we may consider the Fourier series

$$u(t) = \sum_{k=0}^{\infty} u_k \sin\Big(\Big(\frac{\pi}{2} + k\pi\Big)\frac{t}{T}, \quad u_k = \frac{2}{T}\int_0^T u(t) \sin\Big(\Big(\frac{\pi}{2} + k\pi\Big)\frac{t}{T}\, dt,$$

and we define the modified Hilbert transformation [5]

$$(\mathcal{H}_T u)(t) = \sum_{k=0}^{\infty} u_k \cos\Big(\Big(\frac{\pi}{2} + k\pi\Big)\frac{t}{T}.$$

It turns out that $\mathcal{H}_T : H^1_{0,}(0,T) \to H^1_{,0}(0,T)$ is norm preserving, non–negative, i.e., $\langle \mathcal{H}_T v, v\rangle_{L^2(0,T)} > 0$ for all $v \in H^1_{0,}(0,T)$, and the bilinear form $\langle \partial_t u, \mathcal{H}_T v\rangle_{(0,T)}$ is self–adjoint and elliptic, i.e., $\langle \partial_t v, \mathcal{H}_T v\rangle_{(0,T)} = \|v\|^2_{H^{1/2}_{0,}(0,T)}$. Hence we consider the Galerkin–Bubnov variational formulation to find $u \in H^{1,1/2}_{0;0,}(Q)$ such that

$$\langle \partial_t u, \mathcal{H}_T v\rangle_Q + \langle \nabla_x u, \nabla_x \mathcal{H}_T v\rangle_{L^2(Q)} = \langle f, \mathcal{H}_T v\rangle_Q$$

is satisfied for all $v \in H^{1,1/2}_{0;0,}(Q)$. Again we can establish a related inf–sup stability condition [5]. Moreover, for any conforming finite element approximation $X_h \subset X$ we have unique solvability of the space–time finite element scheme, and when consider space–time tensor–product approximations we can prove quasi–optimal a priori error estimates. For a given space–time finite element solution one can define suitable a posteriori error indicators to drive an adaptive refinement simultaeneously in space and time, see the discussion as given in [4]. For the solution of the resulting linear system of algebraic equations one may use parallel iterative solution strategies, in combination with geometric and algebraic multigrid methods, see, e.g., [4].

As a second model problem we consider the Dirichlet problem for the wave equation,

$$\begin{aligned} \partial_{tt} u(x,t) - \Delta_x u(x,t) &= f(x,t) && \text{for } (x,t) \in Q := \Omega \times (0,T), \\ u(x,t) &= 0 && \text{for } (x,t) \in \Sigma := \partial\Omega \times (0,T), \\ u(x,0) = \partial_t u(x,t)_{|t=0} &= 0 && \text{for } x \in \Omega. \end{aligned}$$

The related variational formulation is to find $u \in X := H^{1,1}_{0;0,}(Q)$ such that

$$-\langle \partial_t u, \partial_t v\rangle_{L^2(\Omega)} + \langle \nabla_x u, \nabla_x v\rangle_{L^2(\Omega)} = \langle f, v\rangle_Q$$

is satisfied for all $v \in H^{1,1}_{0;,0}(Q)$. As in the parabolic case we can establish unique solvability of the space–time variational formulation [5], but we have to assume $f \in L^2(Q)$. As in the case of the heat equation we can introduce a modified Hilbert transformation $\widetilde{\mathcal{H}}_T : H^1_{0,}(0,T) \to H^1_{,0}(0,T)$, given as $(\widetilde{\mathcal{H}}_T v)(t) := v(T) - v(t)$. However, for a conforming finite element approximation $X_h \subset X$, and when using space–time tensor–product finite element spaces, we have to assume a CFL condition $h_t \leq h_x/\sqrt{n}$ which restricts the use of adaptive refinements. Instead, we can consider a stabilized variational formulation to find $\widetilde{u}_h \in X_h$ such that

$$\langle \partial_t \widetilde{u}_h, \partial_t v_h\rangle_{L^2(\Omega)} + \langle \nabla_x Q_{h_t} \widetilde{u}_h, \nabla_x \widetilde{\mathcal{H}}_T v_h\rangle_{L^2(\Omega)} = \langle f, \widetilde{\mathcal{H}}_T v_h\rangle_Q$$

is satisfied for all $v_h \in X_h$, where Q_{h_t} is the L^2 projection on the space of functions which are piecewise constant in time. It turns out that this perturbed variational formulation is unconditionally stable, and provides optimal convergence of the space–time finite element error in $L^2(Q)$ and $H^1(Q)$, respectively, see [6].

The approach as given for the scalar wave equation can be generalized when considering the electromagnetic wave equation [2]. Moreover, one may also consider space–time boundary element methods [1], and the coupling of space–time finite and boundary element methods.

References

[1] S. Dohr, K. Niino, O. Steinbach: Space–time boundary element methods for the heat equation. In: Space–Time Methods. Applications to Partial Differential Equations, (U. Langer, O. Steinbach eds.), Radon Series on Computational and Applied Mathematics, vol. 25, de Gruyter, Berlin, pp. 1–60, to appear, 2019.

[2] J. I. M. Hauser, O. Steinbach: Space–time variational methods for Maxwell's equations. Proc. Appl. Math. Mech., published online, 2019.

[3] O. Steinbach: Space–time finite element methods for parabolic problems. Comput. Meth. Appl. Math. 15 (2015) 551–566.

[4] O. Steinbach, H. Yang: Space–time finite element methods for parabolic evolution equations: Discretization, a posteriori error estimation, adaptivity and solution. In: Space–Time Methods. Applications to Partial Differential Equations, (U. Langer, O. Steinbach eds.), Radon Series on Computational and Applied Mathematics, vol. 25, de Gruyter, Berlin, pp. 207–248, to appear, 2019.

[5] O. Steinbach, M. Zank: Coercive space–time finite element methods for initial boundary value problems, submitted, 2018.

[6] O. Steinbach, M. Zank: A stabilized space–time finite element method for the wave equation. In: Advanced Finite Element Methods with Applications. Selected papers from the 30th Chemnitz FEM Symposium 2017, (T. Apel, U. Langer, A. Meyer, O. Steinbach eds.), Lecture Notes in Computational Science and Engineering, vol. 128, Springer, pp. 341–370, 2019.

A structure-preserving finite element method for uniaxial nematic liquid crystals

Juan Pablo Borthagaray

(joint work with Ricardo H. Nochetto, Shawn W. Walker)

We consider a uniaxially-constrained Landau-de Gennes model for nematic liquid crystals. In such a model, a tensor field $\mathbf{Q}(x)$ measures the discrepancy between the probability distribution of the molecular orientation at x and a uniform distribution on $\mathbb{S}^{d-1}$ [5]. We assume that $\mathbf{Q}$ takes the state $\mathbf{Q} = s\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\right)$, where the scalar field s is called the *degree of orientation*.

Formulation of the problem. Let $\mathbf{\Theta} = \mathbf{n}\otimes\mathbf{n}$ above. We study a one-constant model, in which the energy is given by $E_{\text{uni}}[\mathbf{Q}] := E_{\text{uni}-\text{m}}[s,\mathbf{\Theta}] + E_{\text{bulk}}[s]$, with

$$E_{\text{uni}-\text{m}}[s,\mathbf{\Theta}] := \frac{1}{2}\left(\frac{d-1}{d}\int_\Omega |\nabla s|^2\,dx + \int_\Omega s^2|\nabla\mathbf{\Theta}|^2\,dx\right),\ E_{\text{bulk}}[s] := \int_\Omega \psi(s)\,dx.$$

Above, the function $E_{\text{uni}-\text{m}}$ is an elastic energy, whereas E_{bulk} is a bulk energy with a double-well potential ψ that confines the eigenvalues of $\mathbf{Q}$ to a physically meaningful range. Introducing the auxiliary variable $\mathbf{U} = s\mathbf{\Theta}$ yields the identity

$$E_{\text{uni}-\text{m}}[s,\mathbf{\Theta}] = \frac{1}{2}\left(-\frac{1}{d}\int_\Omega |\nabla s|^2\,dx + \int_\Omega |\nabla\mathbf{U}|^2\,dx\right) =: \widetilde{E}_{\text{uni}-\text{m}}[s,\mathbf{U}].$$

This formula shows that $\mathbf{U}$ must be of class H^1 in order to the energy be finite. Motivated by this observation, we consider the admissible class

$$\mathcal{A}_{\text{uni}} := \{(s,\mathbf{\Theta}) \in H^1(\Omega)\times[L^\infty(\Omega)]^{d\times d} : (s,\mathbf{U},\mathbf{\Theta}) \text{ satisfies (1), with } \mathbf{U}\in[H^1(\Omega)]^{d\times d}\},$$

with the structural condition

$$-\frac{1}{d-1} \le s \le 1, \qquad \mathbf{U} = s\boldsymbol{\Theta}, \qquad \boldsymbol{\Theta} \in \mathbf{L}^{d-1} \text{ a.e. in } \Omega, \tag{1}$$

where $\mathbf{L}^{d-1} := \{\mathbf{A} \in \mathbf{R}^{d\times d}\colon \text{ there exists } \mathbf{n} \in \mathbb{S}^{d-1},\ \mathbf{A} = \mathbf{n}\otimes\mathbf{n}\}$. Our problem consists in seeking the minimizer of E_{uni} over $\mathcal{A}_{\text{uni}}$. Naturally, boundary conditions should be incorporated in the model; here, we omit the details for brevity.

Discretization. We assume $\mathcal{T}_h = \{T\}$ is a conforming simplicial triangulation of Ω, and introduce the discrete spaces

$$\begin{aligned}
\mathbb{S}_h &:= \{s_h \in H^1(\Omega) : s_h|_T \text{ is affine for all } T \in \mathcal{T}_h\},\\
\overline{\mathbb{U}}_h &:= \{\mathbf{U}_h \in [H^1(\Omega)]^{d\times d} : \mathbf{U}_h|_T \in \mathcal{P}_1(T), \forall T \in \mathcal{T}_h\},\\
\mathbb{T}_h &:= \{\boldsymbol{\Theta}_h \in \overline{\mathbb{U}}_h : \boldsymbol{\Theta}_h(x_i) \in \mathbf{L}^{d-1}, \text{ for all nodes } x_i\}.
\end{aligned}$$

We consider the discrete admissible class,

$$\mathcal{A}^h_{\text{uni}} := \big\{(s_h, \boldsymbol{\Theta}_h) \in \mathbb{S}_h \times \mathbb{T}_h : (s_h, \mathbf{U}_h, \boldsymbol{\Theta}_h) \text{ satisfies (2), with } \mathbf{U}_h \in \overline{\mathbb{U}}_h\big\},$$

where

$$\mathbf{U}_h = I_h(s_h\boldsymbol{\Theta}_h), \quad -\frac{1}{d-1} \le s_h \le 1 \text{ in } \Omega. \tag{2}$$

We set $\delta_{ij}s_h := s_h(x_i) - s_h(x_j)$, $\delta_{ij}\boldsymbol{\Theta}_h := \boldsymbol{\Theta}_h(x_i) - \boldsymbol{\Theta}_h(x_j)$, and define

$$E^h_{\text{uni}-\text{m}}[s_h, \boldsymbol{\Theta}_h] := \frac{d-1}{4d}\sum_{i,j=1}^n k_{ij}\left(\delta_{ij}s_h\right)^2 + \frac{1}{4}\sum_{i,j=1}^n k_{ij}\left(\frac{s_h(x_i)^2 + s_h(x_j)^2}{2}\right)|\delta_{ij}\boldsymbol{\Theta}_h|^2.$$

Above, the first term corresponds to $\frac{1}{2}\sum_{i,j=1}^n k_{ij}\left(\delta_{ij}s_h\right)^2 = \int_\Omega |\nabla s_h|^2 dx$, while the second term is a first order approximation of $\int_\Omega s^2|\nabla\boldsymbol{\Theta}|^2 dx$. The bulk energy is discretized in a standard fashion, namely, $E^h_{\text{bulk}}[s_h] := \int_\Omega \psi(s_h)dx$.

Our discrete problem consists in finding a minimizer of

$$E^h_{\text{uni}}[s_h, \boldsymbol{\Theta}_h] := E^h_{\text{uni}-\text{m}}[s_h, \boldsymbol{\Theta}_h] + E^h_{\text{bulk}}[s_h]$$

over $\mathcal{A}^h_{\text{uni}}$. Because the discrete spaces consist of piecewise linear functions, the structural condition $\mathbf{U}_h = s_h\boldsymbol{\Theta}_h$ is only satisfied at the nodes (cf. (2)); thus, there is a variational crime that we need to account for. More precisely, if we define

$$\widetilde{E}^h_{\text{uni}-\text{m}}[s_h, \mathbf{U}_h] := \frac{1}{2}\left(-\frac{1}{d}\int_\Omega |\nabla s_h|^2 dx + \int_\Omega |\nabla \mathbf{U}_h|^2 dx\right),$$

then the consistency of the method can be expressed as whether

$$\lim_{h\to 0} E^h_{\text{uni}-\text{m}}[s_h, \boldsymbol{\Theta}_h] - \widetilde{E}^h_{\text{uni}-\text{m}}[s_h, \mathbf{U}_h] = 0.$$

Computation of discrete minimizers. We propose an alternating direction method that, at each step, first performs a tangential variation on the director line field and then a gradient flow step on the degree of orientation. Let

$$\mathbf{V}_h(\mathbf{n}_h) = \{\mathbf{v}_h \in [H^1(\Omega)]^d : \mathbf{v}_h|_T \in \mathcal{P}_1(T)\ \forall T \in \mathcal{T}_h, \\ \mathbf{v}_h(x_i)\cdot\mathbf{n}_h(x_i) = 0 \text{ for all nodes } x_i\}.$$

Given $(s_h^0, \mathbf{\Theta}_h^0) \in \mathcal{A}_{\rm uni}^h$, with $\mathbf{\Theta}_h^0 = \mathbf{n}_h^0 \otimes \mathbf{n}_h^0$, and a time step $\delta t > 0$, we iterate steps **1**–**3** for $k \geq 0$:

1. *(Weighted) tangent flow step for $\mathbf{\Theta}_h$:* find $\mathbf{t}_h^k \in \mathbf{V}_h$ and $\mathbf{T}_h^k = \mathbf{n}_h^k \otimes \mathbf{t}_h^k + \mathbf{t}_h^k \otimes \mathbf{n}_h^k$ such that, for all $\mathbf{V}_h = \mathbf{n}_h^k \otimes \mathbf{v}_h + \mathbf{v}_h \otimes \mathbf{n}_h^k$,

$$\frac{1}{\delta t}\int_\Omega (\nabla \mathbf{t}_h^k \colon \nabla \mathbf{v}_h (s_h^k)^2 + \mathbf{t}_h^k \cdot \mathbf{v}_h) + \delta_{\mathbf{\Theta}} E_{\rm uni-m}^h[s_h^k, \mathbf{\Theta}_h^k + \mathbf{T}_h^k; \mathbf{V}_h] = 0. \tag{3}$$

2. *Projection:* update $\mathbf{\Theta}_h^{k+1} \in \mathbb{T}_h$ at each node x_i by

$$\mathbf{\Theta}_h^{k+1}(x_i) := \frac{\mathbf{n}_h^k(x_i) + \mathbf{t}_h^k(x_i)}{|\mathbf{n}_h^k(x_i) + \mathbf{t}_h^k(x_i)|} \otimes \frac{\mathbf{n}_h^k(x_i) + \mathbf{t}_h^k(x_i)}{|\mathbf{n}_h^k(x_i) + \mathbf{t}_h^k(x_i)|}. \tag{4}$$

3. *Gradient flow step for s_h:* find $s_h^{k+1} \in \mathbb{S}_h$ such that

$$\frac{1}{\delta t}\int_\Omega (s_h^{k+1} - s_h^k)\, z_h + \delta_s E_{\rm uni}^h[s_h^{k+1}, \mathbf{\Theta}_h^{k+1}; z_h] = 0 \quad \forall z_h.$$

The algorithm above is energy-decreasing provided meshes are weakly acute and the time step is sufficiently small [2].

Theorem 1. *If the meshes are weakly acute and $\delta t \leq C h^{d/2}$ then, for all $N \geq 1$,*

$$E_{\rm uni}^h[s_h^N, \mathbf{\Theta}_h^N] + \frac{1}{\delta t}\sum_{k=0}^{N-1}\left(\|s_h^k \nabla \mathbf{t}_h^k\|_{L^2(\Omega)}^2 + \|\mathbf{t}_h^k\|_{L^2(\Omega)}^2 + \|s_h^{k+1} - s_h^k\|_{L^2(\Omega)}^2\right) \leq E_{\rm uni}^h[s_h^0, \mathbf{\Theta}_h^0].$$

Two comments are in order. The weakly acuteness requirement is needed to guarantee that step **2** be energy-decreasing [1]. We also point out that, although our method is implicit, we have a time-step restriction. This is caused by the second-order inconsistency when updating $\mathbf{\Theta}_h^k$ with a non-tangential variation. Indeed, a proper tangential perturbation of $\mathbf{\Theta}_h^k$ would consist in taking $\widetilde{\mathbf{\Theta}}_h^{k+1} = \mathbf{\Theta}_h^k + \mathbf{T}_h^k$. However, this update would not have rank one. Our choice in (4) (before normalization) preserves the rank-one constraint but differs from $\mathbf{\Theta}_h^k + \mathbf{T}_h^k$ by a term $\mathbf{t}_h^k \otimes \mathbf{t}_h^k$. Therefore, we need to bound

$$\frac{1}{2}\sum_{i,j} k_{ij}\left(\frac{s_h^k(x_i)^2 + s_h^k(x_j)^2}{2}\right)|\delta_{ij}(\mathbf{t}_h^k \otimes \mathbf{t}_h^k)|^2 \approx \int_\Omega (s_h^k)^2 |\nabla(\mathbf{t}_h^k \otimes \mathbf{t}_h^k)|^2 dx$$

in terms of the norm induced by the inner product in (3). In the end, this introduces a time-step restriction.

Convergence. Convergence of our numerical scheme is expressed in terms of the Γ-convergence of the energy minimization problems as $h \to 0$. We follow the general principle [3]

equi-coerciveness + Γ-convergence $\Rightarrow$ convergence of minimum problems.

Equi-coercivity of the discrete energies and weak-lower semicontinuity can be proved by essentially the same arguments as in [4]. The construction of a recovery sequence (or lim-sup inequality) depends on the use of Lagrange interpolation: we recall that our discrete admissibility conditions (2) are enforced nodewise. Therefore, because the natural space for $(s, \mathbf{U})$ is $[H^1(\Omega)]^{d\times d}$, a key component of our work is showing that smooth (or at least continuous) pairs $(s, \mathbf{U})$ are dense in $\mathcal{A}_{\rm uni}$. As a final result, we derive the following theorem [2].

Theorem 2. *Let $(s_h, \mathbf{U}_h, \mathbf{\Theta}_h) \in \mathcal{A}^h_{\rm uni}$ be a sequence of global minimizers of the discrete energies $E^h_{\rm uni}$. Then, every cluster point is a global minimizer of the continuous energy $E_{\rm uni}$.*

References

[1] F. Alouges, *A new algorithm for computing liquid crystal stable configurations: The harmonic mapping case*, SIAM Journal on Numerical Analysis, **34** (1997), 1708–1726.

[2] J.P. Borthagaray, R.H. Nochetto, S.W. Walker, *A structure-preserving FEM for the uniaxially constrained* $\mathbf{Q}$*-tensor model of nematic liquid crystals*, in preparation.

[3] A. Braides, *Gamma-Convergence for Beginners*, Oxford Lecture Series in Mathematics and Its Applications Volume 22, Oxford Scholarship, 2002.

[4] R.H. Nochetto, S.W. Walker, W. Zhang, *A finite element method for nematic liquid crystals with variable degree of orientation*, SIAM Journal on Numerical Analysis, **55** (2017), 1357–1386.

[5] E. G. Virga, *Variational Theories for Liquid Crystals*, Chapman and Hall, 1994.

On analysis of discrete exterior calculus

Gantumur Tsogtgerel

(joint work with Erick Schulz)

Among the major applications of discrete exterior calculus (DEC, in the sense of [1]) are a discretization of the Hodge-Laplace operator and various related problems. However, convergence issues for those problems are not completely resolved; as far as we are aware, there is no proof of convergence except for the Poisson equation in two dimensions, which is immediate because the discrete problem is identical to the one that arises from affine finite elements. Moreover, even in two dimensions, there have been some puzzling numerical experiments reported in the literature, apparently suggesting that there is convergence without consistency.

In [2], we developed a general independent framework for analyzing issues such as convergence of DEC without relying on theories established for other discretization methods, and demonstrate its usefulness by proving that DEC solutions to the scalar Poisson problem in arbitrary dimensions converge to the exact solution as the mesh size tends to 0. The proved rate of convergence in H^1-type norms is

$O(h)$, which is consistent with general expectations and numerical experiments. However, our proof only gives the convergence rate $O(h)$ for the L^2-type norms, although numerical experiments and comparison with finite element methods indicate that the true convergence rate is indeed $O(h^2)$.

Since the publication of [2], we have made an attempt to extend our theory to general p-forms, and as a result have collected some evidence that in fact no convergence occurs for general p-forms.

Conjecture: DEC does not converge in general.

However, despite the possibility of this conjecture being true, DEC is thriving in many fields, which provide many interesting theoretical problems. Thus I end this abstract by listing some open problems.

- Prove that DEC converges in L^2 with the rate $O(h^2)$.
- Study convergence of DEC for the $\mathfrak{B}^*$-problem.
- DEC for computing harmonic forms and eigenvalue problems.

References

[1] M. Desbrun, A. N. Hirani, M. Leok, and J. E. Marsden, *Discrete exterior calculus*, arXiv math/0508341 [math.DG], 2005.

[2] R. Schulz and G. Tsogtgerel, *Convergence of discrete exterior calculus approximations for Poisson problems*, arXiv:1611.03955 [math.NA], 2016.

Equilibrated Stress reconstruction for Nonlinear Elasticity

Fleurianne Bertrand

(joint work with Gerhard Starke, Marcel Moldenhauer)

A stress equilibration procedure for hyperelastic material models is presented and analyzed in this talk. Based on the displacement-pressure approximation computed with a stable finite-element pair, it constructs, in a vertex-patch-wise manner an $H(div)$-conforming approximation to the first Piola-Kirchhoff stress. This is done in such a way that its associated Cauchy stress is weakly symmetric in the sense that its anti-symmetric part is zero tested against continuous piecewise linear functions. Our main result is the identifications of the subspace of test functions perpendicular to the range of the local equilibration system on each patch, which turn out to be the rigid body modes associated with the current configuration. Momentum balance properties are investigated analytically and numerically and the resulting stress reconstruction is shown to provide improved results for surface traction faces by computational experiments.

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