Mathematisches Forschungsinstitut Oberwolfach

New Discretization Methods for the Numerical Approximation of PDEs

Organised by
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ABSTRACT. The construction and mathematical analysis of numerical methods for PDEs is a fundamental area of modern applied mathematics. Among the various techniques that have been proposed in the past, some – in particular, finite element methods, – have been exceptionally successful in a range of applications. There are however a number of important challenges that remain, including the optimal adaptive finite element approximation of solutions to transport-dominated diffusion problems, the efficient numerical approximation of parametrized families of PDEs, and the efficient numerical approximation of high-dimensional partial differential equations (that arise from stochastic analysis and statistical physics, for example, in the form of a backward Kolmogorov equation, which, unlike its formal adjoint, the forward Kolmogorov equation, is not in divergence form, and therefore not directly amenable to finite element approximation, even when the spatial dimension is low). In recent years several original and conceptionally new ideas have emerged in order to tackle these open problems.

The goal of this workshop was to discuss and compare a number of novel approaches, to study their potential and applicability, and to formulate the strategic goals and directions of research in this field for the next five years.

Introduction by the Organisers

The workshop *New Discretization Methods for the Numerical Approximation of PDEs* was organized by Stephan Dahlke (Marburg), Gitta Kutyniok (Berlin), Endre Süli (Oxford), and Rob Stevenson (Amsterdam). This meeting was attended by 51 participants from 11 countries.

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 (as in h-version and (h, p)-version adaptive FEMs), and their flexibility in representing computational domains possessing complicated geometries. By now, powerful software packages based on finite element methods have been developed and it is fair to say that the theory of FEMs is an established and mature field of numerical analysis. While it is expected that the range of applications of FEMs will continue to grow (a recent active area being, for example, the development and mathematical analysis of FEMs for geometric PDEs and PDEs on manifolds), it seems unclear whether ground-breaking new theoretical contributions are likely to emerge in the subject.

Contemplating scientific challenges that have arisen in recent years, it is possible to identify problem classes for which the performance of existing numerical techniques (and finite element methods in particular) is not entirely satisfactory. These include PDEs whose solutions develop singularities along lower-dimensional manifolds (e.g. blow-up phenomena in combustion problems and in kinetic models of chemotaxis (Keller–Segel system)), nonlinear hyperbolic conservation laws, for which smooth initial data can evolve into solutions that contain discontinuities (shocks and contact discontinuities), and transport-dominated diffusion equations whose solutions exhibit thin internal and boundary layers. One of the key open questions is in particular whether an adaptive finite element approximation of an elliptic or parabolic transport-dominated diffusion equation realizes the convergence rate that could be obtained with the best possible partition from the class of all partitions generated by, say, the newest vertex bisection technique; as a matter of fact, the convergence rate that could be obtained even with the best possible partition is unlikely to be "optimal" for such equations because of the loss of regularity of the analytical solution (in the scale of Besov spaces relevant for isotropic approximations) in the limit of the Péclet number tending to $+\infty$. Consequently, "anisotropic refinement" techniques will be needed in order to achieve the rate that is "optimal" for a given polynomial degree used in the finite element space.

Recently, several original and conceptionally novel ideas have been proposed whose potentials and scope of applicability are still being investigated. Among those are (adaptive) numerical schemes based on anisotropic ansatz functions, mixed dictionaries/frames or tensor wavelets. Other exemplary classes are low-rank tensor techniques for high-dimensional PDEs, schemes based on compressed sensing, meshless methods, and reduced-basis methods. The main focus of this workshop was to investigate the potentials of these newly developed discretization schemes and to identify and manifest promising future research directions in the field.

The workshop featured 36 talks, thereof 11 longer overview talks. Some highlights of the presentations include:

- **Reduced basis methods:** Wolfgang Dahmen reported on a double greedy algorithm for solving radiative transfer problems. To reduce the dimension of the problem, the angular variables are treated as parameters, and the solution manifold is approximated by the reduced basis method. The expansion coefficients in this basis are determined by solving stable Petrov-Galerkin problems in the reduced space. The test spaces are generated through an interior greedy loop.
- **Low rank tensors:** Reinhold Schneider gave an overview of low rank tensor techniques for the numerical solution of high dimensional PDEs. The recently introduced Hierarchical Tucker tensor formats and Tensor Trains offer stable and robust approximations at low cost. Approximations in those formats can be found by applying matrix low rank factorisation techniques (SVD).
- **Entropy-stable finite difference schemes:** Eitan Tadmor's lecture focussed on the importance of entropy stability in the dynamics of nonlinear systems of conservation laws and related convection-diffusion equations. He presented a general theory of entropy stability for difference approximations of such nonlinear partial differential equations, and illustrated the general theory through a range of first- and second-order accurate finite difference schemes for a variety of scalar problems as well as entropy stable schemes for the Euler and Navier–Stokes equations. Recent computations of entropy-measure-valued solutions based on a class of arbitrarily high order accurate and entropy stable TeCNO schemes were also shown.
- **Ridgelet and shearlet based discretisations for transport problems and wave propagation:** Philipp Grohs presented a ridgelet-based discretization of the kinetic transport equation.Using either a sparse collocation approach in the transport direction, or a tensor product construction, the system was solved in optimal complexity, even in the presence of line singularities in the solution.

   The numerical solution of inverse scattering problems was discussed by Philipp Petersen. In the two-dimensional case, scatterers can be modeled by curves. These curves have optimally sparse representations in shearlet systems. This suggests to solving the inverse problem with a sparsity

promoting Tikhonov regularization term. The approach generalizes to certain linearized inverse problems.

The organizers would like to take the opportunity to thank MFO for providing support and a very inspiring environment for the workshop. The magic of the place (as coined by one of the participants) and the pleasant atmosphere contributed greatly to the success of the workshop.

Workshop: New Discretization Methods for the Numerical Approximation of PDEs

Table of Contents

Abstracts

Reduced basis techniques for multiscale methods
ASSYR ABDULLE

In this report, we consider reduced basis numerical homogenization methods for the numerical solution of *multiscale* partial differential equations (PDEs) in a domain $\Omega \in \mathbb{R}^d$, $1 \leq d \leq 3$. We will consider two classes of multiscale PDEs. First we consider quasilinear problems: find $u^\varepsilon \in H_0^1(\Omega)$ such that

$$(1) \qquad \int_\Omega a^\varepsilon(x, u^\varepsilon) \nabla u^\varepsilon \cdot \nabla w dx = \int_\Omega f w dx \quad \forall \ w \in H_0^1(\Omega),$$

where $f \in L^2(\Omega)$, $a^\epsilon(x, u)$ is a $d \times d$ tensor of Carathéodory type, uniformly elliptic and bounded. Second, we consider Stokes problems in porous media: find $(\mathbf{v}^\varepsilon, p^\epsilon) \in (H_0^1(\Omega_\epsilon))^d \times L^2(\Omega_\epsilon)/\mathbb{R}$ such that

$$(2) \qquad \begin{aligned} a(\mathbf{v}^\epsilon, \mathbf{w}) + b(\mathbf{w}, p^\epsilon) &= \int_\Omega \mathbf{f} \cdot \mathbf{w} dx \quad \forall \mathbf{w} \in (H_0^1(\Omega_\epsilon))^d, \\ b(\mathbf{v}^\epsilon, q) &= 0 \quad \forall q \in L^2(\Omega_\epsilon)/\mathbb{R}, \end{aligned}$$

where $\mathbf{f} \in (L^2(\Omega))^d$, $a(\mathbf{v}, \mathbf{w}) = \int_{\Omega_\epsilon} \nabla \mathbf{v} : \nabla \mathbf{w} dx$, $b(\mathbf{v}, q) = -\int_{\Omega_\epsilon} q(\nabla \cdot \mathbf{v}) dx$. The multiscale nature of the above PDEs has different sources. For the quasilinear problems, the tensor $a^\varepsilon(x, u^\varepsilon)$ oscillates over a small length scale ϵ. For the Stokes problems, the presence of pore structures (solid parts) of size ϵ makes the fluid domain Ω_ϵ highly heterogeneous. Precisely $\Omega_\epsilon = \Omega \backslash \bigcup_{x \in (1/2 + \mathbb{Z})^d} \epsilon(x + \varphi(Y_S; \epsilon x))$, where Y_S is a reference solid domain $\subset \bar{Y}$ with $Y = (-1/2, 1/2)^d$ and $\varphi(\cdot; x) : \overline{Y} \to \overline{Y}$ is a homeomorphism such that $\varphi(\cdot; x)|_{\partial Y}$ is an identity for every $x \in \overline{\Omega}$.

Homogenization. For both problems described above, a direct application of a finite element method (FEM) is computationally prohibitive as such a method needs a mesh size $h < \epsilon$ to converge. However, in many applications one is interested in the macroscale behavior of the solution. Such effective equations have been derived for the considered problems. They involve a macroscale partial differential operator. Under suitable assumptions on the data of the problem, it is possible to show that the family of micro solutions converge (usually in a weak sense, up to a subsequence extraction) towards the solution of the macroscale problem. For (1) the homogenized problem reads [11] : find $u \in H_0^1(\Omega)$ such that

$$(3) \qquad \int_\Omega a(x, u) \nabla u \cdot \nabla w dx = \int_\Omega f w dx, \quad \forall \ w \in H_0^1(\Omega).$$

The effective equation is of the same type as the microscopic equation, but the oscillating tensor has been replaced by an averaged ϵ independent tensor. For (2) the homogenized problem reads [15, 10]: find $p \in H^1(\Omega)/\mathbb{R}$ such that

$$(4) \qquad \int_\Omega a(x) \nabla p \cdot \nabla q dx = \int_\Omega a(x) \mathbf{f} \cdot \nabla q dx, \quad \forall \ q \in H^1(\Omega)/\mathbb{R},$$

where $a(x)$ is a $d \times d$ conductivity tensor. The effective problem is of Darcy type, the domain does not contain "pore scales" anymore (it has been "homogenized"). For both problems, under suitable assumptions on the oscillatory data (respectively the pore structure), the effective conductivity tensor is recovered at a given point $x \in \Omega$ by solving "micro problems" (PDEs involving the original multiscale problem in a unit reference domain where x enters as a parameter).

A brief description of a numerical homogenization method. Given the problems (1) or (2), the goal is to find a numerical approximation of (3) or (4) involving *a priori unknown* homogenized coefficients ($a(x,u)$, or $a(x)$ for our problems). We describe the finite element heterogeneous multiscale method (FE-HMM) [3, 1, 13] (see [4, 7] for an analysis of problems (1),(2)). It relies on

1. A macroscopic FE solver for the effective (homogenized) problem *with a priori unknown data* $\{a^h(x_{K,j}, u(x_{K,j}))\}_{j=1}^{J}$ (quasilinear problem), $\{a^h(x_{K,j})\}_{j=1}^{J}$ (Stokes problem), defined on quadrature points $x_{K,j}$ on each macro element K of a macroscopic partition $\mathcal{T}_H$ of Ω;

2. A microscopic FE solver for "micro" problems based on the differential operators (1) or (2) with right-hand side involving the unit vectors $\{\mathbf{e}_1, \dots, \mathbf{e}_d\}$ in $\mathbb{R}^d$ on sampling domains $K_{\delta_j} = x_{K,j} + \delta(-1/2, 1/2)^d$, $\delta \geq \epsilon$; the outcome of this step are d FE solutions $\xi_{x_{K,j}}^i, i = 1, \dots, d$ for each quadrature point $x_{K,j}$ of each element $K \in \mathcal{T}_H$ (for the Stokes micro problems each micro function is a couple of velocity-pressure solutions).

3. A data recovery process in which the effective data $a^h(x_{K,j}, u(x_{K,j}))$, respectively $a^h(x_{K,j})$, at the point $x_{K,j}$ are computed using a suitable average involving the fine scale functions $\xi_{x_{K,j}}^i, i = 1, \dots, d$ in each K_{δ_j} (for the Stokes problem only the micro velocity (vector) solution enter in the computation of $a^h(x_{K,j})$).

Reduced basis techniques for numerical homogenization. The main computational cost of the FE-HMM comes from the repeated solutions of micro problems around macro quadrature points. One can thus ask if the macroscopic dependence of the micro solutions could be "interpolated" in an appropriate way and if a reduced number of micro solutions could be precomputed and used to compute the effective data at the required quadrature nodes of the macro solver. This question has been addressed for numerical homogenization in the framework of the reduced basis (RB) method [12, 2, 5].

Observe that the effective data computed in the FE-HMM are parameter dependent. For Problem (1) the effective data depend on $x \in \Omega$, on the force field of the micro problems which involves any of the unit vector $\{\mathbf{e}_1, \dots, \mathbf{e}_d\}$ in $\mathbb{R}^d$ and the value of the unknown (numerically) homogenized solution itself (cheap upper and lower bounds $[u_{low}, u_{up}]$ are available for this solution). For Problem (4) the effective data depend on a set of geometrical parameters $(\mu_1(x), \dots, \mu_p(x)) \in \mathcal{D} \subset \mathbb{R}^d$ and on the force field of the micro problem $\{\mathbf{e}_1, \dots, \mathbf{e}_d\}$ in $\mathbb{R}^d$.

A greedy algorithm allows to select (thanks to suitable a posteriori error estimators) among this parameter space an $N-$dimensional set of the parameters for which the corresponding micro functions differ most (measured in a Hilbert norm

corresponding to the PDE). For many problems N turns out to be small. The corresponding $N-$dimensional set of micro functions accurately computed span the reduced basis space. A separation between microscopic variables and parameters variables (either in the tensor for (1) or in the geometry for (4)), called an affine representation is crucial for the efficiency of the Greedy procedure (appropriate interpolation procedures [14] can be applied if this requirement is not satisfied). In an online stage, the precomputed basis (set once for all) is used at the macroscopic quadrature point to compute the actual value of the effective data. Thanks to the affine representation this amounts to solve (small) $N \times N$ linear system (essentially pre-assembled in the offline stage).

A priori error estimates in terms of macro, micro, modeling and reduced basis errors have been derived for the RB-FE-HMM applied to Problems (1) in [6]. An adaptive FE-HMM method for Problem (2) has been analyzed in [7] and reduced basis approximations have been presented in [8, 9].

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Kolmogorov widths and low-rank approximations of parametric elliptic PDEs

MARKUS BACHMAYR

(joint work with Albert Cohen)

We consider parametric diffusion equations

$$- \operatorname{div}_x \big(a(x,y) \nabla u(x,y) \big) = f(x) , \quad x \in D \subset \mathbb{R}^m, \ y \in U := [-1,1]^d,$$

with $m, d \in \mathbb{N}$, where the coefficient a has the form $a(x,y) = \bar{a}(x) - \sum_{i=1}^d y_i \psi_i(x)$ and is assumed to satisfy a uniform ellipticity assumption, that is, there exist $0 < r \le R$ such that $0 < r \le a(x,y) \le R < \infty$ for $x \in D$ and $y \in U$. The weak form of this problem on $V := H_0^1(D)$ reads

$$\Big(\bar{A} - \sum_{i=1}^d y_i A_i \Big) u(y) = f ,$$

where $f \in V'$ and $\bar{A}, A_i \colon V \to V'$, $i = 1, \ldots, d$, are defined by

$$\langle \bar{A} u, v \rangle := \int_D \bar{a} \nabla u \cdot \nabla v \, dx , \quad \langle A_i u, v \rangle := \int_D \psi_i \nabla u \cdot \nabla v \, dx , \qquad u, v \in V .$$

Our aim is to study the performance of low-rank approximations of u of the form

$$\text{(1)} \qquad\qquad \sum_{k=1}^n v_k(x) \, \phi_k(y) ,$$

where the v_k and ϕ_k can be chosen arbitrarily to minimize the error for each n.

Approximations of the type (1) are used implicitly in reduced basis or POD methods and constructed explicitly in methods based on more general tensor decompositions. In all of these approaches, it is of crucial importance that the required number of terms n does not increase too rapidly with a decreasing error tolerance in approximating u. In the reduced basis context, where one is generally interested in uniform error estimates, the relevant measure for assessing the speed of convergence of (1) towards u is the Kolmogorov n-width of $u(U) \subset V$, which is defined for $n \in \mathbb{N}$ by

$$d_n \big(u(U) \big)_V := \inf_{\dim(W)=n} \ \sup_{y \in U} \ \min_{w \in W} \| u(y) - w \|_V ,$$

where we consider u as a map $y \mapsto u(y)$ from U to V. The rank of a $v \in L^2(U, V)$ is defined as the rank of the induced Hilbert-Schmidt operator $\varphi \mapsto \int_U v(y) \, \varphi(y) \, dy$ from $L^2(U)$ to V.

First upper bounds for the n-widths can be obtained from polynomial expansions [1, 2], where the functions ϕ_k are selected from a given basis of tensor product polynomials. However, if the problem has additional structure, one can obtain stronger decay of n-widths when allowing arbitrary ϕ_k.

We consider in particular the case of coefficients that are piecewise constant on some fixed partition $\{D_1, \ldots, D_d\}$ of D, that is,

$$(2) \qquad\qquad \bar{a} := 1, \quad \psi_i := \theta \chi_{D_i},$$

for a fixed $\theta \in (0, 1)$. A simple example of improved bounds under this structural assumption is the one-dimensional case $D = (0, 1)$ with a partition into d subintervals, where one easily finds that $\mathrm{rank}(u) \leq 2d - 1$.

Our further considerations are based on a Neumann series expansion of u with the partial sums

$$(3) \qquad\qquad u_k(y) := \sum_{\ell=0}^{k} \Big(\sum_{i=1}^{d} y_i (\bar{A}^{-1} A_i) \Big)^{\ell} \bar{A}^{-1} f,$$

which satisfy $\|u - u_k\| \leq C\theta^k$. Expanding and grouping terms corresponding to the same multinomials one finds that the u_k are in fact partial sums up to fixed total degrees of the Taylor expansion of u [2], and counting terms one obtains the generic estimate

$$d_n\big(u(U)\big)_V \leq C e^{-c\, n^{1/d}}$$

for the n-widths, which is a consequence of the analyticity of u with respect to y. This estimate can be improved under a further assumption that is in particular implied by (2).

Proposition 1. *If $\sum_{i=1}^{d} A_i = \theta \bar{A}$, then for each k, there exist $v_\ell \in V$ and d-variate polynomials $\phi_{k,\ell}$, $\ell = 1, \ldots, n(k) := \binom{k+d-1}{d-1}$, such that for u_k as in (3) we have $u_k(y) = \sum_{\ell=1}^{n(k)} \phi_{k,\ell}(y)\, v_\ell$, and consequently, $d_n\big(u(U)\big)_V \leq C e^{-c\, n^{1/(d-1)}}$.*

Under a fairly general additional condition, we thus only obtain a reduction in the n-widths that weakens for large d. However, substantially stronger results can be obtained under more specialized further assumptions. To this end, we first describe a reduction to a problem on the skeleton $\Gamma := \bigcup_{i=1}^{d} \partial D_i \setminus \partial D$ of the partition, where we define V_Γ as the space of trace values on Γ of functions in $V = H_0^1(D)$.

Denoting by E the harmonic extension operator from V_Γ to V, we define the Steklov-Poincaré operators $S_i \colon V_\Gamma \to V_\Gamma'$, $i = 1, \ldots, d$, and $\bar{S} \colon V_\Gamma \to V_\Gamma'$, as well as the projected right hand side $\hat{f}$, by

$$\langle S_i v_\Gamma, w_\Gamma \rangle := \int_{D_i} \nabla E v_\Gamma \cdot \nabla E w_\Gamma\, dx, \quad \bar{S} := \sum_{i=1}^{d} S_i, \quad \langle \hat{f}, v_\Gamma \rangle := \int_{D} f\, E v_\Gamma\, dx,$$

for $v_\Gamma, w_\Gamma \in V_\Gamma$. We obtain a Neumann series representation on Γ with partial sums

$$u_{k,\Gamma}(y) := \sum_{\ell=0}^{k} \Big(\sum_{i=1}^{d} y_i\, (\theta \bar{S}^{-1} S_i) \Big)^{\ell} \bar{S}^{-1} \hat{f},$$

which converge in $L^\infty(U, V_\Gamma)$ to the projection of u onto $E V_\Gamma$. Since the component of u in the complement of $E V_\Gamma$ in V is of rank at most d, one has $\mathrm{rank}(u_k) \leq \mathrm{rank}(u_{k,\Gamma}) + d$, and thus the problem is reduced to estimating $\mathrm{rank}(u_{k,\Gamma})$.

We consider this in detail in the case of $D = (-\frac{1}{2}, \frac{1}{2})^2$ and $d = 4$ with the two-by-two checkerboard partition

$$(4) \quad D_1 = \left(-\tfrac{1}{2}, 0\right)^2, \; D_2 = \left(0, \tfrac{1}{2}\right) \times \left(-\tfrac{1}{2}, 0\right), \; D_3 = \left(-\tfrac{1}{2}, 0\right) \times \left(0, \tfrac{1}{2}\right), \; D_4 = \left(0, \tfrac{1}{2}\right)^2,$$

where we set $\Gamma_1 = [-\frac{1}{2}, \frac{1}{2}] \times \{0\}$, $\Gamma_2 = \{0\} \times [-\frac{1}{2}, \frac{1}{2}]$, such that $\Gamma = \Gamma_1 \cup \Gamma_2$. We rewrite $u_{k,\Gamma}$ in terms of the operators

$$G_0 := \theta \bar{S}^{-1} \bar{S} = \theta \, \mathrm{id}, \qquad\qquad G_1 := \theta \bar{S}^{-1}(S_1 - S_2 - S_3 + S_4),$$
$$G_2 := \theta \bar{S}^{-1}(S_1 + S_2 - S_3 - S_4), \qquad G_3 := \theta \bar{S}^{-1}(S_1 - S_2 + S_3 - S_4),$$

which gives, with $z_i(y)$ that are linear combinations of $y_1, \ldots, y_4$,

$$u_{k,\Gamma}(y) = \sum_{\ell=0}^{k} \Big(\sum_{i=0}^{d-1} z_i(y)\, G_i\Big)^{\ell} \bar{S}^{-1} \hat{f}.$$

Introducing the orthogonal decomposition of V_Γ into $\hat{V}_1 := \{v \colon v|_{\Gamma_1}, v|_{\Gamma_2} \text{ even}\}$, $\hat{V}_2 := \{v \colon v|_{\Gamma_1} \text{ odd}, v|_{\Gamma_2} = 0\}$, $\hat{V}_3 := \{v \colon v|_{\Gamma_1} = 0, v|_{\Gamma_2} \text{ odd}\}$, we obtain

$$G_1 \hat{V}_1 = G_2 \hat{V}_2 = G_3 \hat{V}_3 = \{0\} \subset V_\Gamma,$$
$$G_2 \hat{V}_1, G_1 \hat{V}_2 \subset \hat{V}_3, \quad G_3 \hat{V}_1, G_1 \hat{V}_3 \subset \hat{V}_2, \quad G_3 \hat{V}_2, G_2 \hat{V}_3 \subset \hat{V}_1,$$
$$G_2 G_3 v_2 = G_1 v_2, \; G_3^2 v_2 = v_2, \; v_2 \in \hat{V}_2, \quad G_3 G_2 v_3 = G_1 v_3, \; G_2^2 v_3 = v_3, \; v_3 \in \hat{V}_3.$$

Combining these properties, we arrive at the following result.

Theorem 2. *Let D be as in (4) with $d = 4$. Then for each $k \in \mathbb{N}$, and for $n(k) := 8k + 5$, there exist $v_1, \ldots, v_{n(k)} \in V$ and d-variate polynomials $\phi_1, \ldots, \phi_{n(k)}$, each of total degree k, such that*

$$\sup_{y \in U} \Big\| u(y) - \sum_{\ell=1}^{n(k)} \phi_\ell(y)\, v_\ell \Big\|_V \leq \frac{\|\bar{A}^{-1} f\|_V}{1 - \theta}\, \theta^{k+1},$$

and consequently $d_n\big(u(U)\big)_V \leq C \exp(-\frac{|\ln \theta|}{8} n)$.

This explains the numerical observation of exponential convergence in this case. Numerical tests also reveal, however, that this effect is strongly tied to the problem geometry and is lost for less regular subdivisions of the unit square into quadrilaterals, where one only observes subexponential decay of the n-widths.

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Numerical approximation of total-variation regularized problems
Sören Bartels

The numerical treatment of minimization problems defined on functions of bounded variations leads to several difficulties. First, solutions do not exhibit higher regularity properties and typically jump across lower dimensional subsets. Second, the problems are non-linear and non-differentiable, so that the practical iterative solution has to be done appropriately. We discuss a priori and a posteriori error estimates and their practical performance in the context of adaptive mesh refinement. The iterative solution is done by a primal-dual method, for which modifications are addressed that allow for larger time steps under appropriate conditions. Particular attention is paid to the the optimality of convergence rates and restrictions on step sizes.

As a reference model, we consider the Osher–Rudin–Fatemi energy functional, see [7], defined for $u \in BV(\Omega) \cap L^2(\Omega)$ by

$$I(u) = |Du|(\Omega) + \frac{\alpha}{2}\|u - g\|_{L^2(\Omega)}^2.$$

Here, $g \in L^\infty(\Omega)$ is a given noisy image, and $\alpha > 0$ a suitably chosen parameter, so that the minimizer u serves as a regularization of g. By noting that

$$|Du|(\Omega) = \sup\left\{\int_\Omega (-u)\operatorname{div} p\,dx : p \in H_N(\operatorname{div};\Omega),\ |p| \le 1\right\},$$

the minimization problem can be written as a saddle point problem, i.e.,

$$\inf_u \sup_p \int_\Omega (-u)\operatorname{div} p\,dx + \frac{\alpha}{2}\|u - g\|_{L^2(\Omega)}^2 - I_{K_1(0)}(p).$$

The indicator functional $I_{K_1(0)}$ enforces the constraint $|p| \le 1$ on vector fields $p \in H_N(\operatorname{div};\Omega)$. Duality arguments allow us to exchange the order of the infimum and supremum without modifying the value of corresponding saddle points. In particular, we may then eliminate the variable u via the optimality relation $\operatorname{div} p = \alpha(u-g)$. This defines the dual problem, that consists in maximizing the functional

$$D(p) = \frac{-1}{2\alpha}\|\operatorname{div} p + \alpha g\|_{L^2(\Omega)}^2 + \frac{\alpha}{2}\|g\|_{L^2(\Omega)}^2 - I_{K_1(0)}(p)$$

in the set of all $p \in H_N(\operatorname{div};\Omega)$. For admissible functions v and vector fields q we have that $I(v) \ge D(q)$ and equality for the corresponding solutions.

Following [6, 2] the approximation error $u - u_h$ of a conforming numerical method can be bounded via

$$\frac{\alpha}{2}\|u - u_h\|_{L^2(\Omega)}^2 \le I(u_h) - I(u) \le I(u_h) - D(q),$$

for an arbitrary vector field $q \in H_N(\operatorname{div};\Omega)$. For practical error estimation and mesh-refinement, a good choice of q is obtained by an appropriate post-processing of u, noting that formally we have $p = \nabla u/|\nabla u|$, or by a numerical solution of the dual problem. An appropriate choice of a subspace $Q_h \subset H_N(\operatorname{div};\Omega)$ is needed to efficiently solve the non-differentiable dual problem.

The iterative procedure to solve the primal problem follows [5, 1, 4], and realizes a primal-dual iteration via solving the equations

$$\widetilde{u}_h^{k+1} = u_h^k + \tau d_t u_h^k,$$

$$-(d_t p_h^{k+1} + \nabla \widetilde{u}_h^{k+1}, q_h - p_h^{k+1})_a \le 0,$$

$$(d_t u_h^{k+1}, v_h)_b + (p_h^{k+1}, \nabla v_h)_{L^2(\Omega)} = -\alpha(u_h^{k+1} - g, v_h)_{L^2(\Omega)},$$

repeatedly until a stopping criterion is satisfied. Here, $d_t a^{k+1} = (a^{k+1} - a^k)/\tau$ with a step-size $\tau > 0$ is the backward difference quotient. The choice of the scalar products is crucial to obtain efficient iterations. If $(\cdot, \cdot)_a$ is a discrete version of the L^2 inner product, then the equation for $d_t p_h^{k+1}$ can be solved directly. The choice of the L^2 inner product for the equation that defines $d_t u_h^{k+1}$ leads to the step size condition $\tau \le ch$. This can be improved to the condition $\tau \le ch^{1/2}$ if a discrete version of the $H^{1/2}$ norm is used. The choice is justified by the observation that solutions belong to $BV(\Omega) \cap L^\infty(\Omega)$ and hence algebraically to $H^{1/2}(\Omega)$. For details, see [3].

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Multilevel Preconditioning of Discontinuous-Galerkin Spectral Element Methods

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(joint work with Martin Campos Pinto, Claudio Canuto, and Wolfgang Dahmen)

We consider preconditioning techniques for Discontinuous Galerkin (DG) discretizations of elliptic boundary value problems [1]. Since the important effects already arise in a simple model problem, we focus on Poisson's equation. We choose the symmetric interior penalty Galerkin method (SIPG), because symmetry is preserved in the discretization process and the method is dual consistent.

While in previous studies preconditioners for low-order methods have been addressed [2, 3], our goal is now to exploit the full discretization power of DG methods using locally refined meshes and in particular varying polynomial degrees. For preconditioners currently available the condition number grows logarithmically with

the polynomial degree as long as it is kept the same throughout the mesh and it grows quadratically for spatially varying polynomial degrees. Our aim is to construct a preconditioner, which under mild grading conditions on the distribution of the mesh sizes and of the polynomial degrees leads to uniformly bounded condition numbers for arbitrarily large and spatially varying polynomial degrees. Moreover, we require the complexity of each iteration to remain proportional to the number of degrees of freedom. In this presentation we focus on the dependence of the condition number on the polynomial degrees and only consider the case of geometrically conforming meshes [5].

A key ingredient for preconditioning high-order methods is to use the nodal spectral element method on Legendre–Gauss–Lobatto (LGL) grids. The LGL grid $\mathcal{G}_N \subset [-1, 1] \subset \mathbb{R}$ of order $N \in \mathbb{N}$ consists of the two boundary points ± 1 and $N - 1$ inner points, which are the zeros of the first derivative of the Legendre polynomial L_N. These grids do not only provide high-order quadrature rules at low cost in combination with appropriate weights, but give also rise to important norm equivalences, see e.g. [10, 7, 15]. In particular, for the LGL grid $\mathcal{G}_N$ of order N for any polynomial p on $[-1, 1]$ of degree at most N and its piecewise affine interpolant $I_{\mathcal{G}_N} p$ at the points of the LGL grid $\mathcal{G}_N$, one has

$$\|p\|_{L^2(-1,1)} \eqsim \|I_{\mathcal{G}_N} p\|_{L^2(-1,1)} \quad \text{and} \quad |p|_{H^1(-1,1)} \eqsim |I_{\mathcal{G}_N} p|_{H^1(-1,1)},$$

where the constants are independent of the polynomial degree N.

Our main tool for the construction of preconditioners is the auxiliary space method (ASM). Many researchers can claim credit for this technique, see e.g. [14, 16], and it can be seen as an application of Nepomnyaschikh's fictitious space lemma [13]. In the framework of the ASM, we set up an auxiliary problem that is closely related to the original one, but easier to solve. The closeness of the original and the auxiliary problem is expressed by the ASM-conditions [14, 5], which are direct and inverse estimates that involve the bilinear forms arising in the weak formulations of the original and the auxiliary problem, a smoothing operator, and two linear transfer operators that couple the linear spaces underlying both problems. The central ASM result [14] then identifies a symmetric preconditioner such that the spectral condition number of the resulting preconditioned system is up to a constant bounded by the quotient of the largest and smallest eigenvalue of the preconditioned auxiliary problem and the preconditioned smoothing operator.

We construct a multi-stage preconditioner [4, 5] by using three consecutive realizations of the ASM. Formally this concatenation of ASM preconditioners can be interpreted as a single preconditioner with three smoothers. We would like to emphasize that in particular the first and the third application of the ASM are also of interest as standalone components for new preconditioners, see e.g. [8].

In a first application of the ASM, the spectral DG method is preconditioned by a spectral conforming Galerkin method on the same grid. The smoothing operator is obtained from an inverse estimate and its matrix representation is diagonal.

Since LGL grids for different degrees do not match at element interfaces, one cannot use direct low-order finite elements on LGL grids as conforming auxiliary spaces. Therefore, for the second application of the ASM the problem is transferred

from a spectral conforming method to a problem on a space that in each element is given by a tensor product of piecewise linear finite elements on a dyadic subgrid. These dyadic grids, which mimic LGL grids, are constructed [6] such that they are locally quasi-uniform, the grids are locally of a mesh size that is comparable with that of the corresponding LGL grid, and the family of grids is nested at the same time. Due to the anisotropy of the dyadic grids, in order to derive an appropriate smoothing operator an inverse estimate can only be applied in selected parts of the domain. Nevertheless, the matrix representation of the smoothing operator is very sparse and its inverse can be efficiently approximated using a substructuring approach with patchwise block-elimination and finitely many Gauss–Seidel relaxations on the skeleton. Suitable coupling operators for the case of varying polynomial degrees can be obtained using element shape functions and polynomial and piecewise linear interpolation [4, 5].

The third application of the ASM exploits the hierarchical structure inherent to dyadic grids in order to build a multilevel preconditioner based on a composite multiwavelet approach. From [12] we know that in an anisotropic situation a H^1-stable splitting on a single element is obtained by tensorization, when orthogonality of difference spaces is ensured. Therefore, we use piecewise linear orthogonal multiwavelets [11], which are constructed in such a way that the finite element space on a dyadic grid can be embedded into a locally refined wavelet space of comparable dimension. Since the multiwavelets are prepared to be restricted to the interval $[0, 1]$, we obtain a Riesz basis for $L^2([0, 1]^d)$ and by scaling also for $H^1([0, 1]^d)$ and $H_0^1([0, 1]^d)$. Now our idea is to construct a global auxiliary multilevel space with a H^1-stable multilevel decomposition [5]. Following [9], we continuously glue anisotropic wavelet bases in 2D or 3D obtained by tensorization on each element into a global composite basis, such that H^1-stability is preserved. Then we can apply a diagonal wavelet preconditioner and nested iteration techniques to ensure an efficient solution of the auxiliary problem in linear complexity.

Various numerical experiments quantify the theoretical findings [5].

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Regularity of Stochastic Partial Differential Equations in Besov Spaces Related to Adaptive Schemes

Petru A. Cioica

(joint work with S. Dahlke, K.-H. Kim, S. Kinzel, K. Lee, F. Lindner, T. Raasch, K. Ritter, and R.L. Schilling)

We present a result concerning the regularity of the solution to second order stochastic partial differential equations (SPDEs, for short) of the form

$$(\bullet) \quad \begin{cases} \mathrm{d}u = \Big(\sum_{i,j=1}^{d} a^{ij} u_{x^i x^j} + f \Big) \, \mathrm{d}t + \sum_{k=1}^{\infty} \Big(\sum_{i=1}^{d} \sigma^{ik} u_{x^i} + g^k \Big) \, \mathrm{d}w_t^k \\ \qquad\qquad \text{on } \Omega \times [0,T] \times \mathcal{O}, \\ u = 0 \qquad \text{on } \Omega \times (0,T] \times \partial\mathcal{O}, \\ u(0) = u_0 \quad \text{on } \Omega \times \mathcal{O}, \end{cases}$$

where $\mathcal{O} \subset \mathbb{R}^d$ is an arbitrary bounded Lipschitz domain. The equations are driven by a sequence $\{(w_t^k)_{t\in[0,T]} : k \in \mathbb{N}\}$ of real-valued standard Brownian motions w.r.t. a normal filtration $(\mathcal{F}_t)_{t\in[0,T]}$ on a complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$. We use the special scales

$$(\star) \qquad\qquad B_{\tau,\tau}^{\alpha}(\mathcal{O}), \qquad \frac{1}{\tau} = \frac{\alpha}{d} + \frac{1}{p}, \qquad \alpha > 0,$$

of Besov spaces to measure the smoothness w.r.t. the space variable ($p \geq 2$ fixed). This analysis is motivated by some fundamental problems arising in the context of the numerical treatment of Eq. ($\bullet$). By now, the numerical methods for SPDEs discussed in the predominant part of the literature rely on uniform refinements w.r.t. the space variable $x \in \mathcal{O}$. This seems to be suboptimal: It is well-understood that, in general, the convergence rate of classical uniform methods depends on the Sobolev regularity of the target function. Simultaneously, in common settings, the solution to Eq. ($\bullet$) has only poor spatial Sobolev regularity, see, e.g., [6, 7]. Consequently, we cannot expect high convergence rates by refining uniformly in space. Therefore, it would be tempting to use *adaptive* schemes in order to increase efficiency. It is well-known that the approximation order that can be achieved by adaptive and other non-linear approximation schemes depends in many cases on the regularity of the target function in the scale ($\star$), where p indicates the L_p-norm in which the error is measured. In particular, this relationship holds for adaptive schemes based on wavelets. Thus, in order to clarify whether spatial adaptivity really pays for SPDEs, first of all, the regularity of the solution has to be analysed, using the scale ($\star$) to measure the smoothness w.r.t. the space variable. The scales ($\star$) are commonly known as (L_p-)*adaptivity scales*.

Main Results. Our analysis is embedded into the framework of the analytic approach to SPDEs initiated by N.V. Krylov. In particular, we borrow (and extend) the L_p-theory developed in [5] for second order linear SPDEs on general bounded Lipschitz domains. Therein, certain weighted Soblev spaces $H_{p,\theta}^{\gamma}(\mathcal{O})$ are

used to measure the regularity of the equation w.r.t. the space variable. For integer $\gamma \in \mathbb{N}_0$ and $\theta \in \mathbb{R}$, they consist of all measurable functions having finite norm

$$\|u\|_{H_{p,\theta}^\gamma(\mathcal{O})} := \left(\sum_{|\alpha| \leq \gamma} \int_{\mathcal{O}} |\rho(x)^{|\alpha|} D^\alpha u(x)|^p \rho(x)^{\theta-d} \, \mathrm{d}x \right)^{1/p},$$

where $\rho(x)$ denotes the distance of a point x to the boundary of the domain. For fractional and negative smoothness parameters γ, they can be obtained by complex interpolation and duality. In order to give a rigorous meaning to Eq. ($\bullet$), one also needs analogous spaces $H_{p,\theta}^\gamma(\mathcal{O}; \ell_2)$ for ℓ_2-valued functions; we refer, e.g., to [5] for details. The main result of [5] applied to Eq. ($\bullet$) in a simplified setting reads as follows: Assume that the coefficients a^{ij} and σ^{ik} are constant and fulfill the stochastic parabolicity condition

$$(\mathrm{P}) \qquad \delta_0|\lambda|^2 \leq \sum_{i,j=1}^d \left(a^{ij} - \frac{1}{2}\langle \sigma^{i\cdot}, \sigma^{j\cdot}\rangle_{\ell_2} \right) \lambda_i \lambda_j \leq K|\lambda|^2, \qquad \lambda \in \mathbb{R}^d,$$

for some constants $\delta_0, K \in (0, \infty)$. Then, for $p \geq 2$ and $\gamma \in \mathbb{R}$, if

(1) $f \in L_p(\Omega \times [0,T]; H_{p,d+2p-2}^{\gamma-2}(\mathcal{O}))$ and $g \in L_p(\Omega \times [0,T]; H_{p,d+p-2}^{\gamma-1}(\mathcal{O}; \ell_2))$,

then Eq. ($\bullet$) with vanishing initial condition $u_0 \equiv 0$ has a unique solution

$$u \in L_p(\Omega \times [0,T]; H_{p,d-2}^\gamma(\mathcal{O})).$$

From this result, we extract information about the spatial Besov regularity of the solution in the adaptivity scale by proving the following central embedding. It shows that—up to a certain extent—the analysis of the Besov regularity in the adaptivity scale can be traced back to the analysis of the weighted Sobolev regularity. It is worth mentioning that this embedding is not necessarily connected to the SPDE setting. A proof can be found in [1, theorem 4.7] or alternatively in [4, theorem 6.9].

Theorem 1.1. *Let $\mathcal{O} \subset \mathbb{R}^d$ be a bounded Lipschitz domain. For $p \geq 2$, $\gamma, \nu > 0$, we have*

$$H_{p,d-\nu p}^\gamma(\mathcal{O}) \hookrightarrow B_{\tau,\tau}^\alpha(\mathcal{O}), \quad \frac{1}{\tau} = \frac{\alpha}{d} + \frac{1}{p}, \quad \textit{for all} \quad 0 < \alpha < \min\left\{ \gamma, \nu \frac{d}{d-1} \right\}.$$

Using this embedding, we obtain our main result on the spatial Besov regularity of SPDEs in the adaptivity scales ($\star$). For Eq. ($\bullet$), it reads as follows. The result in its full generality has been proven in [1, 2, 4].

Theorem 1.2. *Let $p \geq 2$ and $\gamma \in \mathbb{R}$. Assume the simplified setting from above. Then, if f and $g = (g^k)$ fulfill (1) and $u_0 \equiv 0$, the unique solution u to ($\bullet$) fulfills:*

$$u \in L_p(\Omega \times [0,T]; B_{\tau,\tau}^\alpha(\mathcal{O})), \quad \frac{1}{\tau} = \frac{\alpha}{d} + \frac{1}{p}, \quad \textit{for all} \quad 0 < \alpha < \min\left\{ \gamma, \frac{2}{p}\frac{d}{d-1} \right\}.$$

Let us illustrate the relevance of our result for the question whether adaptivity pays in the SPDE context, by considering a prime example.

Example 1. Let $\mathcal{O} \subset \mathbb{R}^2$ be a bounded two-dimensional polygonal domain. Assume that $(a^{ij}) = (\delta_{ij})$, where (δ_{ij}) denotes the Kronecker delta, and $\sigma^{ik} \equiv 0$, i.e., consider the stochastic heat equation with additive noise. If f and g fulfill (1) with $\gamma = 2$ and $p = 2$, then the unique solution u to Eq. ($\bullet$) with $u_0 \equiv 0$ fulfills

$$u \in L_2(\Omega \times [0,T]; B^{\alpha}_{\tau,\tau}(\mathcal{O})), \quad \frac{1}{\tau} = \frac{\alpha}{2} + \frac{1}{2}, \quad \text{for all} \quad 0 < \alpha < 2.$$

Simultaneously, the analysis in [7] shows that, under similar assumptions, the spatial Sobolev regularity of the solution to Eq. ($\bullet$) is strictly less than 2, if the underlying domain is non-convex. This is a clear theoretical justification for starting to design spatially adaptive wavelet schemes for SPDEs.

Note that, in contrast to the deterministic setting, when considering stochastic PDEs we observe the paradigm that the Besov regularity in the scale ($\star$) exceeds the spatial Sobolev regularity of the solution also in the case of smooth domains, see, e.g., [3, Example 5.2].

Further results obtained so far, in particular, concerning the Hölder regularity of the paths of the solution, considered as a stochastic process taking values in the Besov spaces from the adaptivity scales ($\star$), can be found in [1, 4]. Therein, we also extend the L_p-theory from [5] to an $L_q(L_p)$-theory for the stochastic heat equation, allowing the integrability parameters q and p w.r.t. the time and space variable, respectively, to differ. This is done by a combination of techniques from the analytic approach with results from the semigroup approach to SPDEs.

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Greedy approximation and radiative transfer

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(joint work with Christian Plesken)

The numerical treatment of kinetic models such as radiative or neutron transfer (see e.g. [7]) pose significant challenges because the underlying operator equation involves a global scattering term and the solution is a function of the velocity or angular variables, ranging (in the present context) over a compact set $\mathcal{V}$, and the spatial (and/or temporal) variables in a bounded domain D (as well as possibly further parameters). Thus, one confronts the curse of dimensionality when employing standard discretizations such as finite differences or finite elements. In fact, for a total number of variables p, which even in the stationary case of $d = 3$ spatial variables and two directional parameters amounts to $p = 5$, the size of such standard discretizations with meshsize h would scale like h^{-p} where, due to the scattering term, the system matrices are fully populated. Numerous strategies have been developed to deal with these obstructions such as the method of moments, employing spectral expansions in the angular variables, or the discrete ordinate method in combination with fixed point iterations, see e.g. [6] and the references cited there.

We now sketch a rather different strategy proposed in [4] and highlight the principal underlying conceptual guidelines. It aims at approximating the solution in terms of possibly short sums of products of functions of the spatial variable x and the velocity variable v, respectively. Rather than choosing a fixed expansion system beforehand, the factors in such low-rank tensor approximations have to be determined in the course of the solution process so as to generate possibly few terms needed to realize a given accuracy tolerance. Starting from a large fixed background discretization of the problem, aside from its prohibitive size, would be a delicate matter because of the nature of the PDE, so that the meaning of an accurate solution of the discrete problem is not clear. The construction works therefore from coarse to fine improving on the accuracy of the current iterate in an outer fixed point iteration tracking the solution as a function in $L_2(D \times \mathcal{V})$. Each iteration step is realized approximately within a tolerance ε_n depending on the current fixed-point iteration accuracy level. Rather than viewing an iterate u^{n+1} as a function in $L_2(D \times \mathcal{V})$ though, a key idea is to interpret the set of states $u^{n+1}(\cdot, v) \in L_2(D)$ for each $v \in \mathcal{V}$ as an element of the *solution manifold* $\mathcal{M}_{n+1} = \{u^{n+1}(\cdot, v) : v \in \mathcal{V}\}$ for a *parameter dependent family* of transport equations. The solution manifolds $\mathcal{M}_n$ are approximated by *snapshots* $u^n(\cdot, v_i)$, $v_i \in \mathcal{V}$, for judiciously chosen parameters v_i. In this sense the method shares some common features with the discrete ordinate method. The essential difference lies in the fact that the expansion systems are not fixed beforehand but determined adaptively in the course of the outer fixed-point iteration. Here are a few comments on the actual realization of this process. When approximating $\mathcal{M}_{n+1}$, the right hand sides in the corresponding transport problems involve the application of the scattering operator with input from the preceding approximation to $\mathcal{M}_n$.

A Hilbert-Schmidt expansion of the kernel facilitates on the one hand the application of the scattering operator and also yields a favorable form of the parameter dependence for the main ingredient of the scheme, namely a *reduced basis approximation* to the evolving solution manifolds $\mathcal{M}_n$. Here we make essential use of the results from [5] on *rate-optimal reduced basis methods* for a wide class of parameter dependents PDEs. This class includes singular perturbed and indefinite problems, in particular, convection dominated convection-diffusion problems as well as pure transport problems needed in the present context. Rate-optimality means that the distances of the solution manifold from the reduced spaces tend to zero at the same rate as the respective Kolmogorov n-widths, see [5, 1]. For judiciously chosen tolerances ε_n, $n \in \mathbb{N}$, the fixed-point step at stage n boils then down to extending the reduced basis $\{\phi_j\}_{j=1}^{N_n}$ constructed for $\mathcal{M}_n$ to a basis $\{\phi_j\}_{j=1}^{N_{n+1}}$ for $\mathcal{M}_{n+1}$ so as to meet an accuracy level $\theta\varepsilon_n$ for a suitable $\theta \in (0,1)$ (see above for the role of ε_n). This makes also use of a robustness result in [1] combined with the convergence of the fixed-point iteration to ensure rate-optimality of the successively generated basis. At stage n this gives rise to approximations of the form

$$(1) \qquad\qquad \sum_{j=1}^{N_n} c_{n,j}(v)\phi_j(x)$$

that approximate $u^n(\cdot, v)$, $v \in \mathcal{V}$, in $L_2(D)$ even uniformly in $\mathcal{V}$. In principle, the coefficients $c_{n,j}(v)$ are then not yet given explicitly but can be computed by solving a stable Petrov-Galerkin problem in the reduced space. The corresponding (near-optimal) test spaces are generated through an *interior greedy* loop that can be shown to guarantee an inf-sup constant that stays uniformly away from zero. This in turn, gives rise to an efficient surrogate that can be used to steer the outer greedy search for the next basis function, [5]. This builds in an essential way on the general strategies for contriving *well-conditioned variational formulations* from [2, 3]. In particular, the equivalent formulation of Petrov-Galerkin schemes in terms of *saddle point* problems plays a crucial role in avoiding the computation of explicit near-best test function systems that necessarily depend on the parameters. We also discuss ways of deriving from (1) *explicit* representations for the coefficients $c_{n,j}(v)$ yielding approximations of the exact solution $u(x, v)$ in $L_2(D \times \mathcal{V})$. On the one hand, this can be done by (quasi-)interpolation over $\mathcal{V}$. An alternative is to use Petrov-Galerkin projections this time in $L_2(D \times \mathcal{V})$ from suitable low-dimensional pairs of trial and test spaces which are derived from the pairs in $L_2(D)$ constructed by the greedy procedure. We briefly discuss some relevant norm equivalences between several graph norms that are needed for the stability of these Petrov-Galerkin projections. We conclude with some remarks on the complexity of such a strategy. The only problems to be solved in a sufficiently large *truth space* are the transport problems in $L_2(D)$ needed to determine the reduced basis functions. For a given target accuracy, their number roughly scales like the dimension of a "Kolmogorov-best" linear space that approximates the solution manifold corresponding to $u(\cdot, v), v \in \mathcal{V}$, which is the exact solution $u \in L_2(D \times \mathcal{V})$, within that target accuracy. When these n-widths decay with some algebraic rate,

one expects a finite number of new basis functions in each fixed-point iteration so that the overall number of truth-solves grows logarithmically in the target accuracy. These transport solves employ also stable variational formulations and give rise to rigorous a posteriori bounds, [3]. All other Petrov-Galerkin solves as well as the inner stabilizing greedy loops for finding near-optimal test functions take place in the "small" reduced spaces requiring a computational effort that scales (low-order) polynomially in the reduced dimensions. Finally, the well-conditioned stable formulations used on each level of the scheme provide rigorous a posteriori error bounds that allow one to verify the set target accuracy, see [2, 3, 5].

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Randomized sampling of matrices: three recent results

Laurent Demanet

We briefly review three matrix factorization methods based on randomized sampling: the randomized SVD; the randomized skeleton or CUR factorization; and matrix probing. This note is an aide-memoire for a presentation given at Oberwolfach in January 2015. The author is grateful to the organizers for their work on a very successful event.

1. The randomized SVD

The question is to find the SVD of $A \in \mathbb{R}^{n \times n}$, where A has rank close to k, from $Y = AX$ where $X \in \mathbb{R}^{n \times (k+p)}$ is a gaussian random matrix with iid entries.

Once Y is computed, it can be orthogonalized into a matrix Q. We obtain a low-rank approximation of A from QQ^*A. The following result indicates how accurately the column space information is captured by this random sampling method, as a function of p. In this note, $\|\cdot\|$ is the spectral norm.

Theorem. (Halko, Martinsson, Tropp, 2009 [7])

$$\|A - QQ^*A\| \leq (1 + 11\sqrt{(k+p)n})\,\sigma_{k+1},$$

where σ_k are the singular values of A, and with probability $1 - 6p^{-p}$.

In practice, a slight oversampling of $p = 5$ or 10 suffices. The SVD $A = \tilde{U}\,\Sigma V^T$ can then be obtained as follows:

- Factorize $Q^* A = U\Sigma V^T$.
- Form $Q\,(U\Sigma V^T) = (QU)\,\Sigma V^T = \tilde{U}\,\Sigma V^T$.

This randomized construction of the SVD is potentially useful in any application where the SVD needs to be sped up.

2. THE RANDOMIZED SKELETON OR CUR FACTORIZATION

The question is to factorize A in skeleton form as $A \simeq A_C\,Z\,A_R$, where C and R indicate restriction to subsets of columns and rows, respectively.

The middle matrix can either be formed as $Z_{\mathrm{opt}} = A_C^+ A A_R^+$ (optimal in the Frobenius norm), or $Z_{\mathrm{poor}} = A_{CR}^+$, where the pseudo-inverse is adequately regularized. A first result concern the existence of subsets C and R yielding a good skeleton approximation, though it does not detail a practical algorithm for computing C and R.

Theorem. (Goreinov, Tyrtyshnikov, Zamarshkin, 1997 [5]) There exist C, R, such that

$$\|A - A_C\,Z_{\mathrm{opt}}\,A_R\| \le (\,\sqrt{1 + k(n-k)}\,)\,\sigma_{k+1}.$$

A second result finds C and R constructively via a rank-revealing QR decomposition, at the expense of a slightly worse constant in the error estimate.

Theorem. (Gu, Eisenstat, 1996 [6]) There exist C, R, and Z obtained from a rank-revealing QR algorithm, such that

$$\|A - A_C\,Z\,A_R\| \le (\,\sqrt{1 + 4k(n-k)}\,)\,\sigma_{k+1}.$$

A third result is concerned with the case when C and R are chosen uniformly at random, which allows to lower the complexity of computing the factors below $O(n^2)$ (by not having to even sample every entry of the matrix A). For uniform sampling to be successful, we need to assume the existence of a factorization $A = U\Sigma V^T$ with $\max_{i,j}\{|U_{ij}|, |V_{ij}|\} \le \frac{\mu}{\sqrt{n}}$, where $\mu \ge 1$ is small. Here U and V need not contain the singular vectors, but they are assumed to be isometries.

Theorem. (Chiu, Demanet, 2011 [3]) Sample $\ell = 10\,\mu\,k\log n$ columns and rows uniformly at random to get C and R. Then

$$\|A - A_C\,Z_{\mathrm{poor}}\,A_R\| \le C\,\frac{n}{\ell}\,\sigma_{k+1},$$

with probability $1 - 4kn^{-2}$.

The complexity of forming the middle factor Z_{poor} is $O(k^3)$, up to log factors. Applications of the randomized skeleton factorization include the numerical analysis of operators, and possibly uncertainty quantification.

3. Matrix probing

The question is to recover a matrix $A \in \mathbb{R}^{n \times n}$ from the knowledge of $y_k = Ax_k$, where $x_1, \ldots, x_q \sim N(0, I_n)$. Assume that A belongs to a known p-dimensional linear subspace, i.e., there exist $B_1, \ldots, B_p$ (fixed, given) such that

$$A = \sum_{i=1}^{p} c_i B_i.$$

This assumption on A is very different from the rank-k assumption that underlies the randomized SVD. The vector c can be solved for from the simple least-squares formulation

$$\begin{pmatrix} y_1 \\ \vdots \\ y_q \end{pmatrix} = A \begin{pmatrix} x_1 \\ \vdots \\ x_q \end{pmatrix} = \sum_{i=1}^{p} c_i \begin{pmatrix} Bx_1 \\ \vdots \\ Bx_q \end{pmatrix} = \Psi_x\, c.$$

The matrix Ψ_x is of size $nq \times p$. For this matrix to be left-invertible, is is necessary that it is tall and thin, i.e., $nq \geq p$. Probing will be successful if Ψ_x is furthermore well-conditioned. This will happen if the B_i are properly chosen, and if p is small enough, as we now detail.

The two important properties of the B_i are the "weak condition numbers" λ and κ, defined as follows.

Definition.

$$\lambda = \max_i \frac{\|B_i\| \sqrt{n}}{\|B_i\|_F}$$

Definition.

$$\kappa = \text{cond}(N), \qquad N_{ij} = \text{Tr}(B_i^T B_j).$$

A small λ amount to a *high rank* condition, while a small κ amounts to a *Riesz basis* condition. The recovery result for the vector c is as follows.

Theorem. (Chiu, Demanet, 2011 [2]) For sufficiently large C, if

$$nq \geq C\,p\,(\lambda\kappa \log p)^2,$$

then

$$\text{cond}(\Psi_x) \leq 2\kappa + 1,$$

with probability $1 - O\left(pn^{1-C/C'}\right)$.

Matrix probing is useful for preconditioning large, structured systems of equations [4], and for representing singular and oscillatory kernels in numerical analysis [1].

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Instance optimality of the maximum strategy

LARS DIENING

(joint work with Christian Kreuzer)

For more than forty years adaptive finite element methods (AFEM's) have been a standard tool of engineering and scientific computing for solving PDEs. In contrast to uniform refinements adaptive mesh refinements allow to minimize the required degrees of freedom needed to obtain a given accuracy. Although very successful in the convergence analysis is rather recent.

The basic idea is that based on the discrete solution on some coarse mesh local (per element or edge) a posteriori error indicators are computed. A finer mesh is then constructed by local refinements in areas with large indicators. This process is iterated until the a prescribed error tolerance is met. Up to now there are basically two marking strategies for which optimal convergence has been studied.

(a) Dörfler marking (bulk chasing): The smallest set of elements is marked for refinement such that the indicators on the marked elements are a fixed bulk of the total error estimator.

(b) Maximum strategy: The elements with error indicator comparable to the maximal indicator are marked for refinement.

In the meantime convergence and optimality of the Dörfler marking strategy is well understood. In [4] Dörfler (and later refined in [5]) showed linear convergence of the adaptive finite element method (AFEM):

$$\text{SOLVE} \rightarrow \text{ESTIMATE} \rightarrow \text{MARK} \rightarrow \text{REFINE}$$

In [2], Binev, Dahmen and DeVore proved optimal convergence rates of Dörfler marking introducing an additional coarsening step. This artificial requirement was removed in [7]. Numerous article have appeared since then, extending the results to, various types of error estimators, general elliptic problems and different type

of finite element methods. In summary the development for the theory of Dörfler marking has been very successful in the last years.

For the maximum strategy not much has been known until recently. Under very restrictive assumptions Babuska and Vogelius studied a simple one dimensional problem in [1]. However, in the much more involved multidimensional case there was even no convergence theory until Morin, Sieber and Veeser showed in [6] basic convergence. Very recently Diening, Kreuzer and Stevenson [3] proved *instance optimality* of an AFEM with (modified) maximum strategy for the Dirichlet model problem

$$-\Delta u = f, \qquad \text{in } \Omega$$
$$u = 0, \qquad \text{on } \partial\Omega$$

with $f \in L^2(\Omega)$.

Theorem. *In each iteration an AFEM with (modified) maximum strategy produces a quasi optimal total error with respect to the degrees of freedom (DOFs) up to a constant.*

This result has been obtained in [3] for piecewise linear ansatz functions in two dimensions. The purpose of this talk was to present this result and further generalisations to higher order elements.

In order to explain the main ideas we need to introduce some notation. We denote by $\mathcal{T}_\perp$ a conforming initial triangulation of a polygonal, planar domain Ω. Based on the newest vertex bisection we consider conforming refinements of $\mathcal{T}_\perp$, which have a partial order in the sense that $\mathcal{T}_* \geq \mathcal{T}$ if $\mathcal{T}_*$ is a refinement of $\mathcal{T}$. For a fixed $k \in \mathbb{N}$, let $\mathbb{V}(\mathcal{T})$ denote the subspace of $W_0^{1,2}(\mathcal{T})$ of functions, which are piece wise polynomials of degree at most k on every element of $\mathcal{T}$. For each admissible triangulation $\mathcal{T}$ we denote by $u_\mathcal{T} \in \mathbb{V}(\mathcal{T})$ the Galerkin approximation of the Poisson problem.

Since the estimator is equivalent to the error only up to some additive so called data oscillation term called it is reasonable that optimal convergence of an AFEM can only obtained with respect to the total error

$$\|\nabla u_\mathcal{T} - \nabla u\|_2^2 + \text{osc}_{k-1}^2(\mathcal{T}).$$

The oscillation somehow quantifies the resolution of the data f on the current triangulation $\mathcal{T}$. In particular, we set

$$\text{osc}_\alpha^2(\mathcal{T}) := \sum_{T \in \mathcal{T}} \int_T h_T^2 |f - \Pi_{T,\alpha} f|^2 \, dx.$$

Here $\Pi_{T,\alpha}$ is the local L^2-projection to the space of polynomials of degree at most α and $\Pi_{T,-1} f \equiv 0$.

It is well known that the Galerkin approximation $u_\mathcal{T}$ can be equivalently characterised as the minimiser of the energy functional

$$\mathcal{J}(v) := \int_\Omega \frac{1}{2} |\nabla v|^2 \, dx - \int_\Omega v f \, dx.$$

Therefore, defining $\mathcal{J}(\mathcal{T}) := \mathcal{J}(u_\mathcal{T})$ allows us to reinterpret the AFEM as an energy minimisation process with respect to a sequence of nested admissible refinements.

We use the standard residuum based error estimator organised by edges S of the triangulation, i.e.

$$\mathcal{E}^2(\mathcal{T}; S) := h_S \int_S |[\nabla u_\mathcal{T}]_S|^2 \, ds + \sum_{S \text{ is side of } T} \int_T h_T^2 | -\overline{\Delta} u + f|^2 \, dx,$$

where h_S and h_T are the local mesh sizes of the edge S and the triangle T respectively and $\overline{\Delta}$ denotes the local Laplacian, which is a piece wise polynomial of degree at most $k-2$.

We define a modified energy by

$$\mathcal{G}(\mathcal{T}) := \mathcal{J}(\mathcal{T}) + \mathsf{osc}_{k-2}^2(\mathcal{T}).$$

Note that we have osc_{k-2} here instead of osc_{k-1} different from the definition of the total error. The modified energy satisfies the following crucial properties:

(a) $\mathcal{G}$ is decreasing with respect to refinement.

(b) For $\mathcal{T}_* \geq \mathcal{T}$ we have

$$\mathcal{G}(\mathcal{T}_*) - \mathcal{G}(\mathcal{T}) \sim \sum_{S \text{ refined}} \mathcal{E}^2(\mathcal{T}; S),$$

i.e., the energy difference is equivalent to the error estimators of the refined edges up to fixed constants.

(c) The lower diamond estimate holds: If $\mathcal{T}_1, \ldots, \mathcal{T}_m$ are triangulations with joint refinement $\mathcal{T}_\vee$ and joint coarsening $\mathcal{T}^\wedge$ such that the areas of refinement from $\mathcal{T}_j$ to $\mathcal{T}_\vee$ are disjoint, then the energy differences approximately sum up, i.e.

$$\mathcal{G}(\mathcal{T}^\wedge) - \mathcal{G}(\mathcal{T}_\vee) \sim \sum_{j=1}^m \big(\mathcal{G}(\mathcal{T}_j) - \mathcal{G}(\mathcal{T}_\vee)\big).$$

(d) We have that

$$\mathcal{G}(\mathcal{T}) - \mathcal{J}(u) \sim \|\nabla u_\mathcal{T} - \nabla u\|_2^2 + \mathsf{osc}_{k-1}^2(\mathcal{T}).$$

In other words, up to fixed constants, the difference between the modified energy and the energy of the continuous solution is equivalent to the total error.

These are the main ingredients of the proof of instance optimality in [3], where the case $k = 1$ has been studied. We show that all of these estimates are valid in the case $k \geq 1$, which implies the desired instance optimality result of an higher order AFEM with modified maximum marking strategy.

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Anisotropic mesh adaptation for crack detection in brittle materials

Massimo Fornasier

(joint work with Marco Artina, Stefano Micheletti, and Simona Perotto)

A brittle material, subjected to an external force, first deforms itself elastically, then it breaks without any intermediate phase. A mathematical model of brittle fractures without prescribed path has been proposed by Francfort and Marigo in [6]. The quasi-static evolution of the fracture is based on the successive minimization of an energy designed according to the Griffith's principle of energy balance between elastic energy and a fictitious crack energy:

$$\hat{u}(t) \in \arg \min_{\substack{u \in SBV(\Omega), \\ u|_{\Omega_D} = g(t)|_{\Omega_D}}} \int_{\Omega \setminus S_u} |\nabla u|^2 dx + \kappa \mathcal{H}^{N-1}(S_u),$$

where $\Omega_D \subset \Omega$ is the domain of the force g, κ the elasticity constant, and S_u is the *jump set* of the function u in the special bounded variation function space $SBV(\Omega)$. This approach has the advantage that the functional setting in SBV does not require a pre-defined crack path, but has the drawbacks that it evolves through the minimization of a nonconvex and nonsmooth functional involving unknown functions and sets and any discretization is a bias towards a proper fracture propagation. Bourdin, Francfort, and Marigo [4] used either very fine grids , with consequent very large computational times, or design meshes according to the expected crack evolution, in order to have reliable simulations.
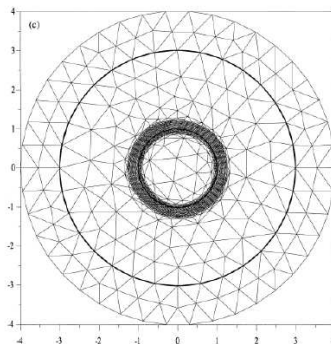
Typical mesh from the experiments of Bourdin, Francfort, and Marigo.

Burke, Ortner, and Süli [5] proposed a fully adaptive scheme based on isotropic mesh refinements, leading though to the generation of extremely fine adapted meshes.
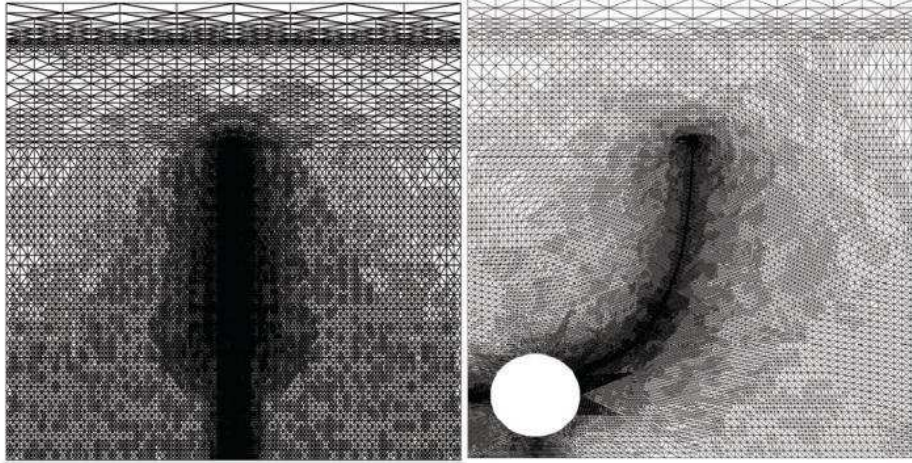
Respectively 300658 and 429116 elements.

In our talk we presented the results included in the papers [1, 2, 3] on the numerical simulation of brittle fractures, building upon the work [5], but using adaptive anisotropic remeshing.
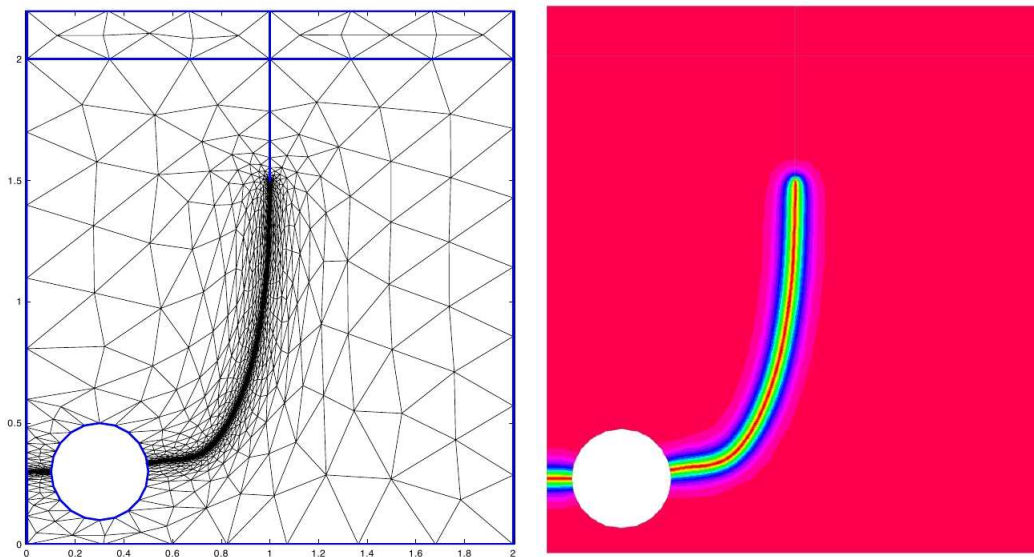
Significantly reduced number of elements (15987) in our simulations.

Relevant features of our adaptive anisotropic remeshing method are:

1. The number of degrees of freedom and the computational times are dramatically reduced, despite the remeshing;
2. The remeshing does not alter the energy profile evolution;
3. On the crack tip the automatically generated mesh is nearly isotropic and does not constitute an artificial bias for the crack evolution.

As a consequence of 2. and 3. we obtain always physically acceptable crack evolutions beyond state of the art simulations. It remains still open to provide

rigorous proofs for the improved complexity 1. as well as for the more fundamental properties 2. and 3.

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Reduced Basis Approximation of Noncoercive Variational Inequalities

Silke Glas

(joint work with Karsten Urban)

Parabolic variational inequalities often occur in industrial or financial problems, e.g. as time dependent obstacle problems or as pricing of swing options on the stock market. Swing options are widely used in electricity markets for the volume and price flexibility reasons they provide. Due to their multiple exercise property, the pricing of swing options requires sophisticated numerical methods. The objective is to price swing options for many different parameters, e.g. calibration of volatility, interest rate or strike price. Using the setting of [12], swing options, which are modeled by a series of parabolic variational inequalities, can be rewritten as a cascade of European and American options. Therefore, one needs to efficiently solve parametrized parabolic equations for European options as well as parametrized parabolic variational inequalities for American options.

Fine discretizations, that are needed for these problems, resolve in large scale problems and thus in long computational times. To reduce the size of these problems, we use the Reduced Basis Method (RBM)[9]. The ambition of the RBM is to efficiently reduce discretized parametrized partial differential equations. Problems are considered, where not only a single solution is needed, but solutions are wanted for a whole range of different parameter configurations. For the European options, we can apply standard RBMs for parabolic equations, e.g. [5, 11], whereas for the American options, we need new methods to treat the reduction of the parabolic variational inequalities.

In the context of variational inequalities, RBM have initially been applied to the elliptic setting [6]. Based on this, [7] applies RBM to parabolic variational inequalities for American options, but does not provide error estimators. Recently, we have been aware of [1], which presents a time stepping error estimator.

Indeed, improved error estimators for parabolic equations could be achieved by linking the RBM with the space-time formulation [11]. Using space-time formulations [10], we do not have a time stepping scheme anymore, but take the time as an additional variable in the variational formulation of the problem. Combining the RBM with the space-time formulation, we derive a noncoercive Petrov–Galerkin variational inequality problem [3]. For this case, the standard theory for the wellposedness does not hold. We derive the necessary conditions for wellposedness and therefore extend the results from [8]. Using this framework, an error estimator based on the residuum. We present numerical results for a parametrized heat inequality model [4], particularly, we perform experiments focusing on rigor and efficiency of the error estimator depending on the shape of the obstacle.

Further research will be devoted to the search for suitable stable reduced test spaces using the double greedy approach [2].

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Ridgelet Discretization of Linear Transport Equations

Philipp Grohs

(joint work with Axel Obermeier)

We presented a novel method for the numerical solution of linear transport equations of the form

$$(1) \qquad s \cdot \nabla u(x) + \kappa(x)u(x) = f(x),$$

where

$$s \in \mathbb{S}^{d-1}, \quad \text{and} \quad \Omega \subset \mathbb{R}^d,$$

and subject to appropriate boundary conditions.

Our motivation comes from the desire to efficiently solve kinetic transport equations (arising for instance in radiative transport or statistical mechanics e.g. the Boltzmann equation) which are in general of the form

$$(2) \qquad s \cdot \nabla u(x,s) + \kappa(x,s)u(x,s) = f(x,s) + Q(u)(x,s)$$

where Q is a scattering or collision operator.

The numerical discretization of such equations is challenging, mainly due to the fact that the above equation is not elliptic (making it difficult to precondition the arising linear system of equations) and singularities can be transported along rays which may result in solutions u which are discontinuous across the transport direction s.

The purpose of this talk was to present a novel, ridgelet-based discretization of (1) and use this discretization for the numerical solution of the full kinetic transport equation (2) either using a (sparse) collocation approach in the direction s or a tensor product construction [1].

Due to the fact that ridgelet systems are well adapted to the structure of linear transport operators, it can be shown that our scheme operates in optimal complexity, even if line singularities are present in the solution [2].

Many questions remain for future work, in particular the problem of good ridgelet constructions for finite domains Ω.

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Hybrid numerical-asymptotic boundary element methods for high frequency wave scattering

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(joint work with Simon Chandler-Wilde, Stephen Langdon, Ashley Twigger, Samuel Groth, Markus Melenk)

There has been considerable interest in recent years in the development of numerical methods for time-harmonic acoustic and electromagnetic wave scattering problems that can efficiently resolve the scattered field at high frequencies. Standard finite or boundary element methods (FEMs and BEMs), with piecewise polynomial approximation spaces, suffer from the restriction that a fixed number of degrees of freedom is required per wavelength in order to represent the oscillatory solution, leading to excessive computational cost when the scatterer is large compared to the wavelength.

The *hybrid numerical-asymptotic* (HNA) approach aims to reduce the number of degrees of freedom required, by enriching the numerical approximation space with oscillatory functions, chosen using partial knowledge of the high frequency (short wavelength) asymptotic behaviour of the solution. The BEM setting is particularly attractive for such an approach, since knowledge of the high frequency asymptotics is required only on the boundary of the scatterer; for a recent review of the HNA methodology in the BEM context see [3]. In this setting one takes the relevant boundary value problem, which in the acoustic case involves the Helmholtz equation

$$(1) \qquad\qquad (\Delta + k^2)u = 0,$$

where the wavenumber k is proportional to the frequency of the incident wave, and reformulates it as a boundary integral equation on the boundary Γ of the scatterer, with frequency dependent solution V. Then, informed by a high frequency asymptotic theory such as the Geometrical Theory of Diffraction (GTD) (see e.g. [11, 2]), one seeks to approximate V using an HNA ansatz of the form

$$(2) \qquad V(x,k) \approx V_0(x,k) + \sum_{m=1}^{M} V_m(x,k)\exp(\mathrm{i}k\psi_m(x)), \quad x \in \Gamma,$$

where V_0 is a known oscillatory function (e.g., the leading order term in GTD approximation), the phases ψ_m are chosen *a-priori* (e.g., from partial knowledge of the higher order GTD components) and the amplitudes V_m, $m = 1, \ldots, M$, are approximated numerically. The key idea is that if V_0 and ψ_m, $m = 1, \ldots, M$, in (2) are chosen wisely, then V_m, $m = 1, \ldots, M$, will be much less oscillatory than V and so can be better approximated by piecewise polynomials than V itself.

The nature and complexity of the HNA ansatz (2) is inherently problem-dependent, being governed by the underlying high frequency asymptotics of the solution, which themselves depend strongly on the geometry of the scatterer and the form of the incident wave. As a result, the HNA approach has been applied so far mainly to problems for which these asymptotics are relatively simple (mostly 2D

problems, with the exception of [6] and [3, §7.6], and mostly convex scatterers, with the exception of [4]). But for many such problems (e.g., scattering by sound-soft smooth convex obstacles in 2D [5, 1], convex [10] and nonconvex [4] polygons and 2D planar screens [9] - see [3] for further examples) the HNA approach has proved to be very effective, providing a dramatic reduction in the number of degrees of freedom at high frequencies, and in some cases even frequency-independent computational cost (when the numerical integration required for practical implementation is carried out using appropriate oscillatory quadrature routines), see, e.g., [9].

In my talk I will outline the basic HNA methodology in the BEM context, and will highlight some of the interesting analytical and numerical challenges it presents. One such challenge is that to design HNA approximation spaces optimally, and to prove their effectiveness by rigorous numerical analysis, one needs to derive regularity estimates for the amplitudes V_m, $m = 1, \ldots, M$, which are explicit in their wavenumber dependence. This requires rigorous high frequency asymptotics of a type not typically available in the asymptotics literature. For instance, the HNA BEMs presented in [10, 4, 8] for scattering of acoustic plane waves by sound-soft polygons adopt an hp approximation strategy for the amplitudes V_m, $m = 1, \ldots, M$, with mesh refinement towards corner singularities (and towards geometrical shadow boundaries in the case of [8]). In order to apply standard hp techniques to obtain best approximation error estimates, one first has to derive non- standard wavenumber-explicit bounds on the analytic continuation of V_m, $m = 1, \ldots, M$, into the complex plane.

I will also give an overview of current research into the development and analysis of HNA methods for more general scattering problems involving nonconvex scatterers [4, 8], 3D scatterers, and transmission problems [7], where complicated multiple scattering and shadowing effects present interesting challenges.

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Sparse BEM for the heat equation

Helmut Harbrecht

(joint work with Christoph Schwab and Johannes Tausch)

1. Introduction

This talk is concerned with the numerical solution of the heat equation

$$\partial_t u - \Delta u = 0 \quad \text{in } \Omega \times I$$
$$u = f \quad \text{on } \Gamma \times I$$
$$u = 0 \quad \text{on } \Omega \times \{0\}$$

via boundary integral equations, where $\Omega \subset \mathbb{R}^3$ is a domain with Lipschitz boundary $\Gamma := \partial\Omega$ and $I = (0, T)$ is a time interval. To this end, we introduce the thermal single layer operator

$$\mathcal{V}g(\mathbf{x}, t) = \int_0^t \int_\Gamma G(\|\mathbf{x} - \mathbf{y}\|, t - \tau) g(\mathbf{y}, \tau) \, \mathrm{d}\sigma_{\mathbf{y}} \, \mathrm{d}\tau$$

where $\mathbf{x} \in \Gamma$ and $G(\cdot, \cdot)$ is the heat kernel, given by

$$G(r, t) = \frac{1}{(4\pi t)^{3/2}} \exp\left(-\frac{r^2}{4t}\right), \ t \geq 0 \quad \text{and} \quad G(r, t) = 0, \ t < 0.$$

Thus, the potential ansatz

$$u(\mathbf{x}, t) = \int_0^t \int_\Gamma G(\|\mathbf{x} - \mathbf{y}\|, t - \tau) g(\mathbf{y}, \tau) \, \mathrm{d}\sigma_{\mathbf{y}} \, \mathrm{d}\tau$$

leads to the boundary integral equation

$$(1) \qquad\qquad \mathcal{V}g = f \quad \text{on } \Gamma \times I.$$

2. Galerkin scheme

The thermal single layer operator is a symmetric, elliptic and continuous operator with respect to the its energy space (see [1] for the details). Hence, we may apply a Galerkin discretization without further restriction.

Consider two sequences of nested ansatz spaces

$$V_0^\Gamma \subset V_1^\Gamma \subset \cdots \subset V_j^\Gamma \subset \cdots \subset L^2(\Gamma),$$
$$V_0^I \subset V_1^I \subset \cdots \subset V_j^I \subset \cdots \subset L^2(I)$$
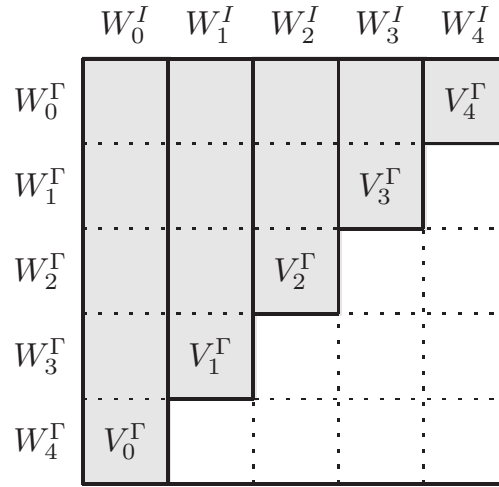
FIGURE 1. Visualization of the sparse tensor product space.

such that

$$|\Delta_j^\Gamma| = \dim V_j^\Gamma \sim 4^j, \quad |\Delta_j^I| = \dim V_j^I \sim 2^j.$$

Instead of using the full tensor product space $U_j^{\Gamma \times I} := V_j^\Gamma \otimes V_j^I$ for the Galerkin discretization of (1), we shall consider the related sparse tensor product space. The starting point are the multilevel decompositions

$$V_j^\Gamma = W_0^\Gamma \oplus W_1^\Gamma \oplus \cdots \oplus W_j^\Gamma,$$
$$V_j^I = W_0^I \oplus W_1^I \oplus \cdots \oplus W_j^I.$$

Then, the sparse tensor product space is given by

$$\widehat{U}_j^{\Gamma \times I} = \bigoplus_{\ell + \ell' \leq j} W_\ell^\Gamma \otimes W_{\ell'}^I = \bigoplus_{\ell'=0}^{j} \left(\bigoplus_{\ell=0}^{j-\ell'} W_\ell^\Gamma \right) \otimes W_{\ell'}^I = \bigoplus_{\ell'=0}^{j} V_{j-\ell'}^\Gamma \otimes W_{\ell'}^I,$$

as illustrated in Figure 1. Notice that only a wavelet basis in time is necessary to obtain a basis in the sparse tensor product space.

The sparse tensor product space contains much less unknowns compared to the full tensor product space: $\dim \widehat{U}_j^{\Gamma \times I} \sim 4^j$ instead of $\dim U_j^{\Gamma \times I} \sim 8^j$. This means that the time discretization is for free. Nevertheless, the approximation property in the sparse tensor product space is essentially the same as in the full tensor product space, provided that we spent some extra smoothness in terms of the mixed Sobolev spaces. Notice that the construction of the sparse tensor product space can be much improved by using generalized sparse grids and ansatz functions with different polynomial orders in space and in time, see [2].

3. FAST MATRIX-VECTOR MULTIPLICATION

For the matrix-vector multiplication, we need to be able to apply the matrix blocks of the form

$$\mathbf{V}_{\boldsymbol{\ell},\boldsymbol{\ell}'} := \langle \mathcal{V}(\Psi^\Gamma_{\ell_1'} \otimes \Psi^I_{\ell_2'}), \Psi^\Gamma_{\ell_1} \otimes \Psi^I_{\ell_2} \rangle_{L^2(\Gamma \times I)},$$

where $\|\boldsymbol{\ell}\|_1, \|\boldsymbol{\ell}'\|_1 \le j$. We aim at approximating such blocks by a low-rank approximation

$$(2) \qquad\qquad \mathbf{V}_{\boldsymbol{\ell},\boldsymbol{\ell}'} \approx \sum_{i=1}^{M} \mathbf{A}^{(i)}_{\ell_2,\ell_2'} \otimes \mathbf{B}^{(i)}_{\ell_1,\ell_1'}$$

where M is at most a power of j. Then, as proposed in [4], the matrix-vector multiplication can be performed in essentially linear complexity provided that $\mathbf{A}^{(i)}_{\ell_2,\ell_2'}$ and $\mathbf{B}^{(i)}_{\ell_1,\ell_1'}$ can be computed in essentially linear complexity. In particular, by use of prolongations and restriction, it suffices to make available quadratic matrices $\mathbf{A}^{(i)}_{\ell_2,\ell_2'}$ and $\mathbf{B}^{(i)}_{\ell_1,\ell_1'}$ with $\ell_1 = \ell_1'$ and $\ell_2 = \ell_2'$.

A semi-discretization of the heat kernel in time leads to an $\mathcal{H}$-matrix, cf. [3]. Exploiting that this $\mathcal{H}$-matrix is a Toeplitz matrix, we arrive at a low-rank approximation of the form (2). In space, we apply the multipole method as proposed in [5]. Putting these ingredients together, we obtain an algorithm which solves the boundary integral equation (1) in the sparse tensor product space in essentially linear complexity.

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hp–Version Discontinuous Galerkin Methods on Polygonal and Polyhedral Meshes

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(joint work with Paola Antonietti, Andrea Cangiani, Emmanuil Georgoulis, and Stefano Giani)

The numerical approximation of partial differential equations (PDEs) posed on complicated domains which contain 'small' geometrical features, or so-called microstructures, is of vital importance in engineering applications. In such situations, an extremely large number of elements may be required for a given mesh generator to

produce even a 'coarse' mesh which adequately describes the underlying geometry. With this in mind, the solution of the resulting system of equations emanating, for example, from a finite element discretization of the underlying PDE of engineering interest on the resulting 'coarse' mesh, may be impractical due to the large number of degrees of freedom involved. Moreover, since this initial 'coarse' mesh already contains such a large number of elements, the use of efficient multi-level solvers, such as multigrid, or domain decomposition, using, for example, Schwarz-type preconditioners, may be difficult, as an adequate sequence of 'coarser' grids which represent the geometry are unavailable.

In recent years, a new class of finite elements, referred to as Composite Finite Elements (CFEs), have been developed for the numerical solution of partial differential equations, which are particularly suited to problems characterized by small details in the computational domain or micro-structures; see, for example, [5, 4], for details. This class of methods are closely related to the Shortley-Weller discretizations developed in the context of finite difference approximations, cf. [6]. The key idea of CFEs is to exploit general shaped element domains upon which elemental basis functions may only be locally piecewise smooth. In particular, an element domain within a CFE may consist of a collection of neighbouring elements present within a standard finite element method, with the basis function of the CFE being constructed as a linear combination of those defined on the standard finite element subdomains. In this way, CFEs offer an ideal mathematical and practical framework within which finite element solutions on (coarse) aggregated meshes may be defined.

In this talk, we consider the generalisation of CFE schemes to the case when hp–version discontinuous Galerkin composite finite element methods (DGCFEMs) are employed, cf. [1]. In particular, we propose a new interior penalty scheme characterized by a careful choice of the discontinuity-penalization parameter, which permits the use of polygonal/polyhedral elements such that

- mesh element faces may have arbitrarily small measure in two dimensions;
- both mesh element faces and edges may have arbitrarily small measure in three dimensions.

The approach is based on exploiting a new inverse inequality relevant to elements with elemental interfaces whose measure is potentially much smaller than the measure of the corresponding element, cf. [3]. On the basis of this inverse inequality, together with appropriate approximation results on general polygons/polyhedra, we derive *a priori* error bounds for the proposed IP DGCFEM. Furthermore, the application of this class of methods within Schwarz-type domain decomposition preconditioners will be considered, cf. [2].

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On low-rank approximability of solutions to operator equations and eigenvalue problems

DANIEL KRESSNER

(joint work with Luka Grubišić, André Uschmajew)

We consider the approximate solution of tensor equations and eigenvalue problems of the form

$$\mathcal{A}(\mathcal{X}) = \mathcal{B}, \qquad \mathcal{A}(\mathcal{X}) = \lambda \mathcal{X}, \tag{1}$$

where $\mathcal{B}, \mathcal{X} \in \mathbb{R}^{n \times \cdots \times n}$ are tensors of order d and $\mathcal{A} \in \mathbb{R}^{n \times \cdots \times n} \to \mathbb{R}^{n \times \cdots \times n}$ is a linear operator. Such problems arise in a variety of applications, including the structured discretization of PDE boundary and eigenvalue problems on a d-dimensional hypercube; we refer to the survey [GraKT13] for a more comprehensive overview.

As d increases, the solution of (1) by standard linear algebra techniques becomes quickly infeasible, due to the exponential growth of the degrees of freedom. Low-rank matrix and tensor approximation techniques have been remarkably successful at obtaining highly accurate solutions to various instances of (1). To understand the success of these techniques and to decide a priori whether they can be applied to a given problem, it appears to be important to study under which conditions on the given data $\mathcal{A}, \mathcal{B}$ one can expect good low-rank approximability of $\mathcal{X}$. In the following, we summarize some new contributions in this direction.

The case $d = 2$ has been studied intensively in the literature, in particular for the special case of a Lyapunov matrix equation:

$$AX + XA^T = -bb^T, \quad A \in \mathbb{R}^{n \times n}, \quad b \in \mathbb{R}^n.$$

The situation is particularly clear when A is a symmetric negative definite matrix, in which case it can be shown that the singular values of X satisfy the following bound [Sab06, GruK14]:

$$\sigma_{r+1}(X) \leq \frac{8}{|\lambda_{\max}(A)|} \exp\left[-\frac{r\pi^2}{\log(8\kappa(A))}\right] \|b\|_2^2, \tag{2}$$

where $\kappa(A) = \|A\|_2 \|A^{-1}\|_2$ and $\lambda_{\max}(A)$ denote the condition number and the largest eigenvalue of A, respectively. The situation is less clear case for nonsymmetric A, in particular when A is highly non-normal; see [BakES14] for a recent discussion.

The exponential decay rate in (2) depends rather mildly on the condition number of A. Nevertheless, the bound deteriorates as $\kappa(A) \to \infty$ and therefore does not admit an extension to Lyapunov operator equations with unbounded coefficients. This question has been addressed in [GruK14], where it is shown that the rth (generalized) singular value of X decays exponentially in $\sqrt{r}$, provided that the involved operator A generates an exponentially stable analytic semigroup, and A is either self-adjoint or diagonalizable with its eigenvalues contained in a strip around the real axis. Numerical experiments with discretizations of 1D and 2D PDE control problems confirm this decay.

It turns out to be difficult to derive decay bounds of the form (2) for more general linear matrix equations, such as

$$AX + XA^T + NXN^T = -bb^T,$$

which play a role in bilinear and stochastic systems, see, e.g., [BenB13, BenD11]. The bound (2) relies on the diagonalization of A and therefore can only be extended if A and N can be diagonalized simultaneously, that is, if they commute with each other. As this condition is usually not satisfied in applications, one needs to resort to completely different techniques.

In [KreU14], a general framework for obtaining low-rank approximability of solutions to matrix and tensor equations has been developed. For $d = 2$, one considers a fixed-point iteration

$$X_{n+1} = \Phi(X_n), \qquad X_n \in HS(H_1, H_2)$$

for Hilbert spaces H_1, H_2 and an appropriately chosen energy functional $F : HS(H_1, H_2) \to \mathbb{R}^+$ for measuring convergence to the fixed point X. The following assumptions are imposed:

(A1) Contraction in energy: There exists $0 < q < 1$ such that

$$F(X_{n+1}) \le q^2 F(X_n).$$

(A2) Finite rank growth: There exists $R > 1$ s.t.

$$\operatorname{rank}(X_{n+1}) \le R \cdot \operatorname{rank}(X_n).$$

(A3) Stability with respect to $\|\cdot\|_{HS}$: There exists $\gamma > 0$ such that

$$\gamma \|X - X_n\|_{HS}^2 \le F(X_n).$$

Under these assumptions, it is shown that the singular values σ_k of X satisfy

$$(3) \qquad \sqrt{\sigma_{r+1}^2 + \sigma_{r+2}^2 + \cdots} \le \sqrt{\frac{\pi_1}{\gamma}} \left(\frac{1}{r}\right)^{\left|\frac{\ln q}{\ln R}\right|},$$

where π_1 is the smallest value of F that can be attained on a certain subset of nonzero rank-1 matrices. This tail bound can be turned into (algebraic) decay

bounds for the singular values, using standard techniques. To apply them to (1) for $d = 2$, standard stationary iterations, like the gradient method, for solving linear systems and eigenvalue problems can be plugged into Φ; see [KreU14] for more details.

The extension of the above result to the case $d > 2$ is fairly straightforward provided that an SVD-based format like the tensor train decomposition [Ose11] or the hierarchical Tucker decomposition [HacK09] is used for the low-rank approximation of the involved tensors. Instead of (A2), one then needs to assume that the application of the fixed point map results in a constant growth of the corresponding tensor ranks (e.g., TT ranks or hierarchical Tucker ranks). Again, we refer to [KreU14] for more details.

It should be noted that (3) results in algebraic decay bounds that are substantially weaker than what is typically observed in applications. Future work will therefore aim at exploiting additional structure of $\mathcal{A}$ for particular classes of applications.

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Adaptive Approximations of Parametric PDE-Constrained Control Problems

ANGELA KUNOTH

(joint work with Christoph Schwab)

Optimization problems constrained by linear PDEs (partial differential equations) are challenging from a computational point of view: one needs to solve a *system of PDEs* coupled globally in space, and, in addition, *globally* in time if the underlying PDE is time-dependent. This global coupling is an unavoidable feature of such

control problems where typically an adjoint PDE comes into place as specified next.

PDE-constrained control problems. Let Y, U be Hilbert spaces over $\mathbb{R}$ which shall host the *state* y of a system and a *control* by which the state can be influenced. Let $J : Y \times U \to \mathbb{R}$ be a twice differentiable functional, and $K : Y \times U \to Y'$ be a (in y, u Fréchet-) differentiable function where Y' denotes the topological dual of Y. Consider the constrained minimization problem

$$(1) \qquad \inf_{(y,u) \in Y \times U} J(y,u) \quad \text{subject to } K(y,u) = 0.$$

For the constraints $K(y,u) = 0$ (which will be the PDE later), we assume that there exists a unique solution $y \in Y$ for the case that $u \in U$ is given. A typical way to solve (1) is to compute the zeroes of the first order Fréchet derivatives of the corresponding Lagrangian functional, defined by introducing a new variable p, the *costate* or *adjoint state* in terms of which the constraints are appended to the functional, i.e., $L(y,u,p) := J(y,u) + \langle K(y,u), p \rangle_{Y' \times Y}$ with $L : Y \times U \times Y \to \mathbb{R}$. Denoting by $L_z(y,u,p) := \frac{\partial}{\partial z} L(y,u,p)$ and $L_{zz}(y,u,p) := \frac{\partial^2}{\partial z^2} L(y,u,p)$ the first and second variation, of L with respect to $z = y, u, p$, and assuming that J is quadratic in both y, u and K linear in y, u, the necessary conditions for optimality yield the linear system of equations

$$(2) \qquad \begin{pmatrix} L_{yy} & L_{yu} & K_y^* \\ L_{uy} & L_{uu} & K_u^* \\ K_y & K_u & 0 \end{pmatrix} \begin{pmatrix} y \\ u \\ p \end{pmatrix} = g \iff: \begin{pmatrix} \mathcal{A} & \mathcal{B}^* \\ \mathcal{B} & 0 \end{pmatrix} \begin{pmatrix} (y,u)^\top \\ p \end{pmatrix} = g \iff: G\, q = g$$

with some right hand side g and C^* denoting the dual of C. The Hessian of L or the Karush-Kuhn-Tucker (KKT) operator G has for such *linear-quadratic problems* constant entries, and the necessary conditions are also sufficient. Moreover, if J or K do not contain products yu, one has $L_{yu} = L_{uy} = 0$ so that $\mathcal{A}$ is a block diagonal operator. Typically, the quadratic functional (1) contains inner products so that the resulting Riesz operators L_{yy}, L_{uu} are symmetric which implies that $\mathcal{A}$ and, thus, G is *symmetric*. Moreover, in all the cases we consider, $\mathcal{A} : \mathcal{V} \to \mathcal{V}, \mathcal{B} : \mathcal{V} \to \mathcal{Q}'$ for some Hilbert spaces $\mathcal{V}, \mathcal{Q}$ are continuous, $\operatorname{Im} \mathcal{B} = \mathcal{Q}'$ and $\mathcal{A}$ is invertible on $\operatorname{Ker} \mathcal{B}$ so that the saddle point problem (2) has for $g \in \mathcal{V}' \times \mathcal{Q}'$ a unique solution $q \in \mathcal{V} \times \mathcal{Q}$ by the Brezzi-Fortin theory. Thus, we can consider constrained linear-quadratic minimization problems as *symmetric saddle point problems* (2) with a boundedly invertible linear mapping $G : \mathcal{V} \times \mathcal{Q} \to \mathcal{V} \times \mathcal{Q}'$ where $\mathcal{V} := Y \times U$ and $\mathcal{V} := Q$. Let me present some standard examples from [6] to which this scenario applies and specify the corresponding system (2).

Dirichlet problem with distributed control. Consider the standard weak formulation of a second order elliptic PDE with homogeneous boundary conditions. Choosing $Y := H_0^1(\Omega)$ and $U := Y'$, we consider for given $f \in Y'$ the linear operator equation

$$(3) \qquad K(y,u) := Ay - f - u = 0$$

and quadratic objective functional

$$(4) \qquad\qquad J(y, u) := \frac{1}{2}\|y - y_*\|_Y^2 + \frac{\omega}{2}\|u\|_{Y'}^2$$

for a given target state $y_* \in Y$ and any fixed weight parameter $\omega > 0$. We assume that $A : Y \to Y'$ is a linear (not necessarily symmetric) boundedly invertible operator. The norms in (4) can be norms on Hilbert spaces as long as the constrained optimization system (1) is well-posed.

Denote by $R : Y \to Y'$ the Riesz operator defined by the inner product $(\cdot, \cdot)_Y$ inducing $\|\cdot\|_Y$, $\langle v, Rw\rangle_{Y\times Y'} := (v, w)_Y$, $v, w \in Y$. Since $(\cdot, \cdot)_Y$ is symmetric, R is also. The Lagrangian is now of the form

$$(5) \quad L(y, u, p) = \frac{1}{2}\langle y - y_*, R(y - y_*)\rangle_{Y\times Y'} + \frac{\omega}{2}\langle u, R^{-1}u\rangle_{Y\times Y'} + \langle Ay - f - u, p\rangle_{Y'\times Y}$$

Thus, the system (2) becomes

$$(6) \qquad\qquad \begin{pmatrix} R & 0 & A^* \\ 0 & \omega R^{-1} & -I \\ A & -I & 0 \end{pmatrix} \begin{pmatrix} y \\ u \\ p \end{pmatrix} = \begin{pmatrix} Ry_* \\ 0 \\ f \end{pmatrix},$$

i.e., $\mathcal{A} = \mathrm{diag}(R, \omega R^{-1})$ and $\mathcal{B} = (A, -I)$. The system matrix G defined in (6) is symmetric since R is. Moreover, $\mathcal{A}$ is positive definite and $\mathcal{B}$ has full rank since, by assumption, the PDE constraints have a unique solution for given u. Thus, the resulting saddle point operator G is symmetric and boundedly invertible.

Parabolic PDE with distributed control. The constraint $K(y, u) = 0$ in (1) is here a linear parabolic evolution PDE in full space-time weak formulation from [9] (in a variation). The parabolic operator equation is formulated such that the resulting operator B is boundedly invertible from $\mathcal{X} := L^2(I) \otimes Y$ to $\mathcal{Y}' := ((L^2(I) \otimes Y) \cap (H_T^1(I) \otimes Y'))'$ where $H_T^1(I)$ is the closure of the functions in $H^1(I)$ which vanish at end time T and $I := (0, T)$ denotes the time interval. The constraints are of the form (3) with the parabolic evolution operator $B = \partial_t + A$ in full weak space-time form in place of A, see [5] for details. Choosing the objective function then as in (4) with the obvious changes for the norms, i.e., using the norms for $\mathcal{X}$, $\mathcal{Y}$, we arrive at a system very similar to (6) with symmetric $\mathcal{A} = \mathrm{diag}(R_1, \omega R_2)$ with the respectively defined Riesz operators. The corresponding operator G is here a boundedly invertible mapping from $\mathcal{Z} := \mathcal{X} \times \mathcal{Y}' \times \mathcal{X}$ onto $\mathcal{Z}'$.

Adaptive wavelet methods for the parabolic pde-control problem. In view of the fully in space *and time* coupled system (2), conventional time-stepping methods require an enormous storage. In contrast, adaptive methods in both space and time which aim at distributing the available degrees of freedom in an a-posteriori-fashion to capture singularities are most promising. Employing wavelet schemes for full weak space-time formulations of the parabolic PDEs, we can prove convergence and optimal complexity for control problems constrained by a linear parabolic PDE [5], generalizing the ideas from [3] for control problems constrained by an elliptic PDEs.

Parametric control problems. Yet another level of challenge are control problems constrained by evolution PDEs involving stochastic or countably many infinite parametric coefficients: for each instance of the parameters, this requires the solution of the complete control problem (2).

Our method of attack is based on the following new theoretical paradigm developed for elliptic PDEs in [1, 2]. It is first shown for control problems constrained by evolution PDEs, formulated in full weak space-time form as in [9], that state, costate and control are *analytic* as functions depending on these parameters. We establish that these functions allow expansions in terms of sparse tensorized generalized polynomial chaos (gpc) bases. Their sparsity is quantified in terms of p-summability of the coefficient sequences for some $0 < p \leq 1$. Resulting a-priori estimates establish the existence of an index set for *simultaneous* approximations of state, co-state and control for which the gpc approximations attain rates of best N-term approximation. This entails corresponding *sparse realizations* in terms of deterministic adaptive Galerkin approximations of state, co-state and control on the entire, possibly infinite-dimensional parameter space, see [6]. We specify in [7] how to realize these Galerkin approximations by the techniques in [8] and the realizations in [4] for a single PDE.

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Recent results on greedy algorithms and the reduced basis method for high-dimensional partial differential equations

Tony Lelièvre

Approximating high-dimensional functions which are defined as solutions to partial differential equations (PDEs) is a problem which appears in many contexts (kinetic models, quantum mechanics, finance, uncertainty quantification, optimization problems, etc...). Many techniques have been proposed in the literature to deal with such problems and we focus here on Proper Generalized Decomposition (greedy algorithms) and reduced basis techniques.

The principle of the Proper Generalized Decomposition (PGD) introduced by A. Nouy and F. Chinesta in different contexts is to approximate the solution to a PDE as a sum of tensor products:

$$u(x_1, \ldots, x_d) \simeq \sum_{k=1}^{n} r_k^1(x_1) \ldots r_k^d(x_d)$$

where the successive terms in the sum are computed in a greedy way, one after the other. As an example, one could think of a Poisson problem in high dimension, which can be written in a variational form as:

$$\text{Find } u \in H_0^1([0,1]^d), \ u \in \operatorname{argmin}_{v \in H_0^1([0,1]^d)} \frac{1}{2} \int_{[0,1]^d} |\nabla v|^2 - \int_{[0,1]^d} fv.$$

Let us denote $\mathcal{E}(v) = \frac{1}{2} \int_{[0,1]^d} |\nabla v|^2 - \int_{[0,1]^d} fv$ the functional involved in the variational formulation. Then, the greedy algorithm (PGD) writes:

$$\forall n \geq 0, \text{compute } (r_n^1, \ldots, r_n^d) \in H^1([0,1])^d \text{ such that}$$

$$(r_n^1, \ldots, r_n^d) \in \operatorname{argmin}_{(s^1, \ldots, s^d) \in H^1([0,1])^d} \mathcal{E}\left(\sum_{k=1}^{n-1} r_k^1(x_1) \ldots r_k^d(x_d) + s^1(x_1) \ldots s^d(x_d) \right).$$

At each iteration, one thus has to compute d functions of a one-dimensional variable (instead of a function of a d-dimensional variable for the original problem): this is why the algorithm can be used even in high dimension (say d of the order of 10). The question then is of course whether one can prove that

$$u_n = \sum_{k=1}^{n} r_k^1(x_1) \ldots r_k^d(x_d)$$

converges to u.

In [1], we prove that under suitable assumptions, the algorithm indeed converge in the sense that u_n strongly converges to u in the norm of the Hilbert space on which the functional $\mathcal{E}$ is defined (namely $H_0^1([0,1]^d)$ for the example above). This requires in particular some convexity assumption on $\mathcal{E}$. The proof is based on ideas developed in the field of nonlinear approximation theory by V. Temlyakov, R. De Vore and co-workers.

In practice, the solution $(r_n^1, \ldots, r_n^d)$ to the minimization problem is approximated by considering the associated Euler equations. In the case of the Poisson

equation presented above, these Euler equations are a system of d one-dimensional Poisson problems, coupled through non-linear terms. Starting from a linear problem, we thus end up with, at each iteration, a non-linear problem to be solved. This is the price to pay in order to reduce the complexity of the problem as a function of the dimension d. This is very much reminiscent to what happens in electronic structure computations, when the Schrödinger equation (high dimensional linear eigenvalue problem) is approximated using a variational principle restricted to Slater determinants, which leads to a low dimensional nonlinear eigenvalue problem.

Among the current open questions on this type of algorithm, let us mention the extension to parameterized eigenvalue problems, or the treatment of non-symmetric problems (which are not naturally associated with a minimization problem as above). From a numerical analysis point of view, it would be interesting to show that if the solution to the PDE admits a rapidly converging separated representation, then the greedy algorithm does indeed also converge very quickly.

The reduced basis technique (proposed and developed by Y. Maday, A. Patera and co-workers) is another technique which is restricted to the setting of parametrized PDEs. To make it concrete, let us consider as an example the parameterized Poisson problem:

$$\text{Find } u \in L^2([0,1]^d, H_0^1([0,1]^2)), \ \mathrm{div}_x(a(\mu,x)\nabla_x u) = f(x)$$

where $\mu \in [0,1]^d$ is the parameter and $x \in [0,1]^2$ is the space variable. Here, and contrary to the previous setting, the differential operators only act on a low-dimensional variables (namely $x \in [0,1]^2$) and the high-dimensionality of the problem comes from the parameter $\mu \in [0,1]^d$. The problem is thus to approximate the solution $u(\mu,x)$ to this problem.

The reduced basis technique consists in: (i) building in an offline stage a reduced basis, namely accurate solutions $u(\mu_i, x)$ for some well chosen values μ_i of the parameters (where $1 \le i \le \hat{N}$ with $\hat{N}$ small compared to the total number of degrees of freedom used to approximate the functions $u(\mu_i, \cdot)$) and then (ii) approximating in the online stage the solution to the original problem using a Galerkin procedure on the linear space spanned by $\{u(\mu_1, \cdot), \ldots, u(\mu_{\hat{N}}, \cdot)\}$. The choice of the parameters $\{\mu_i, 1 \le i \le \hat{N}\}$ is based on a greedy procedure, using some a posteriori estimator which gives a reliable estimate of the error introduced by approximating the solution by a Galerkin procedure on the reduced basis.

While trying to apply this technique to an industrial problem (aeroacoustic problems around an airplane, solved by a coupled boundary element method - finite element method, in collaboration with Airbus), two problems were identified: (i) the a posteriori estimator which is usually used is very sensitive to round-off errors and (ii) the implementation of the method is very intrusive: it requires to enter deeply into the industrial codes in order to retrieve the matrices which are built to construct the linear problem to be solved. Using techniques based on the empirical interpolation method introduced by M. Barrault, Y. Maday, Nguyen

and A. Patera in 2004, we were able to propose solutions to the two problems mentioned above, see [2, 3].

Let us finish this short review by an original and hopefully illuminating presentation of the empirical interpolation method (EIM) (see also the recent work by M. Bebendorf, Y. Maday and B. Stamm for similar ideas). The aim of EIM is to build a seperated representation of a function $f : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ using two ingredients. The first one is the following result: For given interpolation points $(x_1, \ldots, x_d) \in \mathcal{X}^d$ and $(y_1, \ldots, y_d) \in \mathcal{Y}^d$, if the matrix $(f(x_i, y_j))_{1 \leq i,j \leq d}$ is invertible, then there exists an interpolating function $I_d(f) : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ which writes:

$$I_d(f)(x,y) = \sum_{1 \leq i,j \leq d} D_{i,j} f(x_i, y) f(x, y_j)$$

such that,

- $\forall k \in \{1, \ldots, d\}, \forall y \in \mathcal{Y}, f(x_k, y) = I_d(f)(x_k, y)$
- $\forall x \in \mathcal{X}, \forall l \in \{1, \ldots, d\}, f(x, y_l) = I_d(f)(x, y_l)$.

Indeed, it is easy to check that these properties are satisfied by choosing $D = F^{-T}$. The second ingredient is a procedure to choose the interpolation points $(x_1, \ldots, x_d) \in \mathcal{X}^d$ and $(y_1, \ldots, y_d) \in \mathcal{Y}^d$ using a greedy procedure. Let us consider $\|\cdot\|_{\mathcal{Y}}$ a norm on $\mathcal{Y}$. One iterates on $k \geq 0$ the following. Assume that $(x_1, \ldots, x_k) \in \mathcal{X}^k$ and $(y_1, \ldots, y_k) \in \mathcal{Y}^k$ have been built, and assume that the associated matrix $(f(x_i, y_j))_{1 \leq i,j \leq k}$ is invertible. Let us denote $I_k(f)$ the associated interpolated function. Then, the next points (x_{k+1}, y_{k+1}) are defined by:

$$(1) \qquad \begin{cases} x_{k+1} = \arg\max_{x \in \mathcal{X}} \|f(x, \cdot) - I_k(f)(x, \cdot)\|_{\mathcal{Y}} \\ y_{k+1} = \arg\max_{y \in \mathcal{Y}} |f(x_{k+1}, y) - I_k(f)(x_{k+1}, y)|. \end{cases}$$

The greedy procedure stops if $|f(x_{k+1}, y_{k+1}) - I_k(f)(x_{k+1}, y_{k+1})| = 0$.

It can be checked that if the matrix $(f(x_i, y_j))_{1 \leq i,j \leq k}$ is invertible and if

$$|f(x_{k+1}, y_{k+1}) - I_k(f)(x_{k+1}, y_{k+1})| \neq 0,$$

then the matrix $(f(x_i, y_j))_{1 \leq i,j \leq k+1}$ is also invertible. In addition, if (x_{k+1}, y_{k+1}) satisfies (1), then $|f(x_{k+1}, y_{k+1}) - I_k(f)(x_{k+1}, y_{k+1})| = 0$ implies that $f(x, y) = I_k(f)(x, y)$ for all $(x, y) \in \mathcal{X} \times \mathcal{Y}$.

These results imply that either the greedy procedure stops after a finite number k of iterations, which means that $f(x, y) = I_k(f)(x, y)$, or the greedy procedure can be pursued, and one can define recursively a sequence of interpolating functions $(I_k(f))_{k \geq 1}$ such that the interpolation error is non increasing.

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Adaptive Wavelet Schwarz Methods for Nonlinear PDEs

Dominik Lellek

(joint work with Stephan Dahlke, Shaun Lui, Rob Stevenson)

In this talk, we present adaptive wavelet domain decomposition methods for the numerical solution of nonlinear partial differential equations. In the first part, we will be concerned with semilinear elliptic equations of the form

$$\mathcal{A}u + \mathcal{G}(u) = f,$$

where $\mathcal{A} \in L(H_0^t(\Omega), H^{-t}(\Omega))$ is a linear elliptic operator, $\mathcal{G} : H_0^t(\Omega) \to H^{-t}(\Omega)$ is a nonlinear mapping given by a Nemitsky operator and $f \in H^{-t}(\Omega)$. A typical example is the disturbed Poisson equation $-\Delta u + u^3 = f$. With the help of a wavelet Riesz basis $\Psi = \{\psi_\lambda\}_{\lambda \in \Lambda}$ for $H_0^t(\Omega)$, this equation can be rewritten in the sequence space $\ell_2(\Lambda)$ as

$$\mathbf{A}\mathbf{u} + \mathbf{G}(\mathbf{u}) = \mathbf{f},$$

with $\mathbf{A}, \mathbf{G} : \ell_2(\Lambda) \to \ell_2(\Lambda)$ and $\mathbf{f} \in \ell_2(\Lambda)$. Using this discretized version, adaptive wavelet methods based on a Richardson iteration or Newton's method were developed in [1]. It can be shown that, under reasonable assumptions, these methods are convergent and asymptotically optimal. The latter means that if the best N-term tree approximation to the solution converges with a given rate $s > 0$, i.e.,

$$\inf\{\|\mathbf{u} - \mathbf{v}\|_{\ell_2(\Lambda)}, \# \operatorname{supp} \mathbf{v} \le N, \mathbf{v} \text{ tree-structured }\} \lesssim N^{-s},$$

then the method reproduces this convergence rate. The above rate s can be described in terms of the regularity of the solution $u = \sum_{\lambda \in \Lambda} \mathbf{u}_\lambda \psi_\lambda$ in a Besov scale, the restriction to tree-structured index set only has a very little effect on this. In many cases, the rate exceeds the convergence rate of standard uniform methods and therefore justifies the use of adaptive methods.

A difficulty in the application of these methods, however, lies in the construction of suitable wavelet bases. If the domain Ω is not smooth and has reentrant corners such as in the standard example of the L-shaped domain

$$\Omega := (-1, 1)^2 \setminus [0, 1)^2,$$

common wavelet constructions are often very technical and may have large condition numbers. An idea from [7] to circumvent this problem is to decompose the domain into overlapping subdomains that are diffeomorphic to the unit cube. In the case of the L-shaped domain, such a decomposition is given by

$$\Omega_0 := (-1, 0) \times (-1, 1), \quad \Omega_1 := (-1, 1) \times (-1, 0).$$

On the subdomains, we can now make use of known wavelet constructions, for which the problems occurring on the L-shaped domain can be avoided. Under weak conditions on the decomposition, the union of the Riesz bases on the subdomains gives a stable, but overcomplete generating system for $H_0^t(\Omega)$, a so-called

wavelet frame. Moreover, the use of such an overlapping domain decomposition corresponds naturally to Schwarz domain decomposition methods. The basic idea of these methods is to reduce the problem on the domain Ω to a series of subproblems on the subdomains Ω_i. We consider two types of such methods, the multiplicative and the additive Schwarz method. The first algorithm requires a sequential solution of the subproblems, whereas they are independent in the latter type of methods. For linear problems, adaptive wavelet methods applying such techniques have been developed and analyzed in [9]. Besides from being convergent and asymptotically optimal, their numerical performance has encouraged us to generalize such methods to a range of nonlinear problems. In [4], we develop an adaptive additive wavelet Schwarz method for a range of nonlinear problems. For the construction of the algorithm, we adapt ideas and strategies from [3, 5]. We show that the method is convergent and asymptotically optimal. The expected convergence rates can also practically be observed in numerical experiments at realistic scales. Ongoing research is concerned with the generalization to a broader range of nonlinearities and to the multiplicative Schwarz method.

Furthermore, in the second part of the talk, we outline how the principles of the additive Schwarz method carry over to the stationary Navier-Stokes equation,

$$(u \cdot \nabla)u = -\nabla p + \frac{1}{\mathrm{Re}}\Delta u + f \quad \text{on } \Omega, \quad \mathrm{div}\, u = 0 \text{ on } \Omega,$$

at least for small Reynolds numbers Re and with Dirichlet boundary conditions. In [2] we sketch the construction of an additive wavelet Schwarz method for the above equation, using the divergence-free wavelets from [8] and adapting strategies from [6]. For this method as well, we can show convergence and optimality with respect to the degrees of freedom.

Finally, we explain how the adaptive wavelet Schwarz methods can be combined with Newton's method, possibly opening the prospect to cover a broader range of nonlinear problems.

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A global view on adaptivity and sparsity in PDE discretization

VOLKER MEHRMANN

(joint work with C. Carstensen, J. Gedicke, A. Miedlar, S. Quaraishi, C. Schröder)

In the numerical solution of partial differential equations (PDEs) modeling the behavior of real world problems, sparsity is of major importance. Major questions are: What is a good space of ansatz functions so that that the solution can be sparsely represented/approximated in this space, what is a good basis/frame in this space, or what is needed so that the finite dimensional version has a sparse operator or a sparse inverse and leads to a fast method? Typical approaches use local basis functions in the finite element method or, if something more about the physics is known, the finite element space is enriched as in the extended finite element method. One can also use wavelets, shearlets, Fourier, or spectral function methods to sparsely represent the solution.

These questions are discussed in the context of modeling and simulation of brake squeal in disc brakes. Break squeal is usually due to self-excited vibration caused by a flutter-type instability originating from friction forces at the pad-rotor interface [1]. The analysis is based on idealized minimal models, real experiments, and numerical simulations on uniform meshes via the finite element models, see e.g., [6, 11]. But, despite extensive research, fully satisfactory remedies have not been found.

The macroscopic model equations are usually considered in the form

$$M(\alpha)\ddot{u} + D(\alpha)\dot{u} + K(\alpha)u = f,$$

where $M, D, K \in \mathbb{R}^{n,n}$ are mass, damping and stiffness matrices respectively, depending on a set of parameters α, and f is an external force. The function $u : \mathbb{R} \to \mathbb{R}^n$ contains the position variables associated with the degrees of freedom, arising from the FE modeling. In rotating machinery, the matrices D and K are typically non-symmetric. The non-symmetry arises by incorporating phenomenological models of the gyroscopic and circulatory forces and the parameters typically include operating conditions (temperature, pad pressure, etc) and material conditions (friction coefficient, brake geometry and mass distribution, effects of wear and damping etc), as well as the rotational speed of the disc brake disc. For self-excited vibrations it is also customary to include the excitation force in the form of a nonsymmetric matrix which is added to the stiffness matrix.

The vibrational modes (as functions of the parameters) are determined by sampling the parameters via a set of values α_j, $j = 1, \ldots, p$, and computing the right half plane eigenvalues and associated eigenvectors of the quadratic eigenvalue problems

$$(\lambda^2 M(\alpha_j) + \lambda D(\alpha_j) + K(\alpha_j))x = 0, \ j = 1, \ldots, p.$$

Collecting all these eigenvectors in a matrix and using a partial singular value decomposition, one obtains a matrix U consisting of the singular vectors associated with the large singular values above a certain threshold value. There exist a multitude of numerical methods for the numerical solution of quadratic eigenvalues problems, see e.g. [9], however, this problem is still a major computational challenge, when the parameter vector p varies in a large range.

Projecting the full problem by a congruence with the matrix U, the reduced model with coefficients

$$U^T M(\alpha)U, U^T D(\alpha)U + U^T K(\alpha))U,$$

can then be used for optimizing the system with respect to parameter variations. The newly developed method improves current approaches but is not very efficient, because it is based on a fine uniform mesh and a large number of eigenvalue problems have to be solved. Furthermore, although the method works well in practice, the convergence and error analysis is rather difficult.

To obtain better performance and error estimates, we also discuss adaptive finite element methods. We derive error estimates and adaptive refinement techniques for the self-adjoint subproblem and incorporate the non-symmetry via a homotopy. The errors in the adaptation and in the homotopy are balanced to get error estimates.

Recently the discussed work has been complemented with a backward error analysis for the infinite dimensional case [10], a posteriori error estimates for the hp-finite element methods in the non-selfadjoint case [5], as well the treatment of multiple real eigenvalues in the self-adjoint case [4]. However, there are no results for multiple complex eigenvalues or Jordan blocks.

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A Dimensional Reduction Approach Based on the Application of Reduced Basis Methods in the Framework of Hierarchical Model Reduction

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(joint work with Kathrin Smetana)

Many phenomena in nature have dominant spatial directions along which the essential dynamics occur. Examples are blood flow problems, fluid dynamics in pipes or river beds, and subsurface flow. Motivated by a project on adaptive hydrological modelling of coupled hydrological processes [2] we started to investigate a new dimensional reduction approach [5, 7] for problems with dominant direction which is based on the application of reduced basis (RB) techniques in the hierarchical model reduction (HMR) framework (cf. [8] and the references therein). In detail let $\Omega \subset \mathbb{R}^2$ be a computational domain. We define the solution space V such that $H_0^1(\Omega) \subseteq V \subseteq H^1(\Omega)$ and consider the following general elliptic problem:

$$\text{Find } p \in V: \quad a(p, v) = f(v) \quad \forall v \in V,$$

where $a(\cdot, \cdot)$ is a coercive and continuous bilinear form and f a linear form.

The idea of HMR, which goes back to the work of Vogelius and Babuska [10], is to perform a Galerkin projection onto a reduced space of rank m, i.e.

$$V_m = \left\{ v_m(x, y) = \sum_{k=1}^{m} \overline{v}_k(x) \, \phi_k(y), \ \ \overline{v}_k(x) \in X, \right\},$$

which combines the full solution space X in the dominant direction with a reduction space $Y := \text{span}(\phi_1, ..., \phi_m)$ in the transverse direction. The latter is spanned by modal orthonormal basis functions. While so far the basis functions in the HMR approach have been chosen a priori, for instance, as Legendre or trigonometric polynomials, in this work a highly nonlinear approximation is employed for the construction of the reduction space. To this end we first derive a lower dimensional parametrized problem in the transverse direction from the full problem where the parameters reflect the influence from the unknown solution in the dominant direction. For the derivation of a suitable 1D PDE in transverse direction, we first make the following tensor product ansatz

$$p(x, y) \approx U(x) \cdot \mathcal{P}(y).$$

Here, $U(x)$ represents the behavior of the full solution in the dominant direction, which is unknown at this stage. By choosing the test functions as $v(x, y) = U(x) \cdot v(y)$ for any $v \in Y$ we obtain a parameterized reduced problem: Given any $U \in X$, find $\mathcal{P} \in Y$ such that

$$a(U\mathcal{P}, Uv) = f(Uv) \ \forall v \in Y.$$

Exploiting the good approximation properties of RB methods, we then construct a reduction space by applying a proper orthogonal decomposition to a set of snapshots of the parametrized partial differential equation. For an efficient construction of the snapshot set we apply adaptive refinement in parameter space (cf. [4]) based on an a posteriori error estimate that is also derived in this article. We introduce our method for general elliptic problems such as advection-diffusion equations in two space dimensions. Numerical experiments demonstrate a fast convergence of the proposed dimensionally reduced approximation to the solution of the full dimensional problem and the computational efficiency of our new adaptive approach.

In a next step, we extend the reduced basis-hierarchical model reduction framework for the application to nonlinear partial differential equations [9]. The major new ingredient to accomplish this goal is the introduction of an adaptive Empirical Projection Method, which is an adaptive integration algorithm based on empirical interpolation [1, 3]. In detail, let $u(\mu, \cdot) \in L^2(\omega)$ be given, e.g. as the image of a nonlinear operator A, i.e. $u(\mu, \cdot) = A(v(\mu, \cdot))$. By $\mathcal{M}_\Xi := \{u(\mu, \cdot), \mu \in \Xi\}$ we denote a snapshot set, where $\Xi \subset \mathcal{D}$ is a training set of size $|\Xi| = n$. The collateral space $W_k = \text{span}\{\kappa_1, ..., \kappa_k\}$ with $(\kappa_i, \kappa_j)_{L^2(\omega)} = \delta_{ij}$ is then defined through a POD of the snapshot set. By projection of u into W_k, we obtain

$$P_k[u](\mu, y) := \sum_{l=1}^{k} \int_\omega u(\mu, z) \, \kappa_l(z) \, dz \, \kappa_l(y)$$

For the usage of such a projection in our dimension reduction approach we need a separation of variables in $u(\mu, z)$ in order to be able to precompute the integral on ω independent of μ. To achieve this goal, the adaptive EPM subdivides ω into subintervals and applies locally a generalized empirical interpolation (GEIM), i.e.

$$P_k^L[u](\mu, y) \quad := \quad \sum_{l=1}^{k} \int_\omega \mathcal{I}_L[u](\mu, z) \, \kappa_l(z) \, dz \, \kappa_l(y)$$

$$\text{with} \quad \mathcal{I}_L[u](\mu, z) \quad := \quad \sum_{I \in \mathfrak{I}} \mathcal{I}_{k_I}^I[u](\mu, z) = \sum_{I \in \mathfrak{I}} \sum_{j=1}^{k_I} \sigma_j^I(u(\mu, \cdot)) \vartheta_j^I(z).$$

Here $(\vartheta_l^j)_j$ is a basis of the localized spaces W_k^I, and $(\sigma_j^I)_j$ a corresponding nodal basis of the dual space, generated by the GEIM (cf. [1, 3]). Using the adaptive EPM, we project both the variational formulation and the range of the nonlinear operator onto reduced spaces. Those combine the full dimensional space in an identified dominant spatial direction and a reduction space or collateral basis space spanned by modal orthonormal basis functions in the transverse direction. Both the reduction and the collateral basis space are constructed in a highly nonlinear fashion by introducing a parametrized problem in the transverse direction and associated parametrized operator evaluations, and by applying reduced basis methods to select the bases from the corresponding snapshots as in the linear case. Rigorous a priori and a posteriori error estimators which do not require

additional regularity of the nonlinear operator are proven for the Empirical Projection Method and then used to derive a rigorous a posteriori error estimator for the resulting hierarchical model reduction approach. Numerical experiments for an elliptic nonlinear diffusion equation demonstrate a fast convergence of the proposed dimensionally reduced approximation to the solution of the full-dimensional problem. Run-time experiments verify a linear scaling of the reduction method in the number of degrees of freedom used for the computations in the dominant direction.

Finally, we also investigate the application of our HMR-RB approach in the presence of interfaces or strong gradients in the solution which are skewed with respect to the coordinate axes [6]. Usually, tensor-based model reduction procedures show bad convergence rates for such situations. The key ideas to recover the good approximation properties are the detection of the interface and a subsequent removal of the interface from the solution by choosing the determined interface as the lifting function of the Dirichlet boundary conditions. For prescribed interfaces we demonstrate in numerical experiments that the proposed procedure yields a significantly improved convergence behavior even in the case when we only consider an approximation of the interface.

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Solution of high-dimensional partial differential equations using tensor decompositions

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High-dimensional partial differential equations appear in many applications: electronic structure calculations, financial modelling, stochastic partial differential equations, chemical master equations and many others. The main problem with the solution of such equation is that it is not possible to represent the solution directly in the tensor-product basis due to the underlying exponential complexity. Different strategies can be used, which can be summarized in three different approaches:

- (Sparsity) We find a basis set $\varphi_1, \ldots$ such that the solution can be well approximated by a sparse linear combination of such functions.
- (Low rank) The main approximation anzatz in this strategy is the approximation of the solution in the sum-of-products (separable, canonical) format

$$f(x_1, \ldots, x_d) \approx \sum_{k=1}^{r} \prod_{s=1}^{d} f_s(x_s, \alpha)$$

- (Composition) This idea is not yet fully understood, but is used implicitly in many cases and may be traced back to Kolmogorov: the function is represented as a superposition of several simpler functions of fewer variables. For example, the *active subspaces* approach has the form

$$f(x) = g(Wx),$$

  where $x \in \mathbb{R}^d$ and W is a $k \times d$ matrix, and function g depends on k variables.

In this talk we focused on the ideas of low-rank approximation, which in two dimension reduces to the Hilbert-Schmidt decomposition and in the discrete case - to low-rank approximation of matrices, which can be computed using singular value decomposition (SVD).

It is now well understood, that for $d > 3$ the separated representation may not be the optimal choice due to several reasons. The computation of the minimal number of summands (r) is an NP-complete problem, and the best approximation with fixed rank may not exist. A powerful alternative to the canonical representation are the novel tensor formats, namely Hierarchical Tucker (H-Tucker) [3] and Tensor Train (TT) formats [2]. The TT-format has a very simple structure (it was known for many years in physics under the name *matrix product states*). Suppose we have chosen some discretization in each of the variables x_k and obtained

a virtual tensor $A(i_1, \ldots, i_d)$ of the coefficients. The tensor is said to be in the TT-format, if it can be represented as

$$A(i_1, \ldots, i_d) = G_1(i_1) \ldots G_d(i_d),$$

where $G_k(i_k)$ is a matrix of size $r_{k-1} \times r_k$ for each fixed i_k and $r_0 = r_d = 1$. This representation inherits many of the properties of the SVD, whereas in the worst case the number of parameters with respect to the canonical format is $\mathcal{O}(dnr^2)$, where r is the canonical rank (however, the canonical representation can be difficult to compute). So if we have an apriori knowledge that the tensor can be represented in the TT-format (or approximated well in this format) it is possible in the robust way to compute the approximation (for example, if we have access to the individual elements of the tensor)

In the PDE setting the function is given explicitly as a solution of a certain equation,

$$A(f) = g,$$

where $A(f)$ is some operator. We require that this equation can be reformulated as a minimization of a certain functional

$$F(f) = \min,$$

and define the solution as a minimizer of F over the set of all tensor of bounded ranks. This set $\mathcal{M}_r$ forms an embedded manifold in the space of all tensors, and we have a non-quadratic and non-convex optimization problem (even if the original functional was quadratic, as in the case of a linear operator A).

There are several technique for the minimization of functionals over low-rank tensor manifolds (and new ones are now in active development). The most straightforward way is the idea of *alternating least squares*. The low-rank structure is polylinear, so if we fix all cores except one, it gives a quadratic minimization problem which can be efficiently solved. This is a block Gauss-Seidel method. ALS has well-known problems: it is not adaptive in the sense that the ranks should be chosen in advance, and it may suffer from a bad convergence. A more sophisticated approaches directly use the "train" structure of the format by merging two adjacent cores into one:

$$W(i_k, i_{k+1}) = G_k(i_k)G_{k+1}(i_{k+1}),$$

optimizing over it and splitting the indices again via the SVD; this is the core of the *density matrix renormalization group* (DMRG) approach [5]. The problem is that we have to work with squared mode sizes and it may not be the case. Another approaches have been proposed as well.

A different idea is to use the geometry of the manifold and to optimize in the tangent space to the manifold; this requires a special machinery, but may lead to the quite efficient methods. The "best" method is yet to be found.

If the solution can be well-approximated in the TT-format, then there are several approaches how to find it efficiently. The main problem now lies in the selection of the parametrization in such a way that the solution can be represented as a low-rank tensor, which is not always the case: consider a two-dimensional front

going along the diagonal $x = y$. By making a variable change, $z = x - y, w = x + y$ we arrive at a low-rank function. The idea of active subspaces [4](linear transformation of coordinates) may be very useful in this case, but it is a special case of a more general anzatz of composition of simpler mappings); so, the question is, can we provide efficient numerical tools for finding such compositions?

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Schwarz Iterative Methods: New Developments

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(joint work with Michael Griebel, Weiqi Zhou)

The name Schwarz iterative methods has been coined in the late 1980ies as a theoretical framework for investigating domain decomposition and multilevel methods for PDEs. They are based on the notion of stable space splittings of finite- and infinite-dimensional Hilbert spaces, and in essence represent a more constructive version of the method of alternating projections, see [2] for details and historical remarks. In a nutshell, a stable space splitting of a Hilbert space H equipped with a coercive Hermitean form $a(\cdot, \cdot)$ is given by a finite or countably infinite family of Hilbert spaces H_i (each equipped with its own coercive Hermitean form $a_i(\cdot, \cdot)$) and a family of bounded linear operators $R_i : H_i \to H$ such that the energy norm $\|u\|_a^2 = a(u, u)$ and the splitting-related norm

$$\||u\||^2 = \inf_{u_i \in H_i : u = \sum_i R_i u_i} \sum_i a_i(u_i, u_i)$$

are equivalent on H. Infimum and supremum of the quotient $a(u, u)/\||u\||^2$ over H are denoted by $\lambda_{\min}$ and $\lambda_{\max}$, respectively, and their quotient $\kappa = \lambda_{\max}/\lambda_{\min}$ is called condition number of the splitting. These constants govern the convergence theory of iterative solvers for elliptic variational problems,

$$(1) \qquad \text{find } u \in H \text{ such that } \quad a(u, v) = (f, v)_H \qquad \forall\, v \in H,$$

based on the splitting. We consider only the multiplicative Schwarz iteration

$$(2) \qquad\qquad u^{j+1} = u^j + \omega_j R_i w_i^j,$$

where finding the update direction $w_i^j \in H_i$ involves solving the i-th subproblem

$$(3) \quad a_i(w_i^j, v_i) = a(u - u^j, R_i v_i) = (f, R_i v_i)_H - a(u^j, R_i v_i) \qquad \forall\, v_i \in H_i.$$

Which $i = i_j$ is chosen for the update matters, until recently only deterministic orderings have been considered. More recently, greedy and random orderings (and their combinations) received much attention, both due to the simplicity of their error analysis and their sometimes much better performance.

Here is a short account of our recent contributions to the convergence analysis of multiplicative Schwarz methods (references to the history of the subject and related (earlier and parallel) work by other authors, especially in optimization literature, can be found in the papers cited below). To correctly state them, we assume uniform boundedness of the operators R_j with respect to the involved energy norms: Let $\gamma_i \leq \Lambda < \infty$ for all i, where

$$\|R_i u_i\|_a \leq \gamma_i \|v_i\|_{a_i} \qquad \forall\, v_i \in H_i.$$

- The early results [1, 2, 3] concern finite splittings with J subproblems ($i \in \{1, 2, \ldots, J\}$) and cyclic orderings $i_j = j \pmod{J} + 1$. For properly chosen, fixed $\omega_j = \omega \in (0, 2/\Lambda)$, the convergence rate per cycle of (2) is upper-bounded by

(4) $$\|u - u^{\ell J}\|_a^2 \leq (1 - 1/(\log_2(4J)\kappa))^\ell \|u - u^0\|_a^2, \quad \ell \geq 1.$$

  The logarithmic dependence on J cannot be removed [1] in general. In the special case of the Kaczmarz method for solving the least-squares problem for linear systems $Ax = b$ with general $m \times n$ matrix A, where the associated subspace splitting involves m one-dimensional H_i, W. Zhou recently improved this bound by replacing the logarithmic dependence on $J = m$ by a logarithmic dependence on the rank $r \leq \min(m, n)$ of A, see [5, Theorem 4].

- Greedy orderings, where $i = i_j$ is chosen depending on the current residual, e.g., such that

$$\gamma_{i_j}^{-1} \|w_{i_j}^j\|_{a_{i_j}} \geq \beta \sup_i \gamma_i^{-1} \|w_i^j\|_{a_i}$$

  for some $0 < \beta \leq 1$, have been treated in [4] for finite splittings. The error reduction per single step in (2) with $\omega_j = \omega/\gamma_i$, $\omega \in (0, 2)$, is upper-bounded by

(5) $$\|u - u^{j+1}\|_a^2 \leq (1 - \beta^2 \omega(2 - \omega)\lambda_{\min}/(\gamma_1 + \ldots \gamma_J))\|u - u^j\|_a^2, \quad j \geq 0.$$

  A rough comparison with (4) indicates the superiority of this bound (e.g., there is no dependence on J).

- The recent interest in investigating random orderings was triggered by a 2009 paper by Strohmer and Vershynin on the convergence of a randomized Kaczmarz method. In [4], the exact counterpart of (5) (with $\beta = 1$) was established for the expected square energy norm error of a randomized iteration (2), where in the j-th step $i = i_j$ was chosen randomly and independently with probability $\pi_i = \gamma_i/(\gamma_1 + \ldots \gamma_J)$. Even though the a priori bounds for greedy and random orderings are identical, the numerical tests reported in [4] show that the greedy version leads to faster convergence in practice, and that combinations of randomization and greedy approaches

can remedy slow convergence of the cheaper randomized (2). A complementary estimate was proved in [5, Theorem 3] for a block version of (2) with random orderings.

- Finally, (2) can be executed also for infinite space splittings, where it turns from an iterative solver into an approximation algorithm for the solution u of (1) by finite linear combinations of $R_i u_i$. In [6], convergence of a modified version of (2) to the solution $u \in H$ of (1) for both greedy and random orderings has been established, together with quantitative convergence rates under additional assumptions for u. The greedy case is a direct generalization of earlier work by Temlyakov et al. on greedy algorithms in Hilbert spaces. We state the quantitative error bound for random orderings from [6, Theorem 1 b)] which seems to be new: Let $\pi_i > 0$, $\sum_{i=1}^{\infty} \pi_i = 1$, be an arbitrary discrete probability distribution, and assume u can be expanded as

$$u = \sum_{i=1}^{\infty} R_i u_i, \qquad \|u_i\|_{a_i} \leq M\pi_i, \quad i = 1, 2, \dots,$$

for some $M < \infty$. If in the j-th step $i = i_j$ is chosen randomly and independently with probability π_i then the modified version of (2)

$$u^{j+1} = \frac{j+1}{j+2} u^j + \omega_j R_i w_i^j,$$

where ω_j is chosen such that $\|u - u^{j+1}\|_a^2$ is minimized, converges in expectation at a guaranteed rate of

(6) $$E(\|u - u^j\|_a^2) \leq 2(\|u\|_a^2 + \Lambda^2 m^2)(j+1)^{-1}, \quad j \geq 0.$$

Simple examples show that faster convergence cannot be expected under these general assumptions. Further evaluation of the potential of greedy and randomized versions of the multiplicative Schwarz method for applications to adaptive algorithms, reduced order modeling, and regularization theory is underway.

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Regularization and Numerical Solution of Inverse Scattering Problems using Shearlet Frames

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(joint work with Gitta Kutyniok, Volker Mehrmann)

Scattering problems are concerned with the behavior of acoustic waves, radiation, or particles, which are transmitted in a medium and are scattered at inhomogeneities of this medium, so called scatterers. The associated inverse problems aim to determine characteristics of the inhomogeneities from the asymptotic behavior of such scattered waves. This problem appears in various flavors in different application areas, e.g. non-destructive testing, ultrasound tomography, and echolocation.

The numerical solution of these problems usually suffers from the ill-posedness of the problems. Hence a regularization is necessary. For this, some a priori knowledge of the solutions of the inverse problems shall be employed. Indeed we will model the inhomogeneities of the medium by functions from a special function class.

Modeling of the Scatterer: Typically, a scatterer is a natural structure, which distinguishes itself from the surrounding medium by a change in density. In the 2D setting, this inhomogeneity can be regarded as a curve with, presumably, certain regularity properties. The interior as well as the exterior of this curve is usually assumed to be homogenous.

In the area of imaging sciences, the class of *cartoon-like functions* [2] is frequently used as model for images governed by anisotropic structures such as edges.

A *cartoon-like function* is a function $f \in L^2(\mathbb{R}^2)$ such that there exists a domain $D \subset (0,1)^2$ such that ∂D can be parametrized by a C^2 curve and there exists $f_1, f_2 \in C^2(\mathbb{R}^2)$ such that $\mathrm{supp}\, f_1 \subset (0,1)^2$ and $f = f_1 + \chi_D f_2$.

This cartoon-like model is well-suited for many inverse scattering problems, where the discontinuity curve models the boundary of a homogeneous domain.

Directional Representation Systems: Having agreed on a model, one needs a suitably adapted representation system which ideally provides optimal approximation rates for cartoon-like functions in the sense of the decay of the L^2-error of best N-term approximation. Such a system can then be used for the regularization term of a Tikhonov functional.

In [1] shearlet systems were introduced, which almost achieve the optimal approximation rate [3]. The sparse approximation properties of shearlets were already used for different inverse problems such as separation of morphologically distinct components [4], or reconstruction from the Radon transform [7].

In view of this discussion, shearlet systems seem a good candidate as a regularizer for inverse scattering problems, and in fact this will be key to our approach.

Application to inverse Scattering Problems: We examine two conceptually different approaches to numerically solve inverse scattering problems. In particular, we study a method to directly tackle the nonlinear problem, as well as a linearization approach. As problem cases we focus on two inverse scattering problems, see e.g. [5], which are the *acoustic inverse scattering problem*, and the *inverse scattering problem of the Schrödinger equation*, for which we analyze the strategy to linearize the inverse scattering problem by means of the so-called Born approximation.

The *acoustic inverse scattering problem* aims to reconstruct a contrast function which encodes the scatterer by emitting an acoustic wave and measuring the scattered waves.

The minimization of a suitable Tikhonov functional is a common approach to directly solve this nonlinear inverse problem. In [6] a sparsity-based regularization term is introduced which uses the L^p-norm with p close to 1 directly on the function to-be-recovered. This regularization scheme is very successful when the object under consideration has small support.

Following our methodological concept, and assuming that cartoon-like functions are an appropriate model for the scatterer, we instead choose as regularization term the ℓ_p-norm of the associated shearlet coefficient sequence with p larger or equal to 1. We compare the two reconstruction approaches numerically and observe, that the regularization based on shearlets yields superior results over the L^p based regularization for cartoon-like scatterers see Figure 1.

In the second numerical approach we first introduce a linearization of an inverse scattering problem. The *inverse scattering problem of the Schrödinger equation* aims to determine a quantum mechanical scattering potential from measurements of *backscattering data*.

A prominent method to linearize the inverse scattering problem is by means of the Born approximation.

Modeling the scatterer by cartoon-like functions, shearlets can be used again as a regularizer, provided that the transition from the nonlinear towards the linear problem does not influence the fact that the solution belongs to the class of cartoon-like functions. It has been shown in [8, 9] that certain singularities of the scatterer can still be found in the solution of the associated linearized problem. However, all
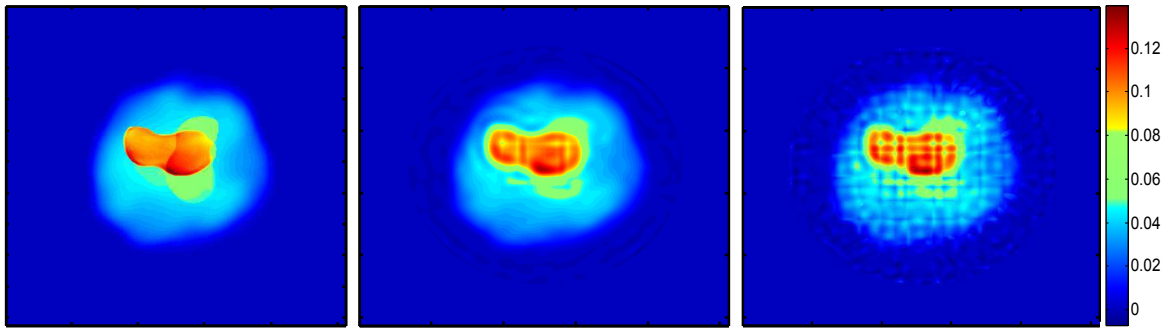
FIGURE 1. **Left:** Contrast function with overlapping discontinuity curves, **Middle:** Reconstruction using the shearlet regularization, **Right:** L^1 Tikhonov regularization.

these results require a global regularity of the scatterer to describe the regularity of the inverse Born approximation. On the other hand, in the case of cartoon-like functions we have strong local but poor global regularity and therefore the results of [8, 9] can not be applied to our situation. To provide a theoretical basis for the application of shearlet frames, we prove that indeed the Born approximation to the Schrödinger equation gives rise to a scattering problem that exhibits sharp edges in the solution of the linearized problem. In particular, we show that the cartoon model is almost invariant under the linearization process by proving the following results.

Theorem 1.1. [10] *Let $\epsilon > 0$, let $s \in \mathbb{N}, s \geq 2$, and let, for some $x_0 \in \mathbb{R}^2$, $f \in L^2(\mathbb{R}^2) \cap H^{s+\epsilon}(x_0)$ be compactly supported and real valued. Then the inverse Born approximation f_B satisfies $f_B \in H^s(x_0)$.*

Corollary 1.2. [10] *If $f_1, f_2 \in H^3(\mathbb{R}^2)$, $D \subset (0,1)^2$ and*

$$f = f_1 + \chi_D f_2,$$

then the inverse Born approximation from backscattering data can be written as

$$f_B = f_1^\delta + \chi_D f_2^\delta + v^\infty + h^\delta,$$

where $f_1^\delta, f_2^\delta \in C^2$, $v \in C^\infty$ and $h^\delta \in H^{\frac{1}{2}-\epsilon}$ for every $\epsilon > 0$ and h^δ is only supported on a δ neighborhood of ∂D.

Theorem 1.1 and Corollary 1.2 describe the regularity of the inverse Born approximation from backscattering data, such that common approaches using sparsity in the shearlet representation can be applied.

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Recent Developments in Entropy Viscosity

Bojan Popov

(joint work with Jean-Luc Guermond, Murtazo Nazarov, and Yong Yang)

We consider the case of a scalar conservation law

$$u_t + \nabla \cdot \mathbf{f}(u) = 0$$

with initial condition $u(\mathbf{x}, 0) = u^0(\mathbf{x})$ in the domain $(\mathbf{x}, t) \in \Omega \times \mathbb{R}_+$. The initial data u^0 is assumed to be bounded and the flux f is assumed to be Lipschitz continuous. We also assume that the boundary conditions are either periodic or the initial data is compactly supported. In the second case we are interested in the solution in a time interval [0; T] such that the domain of influence of u^0 over $[0, T]$ does not reach the boundary of Ω. The purpose of these assumptions is to avoid unnecessary technical difficulties induces by boundary conditions. Following the seminal work of Kruskov [8], it is now well understood that this problem has a unique entropy solution.

Maximum principle, entropy stability and convergence of viscosity approximations for scalar conservation laws have been established a long time ago. However, on discrete level the same questions sometimes are a lot harder and many results were proven on uniform/restricted meshes and only for first order schemes, see [9]. In this talk, we present two recent results in the case of scalar nonlinear conservation laws. First, we will derive a maximum principle preserving second order scheme based on entropy viscosity. The new method preserves maximum principle on a large variety of finite element spaces general unstructured meshes in arbitrary space dimensions, see [6] for all results. This is a joint work with Jean-Luc Guermond, Murtazo Nazarov, and Yong Yang. Second, we will present a general convergence framework for numerical methods for approximating scalar nonlinear conservation laws. Our approach is similar to the one of Bouchut and Perthame in [1] but we relax their arguments using techniques inspired by [3, 4]. As an application of this framework, we will give a convergence proof of a finite element based

numerical method with graph viscosity as a stabilization. This result is valid for a large variety of finite element spaces on general unstructured meshes in arbitrary space dimensions. The main result is as follows.

Theorem. [Guermond and P.] Let f be Lipschitz continuous, $u^0 \in BV(\Omega)$ and $\tilde{u}_h$ be the numerical solution generated by the graph viscosity stabilization. Then, under a standard CFL condition (see [7] for details) we have the following convergence result. If we have a BV bound on $u_h(\cdot, t)$, we have

$$\|u(\cdot, T) - u_h(\cdot, T)\|_{L^1(\Omega)} \leq c(T) h^{1/2} |u_0|_{BV(\Omega)}$$

Otherwise, we have

$$\|u(\cdot, T) - u_h(\cdot, T)\|_{L^1} \leq c(T) h^{1/4} |u_0|_*$$

where $|u_0|_*^2 := |u_0|_{BV(\Omega)} |\Omega| (|u_0|_{L^2(\Omega)}^2 - |\bar{u}_0|_{L^2(\Omega)}^2)$.

Note that, the the BV bound is well known in one space dimension but in the multidimensional case it is not know if it holds. Therefore, the general convergence result is with a rate of $\frac{1}{4}$ which is similar to the estimates in the finite volume setup, see for example [2, 5]. This is a joint work with Jean-Luc Guermond, see [7] for a complete description of the method and full details.

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Quarkonial frames and their connection to high-order schemes

Thorsten Raasch

(joint work with Stephan Dahlke, Peter Oswald)

We are concerned with quarkonial or subatomic decompositions of function spaces, as introduced by Triebel in [11, 12], and their connection to popular high-order ansatz systems, like conforming p- or hp-finite element frames. The design of quarkonial systems on a given domain $\Omega \subseteq \mathbb{R}^n$ merges spectral and multiscale approximation strategies, e.g., by locally enriching a given hierarchy of partitions of unity with polynomial or trigonometric frames [6, 11]. Similar approaches are well-known from the context of partition of unity methods [1, 5] and their multilevel variants [9], as well as from the theory of fusion frames [2]. So far, the concept of quarkonial decompositions has only rarely been exploited in numerical applications. We hope that the stability and approximation properties of quarkonial systems might be helpful, e.g., in the convergence analysis of adaptive hp-FEM and in solving preconditioning issues, similar to the impact of stable subspace splitting approaches [7] on the development of hierarchical preconditioners.

In the univariate, shift-invariant case, one may consider translated, dilated and locally enriched cardinal B-splines $\varphi := N_m(\cdot + \lfloor m/2 \rfloor)$ of order m, e.g.,

$$(1) \qquad \varphi_{p,j,k}(x) := \varphi_p(2^j x - k), \quad \varphi_p(x) := g_p(x)\varphi(x), \quad p, j \geq 0, \quad k \in \mathbb{Z},$$

where the enrichment functions g_p are globally or piecewise polynomial of degree p. We refer to Figure 1 for an example of monomial B-spline quarks. Similar to the

(a) φ_0 (b) φ_1 (c) φ_2 (d) φ_3
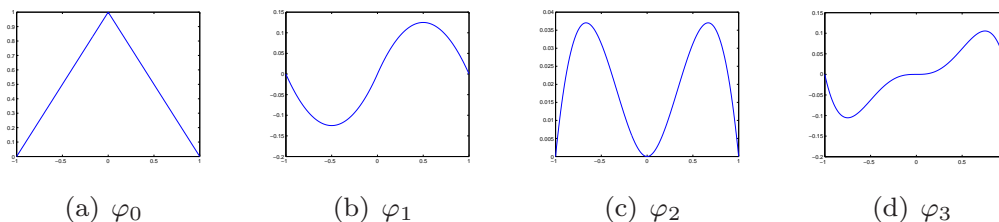
Figure 1. B-spline quarks φ_p with $m = 2$ and $g_p(x) = x^p$, $p \geq 0$.

case of multilevel finite element systems [7], one can show [6, 11] that appropriately weighted quarkonial systems $\Phi := \{w_{p,j,k}\varphi_{p,j,k} : p, j \geq 0, k \in \mathbb{Z}\}$ can be a frame for positive-order Sobolev and Besov spaces $B_q^s := B_q^s(L_q(\Omega))$, where $s, q > 0$, i.e., the span of Φ is dense in B_q^s and we have with frame constants $c_1, c_2 > 0$

$$(2) \qquad c_1\|f\|_{B_q^s}^q \leq \inf_{\mathbf{c}^\top \Phi = f} \sum_{p,j,k} |c_{p,j,k}|^q \leq c_2\|f\|_{B_q^s}^q, \quad f \in B_q^s.$$

The proof of (2) typically relies on approximation and regularity properties of

$$(3) \qquad V_{j,p} := \text{span}\{\varphi_{\mu,\nu,k} : 0 \leq \mu \leq p, 0 \leq \nu \leq j, k \in \mathbb{Z}\}, \quad p, j \geq 0.$$

In the original work [11], (2) was shown via Fourier techniques, assuming a C^∞ partition generator φ and weights $w_{p,j,k}$ with exponential decay in p. An inspection

of the proof from the viewpoint of stable subspace splittings [7] reveals that these assumptions can be relaxed considerably. The necessary approximation properties of $V_{j,p}$ can be ensured by direct estimates of Jackson type. Moreover, the weights $w_{p,j,k}$ only have to overcompensate the asymptotic behavior of $\|v\|_{B_q^s}/\|v\|_{L_q}$, $v \in V_{j,p}$, as $j, p \to \infty$, which can be measured by Bernstein inequalities like

$$(4) \qquad \|v\|_{B_q^s} \leq C B_{p,s} 2^{js} \|v\|_{L_q}, \quad v \in V_{j,p}.$$

In the case of partition generators φ of spline type and polynomial enrichment, the constants $B_{p,s}$ scale like $(1+p)^{2s}$, as $p \to \infty$, which is essentially due to the Markov inequality.. Based on these observations, we showed in [6] that p-algebraic decay $w_{p,j,k} \sim (1+p)^\beta 2^{-js}$, $\beta \in \mathbb{R}$, is sufficient to verify the frame property of Φ in B_q^s, with positive impact on the numerical conditioning of finite subsets of Φ.

Moreover, we would like to point to the close link between B-spline quarks and the Babuška-Shen basis [8] which is widely used in p-finite element methods,

$$(5) \quad \varphi_0(x) = \frac{x+1}{2}, \ \varphi_1(x) = \frac{1-x}{2}, \ \varphi_p(x) = \sqrt{p - \frac{1}{2}} \int_{-1}^{x} l_{p-1}(y)\,\mathrm{d}y, \quad p \geq 2.$$

Here l_p are the L_2-normalized Legendre polynomials on $(-1, 1)$, see also Figure 2. The set of *interior shape functions* ("bubble functions") $\{\varphi_p\}_{p \geq 2}$ is an $H_0^1(-1, 1)$-

(a) φ_0 (b) φ_1 (c) φ_2 (d) φ_3
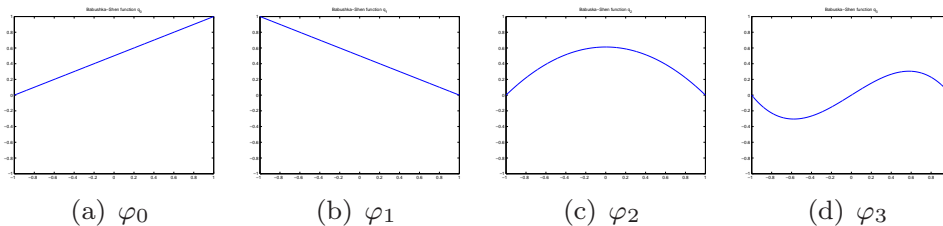
FIGURE 2. Babuška-Shen basis functions φ_p on $(-1, 1)$.

orthonormal basis. The *outer shape functions* φ_0 and φ_1 can be used to extend the bubble functions to a Riesz basis of $H^1(-1, 1)$ where exactly one basis function is nonzero at each of the endpoints ± 1. Therefore, by glueing together φ_0 and $\varphi_1(\cdot - 2)$ to the hat function $\varphi := N_2(\frac{\cdot+1}{2})$ on $(-1, 3)$, the system

$$\left\{\varphi_p(\cdot - 2k) : p \geq 2, k \in \mathbb{Z}\right\} \cup \left\{\varphi(\cdot - 2k) : k \in \mathbb{Z}\right\}$$

is a Riesz basis for $H^1(\mathbb{R})$. We have the factorization $\varphi_p(x) = g_p(x)\varphi(x)$ with continuous splines g_p, $g_p|_{(2k-1,2k+1)} \in \mathbb{P}_{p-1}$, $p \geq 2$. In other words, the Babuška-Shen system is indeed of quarkonial type, with enrichment by C^0 spline functions.

A natural question arises whether quarkonial frames can be made stable in L_q or even in negative-order Sobolev or Besov spaces. Similar to the case of wavelet systems [3], frame elements can be endowed by vanishing moment properties. In the univariate, shift-invariant case (1), one may take a wavelet mask $\{b_k\}_{k \in \mathbb{Z}} \subset \mathbb{R}$ with m discrete vanishing moments and define the *quarklets*

$$(6) \qquad \psi_p(x) := \sum_{k \in \mathbb{Z}} b_k \varphi_p(2x - k), \quad p \geq 0,$$

which then have m vanishing moments as well, regardless of p. We refer to Figure 3 for an example of linear, monomial B-spline quarklets based on the wavelet mask

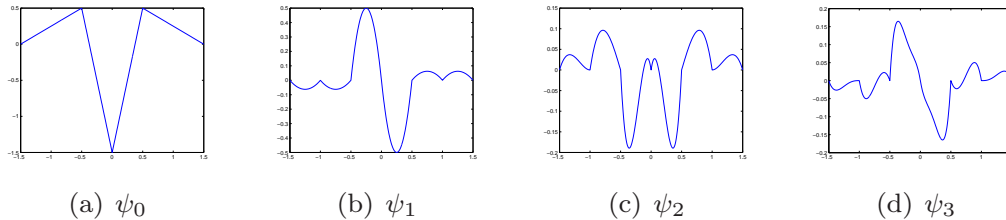(a) ψ_0 (b) ψ_1 (c) ψ_2 (d) ψ_3

FIGURE 3. Monomial B-spline quarklets for the CDF(2,2) wavelet mask.

from [4] with two vanishing moments. Thanks to the vanishing moment property, an appropriately weighted system

$$\{w_{p,k}\varphi_p(\cdot - k) : p \geq 0, k \in \mathbb{Z}\} \cup \{w_{p,j,k}\psi_p(2^j \cdot -k) : p, j \geq 0, k \in \mathbb{Z}\}$$

is indeed a frame for $L_q(\mathbb{R})$, where $1 < q < \infty$ and the weights $w_{p,k}$ and $w_{p,j,k}$ decay algebraically in p.

Current research focuses on the compressibility of differential and integral operators in quarklet coordinates, in the spirit of [10], aiming at the design of adaptive discretization schemes for operator equations with guaranteed exponential convergence.

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Hierarchical tensor representations and tensor networks

Reinhold Schneider

We consider tensor techniques for the numerical solution of high dimensional PDEs. Examples are Schrödinger, Fokker Planck and boundary value problems with uncertain parameters, which, by Wiener Ito chaos polynomials is turned into a parametric PDE setting. We highlight the second quantization for the fermonic multi-particle Schrödinger in a (discrete) Fock space setting.

Although several statements are valid in the infinite-dimensional setting, we often consider a fixed discretization of the operator equations. Let $\mathcal{V}_1, \ldots, \mathcal{V}_d$ Hilbert spaces, or $\mathcal{V}_i = L^2(\mathbb{R})$ or $V_0 = H_0^1(D)$. When we invoke a discretization $\mathcal{V}_i = \mathbb{R}^{n_i}$. An order-d tensor over these spaces is then given by any $U \in \otimes_{i=1}^{d} \mathcal{V}_i$. Let us interpret such tensors as multivariate functions

$$U : \mathcal{I}_1 \times \cdots \times \mathcal{I}_d \ \to \ \mathbb{R}, \ \underline{x} = (x_1, \ldots, x_d) \ \mapsto \ U(x_1, \ldots, x_d),$$

with index sets $\mathcal{I}_i$ to be either discrete, e.g. $\mathcal{I}_i = \{1, \ldots, n_i\}$ in case that $\mathcal{V}_i = \mathbb{R}^{n_i}$, or continuous, e.g. $\mathcal{I}_i = \mathbb{R}$ in the case that, for instance, $\mathcal{V}_i = L^2(\mathbb{R})$. Such tensors play an important role in the description of many complex systems. At the latest after a discretization, tensor quantities take on n^d different values $(x_1, \ldots, x_d)$, assuming $n = \max\{n_i; i = 1, \ldots, d\}$. The complexity $\mathcal{O}(n^d)$ grows at least exponential in d, known as the curse of dimensionality. Even if n is small. e.g. $n = 2$, for large d, e.g $d = 300$ it is impossible to handle the full tensor. Tensor product approximation aims to approximate these tensors by sum of products of univariate functions. Such a multi-linear representation may reduce the number of parameters, from n^d to $\mathcal{O}(nd)$ with a constant depending on the number of terms in the sum. This seems to be appealing, nevertheless there are fundamental problems with this rather simple and canonical idea. The parametrization of the canonical form is no longer linear and does also destroy an original convexity of the problem. Instead of a *curse of dimensions* there appears a *curse of non-linearity* or *curse of non-convexity.*

The *Hierarchical Tucker tensor format (HT)* (Hackbusch-Kühn) and *Tensor Trains (TT)* (Tyrtyshnikov-Oseledets), introduced recently offering stable and robust approximation by a low order cost, see [3]. The representation of these tensors can be described by *tensor networks* with tree structure, already known in quantum physics. We would like to demonstrate that with this approach we can overcome most of the obstructions mentioned above.

We consider mainly TT tensors, known as matrix product states in physics, as a prototype example. The appearing component tensors are of low order, e.g. for binary trees they are of order 3, independent of the original order d. For example, the TT format provides a special case of hierarchical tensor formats. Here $U(x_1, \ldots, x_d)$ is represented in terms of d component matrices $U_1(x_1), U_2(x_2), \ldots, U_d(x_d)$. A value of U at point $(x_1, \ldots, x_d)$ can be computed by

$$U(x_1, \ldots, x_d) = U_1(x_1)U_2(x_2) \cdots U_d(x_d) \ ,$$

or explicitly

$$= \sum_{k_1=1}^{r_1} \dots \sum_{k_{d-1}=1}^{r_{d-1}} U_1(x_1, k_1) U_2(k_1, x_2, k_2) \dots U_{d-1}(k_{d-2}, x_{d-1}, k_{d-1}) U_d(k_{d-1}, x_d).$$

The numbers r_i, define the rank numbers of the TT decomposition or the rank vector $\underline{r} = (r_1, \dots, r_{d-1})$ that mainly governs the complexity of the representation. Letting $r = \max r_i$, storage of the TT decomposition is $\mathcal{O}(r^2 nd)$ and is thus formally free from the curse of dimensionality.

The important observation is that the hierarchical tensors inherit major properties from low rank factorization of matrices. In other words one applies matrix analysis to treat the tensor case. Given a partition tree, then the optimal ranks are defined by the rank of the corresponding *matricisation* or *matrix unfolding* $\mathbf{A}_t$, see [3]. This observations holds for most operators, can be assumed for right hand sides. Even more operation like Summation, application of operators to tensors can be performed in this format. We are looking for those solutions which can be approximated sufficiently accurate in the present form.

The set of tensors of prescribed rank is neither a linear space nor convex. It has been shown, partly by the author [7], that given a tree, the set hierarchical tensor of optimal rank forms smooth (open) manifolds $\mathcal{M}_{\underline{r}}$. For numerical computations, we cast the computation of an approximate solution into an optimization problems constraint to this manifold. In particular, for approximation by elements from this highly nonlinear manifold , we apply the well known *Dirac Frenkel variational principle*, see e.g [5],

$$\dot{U}(t) = \operatorname{argmin}\{\|V - (-\mathcal{A} + \mathcal{B})\Psi(t) + f(t)\| : V \in \mathcal{T}_U\} .$$

By straightforward manipulations, this provides the equations of motion in weak form,

$$\langle \dot{U} + (\mathcal{A} - \mathcal{B})\Psi - f, V \rangle , \ \forall V \in \mathcal{T}_U, U(0) = \Psi_0 \in \mathcal{M}_{\underline{r}} .$$

In [6], we have analysed the (open) manifold of such tensors and its projection onto the tangent space $\mathcal{T}_U$ at point $U(t) \in \mathcal{M}_{\underline{r}}$. First convergence estimates in L_2 has been derived, providing quasi-optimal converge local in time, i.e. for $0 \leq t \leq T, T$ sufficiently small. The Dirac Frenkel principle is a Galerkin approximation, where the differential equation has to be satisfied in weak form on the tangent space $\mathcal{T}_U$ at each time $U(t)$. The Lojasiewich inequality allows to prove convergence of the Riemannian gradient iteration [9] to stationary points, only.

Therefore there remains still a curse of non-convexity. In $\ell_2(\mathcal{I})$ a quasi-optimal approximation can be found from the singular value decomposition of these matrices, the HSVD, originally derived by Vidal, and afterwards independently by Oseledets and Grasedyck, see e.g. [3, 4]. This can be used to construct (adaptive) iterative methods by hard (Dahmen & Bachmayr) and soft thresholding operations [1]. These methods are shown to converge to the exact solution still retaining quasi-optimal approximations bounds.

However the analysis of the these bounds is still fairly open. Best N-term approximation results has been derived from this observation in a recent paper

[8]. Let $\mathbf{A}_t = \mathbf{U}^T \Sigma \mathbf{V}$, (SVD) $\Sigma = \text{diag}(\sigma_i)$ be the singular value decomposition of the unfolding at a node t in the tree. For $0 < p \le 2$, we refer to the the nuclear norm $p = 1$ and Schatten class quasi-norms $\|\mathbf{A}_t\|_{*,p} := \left(\sum_i \sigma_{t,i}^p \right)^{\frac{1}{p}}$. Assuming that $\|\mathbf{A}\|_{*,p} := \max_t \|\mathbf{A}_t\|_{*,p} < \infty$, and $|\underline{r}| := \max\{r_t\}$. Then, by Stechkins lemma it follow that the best rank r_t, for $s := \frac{1}{p} - \frac{1}{2}$, best N-term approximation by rank $\underline{r}$ can be estimated by

$$\inf_{\{V:\text{ranks of } V \le \underline{r}\}} \|U - V\|_2 \lesssim C(d)|\underline{r}|^{-s}\|\mathbf{A}\|_{*,p}$$

with a prefactor $C(d) \lesssim \sqrt{d}$, scaling mildly with d. Notice that the complexity scales $\sharp U \lesssim d|\underline{r}|^3$ (HT), ($\lesssim nd|\underline{r}|^2$ (TT)). It has been shown [8] that *mixed Sobolev spaces* are embedded in these classes. Perhaps, due to the complexity scaling $\mathcal{O}(r^3)$, these results are only suboptimal for these classes.

A comparison of different formats is summarized in the following table

	canonical	Tucker	HT
complexity	$\mathcal{O}(ndr)$	$\mathcal{O}(r^d + ndr)$	$\mathcal{O}(ndr + dr^3)$
			TT- $\mathcal{O}(ndr^2)$
	$++$	$-$	$+$
rank	no	defined	defined
	$r_c \ge$	r_T	$r_T \le r_{HT} \le r_c$
(weak) closedness	no	yes	yes
ALS (1site DMRG)	yes - but slow	yes	yes
H (O) SVD	no	yes	yes
embedded manifold	no	yes	yes
Dirac Frenkel	no	yes	yes
algebraic var. $\mathcal{M}_{\le \mathbf{r}}$	no	yes	yes
recovery	??	yes	yes
quasi best approx.	no	yes	yes
best approx.	no	exist	exist
		but NP hard	but NP hard

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High Order, Quasi Monte-Carlo Petrov-Galerkin Discretization for countably-parametric operator equations

CHRISTOPH SCHWAB

(joint work with J. Dick, F.Y. Kuo, T. LeGia, I.H. Sloan)

We construct quasi-Monte Carlo methods to approximate the expected values of linear functionals of Petrov-Galerkin discretizations of parametric operator equations which depend on a possibly infinite sequence of parameters.

Such problems arise among others in the numerical solution and in computational uncertainty quantification for differential and integral equations with so-called "distributed random input data" (random field inputs) cp. eg. [1, 2, 3]. Affine-parametric, infinite-dimensional deterministic operator equations result from uncertainty parametrization by, eg., Karhunen-Loeve expansion of the random input data. We analyze the regularity of the corresponding parametric solutions with respect to the parameters in terms of the rate of decay of the fluctuations of the input field. Based on analytic continuation or on a real-variable, "bootstrapping" argument, we show in [8] that if $p \in (0,1]$ denotes the "summability exponent" corresponding to the fluctuations in affine-parametric families of operators, then deterministic "interlaced polynomial lattice rules" of order $\alpha = \lfloor 1/p \rfloor + 1$ in s dimensions with N points can be constructed using a fast component-by-component algorithm, in $\mathcal{O}(\alpha\, s\, N \log N + \alpha^2\, s^2 N)$ operations, to achieve a convergence rate of $\mathcal{O}(N^{-1/p})$, with the implied constant independent of s. This dimension-independent convergence rate is superior to the rate $\mathcal{O}(N^{-1/p+1/2})$ for the range $2/3 \leq p \leq 1$, with implied constants that are independent of the dimension s, recently established in [12] for randomly shifted lattice quadrature rules under analogous assumptions. The Quasi Monte-Carlo quadrature error analysis in [6, 4, 8] is developed for affine-parametric operator equations with bounded parameter domains. Extensions to holomorphic-parametric operators are in [6], with regularity results from [5]. Partial extensions of the theory for first order Quasi Monte-Carlo quadratures to elliptic PDEs with log-gaussian random inputs are provided in [10].

Multi-Level versions of the presented algorithms were first analyzed in the affine-parametric, uniform case for first order lattice rules in [11] where it was shown the judicious combination of mesh-dependent Quasi Monte-Carlo quadratures can provide substantial gains in complexity, subject to suitable regularity.

The Quasi Monte-Carlo quadrature error analysis is based on a novel, non-standard Banach space setting for the error analysis of Quasi Monte-Carlo proposed recently in [14] and on "smoothness-driven product and order dependent (SPOD)" weights proposed for higher order Quasi Monte-Carlo integration in [8].

A new, so-called fast CBC construction (quadratically scaling in the dimension s of the integration domain) proposed in [8] shows that the asymptotic error bounds are attained already for moderate dimensions $s \simeq 10, ..., 1000$, and for as few as $N = \mathcal{O}(10^2)$ lattice points.

The implementation of the finite field algorithms in [9] for the fast Component-by-Component construction of the generating vectors, based on original ideas of [13] of the lattice rule is shown to exhibit the asymptotic complexity bounds already from dimension $s = 10$ upwards.

Detailed numerical experiments in [9] show, in a number of countably-parametric model elliptic PDE integration problems, the predicted, dimension-independent convergence rate $\mathcal{O}(N^{-1/p})$ where the exponent $1/p$ depends only on the sparsity parameter $p \in (0, 1]$ of the distributed, parametric input.

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Discontinuous Galerkin finite element approximation of Hamilton–Jacobi–Bellman equations with Cordes coefficients

IAIN SMEARS

(joint work with Endre Süli)

We propose a novel approach to the numerical analysis of fully nonlinear second-order elliptic and parabolic Hamilton–Jacobi–Bellman (HJB) partial differential equations. For example, consider the Dirichlet boundary value problem

$$
(1) \qquad
\begin{aligned}
\sup_{\alpha \in \Lambda} \left[L^\alpha u - f^\alpha \right] &= 0 \quad \text{in } \Omega, \\
u &= 0 \quad \text{on } \partial\Omega,
\end{aligned}
$$

where Ω is a convex domain in $\mathbb{R}^d$, $d \geq 2$, Λ is a compact metric space, and the nondivergence form elliptic operators L^α, $\alpha \in \Lambda$, are defined by

$$
(2) \qquad L^\alpha v = a^\alpha \colon D^2 v + b^\alpha \cdot \nabla v - c^\alpha \, v.
$$

These equations arise from models for the optimal control of stochastic processes. Stochastic control problems encompass a diverse set of applications from engineering, economics and finance, including examples such as industrial production planning, option pricing, and portfolio investment. The study of HJB equations thus continues to be an active research area.

Furthermore, HJB equations constitute an important example of fully nonlinear second-order elliptic equations. The theory of viscosity solutions provides a general solution theory for this family of equations, and its relevance to HJB equations was among the main motivations for developing the theory [3, 8, 9]. Recall that the regularity theory centered around the celebrated Evans–Krylov Theorem establishes interior $C^{2,\beta}$-regularity of the viscosity solution of fully nonlinear uniformly elliptic equations with convex nonlinearities [1, 4, 7]; this applies to (1) provided that the diffusion coefficients a^α satisfy the usual uniform ellipticity condition.

We summarise here the contributions of our papers [11, 12, 13, 14] on hp-version discontinuous Galerkin finite element methods (DGFEM) for uniformly elliptic and uniformly parabolic HJB equations with Cordes coefficients. In order to focus the

discussion, we concentrate on elliptic HJB equations of the form (1), although we note that we have extended our method and analysis to parabolic equations in [14].

The Cordes condition is an algebraic assumption on the coefficients of the equation, and it encompasses a large range of possibly strongly anisotropic applications. The Cordes condition requires that there exist a $\lambda > 0$ and an $\varepsilon \in (0, 1]$ such that, for each $\alpha \in \Lambda$,

$$(3) \qquad \frac{|a^\alpha|^2 + |b^\alpha|^2/2\lambda + (c^\alpha/\lambda)^2}{(\operatorname{Tr} a^\alpha + c^\alpha/\lambda)^2} \leq \frac{1}{d+\varepsilon} \quad \text{in } \overline{\Omega},$$

where $|\cdot|$ represents the Euclidian norm for vectors and the Frobenius norm for matrices.

The motivation for applying the Cordes condition to HJB equations stems from the literature on nondivergence form PDEs, for which it is well-known that uniform ellipticity alone is generally not sufficient to guarantee well-posedness [2, 5, 10] in more than two dimensions. Moreover, it is also known that HJB equations are naturally related to nondivergence form PDE through the fact that linearisations of HJB operators are in nondivergence form.

Although the PDE (1) does not admit a weak formulation, it does admit an equivalent formulation as a variational problem $A(u; v) = 0$ for all $v \in H^2(\Omega) \cap H_0^1(\Omega)$, with A a nonlinear form defined by

$$(4) \qquad A(u; v) := \int_\Omega F_\gamma[u] \, L_\lambda v \, \mathrm{d}x, \quad L_\lambda v := \Delta v - \lambda v,$$

where F_γ is a renormalisation of the nonlinear operator of (1). The Cordes condition leads to a key stability result in the form of a *strong monotonicity bound*:

$$(5) \qquad \|u - v\|_{H^2(\Omega)}^2 \lesssim A(u; u - v) - A(v; u - v) \quad \forall u, v \in H^2(\Omega) \cap H_0^1(\Omega).$$

This enables the application the Browder–Minty theorem to show existence and uniquness of a solution $u \in H^2(\Omega) \cap H_0^1(\Omega)$ of (1).

In [13], we construct a discrete analogue A_h of the nonlinear form A, leading to the numerical scheme of finding $u_h \in V_{h,\mathbf{p}}$ such that $A_h(u_h; v_h) = 0$ for all $v_h \in V_{h,\mathbf{p}}$, where $V_{h,\mathbf{p}}$ is the DG finite element space. The method is *consistent* in the usual sense of Galerkin type methods. The main challenge however is to achieve *stability* through a discrete analogue of the strong monotonicity bound (5). This is achieved by relating the residual of the equation to terms measuring the lack of H^2-conformity of the numerical solution.

The stability and consistency properties enable the derivation of error bounds. In the special case of quasi-uniform meshes of size h and quasi-uniform polynomial degrees p, provided that $u \in H^s(\Omega; \mathcal{T}_h)$, $s > 5/2$, the error bound is of the form

$$(6) \qquad \|u - u_h\|_h \lesssim \frac{h^{\min(p+1,s)-2}}{p^{s-5/2}} \|u\|_{H^s(\Omega)}.$$

where the norm $\|\cdot\|_h$ is the broken H^2-norm. Importantly, these bounds do not depend on the anisotropy of the problem, except through the constants appearing in the Cordes condition. Therefore, our method is able to exploit any available

regularity of the solution and yield high-order accuracy for strongly anisotropic problems, as shown by our numerical experiments in [13]. If hp-refinement is employed, it is even possible to achieve exponential convergence rates of the form $\|u - u_h\|_h \simeq \exp(-c \sqrt[3]{\mathrm{DoF}})$, where DoF is the number of degrees of freedom, even for rough solutions with singularities in parts of the domain.

In practical terms, the implementation and algorithmic aspects of the method, such as memory costs, are the same as those of usual DGFEM for elliptic problems. In [11, 13], it is shown that a combination of a semismooth Newton method and nonoverlapping domain decomposition preconditioners allows the fast and efficient solution of the discrete nonlinear problem.

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A perturbation-method-based post-processing of planewave approximations of nonlinear Schrödinger equations

Benjamin Stamm

(joint work with Eric Cancès, Geneviève Dusson, Yvon Maday, Martin Vohralìk)

In this talk, the Gross-Pitaevskii equation serves as a toy problem for methods arising from the Density-Functional-Theory (DFT). Indeed, the following theory can be generalized to some planewave approximations of DFT-models. We use this simpler problem to illustrate the technical key-arguments of the theory which are identical to those for the DFT Kohn-Sham LDA-models. We note also that the Gross-Pitaevskii equation plays also an important role in the simulation of particle-systems consisting of Bosons.

We consider the minimization problem

$$\inf \left\{ E(v) \ \middle| \ v \in H^1_\#(\Omega), \ \|v\|_{L^2} = 1 \right\},$$

where the energy functional is given by

$$E(v) = \int_\Omega \left[|\nabla v|^2 + V v^2 + \tfrac{1}{4} v^4 \right],$$

for some real-valued potential $V \in H^s_\#(\Omega)$, $s > d/2$. Then, there exists a unique real-valued positive minimizer $u \in H^2_\#(\Omega)$. The Euler-Lagrange equations are then given by: find $\lambda \in \mathbb{R}$, $u \in H^1_\#(\Omega)$ such that $\|u\|_{L^2} = 1$ and

$$(1) \qquad\qquad -\Delta u + V u + u^3 = \lambda u, \qquad \text{in } \Omega.$$

We consider the ground state so that λ denotes the lowest eigenvalue of the mean-field operator $H_u = -\Delta + V + u^2$ and plays the role of the Lagrange multiplier associated to the constraint $\|v\|_{L^2} = 1$. Let us denote by X_N the space spanned by planewaves up to a certain wavenumber $|k| < N$ and $\Pi_N : H^s_\#(\Omega) \to X_N$ the orthogonal projection onto X_N. The planewave approximation to (1) is then given: find $\lambda_N \in \mathbb{R}$, $u_N \in X_N$ such that $\|u_N\|_{L^2} = 1$ and

$$(2) \qquad\qquad -\Delta u_N + \Pi_N \big[V + |u_N|^2 \big] u_N = \lambda_N u_N, \qquad \text{in } \Omega.$$

Again, λ_N is the lowest eigenvalue of the discrete Hamiltonian $H_N = -\Delta + \Pi_N \big[V + |u_N|^2 \big] \Pi_N$.

In this talk, we presented the key-arguments of a post-processing upon u_N defined by

$$(3) \qquad\qquad \tilde{u}_N := u_N - (-\Delta - \lambda_N)^{-1} r_N,$$

where r_N is the residual defined by

$$r_N := -\Delta u_N + V u_N + |u_N|^2 u_N - \lambda_N u_N \in X_N^\perp.$$

The second term of the right-hand side of (3) denotes the leading term of the first order correction of an underlying perturbation argument. Indeed, we consider the exact solution (λ, u) as a perturbation of the discrete planewave approximation

(λ_N, u_N) and apply Kato's perturbation theory in order to show that the Rayleigh-Schrödinger series in the perturbed system

$$\Big(H_N + \beta(H_u - H_N)\Big)\Big(\sum_j \beta^j u_N^{(j)}\Big) = \Big(\sum_j \beta^j \lambda_N^{(j)}\Big)\Big(\sum_j \beta^j u_N^{(j)}\Big),$$

converge for $\beta = 1$ if N is sufficiently large.

From a practical viewpoint, we observe that $r_N \in X_N^\perp$ so that we need to compute the residual in a larger space $X_{N_{res}}$. The most expensive part in terms of operations is to compute $Vu_N + |u_N|^2 u_N$ which requires applying twice a Fast Fourier Transform (FFT) on a larger grid based on $X_{N_{res}}$. Finally we presented the main theorem.

Theorem. [1] *There exists a positive real constant C, independent of N and s, such that for all N sufficiently large, there holds*

$$\|u - \tilde{u}_N\|_{H_\#^1} \leq CN^{-2}\|u - u_N\|_{H_\#^1} + C\|u - u_N\|_{H_\#^{-1}}.$$

In combination with *a priori* results developed in [2] we obtain that

$$\|u - \tilde{u}_N\|_{H_\#^1} \leq CN^{-(s+3)},$$

in the asymptotic limit. We ended the presentation by showing some numerical example in the case of DFT Kohn-Sham LDA-models showing an decrease in the error already from a pre-asymptotic stage on.

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From Perfect Derivatives to Conservative Differences
EITAN TADMOR

Entropy stability plays an important role in the dynamics of nonlinear systems of conservation laws and related convection-diffusion equations. What about the corresponding numerical framework? we present a general theory of entropy stability for difference approximations of such nonlinear equations. We demonstrate this approach with a host of first- and second-order accurate schemes ranging from scalar examples to Euler and Navier-Stokes equations and we conclude with recent computations of entropy measure valued solutions based on the class of arbitrarily high-order accurate and entropy stable TeCNO schemes.

Entropy-conservative and entropy-stable schemes. We consider semi-discrete conservative schemes of the form

$$(1) \qquad \frac{d}{dt}\mathbf{u}_\nu(t) = -\frac{1}{\Delta x_\nu}\Big[\mathbf{f}_{\nu+\frac{1}{2}} - \mathbf{f}_{\nu-\frac{1}{2}}\Big],$$

serving as consistent approximations to systems of conservation laws $\mathbf{u}_t + \mathbf{f}(\mathbf{u})_x = 0$. Here, $\mathbf{u}_\nu(t)$ denotes the discrete solution along the grid line (x_ν, t) with $\Delta x_\nu := \frac{1}{2}(x_{\nu+1} - x_{\nu-1})$ being the variable meshsize, and $\mathbf{f}_{\nu+\frac{1}{2}}$ being the Lipschitz-continuous numerical flux consistent with the differential flux, $\mathbf{f}_{\nu+\frac{1}{2}} = \mathbf{f}(\mathbf{u}_{\nu-p+1}, \ldots, \mathbf{u}_{\nu+p})$. The numerical flux, $\mathbf{f}(\cdot, \cdot, \ldots, \cdot)$, involves a stencil of $2p$ neighboring grid values.

We are concerned here with the question of *entropy stability* of such schemes. Let (η, F) be an entropy pair associated with the system $\mathbf{u}_t + \mathbf{f}(\mathbf{u})_x = 0$. We ask whether the scheme (1) is *entropy-stable* with respect to such a pair, in the sense of satisfying a discrete entropy *inequality* $\frac{d}{dt}\eta(\mathbf{u}_\nu(t)) + \frac{1}{\Delta x_\nu}\Big[F_{\nu+\frac{1}{2}} - F_{\nu-\frac{1}{2}}\Big] \leq 0$, analogous to the entropy inequality $\eta(\mathbf{u})_t + F(\mathbf{u})_x \leq 0$. Here, $F_{\nu+\frac{1}{2}} = F(\mathbf{u}_{\nu-p+1}, \ldots, \mathbf{u}_{\nu+p})$ is a consistent numerical entropy flux, $F(\mathbf{u}, \mathbf{u}, \ldots, \mathbf{u}) = F(\mathbf{u})$. In the particular case that equality holds, we say that the scheme (1) is *entropy-conservative*.

The answer to this question of entropy stability provided in [7] consists of two main ingredients: (i) the use of the entropy variables and (ii) the comparison with appropriate *entropy-conservative* schemes. We conclude this section with a brief overview. Define the entropy variables $\mathbf{v} := \eta'(\mathbf{u}) \leftrightarrow \mathbf{u}$. Making the changes of variables $\mathbf{u}_\nu = \mathbf{u}(\mathbf{v}_\nu)$, the scheme (1) recasts into the equivalent form

$$(2) \qquad \frac{d}{dt}\mathbf{u}_\nu(t) = -\frac{1}{\Delta x_\nu}\Big[\mathbf{f}_{\nu+\frac{1}{2}} - \mathbf{f}_{\nu-\frac{1}{2}}\Big], \quad \mathbf{u}_\nu(t) = \mathbf{u}(\mathbf{v}_\nu(t)),$$

with a numerical flux $\mathbf{f}_{\nu+\frac{1}{2}} = \mathbf{f}(\mathbf{v}_{\nu-p+1}, \ldots, \mathbf{v}_{\nu+p}) := \mathbf{f}(\mathbf{u}(\mathbf{v}_{\nu-p+1}), \ldots, \mathbf{u}(\mathbf{v}_{\nu+p}))$, consistent with the differential flux, $\mathbf{f}(\mathbf{u}(\mathbf{v}))$. We ask whether (2) is *entropy conservative*, that is — given an entropy η, find a numerical flux $\mathbf{f}^*_{\nu+\frac{1}{2}}$ such that

$$\frac{d}{dt}\mathbf{u}_\nu(t) + \frac{\mathbf{f}^*_{\nu+\frac{1}{2}} - \mathbf{f}^*_{\nu-\frac{1}{2}}}{\Delta x} = 0 \stackrel{?}{\implies} \frac{d}{dt}\eta(\mathbf{u}_\nu(t)) + \frac{F_{\nu+\frac{1}{2}} - F_{\nu-\frac{1}{2}}}{\Delta x} = 0.$$

In other words, we are looking for a recipe of entropy conservative fluxes $\mathbf{f}^*_{\nu+\frac{1}{2}}$ such that $\big\langle \eta'(\mathbf{u}_\nu)\,,\,\mathbf{f}^*_{\nu+\frac{1}{2}} - \mathbf{f}^*_{\nu-\frac{1}{2}}\big\rangle \stackrel{?}{\longrightarrow} F_{\nu+\frac{1}{2}} - F_{\nu-\frac{1}{2}}$, which in turn would imply the entropy conservation $\sum_\nu \eta(\mathbf{u}_\nu(t))\Delta x = \sum_\nu \eta(\mathbf{u}_\nu(0))\Delta x$. Expressed in terms of the entropy variables, the entropy conservation requirement $\big\langle \eta'(\mathbf{u}_\nu)\,,\,\mathbf{f}^*_{\nu+\frac{1}{2}} - \mathbf{f}^*_{\nu-\frac{1}{2}}\big\rangle = F_{\nu+\frac{1}{2}} - F_{\nu-\frac{1}{2}}$, reads

$$\overbrace{\big\langle \mathbf{v}_\nu\,,\,\mathbf{f}^*_{\nu+\frac{1}{2}} - \mathbf{f}^*_{\nu-\frac{1}{2}}\big\rangle}^{\text{perfect difference}} \quad \text{if and only if} \quad \overbrace{\big\langle \mathbf{v}_{\nu+1} - \mathbf{v}_\nu\,,\,\mathbf{f}^*_{\nu+\frac{1}{2}}\big\rangle}^{\text{perfect difference}}:$$

and we conclude that $\mathbf{f}^*_{\nu+\frac{1}{2}}$ is entropy conservative if $\big\langle \mathbf{v}_{\nu+1} - \mathbf{v}_\nu, \mathbf{f}^*_{\nu+\frac{1}{2}}\big\rangle = \psi(\mathbf{v}_{\nu+1}) - \psi(\mathbf{v}_\nu)$, where $\psi(\mathbf{v})$ is the entropy flux potential, $\psi(\mathbf{v}) := \big\langle \mathbf{v}\,,\,\mathbf{f}(\mathbf{v})\big\rangle - F(\mathbf{u}(\mathbf{v}))$. This brings us to the following.

Theorem 1.1 (Tadmor, 1987 [7]). *The conservative scheme (2) is entropy-stable if* $\left\langle \Delta \mathbf{v}_{\nu+\frac{1}{2}}, \mathbf{f}_{\nu+\frac{1}{2}} \right\rangle \leq \Delta \psi_{\nu+\frac{1}{2}}$, *and entropy-conservative if* $\left\langle \Delta \mathbf{v}_{\nu+\frac{1}{2}}, \mathbf{f}_{\nu+\frac{1}{2}}^* \right\rangle = \Delta \psi_{\nu+\frac{1}{2}}$.

Scalar examples. We begin by noting that in the scalar case, $\eta'(u)f(u)_x = (\ldots)_x$ — all convex η's are entropy functions, and the corresponding entropy conservative fluxes are given by $f_{\nu+\frac{1}{2}}^* = \dfrac{\psi(v_{\nu+1}) - \psi(v_\nu)}{v_{\nu+1} - v_\nu}$.

Example 2 (Burgers' equation). Consider the inviscid Burgers' equation $u_t + (\frac{1}{2}u^2)_x = 0$ augmented with the quadratic entropy $(\frac{1}{2}u^2)_t + (\frac{1}{3}u^3)_x = 0$. The entropy variable $v(u) = u$ and entropy potential $\psi(v) := vf - F = \frac{1}{6}u^3$ yield the entropy conservative flux which is the "$\frac{1}{3}$-rule"

$$\frac{d}{dt}u_\nu(t) = -\frac{2}{3}\left[\frac{u_{\nu+1}^2 - u_{\nu-1}^2}{4\Delta x}\right] - \frac{1}{3}\left[u_\nu \frac{u_{\nu+1} - u_{\nu-1}}{2\Delta x}\right] \rightsquigarrow \sum u_\nu^2(t)\Delta x = Const.$$

The point we make here, is that the same derivation applies to any scalar conservation law and any convex entropy. Consider the *linear* case $f(u) = u$ with the quartic entropy $\eta(u) = u^4/4$. Here, $v = u^3$ and $\psi(u) = \frac{3}{4}u^4$ yield the second-order conservative flux $u_{\nu+\frac{1}{2}}^* = \dfrac{\Delta \psi}{\Delta u} = \dfrac{3}{4}\dfrac{u_{\nu+1}^4 - u_\nu^4}{u_{\nu+1}^3 - u_\nu^3}$. Observe that this is a second-order accurate difference $u_{\nu+\frac{1}{2}}^* \approx u_{\nu+\frac{1}{2}}$ such that *both* $\sum(u_{\nu+\frac{1}{2}}^* - u_{\nu-\frac{1}{2}}^*)$ and $\sum u_\nu^3(u_{\nu+\frac{1}{2}}^* - u_{\nu-\frac{1}{2}}^*)$ are conserved.

Systems of conservation laws. Our study of entropy stability is based on comparison with entropy-conservative schemes. In the scalar case, entropy-conservative schemes are unique (for a given entropy pair). For systems, there are various choices for numerical fluxes which meet the entropy conservation requirement in theorem 1.2. In this section we present the general framework developed in [8]. We present a family of entropy-conservative schemes which enjoys an *explicit, closed-form formulation*. To this end, at each cell consisting of two neighbouring values $\mathbf{v}_\nu$ and $\mathbf{v}_{\nu+1}$, we let $\left\{\mathbf{r}_{\nu+\frac{1}{2}}^j\right\}_{j=1}^N$ be an *arbitrary* set of N linearly independent N-vectors, and let $\left\{\boldsymbol{\ell}_{\nu+\frac{1}{2}}^j\right\}_{j=1}^N$ denote the corresponding orthogonal set, $\left\langle \boldsymbol{\ell}_{\nu+\frac{1}{2}}^j, \mathbf{r}_{\nu+\frac{1}{2}}^k \right\rangle = \delta_{jk}$. Next, we introduce the intermediate states, $\left\{\mathbf{v}_{\nu+\frac{1}{2}}^j\right\}_{j=1}^N$, starting with $\mathbf{v}_{\nu+\frac{1}{2}}^1 = \mathbf{v}_\nu$, and followed by $\mathbf{v}_{\nu+\frac{1}{2}}^{j+1} = \mathbf{v}_{\nu+\frac{1}{2}}^j + \left\langle \boldsymbol{\ell}_{\nu+\frac{1}{2}}^j, \Delta \mathbf{v}_{\nu+\frac{1}{2}} \right\rangle \mathbf{r}_{\nu+\frac{1}{2}}^j$, $j = 1, 2, \ldots, N$, thus defining a path in phase space, connecting $\mathbf{v}_\nu$ to $\mathbf{v}_{\nu+1}$,

$$(3) \qquad \mathbf{v}_{\nu+\frac{1}{2}}^{N+1} = \mathbf{v}_{\nu+\frac{1}{2}}^1 + \sum_{j=1}^N \left\langle \boldsymbol{\ell}_{\nu+\frac{1}{2}}^j, \Delta \mathbf{v}_{\nu+\frac{1}{2}} \right\rangle \mathbf{r}_{\nu+\frac{1}{2}}^j = \mathbf{v}_\nu + \Delta \mathbf{v}_{\nu+\frac{1}{2}} \equiv \mathbf{v}_{\nu+1}.$$

Since the mapping $\mathbf{u} \mapsto \mathbf{v}$ is one-to-one, the path is mirrored in the usual phase space of conservative variables, $\{\mathbf{u}_{\nu+\frac{1}{2}}^{j} := \mathbf{u}(\mathbf{v}_{\nu+\frac{1}{2}}^{j})\}_{j=1}^{N+1}$, starting with $\mathbf{u}_{\nu+\frac{1}{2}}^{1} = \mathbf{u}_{\nu}$ and ending with $\mathbf{u}_{\nu+\frac{1}{2}}^{N+1} = \mathbf{u}_{\nu+1}$.

Theorem 1.2 (Tadmor , 2003 [8]). *Fix an entropy pair (η, F) and let ψ denote the corresponding entropy flux potential $\psi(\mathbf{v}) := \langle \mathbf{v}, \mathbf{f}(\mathbf{v}) \rangle - F(\mathbf{u}(\mathbf{v}))$. Then the numerical flux, $\mathbf{f}_{\nu+\frac{1}{2}}^{*}$, given by*

$$(4) \qquad \mathbf{f}_{\nu+\frac{1}{2}}^{*} := \sum_{j=1}^{N} \frac{\psi(\mathbf{v}_{\nu+\frac{1}{2}}^{j+1}) - \psi(\mathbf{v}_{\nu+\frac{1}{2}}^{j})}{\langle \boldsymbol{\ell}_{\nu+\frac{1}{2}}^{j}, \Delta\mathbf{v}_{\nu+\frac{1}{2}} \rangle} \boldsymbol{\ell}_{\nu+\frac{1}{2}}^{j},$$

is an η-entropy conservative such that $\dfrac{d}{dt}\eta(\mathbf{u}_{\nu}(t)) + \dfrac{1}{\Delta x_{\nu}}\left[F_{\nu+\frac{1}{2}} - F_{\nu-\frac{1}{2}}\right] = 0$.

We demonstrate our approach in the context of Euler equations. We begin with the entropy decay in the Navier-Stokes equations

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho \\ m \\ E \end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix} m \\ qm + p \\ q(E + p) \end{bmatrix} = (\lambda + 2\mu)\frac{\partial^2}{\partial x^2}\begin{bmatrix} 0 \\ q \\ q^2/2 \end{bmatrix} + \kappa\frac{\partial^2}{\partial x^2}\begin{bmatrix} 0 \\ 0 \\ \theta \end{bmatrix}$$

The viscosity and heat dissipation of the right dictate an entropy dissipation

$$\overbrace{(-\rho S)_t}^{\eta(\mathbf{u}^\epsilon)} + \overbrace{(-\rho q S + \epsilon \ln(\theta)_x)_x}^{F_\epsilon(\mathbf{u}^\epsilon)} = \overbrace{-(\lambda + 2\mu)\frac{(q_x)^2}{\theta}}^{\text{viscosity}} \overbrace{-\kappa\frac{|\theta_x|^2}{\theta^2}}^{\text{heat conduction}} \leq 0$$

We now seek the entropy conservative flux, $\mathbf{f}_{\nu+\frac{1}{2}}^{*}$ which produces no *artificial numerical viscosity*; namely, we should end with the precise entropy balance[1],

$$\frac{d}{dt}\eta(\mathbf{u}_\nu) + \frac{F_{\nu+\frac{1}{2}} - F_{\nu-\frac{1}{2}}}{\Delta x} = \begin{cases} 0, & \text{Euler eq's,} \\ -\epsilon\left[\left(\frac{\Delta q}{\Delta x}\right)^2 \overline{\left(\frac{1}{\theta}\right)} + \left(\frac{\Delta\theta}{\Delta x}\right)^2 \widetilde{\left(\frac{1}{\theta}\right)}^2\right] \leq 0, & \text{NS eq's.} \end{cases}$$

An entropy conservative flux for Euler equations was computed in [9]. The entropy variables associated with $\eta(\mathbf{u}) = -\rho S$ are $\eta_{\mathbf{u}}(\mathbf{u}) = [-E/e - S + \gamma + 1, q/\theta, -1/\theta]^{\top}$; the corresponding entropy flux potential amounts to $\psi(\mathbf{v}) = \langle \mathbf{v}, \mathbf{f} \rangle - F(\mathbf{u}) = (\gamma - 1)m$. We choose a path in phase-space along the eigensystem of the Jacobian — an approximate Riemann path. We end up with the entropy conservative flux, given in an explicit form $\mathbf{f}_{\nu+\frac{1}{2}}^{*} = (\gamma - 1)\sum_{j=1}^{3} \frac{m^{j+1} - m^{j}}{\langle \boldsymbol{\ell}^j, \Delta\mathbf{v}_{\nu+\frac{1}{2}} \rangle}\boldsymbol{\ell}^j$.

No artificial numerical viscosity is present.

Higher-order extensions — the class of TeCNO schemes. In [2] we introduced the class *arbitrarily high-order* entropy-stable schemes — the TeCNO

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[1]The notations $\overline{\{\cdot\}}$ and $\widetilde{\{\cdot\}}$ denote proper average values.

schemes. This was achieved by coupling entropy-conservative fluxes coupled with high-order diffusion based on ENO reconstruction of cell-interfaces $\mathbf{v}^{\pm}_{\nu+\frac{1}{2}}$. The resulting class of *arbitrarily* high-order entropy-stable fluxes take the form $\mathbf{f}_{\nu+\frac{1}{2}} :=$ $\mathbf{f}^*(\mathbf{v})_{\nu+\frac{1}{2}} - \frac{1}{2} D_{\nu+\frac{1}{2}} \langle\!\langle \mathbf{v} \rangle\!\rangle_{\nu+\frac{1}{2}}$ where $\langle\!\langle \mathbf{v} \rangle\!\rangle_{\nu+\frac{1}{2}} := \mathbf{v}^-_{\nu+1} - \mathbf{v}^+_{\nu}$ is the jump across the cell interface. The ENO reconstruction has an important *sign property* $\langle\!\langle \mathbf{v} \rangle\!\rangle_{\nu+\frac{1}{2}} \sim \Delta \mathbf{v}_{\nu+\frac{1}{2}}(!)$ which was judiciously used in [2] to tune the entropy stability of any order. These schemes were used in recent computations of *entropy measure valued* solutions of 2D Euler equations [3]. The point we make here is that these *failthful* computations require high-resolution without artificial numerical viscosity. This is precisely what the TeCNO schemes provide. They enable us to explore the question of what computed quantities are encoded in *unstable* 2D Euler computations.

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A fast-marching method for non-monotonically evolving fronts

ALEXANDRA TCHENG

(joint work with Jean-Christophe Nave)

The following treats the development of a new algorithm tracking non-monotonically evolving fronts using finite-differences. This is the subject of my PhD thesis, supervised by Prof. Dr. Jean-Christophe Nave.

Front propagation is a time-dependent phenomenon occurring when the boundary between two distinct regions of space is evolving. It is possible to make the distinction between *monotone* and *non-monotone* motion of fronts. For example, a

fire evolves monotonically in that, if a point $\mathbf{x}$ of space belongs to a burnt region, then it cannot belong to an unburnt region at a later time [1]. Given an initial front $\mathcal{C}_0$ as a codimension-one C^1 subset of $\mathbb{R}^n$, let each point of the front evolve with a given speed $F : \mathbb{R}^n \times [0, T] \to \mathbb{R}$ in the direction of the outward normal to the front $\hat{\nu}_t : \mathcal{C}_t \to \mathbb{R}^n$. The resulting non-linear evolution is such that even if F and $\mathcal{C}_0$ are smooth, the front may become C^0 and undergo topological changes [2]. Numerical algorithms tracking interface propagation aim to recover the front $\mathcal{C}_t$ at later times $t > 0$.

On the one hand, a robust but computationally expensive numerical method for tracking either kind of evolution is the Level-Set Method (LSM) [1]. On the other hand, the Fast Marching Method (FMM) [3, 4] may be used when $F(\mathbf{x}) \geq \delta > 0$, and is therefore suited for monotone propagation. This approach builds the *first arrival time function* ψ, i.e., $t = \psi(\mathbf{x})$ gives the unique time at which the front reaches the point $\mathbf{x} \in \mathbb{R}^n$. The FMM finds ψ by marching the front at a computational speed that is *optimal*. The purpose of the work described below was to develop an algorithm able to handle speed functions changing sign *while* featuring a computational complexity comparable to that of the FMM.

In [5] and [6], we consider the set $\mathcal{M} := \{(\mathbf{x}, t) : \mathbf{x} \in \mathcal{C}_t\}$ consisting of the surface traced out by the fronts as they evolve. If $\mathcal{M}$ embeds in $\mathbb{R}^n \times (0, T)$ as a C^k-manifold of dimension n, then each point $(\mathbf{x}, t) \in \mathcal{M}$ belongs to a neighbourhood that is locally the image of a C^k-function of n variables. We describe $\mathcal{M}$ locally with functions of the form $\psi(\mathbf{u})$ where the n variables $\mathbf{u} = (u_1(\mathbf{x}, t), \ldots, u_n(\mathbf{x}, t))$ parameterise *some hyperplane* lying in $\mathbb{R}^n \times [0, T]$. We show that $\psi : \mathbb{R}^n \to \mathbb{R}$ solves a Dirichlet problem of the form:

$$(1) \qquad \begin{cases} H(\mathbf{u}, \psi(\mathbf{u}), \nabla\psi(\mathbf{u})) & = & 0 & \text{in } \mathcal{U} \subset \mathbb{R}^n \\ \psi(\mathbf{u}(\mathbf{x}, t)) & = & u_{n+1}(\mathbf{x}, t) & \text{on } \mathbf{x} \in \mathcal{C}_t \cap \mathcal{V} \end{cases}$$

for appropriate neighbourhoods $\mathcal{U}$ and $\mathcal{V}$, where u_{n+1} is normal to the plane. As with the FMM, points sampling $\mathcal{M}$ first belong to the *narrow band* set $\mathcal{N}$ before they are moved to the *accepted* set $\mathcal{A}$. However the points $p \in \mathcal{M}$ are no longer required to lie on any grid. Rather, when the point $p_a \in \mathcal{N}$ with the smallest time value is accepted, the algorithm works in the $\mathbf{u}$-u_{n+1}-coordinate system to find a new point belonging to $\mathcal{M}$. To this end, the relation $H(\mathbf{u}, \psi(\mathbf{u}), \nabla\psi(\mathbf{u})) = 0$ is discretized using finite-differences. Then, given a location $\mathbf{u}_c$ and another point $p_b \in \mathcal{M}$, we may solve for $(u_{n+1})_c$ using either a direct or an iterative solver. To determine the coordinates $\mathbf{u}_c$, a constrained optimisation problem is solved. The objective function f captures the *accuracy* of the solvers, whereas the constraints ensure that both *causality* is enforced into the solution, and the sampling of $\mathcal{M}$ is *even*. The final output is a discrete sampling of the manifold $\mathcal{M}$. Figure 1 (a) & (b) features one such set, where it is visible that the sampling of $\mathcal{M}$ is highly regular. First order convergence is observed; see Figure 1 (c).

If my talk, I will elaborate on the non-linear optimisation problem lying at the heart of this algorithm and present more results.
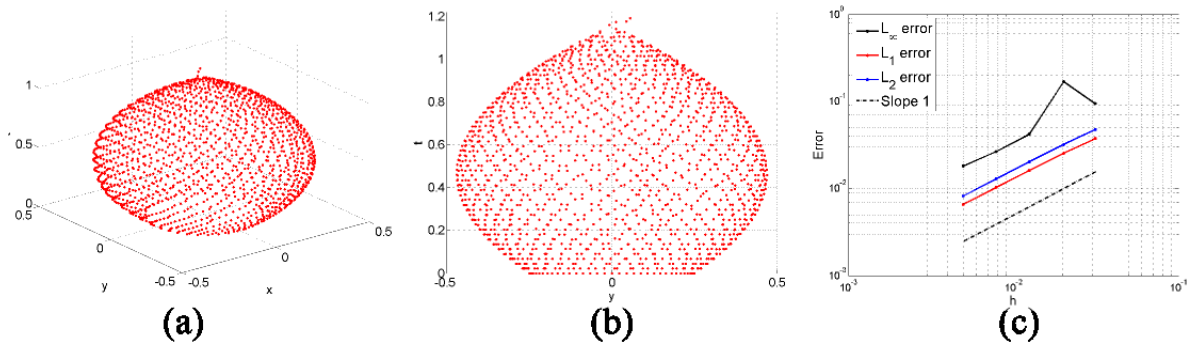
FIGURE 1. **(a) & (b)** In this example, $F = 1 - 2t$, and $\mathcal{C}_0$ consists of a circle. **(c)** Convergence results for the example illustrated on (a) & (b) (global truncation error).

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Adaptive Wavelet BEM

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(joint work with Helmut Harbrecht)

INTRODUCTION

We consider the adaptive wavelet boundary element method for the solution of boundary integral equations in three dimensions. Partial differential equations are frequently encountered in science and engineering, some of which can be formulated as boundary integral equations. Apart from reducing the dimensionality of the problem, this is also a way to handle the infinite expansion of the domain in case of an exterior problem. Some situations (e.g. domains with edges and vertices) require a strong refinement in certain parts of the geometry. Where uniform refinement would lead to huge systems, an adaptive approach saves a large amount of computation power and memory. Even though the dimensionality of the problem is reduced drastically, the involved linear system of equations is densely populated. By applying the wavelet compression [4, 6], we end up with a quasi-sparse system

matrix. This means that the matrix is not sparse per se, but many matrix entries can be neglected without compromising the accuracy. Thus, after compression, only $\mathcal{O}(N)$ relevant matrix entries remain.

Exterior Dirichlet Problem for the Helmholtz Equation

Acoustic scattering at a three dimensional object $\Omega \subset \mathbb{R}^3$ can be described by the exterior Helmholtz equation

$$\Delta U + \kappa^2 U = 0 \quad \text{in } \Omega_{\text{ext}} := \mathbb{R}^3 \setminus \bar{\Omega},$$

with $k = 2\pi/\lambda$ being the wavenumber and λ the wavelength, describing the oscillation of the incoming and the scattered wave. Depending on the characteristics of the scatterer, the boundary conditions are chosen appropriately. Additionally, in order to be a solution to the Helmholtz equation, the function U must fulfill the Sommerfeld radiation condition, ensuring the uniqueness of the solution U. We reformulate the problem by using the fundamental solution

$$E(x, y) = \frac{1}{4\pi} \frac{e^{i\kappa\|x-y\|}}{\|x - y\|}$$

for x and y in $\mathbb{R}^3$. With the acoustic single layer and the acoustic double layer potential

$$(\mathcal{S}u)(x) = \int_\Gamma E(x, y)\, u(y)\, \mathrm{d}\sigma_y \quad \text{and} \quad (\mathcal{D}u)(x) = \int_\Gamma \frac{\partial E(x, y)}{\partial n_y}\, u(y)\, \mathrm{d}\sigma_y$$

we end up with the boundary integral equation

$$\left(\mathcal{D} + \frac{1}{2}\mathcal{I}\right) u = f$$

for Dirichlet problems. If κ^2 is an eigenvalue of the interior Neumann problem, then the solution is not unique anymore. Brakhage and Werner [1] thus came up with the ansatz $U = (\mathcal{D} - i\eta\mathcal{S})u$, leading us to the boundary integral equation

$$\mathcal{L}u = \left(\frac{1}{2} + \mathcal{D} - i\eta\mathcal{S}\right) u = f \quad \text{on } \Gamma$$

with $\eta > 0$.

After introducing the variational formulation and the Galerkin projection, we arrive at a linear system of equations to solve. Depending on how we choose the basis functions in our ansatz space, the resulting structure of matrix differs. Namely, if we choose a wavelet basis, many matrix entries can be neglected without compromising the accuracy. This is because the wavelets are supposed to have vanishing moments of a certain order m, meaning that

$$\int_\square x^\alpha\, \psi_{j,k}(x)\, \mathrm{d}x = 0 \quad \text{for } |\alpha| < m.$$

This property, together with the asymptotic smoothness of the kernel, implies the following estimate for the matrix entries

$$|\langle \mathcal{L}\psi_k, \psi_i \rangle_{L^2(\Gamma)}| \leq C \frac{\text{diam}(\text{supp } \psi_i)^{m+1}\text{diam}(\text{supp } \psi_k)^{m+1}}{\text{dist}(\text{supp } \psi_i, \text{ supp } \psi_k)^{2+2q+2m}}.$$

From this estimate, we see that wavelets having a large distance from each other result in a small matrix entry. To make the compression even more efficient, we use a second compression, having an effect on the other wavelets as well.

Adaptive Wavelet Schemes

With adaptivity, there comes a whole new theory [3, 5]. Without going too much into detail, we just want to mention one estimate and to introduce the basic idea of what our goal is. Let $\mathbf{u} \in \ell^2(\mathcal{J})$ (with respect to some index set $\mathcal{J}$), $\mathbf{u}_N \in \ell^2(\mathcal{J})$ its best N-term approximation and $\mathbf{\Psi}$ an $H^t(\Gamma)$-normalized wavelet basis. Obviously, there holds that $u := \mathbf{\Psi}\mathbf{u}$. For $u \in H^{t+2s}(\Gamma)$, where $s \leq \bar{s} := \frac{1-t}{2}$, there holds the estimate $\|\mathbf{u} - \mathbf{u}_N\| \leq CN^{-s}$. Now, if $u \in B_\tau^{t+2s}(\Gamma)$ with $\tau = (s + 1/2)^{-1}$, then

$$\|\mathbf{u} - \mathbf{u}_N\| \leq CN^{-s}$$

with $B_\tau^{t+2s}(\Gamma)$ being a Besov space.

In order to get an adaptive data structure for the adaptive code, we use wavelet and element trees instead of arrays. To preserve the tree structure of the wavelet basis, we use the best N-term tree approximation which is nearly as good as the pure N-term approximation. Our aim is to find the approximate solution in optimal computational complexity $\mathcal{O}(N)$.

The adaptive algorithm works in the steps:

$$\boxed{\text{solve}} \rightarrow \boxed{\text{estimate}} \rightarrow \boxed{\text{mark}} \rightarrow \boxed{\text{refine}}.$$

Starting with a small set of wavelets, we solve the linear system of equations. With this and an estimated residuum at hand, we start an iteration where our goal is to add the required new wavelets. In each step of the iteration, we coarse the developed index set by a fixed percentage. After the set of wavelets has been increased in this growth process, we solve the newly formed linear system of equations. With this newly developed algorithm, we are able to refine 15 times or more where it is necessary, which would be unthinkable (in terms of memory) for a uniform scheme.

Numerical examples

To conclude, we present a numerical result. On the Fichera vertex we solve the exterior Helmholtz problem with the Brakhage-Werner formulation. We use piecewise constant wavelets with three vanishing moments and the Dirichlet data is chosen as the function $g(x) = E(x, a)$ with $a = (0.55, 0.55, 0.55)$ and $\kappa = 1$ for the wavenumber.
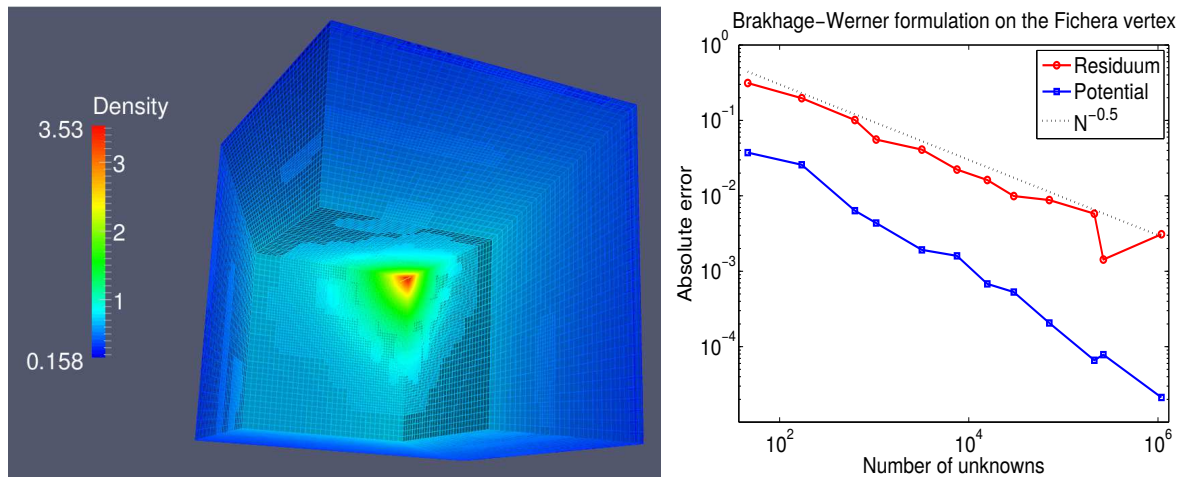
The left figure shows us the density on the geometry, whereas in the figure on the right side we see the norm of the evaluated potential and the residual error versus the unknown, showing the expected rate of convergence.

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hp-Discontinuous Galerkin Time Stepping Discretizations

Thomas P. Wihler

The discontinuous Galerkin (dG) time stepping scheme has been investigated in various works (see, e.g., [1, 9]), and studied within the *hp*-context in, e.g., [6, 7, 8]. Due to its great flexibility with respect to the local time steps and to the approximation orders, the *hp*-version dG scheme is well-known to be capable of resolving both local singularities as well as areas of smooth behavior at high-order algebraic or even exponential convergence rates.

*hp***-Setting.** In order to define the dG scheme, let us consider time nodes $0 = t_0 < t_1 < \ldots < t_{M-1} < t_M = T$ on an interval $[0, T]$, $T > 0$, which introduce a time partition into local intervals $I_m = (t_{m-1}, t_m)$ of (possibly varying) length $k_m = t_m - t_{m-1}$, $m = 1, 2, \ldots M$. Furthermore, to each time interval I_m,

we associate a polynomial degree $r_m \geq 0$, and collect these quantities in a vector $r = \{r_1, r_2, \ldots, r_M\}$. Based on this setup, let us define, for $s \in \mathbb{N}_0$, the polynomial space

$$\mathbb{P}^s(J; H) = \left\{ v \in C^0(J; H) : v(t) = \sum_{j=0}^{s} a_j t^j, a_j \in H \right\}$$

on an interval $J \subset \mathbb{R}$, with values in a real Hilbert space H (with inner product denoted by $(.,.)_H$, and norm $\|.\|_H$). Moreover, for $p \in [1, \infty]$ and $u \in L^p(J; H)$, we define the Bochner norms $\|u\|_{L^p(J;H)} = (\int_J \|u(t)\|_H^p \, dt)^{\frac{1}{p}}$ for $p \in [1, \infty)$, and $\|u\|_{L^\infty(J;H)} = \operatorname{ess\,sup}_{t \in J} \|u(t)\|_H$ for $p = \infty$.

The dG Derivative Operator [3]. On a time interval I_m define the *dG time derivative operator* $\chi_m^{r_m} : \mathbb{P}^{r_m}(I_m; H) \to \mathbb{P}^{r_m}(I_m; H)$ by

$$\int_{I_m} (\chi_m^{r_m}(U), V)_H \, dt = \int_{I_m} (U', V)_H \, dt + (U_{m-1}^+, V_{m-1}^+)_H \qquad \forall V \in \mathbb{P}^{r_m}(I_m; H).$$

Here, we introduce the right-sided limit of a piecewise continuous function U at each time node t_{m-1} by $U_{m-1}^+ = \lim_{s \downarrow 0} U(t_{m-1} + s)$, $m = 1, \ldots, M$.

For the analysis of the dG time discretization scheme it is important to note that the operator $\chi_m^{r_m} : \mathbb{P}^{r_m}(I_m; H) \to \mathbb{P}^{r_m}(I_m; H)$ is an isomorphism, and that, for any $p \in [1, \infty]$, there exists a constant $0 < C_\chi \leq 2$ independent of k_m and r_m such that

$$\|[\chi_m^{r_m}]^{-1}(u)\|_{L^\infty(I_m;H)} \leq C_\chi k_m^{1-\frac{1}{p}} \|u\|_{L^p(I_m;H)} \qquad \forall u \in \mathbb{P}^{r_m}(I_m; H).$$

In particular, the operator $[\chi_m^{r_m}]^{-1}$ is *unconditionally stable* with respect to the polynomial degree r_m.

Application to Nonlinear Initial Value Problems [3]. For $T > 0$ consider a *nonlinear continuous* operator $\mathcal{F} : (0, T) \times H \to H$. Then, for a given initial value $u_0 \in H$, we consider the nonlinear initial value problem

$$u'(t) = \mathcal{F}(t, u(t)), \quad t \in [0, T], \qquad u(0) = u_0,$$

for an unknown solution $u : (0, t) \to H$.

In order to discretize this problem, we introduce finite dimensional subspaces $H_m \subset H$, $\dim(H_m) < \infty$, on each time interval I_m, $m = 1, \ldots, M$. Then, using the dG derivative operator, the m-th time step of the dG time discretization scheme can be formulated as follows: Given an initial value

$$u_{\mathsf{dG},m-1}^- := u_{\mathsf{dG}}|_{I_{m-1}}(t_{m-1}) \qquad (\text{with } u_{\mathsf{dG},0}^- := u_0),$$

find $u_{\mathsf{dG}}|_{I_m} \in \mathbb{P}^{r_m}(I_m; H_m)$ such that

$$\int_{I_m} (\chi_m^{r_m}(u_{\mathsf{dG}} - \pi_m u_{\mathsf{dG},m-1}^-), v)_H \, dt = \int_{I_m} (\mathcal{F}(u_{\mathsf{dG}}), v)_H \, dt,$$

for any $v \in \mathbb{P}^{r_m}(I_m; H_m)$, where $\pi_m : H \to H_m$ signifies the H-orthogonal projection. Then, employing the L^2-projection $\Pi_m^{r_m} : L^2(I_m; H) \to \mathbb{P}^{r_m}(I_m; H_m)$, we obtain the *strong form* of the dG method:

$$\chi_m^{r_m}(u_{\mathsf{dG}} - \pi_m u_{\mathsf{dG},m-1}^-) = \Pi_m^{r_m}(\mathcal{F}(u_{\mathsf{dG}})) \qquad \text{in } \mathbb{P}^{r_m}(I_m; H_m).$$

Thence, introducing the auxiliary variable $Z_{\mathsf{dG}} := u_{\mathsf{dG}} - \pi_m u_{\mathsf{dG},m-1}^-$, and defining the (continuous) operator $\mathsf{T}_m^{\mathsf{dG}} : \mathbb{P}^{r_m}(I_m; H_m) \to \mathbb{P}^{r_m}(I_m; H_m)$ by

$$\mathsf{T}_m^{\mathsf{dG}}(Z) := [\chi_m^{r_m}]^{-1}\left(\Pi_m^{r_m}(\mathcal{F}(Z + \pi_m u_{\mathsf{dG},m-1}^-))\right),$$

yields the fixed point formulation $\mathsf{T}_m^{\mathsf{dG}}(Z_{\mathsf{dG}}) = Z_{\mathsf{dG}}$. This formulation allows the application of Brouwer's fixed point theorem, which implies that, if the local time step $k_m > 0$ is chosen sufficiently small (*independently of the polynomial degree* r_m), then the hp-dG time stepping method possesses at least one solution in $\mathbb{P}^{r_m}(I_m; H_m)$; see [3] for a detailed analysis.

Application to Linear Parabolic Problems [2]. Given two separable Hilbert spaces $X \hookrightarrow H$ with dense embedding, we consider a linear elliptic operator $\mathsf{A} : X \to X^\star$ that is associated with a bounded, coercive bilinear form $a : X \times X \to \mathbb{R}$,

$$a(u,v) = \langle \mathsf{A}u, v \rangle_{X^\star \times X} \qquad \forall u, v \in X.$$

Here, $X^\star$ signifies the dual space of X, and $\langle \cdot, \cdot \rangle_{X^\star \times X}$ is the duality pairing in $X^\star \times X$. Then, we focus on the parabolic evolution problem in $X^\star$:

$$u'(t) + \mathsf{A}u(t) = g(t), \quad t \in (0,T), \qquad u(0) = u_0,$$

with given data $u_0 \in H$, and $g \in L^2((0,T); X^\star)$.

To discretize the above problem, we introduce conforming discrete spaces $X_m \subset X$, $Y_m = \mathbb{P}^{r_m}(I_m; X_m)$, on each time interval I_m, $m = 1, 2, \ldots, M$. Then, the (fully discrete) dG time stepping method can be written as follows: For each $m = 1, 2, \ldots, M$ find $U_{\mathsf{dG}}|_{I_m} \in Y_m$ such that

$$\int_{I_m} \left\{ (\chi_m^{r_m}(U_{\mathsf{dG}} - \pi_m U_{\mathsf{dG},m-1}^-), V)_H + a(U_{\mathsf{dG}}, V) \right\} dt = \int_{I_m} \langle g, V \rangle_{X^\star \times X} \, dt$$

for all $V \in Y_m$, with $\pi_m : X \to X_m$ being the X-orthogonal projection from X to X_m, and $U_{\mathsf{dG},0}^- := \widehat{u}_0 \in X_m$ some projection of $u_0 \in H$.

In order to derive a strong formulation of the above dG scheme, we first define the *time reconstruction* of U_{dG} by

$$\widehat{U}_{\mathsf{dG}}(t) = U_{\mathsf{dG},m-1}^- + \int_{t_{m-1}}^t \chi_m^{r_m}(U_{\mathsf{dG}}) \, d\tau, \qquad t \in I_m;$$

cp., e.g., [5]. Incidentally, there holds $\widehat{U}_{\mathsf{dG}}(t) \in H^1(0,T; X)$, and the difference $\widehat{U}_{\mathsf{dG}} - U_{\mathsf{dG}}(t)$ can be bound explicitly in terms of the discontinuity jump of $U_{\mathsf{dG}}(t)$ at t_{m-1}; see [8]. In addition, to deal with the elliptic part of the discrete formulation, we define the discrete operator $\mathsf{A}_m : X_m \to X_m$ by

$$v \in X_m : \quad (\mathsf{A}_m v, \phi)_H = \langle \mathsf{A}v, \phi \rangle_{X^\star \times X} \qquad \forall \phi \in X_m.$$

Then, we use an *elliptic reconstruction* approach [4] to find $\widetilde{U}$ such that

$$U \in Y_m : \quad \langle \mathsf{A}\widetilde{U}, w \rangle_{X^\star \times X} = (A_m U, w)_H \qquad \forall w \in X.$$

The difference $\widetilde{U}_{\mathsf{dG}} - U_{\mathsf{dG}}(t)$ can be bounded by means of a suitable *a posteriori* error estimate for elliptic problems.

Based on these reconstructions, we infer the strong form of the dG method,

$$\widehat{U}'_{\mathsf{dG}} + A\widetilde{U}_{\mathsf{dG}} = \Pi^\star_m g, \qquad \text{on } I_m,$$

where $\Pi^\star$ is the orthogonal projection from $X^\star$ to X_m. In a subsequent step, estimating the differences between the dG solution U_{dG} and its reconstructions, $L^2(0, T; X)$- and $L^\infty(0, T; H)$-type *a posteriori* error estimates can be derived; see [2] for details.

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The approximation of wavefunctions by anisotropic Gauss functions

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(joint work with Stephan Scholz)

The approximation of high-dimensional problems whether they be given explicitly or implicitly as solutions of differential equations, represents one of the grand challenges of applied mathematics. This field made great progress during the past years, mainly due to the emergence of modern tensor product methods. The astonishing efficiency of such methods for the numerical solution of certain partial differential equations and their obviously often rapid convergence can meanwhile be explained theoretically. Adaptive techniques have been developed that enable to exploit this convergence behavior in practical computations. One of the most

notorious and complicated problems of this type, the electronic Schrödinger equation, however largely resists such approaches. The Schrödinger equation forms the basis of quantum mechanics and is of fundamental importance for our understanding of atoms and molecules. It links chemistry to physics and describes a system of electrons and nuclei that interact by Coulomb attraction and repulsion forces. As proposed by Born and Oppenheimer in the nascency of quantum mechanics, the slower motion of the nuclei is mostly separated from that of the electrons. This results in the electronic Schrödinger equation, the problem to find the eigenvalues and eigenfunctions of the electronic Hamilton operator

$$(1) \qquad H \; = \; - \sum_{i=1}^{N} \Delta_i \; - \; \sum_{i=1}^{N} \sum_{\nu=1}^{K} \frac{Z_\nu}{|x_i - a_\nu|} \; + \; \sum_{i<j} \frac{1}{|x_i - x_j|}.$$

It acts on functions with arguments $x_1, \ldots, x_N$ in $\mathbb{R}^3$, which are associated with the positions of the considered electrons. The $a_1, \ldots, a_K$ in $\mathbb{R}^3$ are the fixed positions of the nuclei and the values $Z_\nu > 0$ the charges of the nuclei in multiples of the electron charge. The reason for the comparatively low performance of tensor product methods when applied to the electronic Schrödinger equation is that such methods fix a set of directions. It is not possible with tensor product methods to capture simultaneously and equally well the singularities arising from the interaction of the electrons and the nuclei aligned with the coordinate directions and the electron-electron singularities aligned with the diagonals.

Therefore we propose a different nonlinear ansatz that is invariant to rotations of the coordinate system and is inspired by the almost exclusive use of Gauss functions in quantum chemistry, that is partly motivated by the fact that the arising integrals can be evaluated without problems but has also to do with the good approximation properties of Gauss functions. We propose to approximate the electronic wavefunctions by linear combinations of anisotropic Gauss functions

$$\exp \left(- \frac{1}{2} \, (x - a) \cdot Q(x - a) \right).$$

The symmetric positive definite matrices Q are arbitrary and are not fixed in advance. The same holds for the points $a \in \mathbb{R}^{3N}$ around which the Gauss functions are centered and which are only indirectly determined by the positions of the nuclei. Basically we show that electronic wavefunctions can be approximated with arbitrary order by linear combinations of such Gauss functions.

The key to our approximation of the wavefunctions is the extremely accurate approximation of the functions $1/\sqrt{r}$ and $1/r$ by exponential functions and with that indirectly also that of $1/r$ by Gauss functions. Approximations of this kind form a rather universal tool that received much attention during the past years, due to the work of Braess and Hackbusch and others. Our central idea is to approximate and replace the Coulomb potentials in the operator (1) and the inverse of the correspondingly shifted Laplace operator, expressed in terms of the Fourier transform, by series of Gauss functions. The eigenvalue problem is first rewritten as a linear equation with the convolution $f = K * u$ of the eigenfunction u under

consideration with a Gaussian kernel K of sufficiently small width as right hand side. The corresponding approximate equation is then solved via a Neumann series. The crucial point is that this series is, after reordering and expansion of the right hand side into a series of Gauss functions, itself a series of Gauss functions that is then truncated in an appropriate manner. The main hurdle, to which most of our work is devoted, is the control of this truncation process.

Our main result is easily sketched. Assume that there exists a sequence of scalar multiples $g_1, g_2, \ldots$ of Gauss functions such that for every $\varepsilon > 0$

$$\Big\| f - \sum_{j=1}^{n} g_j \Big\|_{\vartheta} \leq \varepsilon, \quad n \leq \Big(\frac{\kappa}{\varepsilon}\Big)^{1/r},$$

where r is a given approximation order and the norm an L_2-like fractional order Sobolev norm with a regularity index ϑ a bit greater than one. Expansions of this type can be constructed using that the Fourier transform of an electronic wavefunction for an eigenvalue below the ionization threshold is real-analytic and its partial derivatives of arbitrary order are bounded. The solution of the approximate equation, that serves as a quasi-exact substitute of the original wavefunction, can then, for arbitrarily small $\varepsilon > 0$, be approximated by a linear combination of

$$n \leq 2 \Big(\frac{2\kappa}{\varepsilon}\Big)^{1/r}$$

Gauss functions up to an H^1-error ε, provided the width of the smoothing kernel K is sufficiently small in dependence of the approximation order r aimed for. The approximation of the original, singular wavefunction up to a very small, completely negligible residual error determined by the approximations of the Coulomb potentials and the inverse of the shifted Laplace operator requires therefore only insignificantly more effort than that of its smoothed variant.

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