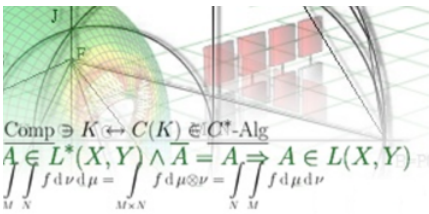

GESELLSCHAFT für
ANGEWANDTE MATHEMATIK und MECHANIK
INTERNATIONAL ASSOCIATION of APPLIED MATHEMATICS and MECHANICS
Fachausschuss
Computational Science and Engineering (CSE)

GAMM CSE Workshop Ulm/Reisensburg Nov. 21-22, 2019

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Welcome!

Welcome to the 2019 workshop of GAMM (Gesellschaft für Angewandte Mathematik und Mechanik) activity group on CSE (Computational Science and Engineering) at Schloss Reisensburg, Günzburg, the science center of Ulm University. It has been organized by the Institute of Numerical Mathematics of Ulm University together with the Scientific Computing Centre Ulm (UZWR) and the GAMM Student Chapter Ulm.

In the tradition of the GAMM, the workshop especially is a good opportunity for young researchers to present and discuss their work in a friendly and productive atmosphere. Together with a long-standing tradition of research on computational mechanics, the fields of Mathematical Modelling, Numerical Mathematics and Scientific Computing are key topics of the GAMM.

The focus of this event is on interdisciplinary collaboration in the best sense of CSE: To combine the complimentary expertise in engineering, modelling, computational science and high-performance computing. This forms a new branch in science for the solution of multi-physical and engineering challenges, requiring an integrative and cross-disciplinary understanding of computational science.

CSE in Ulm goes back to 2011, when the first Bachelor program was started. Since these early days, both the Bachelor and the Masters program in Ulm have been unique in their spirit: They are jointly covered by Ulm University and Ulm University of Applied Sciences (Technische Hochschule Ulm, THU); it is strongly supported by the Chamber of Commerce (Industrie- und Handelskammer, IHK Ulm) and particularly in very close cooperation with several small and medium sized companies in the area. Those companies are hidden champions in their respective field, which is the reason why Modeling, Simulation, Optimization and Visualization, i.e. CSE, is an important factor for their economic success.

Of course, CSE is also a field of academic research, which is the focus of the current workshop. I hope for interesting presentations, fruitful discussions and inspiring meeting in the nice environment of Schloss Reisensburg.

I would like to thank the members of the local organizing committee, namely Dr.-Ing. Ulrich Simon, Lucas Engelhardt, Constantin Greif, Stefan Hain, Petra Hildebrand, Mazen Ali and Tim Wagner. This workshop would not have been possible without their great support!

Karsten Urban

Nonlinear Eigenvalue Problems on Graphs and Images

Martin Burger

Friedrich-Alexander Universität Erlangen-Nürnberg, Department Mathematik

This talk will present recent work on Eigenvalue Problems for nonlinear operators in Banach spaces, in particular focusing on operators arising as the subdifferential of a p-homogeneous functional. The canonical examples are p-Laplacian operators and their analogues on graphs, it turns out the most interesting cases being the limit $p=1$ and $p=$infinifty. We will discuss connections to variational problems and evolution equations, with applications in image and data analysis. Moreover we highlight the issues arising in computing eigenfunctions and solutions of variational problems on large graphs. We discuss the use of cut pursuit algorithms for this sake, which can be interpreted as an abstraction of adaptive discretization methods to graph structures.

The talk is based on joint work with Leon Bungert, Daniel Tenbrinck (FAU) and Fjedor Gaede (WWU Muenster)

Preconditioning the Cahn-Hilliard Equation

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We consider electrode particles of lithium ion batteries during the discharge process. The separation into lithium poor and lithium rich phases due to changes in the host material can be described with a phase-field model, resulting in the fourth order Cahn-Hilliard equation [1].

Difficulties solving this initial boundary value problem are on the one hand the highly nonlinear character of the equations and on the other hand the almost sharp moving phase boundary and the different time scales on which the separation process take place. In particular for three-dimensional electrode particles we need a robust solver overcoming these problems.

For the spatial discretization we employ a finite element method. The semi-discrete problem is linearized with Newton's method and for the time stepping we use an adaptive second order scheme [2]. For the fast solution of the large linear systems arising in each Newton step we use the matrix-free framework within the open-source finite element library deal.II [3, 4]. Based on the work [5] we developed a preconditioner, which is applicable also in the matrix-free framework.

We have implemented and tested an efficient finite element solver for the Cahn-Hilliard equation. The matrix-free solver is fast and does not need to store any matrices, in particular it can be run in parallel using MPI. Analyzing our developed preconditioner, the number of GMRES steps show only a moderate dependence on the time step and the mesh size. A comparison to a standard Jacobi preconditioner is shown.

Acknowledgments

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References

[1] M. Huttin, M. Kamlah: Phase-field modeling of stress generation in electrode particles of lithium ion batteries. Appl. Phys. Lett. 101(13), pp. 133902/1–133902/4, 2012.
[2] H. Gomez, T.J.R. Hughes: Provably unconditionally stable, second-order time-accurate, mixed variational methods for phase-field models. J. Comput. Phys. 230(13), pp. 5310–5327, 2011.
[3] W. Bangerth, R. Hartmann, G. Kanschat: deal.II—a general-purpose object-oriented finite element library. ACM Trans. Math. Software 33(4), pp. 24/1–24/27, 2007.
[4] M. Kronbichler, K. Kormann: A generic interface for parallel cell-based finite element operator application. Comput. & Fluids 63, pp. 135–147, 2012.
[5] S.C. Brenner, A.E. Diegel, L.-Y. Sung: A robust solver for a mixed finite element method for the Cahn-Hilliard equation. J. Sci. Comput. 77(2), pp. 1234–1249, 2018.

Communication-avoiding TT-tensor orthogonalization and rounding procedures

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High dimensional data arise in various areas of scientific computing. Parametric PDEs, molecular simulations, and classification are examples among many others [2–4]. For this reason, low-rank tensor approaches gained intensive attention of researchers in recent years. These methods allow to store the data implicitly and perform arithmetic operations on them with a reasonable complexity avoiding the curse of dimensionality. Most of the research focused on the establishment of representation formats and their corresponding arithmetic operations that reduce the floating point operations complexity [1, 3, 5]. However, few work considered efficient parallel algorithms for tensor computations.

In this work, we present communication-avoiding algorithms for tensors represented in tensor train (TT) format. Left and right orthogonalization procedures play an important role in most computations with TT tensors, e.g., during the projection step in the Alternating Least Squares method, rounding of formal structures, etc. We analyze data distribution and communication cost of the orthogonalization and rounding procedures. Due to the sequential scheme of TT tensors with respect to the modes, the performance of parallel algorithms becomes quickly communication bounded when increasing the number of modes, d. To tackle this issue, we use a mixed representation TT-Tucker to which it was pointed out in the literature [5] and introduce a communication-avoiding orthogonalization and rounding corresponding procedures.

A factor of d in terms of number of messages is saved with respect to the TT variant. Numerical experiments on large number of processes demonstrate the scalability of the proposed methods.

References

[1] W. Hackbusch and S. Kühn. A new scheme for the tensor representation. *J. Fourier Anal. Appl.*, 15(5):706–722, 2009.

[2] Boris N. Khoromskij. *Tensor numerical methods in scientific computing*, volume 19 of *Radon Series on Computational and Applied Mathematics*. De Gruyter, Berlin, 2018.

[3] Tamara G. Kolda and Brett W. Bader. Tensor decompositions and applications. *SIAM Rev.*, 51(3):455–500, 2009.

[4] Daniel Kressner and Christine Tobler. Krylov subspace methods for linear systems with tensor product structure. *SIAM J. Matrix Anal. Appl.*, 31(4):1688–1714, 2009/10.

[5] I. V. Oseledets. Tensor-train decomposition. *SIAM J. Sci. Comput.*, 33(5):2295–2317, 2011.

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Matrix-Less Methods for Computing Eigenvalues of Structured Matrices

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Eigenvalues (and singular values) of matrices are of great importance in applications, both in themselves (e.g., generalized eigenvalue problems) and as tools for designing fast solvers (e.g., preconditioning). When we discretize partial differential equations (PDE), or fractional differential equations, by standard methods (FDM, FVM, FEM, DGM, IgA, etc.) we obtain structured matrices, specifically **Toeplitz-like** matrices [6]. In the simplest case, we find Toeplitz matrices of the form

$$T_n(f) = \left[\hat{f}_{i-j}\right]_{i,j=1}^{n}, \qquad f(\theta) = \sum_{k=-\infty}^{\infty} \hat{f}_k \mathrm{e}^{k\mathbf{i}\theta}, \qquad \hat{f}_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\theta)\mathrm{e}^{-k\mathbf{i}\theta}\mathrm{d}\theta, \qquad k \in \mathbb{Z},$$

where $f(\theta)$ is a 2π-periodic function, called the **symbol** of the sequence $\{T_n(f)\}_n$. Assuming that the symbol f is real and smooth, the Szegő first limit theorem intuitively says that

$$E_{j,n} = \lambda_j(T_n(f)) - f(\theta_{j,n}) = \mathcal{O}(h),$$

where $\{\theta_{j,n} : \ j = 1, \ldots, n\}$ is a uniform grid in the domain of f. In a series of papers (see [1, 2] and the references therein), and under suitable assumptions, Böttcher et al. derived an asymptotic expansion of the form

$$E_{j,n} = \sum_{k=1}^{\alpha} c_k(\theta_{j,n})h^k + E_{j,n,\alpha}, \qquad E_{j,n,\alpha} = \mathcal{O}(h^{\alpha+1}). \tag{1}$$

Typically the functions $c_k(\theta)$ in (1) are not known, and knowing them would yield extremely accurate and fast approximations of $\lambda_j(T_n(f))$ for any matrix size n.

In a number of papers (see [3, 4, 5] and [7] for all references and co-authors) we developed the so-called **matrix-less** methods (not to be confused with matrix-free methods) to find approximations $\tilde{c}_k(\theta_{j,n_0})$ of $c_k(\theta_{j,n_0})$ on a coarse grid θ_{j,n_0} for all $k = 0, \ldots, \alpha$. These approximations can then be interpolated–extrapolated [5] to a finer grid $\theta_{j,n}$ in order to obtain fast and accurate approximations of the eigenvalues

$$\lambda_j(T_n(f)) \approx \sum_{k=0}^{\alpha} \tilde{c}_k(\theta_{j,n})h^k = \sum_{k=0}^{\alpha} \left(\tilde{c}_k^{\Re}(\theta_{j,n}) + \mathbf{i}\tilde{c}_k^{\Im}(\theta_{j,n})\right) h^k. \tag{2}$$

The proposed interpolation–extrapolation algorithm works even if the simple Toeplitz matrix $T_n(f)$ in (2) is replaced by a more general Toeplitz-like matrix (such as a preconditioned or block Toeplitz matrix, a PDE discretization matrix, a generalized locally Toeplitz matrix, etc.). Moreover, the algorithm is applicable even if the symbol f is not known or does not describe the eigenvalue distribution of $\{T_n(f)\}_n$.

We show examples where matrix-less methods yield machine precision accuracy "instantaneously" (i.e., seconds vs. days for standard solvers) when approximating eigenvalues. The necessity for high precision computations, as opposed to double precision, will also be demonstrated with multiple examples.

In future research, we will focus on matrices with non-monotone, multivariate, non-Hermitian, and diagonal sampling symbols. Developing the same techniques for eigenvectors is also an interesting extension. Collaborations for the use of matrix-less methods for solving real-world physical problems are welcome.

[1] Barrera M., Böttcher A., Grudsky S.M., and Maximenko E.A., *Eigenvalues of even very nice Toeplitz matrices can be unexpectedly erratic.* In: Böttcher A., Potts D., Stollmann P., Wenzel D. (eds) The Diversity and Beauty of Applied Operator Theory. Operator Theory: Advances and Applications, 268. Birkhäuser, Cham, 2018

[2] A.A. Batalshchikov, S.M. Grudsky, I.S. Malisheva, S.S. Mihalkovich, E. Ramírez de Arellano, and V.A. Stukopin, *Asymptotics of eigenvalues of large symmetric Toeplitz matrices with smooth simple-loop symbols*, Linear Algebra and its Applications, 580 pp. 292–335 (2019)

[3] S.-E. Ekström, I. Furci, and S. Serra-Capizzano, *Exact formulae and matrix-less eigensolvers for block banded symmetric Toeplitz matrices*, BIT Numerical Mathematics, 58(4), pp. 937–968 (2018)

[4] S.-E. Ekström and C. Garoni, *A matrix-less and parallel interpolation–extrapolation algorithm for computing the eigenvalues of preconditioned banded symmetric Toeplitz matrices*, Numerical Algorithms, 80, pp. 819–848 (2019)

[5] S.-E. Ekström, C. Garoni, and S. Serra-Capizzano, *Are the Eigenvalues of Banded Symmetric Toeplitz Matrices Known in Almost Closed Form?*, Experimental Mathematics, 27(4), pp. 478–487 (2017)

[6] C. Garoni and S. Serra-Capizzano, *Generalized Locally Toeplitz Sequences: Theory and Applications (Volume I)*, Springer, Cham, 2017

[7] `https://www.2pi.se/publications`

Algorithmic differentiation:
Sensitivity analysis and the computation of adjoints

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The provision of exact and consistent derivative information is important for numerous applications arising from optimisation purposes as for example optimal control problems. However, even the pure simulation of complex systems may require the computation of derivative information. Implicit integration methods are prominent examples for this case.

The talk will present the technique of algorithmic (or automatic) differentiation (AD) [1] to compute exact derivative information for function evaluations given as computer programs. This includes a short overview of the history of AD and a description of the main variants of AD, namely the forward mode to compute sensitivities and the reverse mode for the provision of adjoints. A discussion of complexity estimates follows yielding the important cheap gradient result.

To illustrate the importance of structure exploitation also for the use of AD an example from an industrial application will be presented, see [2]. It covers the complete design chain in Computational Fluid Dynamics (CFD), i.e., incorporates the parameterization of the object to be optimized like, e.g., a turbine blade, the usage of a Computer Aided Design (CAD) tool to actually construct the air foil and a flow solver to compute the flow around the air foil. The optimization of such a complete design chain that includes a CAD tool is still a severe challenge. We discuss how AD can be applied to the CAD kernel and a suitable flow solver taking also the complexity of the derivative information into account. We will see that a gradient-based optimization using adjoint information is the only tractable way. Numerical results for the optimization of the TU Berlin stator as one example from turbo machinery are shown. This includes also a verification of the computed derivatives.

References

[1] A Griewank and A Walther: *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation, Second Edition. SIAM (2008).*.

[2] M Banović, I Vasilopoulos, A Walther, and M Meyer: *Algorithmic differentiation of an industrial airfoil design tool coupled with the adjoint CFD method*. Optimization and Engineering, to appear.

Recent Advances in Riccati-Feedback Stabilization of a Two-Phase Stefan Problem

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Our goal is the linear-quadratic feedback stabilization of a two-dimensional two-phase Stefan problem. The Stefan problem can model solidification and melting of pure materials and gets its name from the purely algebraic Stefan condition which describes the coupling between the temperature of the material and its melting process.

After linearization and discretization, the stabilization problem results in anon-autonomous differential Riccati equation (DRE) with differential-algebraic structure. The two phases in the domain evolve, which causes all coefficients of the resulting DRE to be time-varying. The problem specific collocation of Dirichlet conditions and outputs require special techniques for the finite element discretization.

Since all coefficients are time-varying, existing DRE solvers have to be adapted to this highly non-autonomous case which has significantly increased computational costs and memory requirements. We present the most recent techniques to tackle the difficulties and show first results of the application of our feedback stabilization.

A benchmark for fluid rigid body interaction with standard CFD packages

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The interaction between a fluid flow and rigid bodies appears in many physical applications. The flow around a free rigid body causes both displacement and rotation of that body while the motion of the body causes changes in the flow. The complexity that comes with coupling models for fluid and rigid bodies and the numerical challenges due to the interaction make reliable and benchmark computations necessary though difficult to perform. The presented benchmark targets the free rotation of a spherical object in a flow channel. This setup extends the benchmark *flow past a cylinder* [1] and is accessible to standard CFD software.

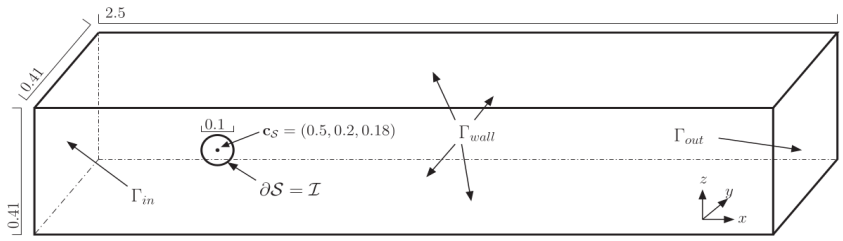

Figure 1: Spatial configuration of the 3D setup.

In this setup the flow applies a torque force on the object. The induced rotation then couples back to the flow via the boundary conditions. The proposed benchmark configurations comprise two and three spatial dimensions and quasi-stationary (low Reynolds-number) and periodic (high Reynolds-number) regimes. For a discretization independent comparison of the results, we also propose a set of significant, nondimensionalized characteristic values. The benchmark cases were solved numerically with various approaches and software tools so that the computed characteristic values could be reported within a reasonable confidence interval.

In this talk, we introduce the mathematical model, discuss the characteristic and challenges of the benchmark cases, and present the various implementation and their particular advantages. The codes that were reported on in our work [2] as well as the raw data and postprocessing routines are available [3] for further exploration and for reproduction.

References

[1] M Schäfer and S Turek: *Benchmark computations of laminar flow around a cylinder.* Flow Simulation with HPC II. DFG priority research program results 1993-1995, 1996.

[2] H von Wahl et al.: *Numerical benchmarking of fluid-rigid body interactions*. Computers & Fluids, 2019.

[3] DOI:10.5281/zenodo.3253455

Data-Efficient Convolution on Irregular FE-Meshes Applied to a 3D Fracture Healing Simulation

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The present work deals with a specific step of a fracture healing simulation (see e.g. [1], [2]). In this step, the given concentration distribution of a biological tissue, such as bone, is *smoothed* (i.e. *smeared* over the three-dimensional healing domain). The current implementation of this *smoothing* operation in the form of a matrix-vector multiplication turns out to be a runtime-critical component in *large* simulation scenarios.

We therefore transfer the original problem definition step by step into an alternative problem definition. Ultimately, this leads to an algorithm in which the smoothing is performed in multiple steps, i.e. iteratively. In each of these steps, a matrix vector product is evaluated. The advantage of this approach over the original approach is that the matrix used here requires significantly less memory space. An analytical estimation indicates that a considerable increase in performance can be expected.

Extensive numerical experiments reveal some characteristics of the different methods and confirm theoretical considerations. Here we focus especially on the numerical errors and the runtime of the algorithms. By using the iterative approach, acceleration factors in the order of 70 can be observed, which is primarily due to the reduction of the memory consumption for the matrix.

Final critical considerations show in particular the influence of the row-wise normalization of the matrix on the result of the smoothing. In addition, some disadvantages of the currently used matrix class with respect to the flexibility in the choice of data types are presented, which suggest a modification of our implementation. This would lead to a further drastic reduction in memory consumption and thus to an additional increase in performance.

Acknowledgements

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References

[1] U. Simon, P. Augat, M. Utz & L. Claes (2011): *A numerical model of the fracture healing process that describes tissue development and revascularisation*, Computer Methods in Biomechanics and Biomedical Engineering, 14:1, 79-93.

[2] F. Niemeyer, L. Claes, A. Ignatius, N. Meyers, U. Simon (2018): *Simulating lateral distraction osteogenesis*. PLOS ONE 13(3): e0194500.

Numerical Algorithms for Forward-Backward Parabolic PDEs

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Partial differential equations (PDEs) of forward-backward parabolic type have been advocated for image enhancement since more than five decades [1,2]. The ill-posedness of the backward parabolic term, however, makes it challenging to design adequate numerical algorithms. Further difficulties can arise from pronounced anisotropies and specific application-driven requirements such as stability in the maximum norm or a high degree of rotation invariance.

In this talk we discuss a number of fairly general numerical ideas to handle these challenges [3,4]. This includes nonstandard finite difference approximations and sequential splittings into highly localised processes, but also ideas from the numerics of hyperbolic PDEs such as upwinding, minmod schemes, and curvature limiters. Combining these concepts in an appropriate way allows to come upwith stability guarantees that reflect key properties of the continuous models.

Our experiments with forward-and-backward (FAB) diffusion and evolutions of Gabor type demonstrate the practical usefulness and the good performance of the resulting algorithms.

Joint work with Martin Welk (UMIT, Hall, Austria) and Guy Gilboa (Technion, Haifa, Israel).

References:

[1.] D. Gabor: Information theory in electron microscopy. Laboratory Investigation, Vol. 14, pp. 801-807, 1965.

[2.] G. Gilboa, N.A. Sochen, Y.Y. Zeevi: Forward-and-backward diffusion processes for adaptive image enhancement and denoising. IEEE Transactions on Image Pocessing, Vol. 11, No. 7, pp. 689-703, 2002.

[3.] M. Welk, J. Weickert, G. Gilboa: A discrete theory and efficient algorithms for forward-and backward diffusion filtering. Journal of Mathematical Imaging and Vision, Vol. 60, No. 9, pp. 1399-1426, Nov. 2018.

[4.] M. Welk, J. Weickert: PDE evolutions for M-Smoothers: From common myths to robust numerics. In J. Lellmann, M. Burger, J. Modersitzki (Eds.): Scale Space and Variational Methods. Springer Lecture Notes in Computer Science, Vol. 11603, pp. 236--248, 2019.

2D Simulations of Piezoelectric PDEs as a Basis for Electrode Shape Optimization

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Piezoelectric materials are nowadays present in many areas from high-end to everyday life applications. Their ability, the so-called piezoelectric effect, is to generate an electrical discharge as a response to mechanical stresses and vice-versa. This piezoelectric effect depends on material parameters. Therefore it is of crucial importance to determine these parameters. One possibility to obtain this information is via measurements, however this implies large experimental costs. A more efficient approach is to employ only electrical impedance and the sensitivities with respect to the parameters of the piezoceramic and use this information to solve an inverse problem to obtain the material parameters.

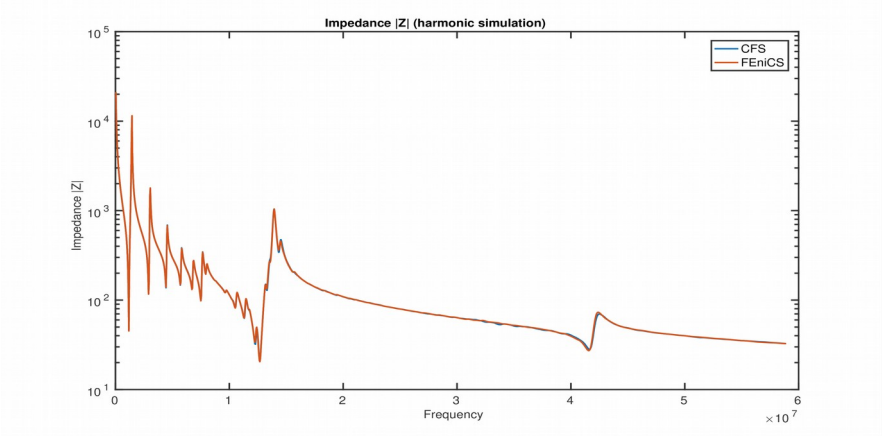

Figure 1: Impedance simulation of a 2D piezoceramic disk model.

We consider a rotationally symmetric 2D representation of a piezoelectric ceramic disk which behaviour can be described by a damped 2nd order PDE system with neglected thermal effects. As the first step two different FEM-based simulations are performed using FEniCS and CFS++, in order to compute the impedance for given material data, see Figure 1. Next, by using the measured or simulated impedance, we are able to compute the sensitivities with respect to the material parameters. Certain sensitivities are too low and have to be increased.

For this reason we employ shape or topology optimization approaches for electrodes on top and bottom of the piezoceramic, to increase the sensitivities for an improved solution of the inverse problem.

Acknowledgments

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Simulation of a two-dimensional induction machine with Multigrid-reduction-in-time (MGRIT)

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Due to modern developments in traffic, global warming, and the energy transition, efficient and robust designs of electrical machines are again becoming increasingly important. A major time factor in the design process is the simulation of the behavior of the electrical machine, which is in general based on the so-called magnetoquasistatic approximation or eddy current problem [1]. The discretization of the eddy current problem yields an initial value problem (IVP) for a system of differential-algebraic equations (DAEs), that can be solved by computing one time step after the other. For long time simulations, computational costs are high.

Parallel-in-time methods make use of modern parallel computers and allow us to reduce the time-to-solution for time-dependent evolutionary problems, such as the eddy current problem. The Multigrid-reduction-in-time (MGRIT) [2] algorithm, one parallel-in-time method, uses a time-grid hierarchy for calculating multiple time steps simultaneously. One key advantage of MGRIT compared to other parallel-in-time approaches is its non-intrusiveness, i.e., MGRIT allows reusing existing time propagators and their integration into a parallel framework.

In this talk, we apply the MGRIT algorithm to the eddy current problem of a two-dimensional induction machine and compare the runtime of the time-parallel MGRIT algorithm with the runtime of the sequential forward solve. Furthermore, we add spatial coarsening to the temporal-coarsening strategy of the MGRIT algorithm and investigate the behavior for different relaxation and coarsening strategies. Results demonstrate a significant speedup in comparison with sequential timestepping. Moreover, the use of spatial-coarsening allows efficient simulation of more accurate models.

Acknowledgments

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References

[1] Haus, H.A., Melcher, J.R.: Electromagnetic Fields and Energy. Prentice-Hall (1989)
[2] R. Falgout et al.: Parallel time integration with multigrid. SISC, 2014

Optimizing MGRIT and Parareal coarse-grid operators for linear advection

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Hardware trends and scaling limits have driven the development of algorithms that allow space-time parallelism. These methods consider the solution of time-dependent systems of partial differential equations (PDEs), and allow simultaneous solution across multiple time steps, in contrast to classical time-stepping approaches considering the sequential solution of one time step after the other. While parallel-in-time methods, such as multigrid-reduction-in-time (MGRIT) [1] and Parareal [2] have been very successful for parabolic equations, it has often been observed that their performance suffers dramatically when applied to advection-dominated problems or purely hyperbolic PDEs using standard rediscretization approaches on coarse grids.

In this talk, we apply MGRIT or Parareal to the coonstant-coefficient linear advection equation, appealing to existing convergence theory to provide insight into the typically non-scalable or even divergent behavior of these solvers for this problem. To overcome these failings, we replace rediscretization on coarse grids with near-optimal coarse-grid operators that are computed by applying optimization techniques to approximately minimize error estimates from the convergence theory.

Our approach is tested on discretizations of various orders that use explicit or implicit Runge-Kutta time integration with upwind-finite-difference spatial discretizations, for which we obtain fast and scalable solvers in all cases. Parallel tests also demonstrate significant speed-ups over sequential time-stepping. Our main finding is that, in order to obtain fast convergence as for parabolic problems, coarse-grid operators should take into account the behavior of the hyperbolic problem by tracking the characteristic curves. Our insight is implemented for linear advection using an optimization approach, but the principle is general, and provides a key idea for solving the long-standing problem of efficient parallel-in-time integration for hyperbolic PDEs.

References

[1] R. Falgout et al.: *Parallel time integration with multigrid.* SISC, 2014.
[2] J.-L. Lions et al.: *Résolution d'EDP par un schéma en temps pararéel.* C. R. Acad. Sci., 2001.

Inverse iterations for the non-linear Schrödinger eigenvalue problem

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This talk presents a new generalized inverse iteration for nonlinear eigenvector problems of Gross-Pitaevskii (or nonlinear Schrödinger) type. On the one hand, a simple damping strategy inspired by energy-decreasing discrete gradient flows yields global qualitative convergence towards an eigenfunction. On the other hand, a local linear rate of convergence is established. The latter quantitative convergence analysis is closely connected to the method's unique feature of sensitivity with respect to spectral shifts. Contrary to classical gradient flows this allows both the selective approximation of excited states as well as the amplification of convergence beyond linear rates in the spirit of the Rayleigh quotient iteration for linear eigenvalue problems. These advantageous convergence properties are demonstrated in a series of numerical experiments involving exponentially localized states under disorder potentials and vortex lattices in rotating traps.

References

[1] R. Altmann, P. Henning and D. Peterseim. The J-method for the Gross-Pitaevskii eigenvalue problem. *ArXiv e-prints*, 1908.00333, 2019.

[2] P. Henning and D. Peterseim. Sobolev gradient flow for the Gross-Pitaevskii eigenvalue problem: global convergence and computational efficiency. *ArXiv e-prints*, 1811.06319, 2018.

[3] R. Altmann, P. Henning, and D. Peterseim. Quantitative Anderson localization of Schrödinger eigenstates under disorder potentials. *ArXiv e-prints*, 1803.09950, 2018.

Assembly constraint fit during gradient-based shape optimization of the TU Berlin Stator

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Shape optimization in industrial workflows is usually performed on individual components of a product rather than considering complex CAD (*Computer Aided Design*) models that define the complete product's assembly. However, the optimal shape of a component may cause a collision with adjacent components when re-inserting it in the assembly CAD model. This would imply further changes on the component's geometry which would impair the optimality of the shape. Therefore, it is of crucial importance to respect assembly constraints during the optimization. One type of assembly constraint is related to fasteners such as bolts and screws, that serve to connect various components in the product's assembly. Such a constraint is defined for the TU Berlin (TUB) *TurboLab* Stator test-case, which is a component used in modern jet-engine compressors. In particular, the optimal blade has to accommodate four mounting bolts (cylinders) that serve to mount the blade to its casing. To tackle this requirement, a gradient-based workflow has been developed in this study in order to integrate a CAD kernel into an optimization loop. However, computing CAD gradients is a challenging task and typically this information is not provided within CAD systems.

For this reason, algorithmic differentiation (AD) is applied to the open-source CAD kernel Open CASCADE Technology (OCCT) to obtain the so-called *geometric sensitivities*, e.g. derivatives of a surface point with respect to design parameters of the CAD model to be optimized. Next, the differentiated OCCT is coupled with a discrete adjoint CFD (*Computational Fluid Dynamics*) solver developed at Queen Mary University of London, also produced by AD. This completely differentiated design chain is employed to perform the aerodynamic shape optimization of the TUB stator blade, with the aim to minimize the total pressure loss. Moreover, an automatic positioning of the cylinders during the optimization is accomplished using the derivative information from the differentiated OCCT.

The gradient-based optimization with a high-fidelity CFD simulation converged after 42 iterations and yields 14% reduction of the objective function. Moreover, the developed approach ensures there is no collision between the optimal blade and the cylinders.

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REDUCED BASIS METHOD FOR PARAMETER FUNCTIONS WITH APPLICATION IN QUANTUM MECHANICS

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Often Quantum systems are studied under isolated conditions. However, the influence of external potentials on quantum systems are of major interest, both for quantum physics and quantum chemisty. For instance, controlling chemical reactions leads to a PDE constrained bilinear optimal control problem, where the the external potential arises in the time-dependent linear Schrödinger equation as a reaction term, or more precisely: Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with smooth boundary, $\mathscr{I} := (0,T)$ a time interval and $\mu_d \in L_2(\Omega,\mathbb{C})$ a desired state. Then, following [1], for suitable seperable Hilbert spaces $\mathscr{X}$ and $\mathscr{P}$, the PDE constrained bilinear optimal control problem reads:

$$\min_{(\psi,\mu)\in(\mathscr{X},\mathscr{P})} J(\psi,\mu) = \frac{1}{2}\|\psi(T,x)-\mu_d\|^2_{L_2(\Omega,\mathbb{C})} + \frac{\alpha}{2}\|\mu\|^2_{\mathscr{P}}$$

such that $(\psi,\mu) \in (\mathscr{X},\mathscr{P})$ solves

$$\mathrm{i}\,\partial_t\psi(t,x) = -\frac{1}{2}\Delta_x\psi(t,x) + \mu(t,x)\psi(t,x) + g(t,x), \qquad (t,x) \in \mathscr{I}\times\Omega$$

together with suitable boundary conditions. Aim of this project is to solve the PDE constrained bilinear optimal control problem in a real-time context by reducing the so called *control-to-state operator* within the *Reduced Basis Method* (RBM), where the external potential is interpreted as a variable reaction coefficient and therefore - in the language of the RB theory - as a parameter function. Typically, in the theory of the RBM the parameter space $\mathscr{P}$ is given by a finite-dimensional subset of $\mathbb{R}^P$, $P \in \mathbb{N}$. However, in our case it holds $\dim(\mathscr{P}) = \infty$. While finite-dimensional parameter spaces have been extendively studied in recent decades, there has been done little work on the infinite-dimensional setting so far. First progress in this direction has been made by [3], where the initial condition of a parabolic partial differential equation is interpreted as a parameter function. The main idea used in [3] is to split the problem into two subproblems and dealing with this subproblems by using a so called *Two-Step-Greedy-Algorithm*. However, since the parameter function arises in the reaction term this approach is not employable in our case.

It is well-known that if the constrained equation is well-posed according to the Banach-Nĕcas theorem we get both, the existence of an optimal control and the existence of a control-to-state operator. In our work we want to consider a space-time variational formulation of the constrained equation. Although there are existing many well-posedness results for the Schrödinger equation in the literature, see e.g. [2], all results, known to us, provide no basis to construct a well-posed space-time variational formulation according to the Banach-Nĕcas theorem. In this talk we want to present a well-posedness result, which provides a basis for a well-posed space-time variational formulation, along with the theory of dealing with parameter function arising as coefficient varaibles. Numerical experiments according to a stable space-time finite element discretization will be also presented.

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References

[1] L. Baudouin, O. Kavian, and J.-P. Puel. Regularity for a schroedinger equation with singular potentials and application to bilinear optimal control. *Journal of Differential Equations*, 216(1):188 – 222, 2005.

[2] R. Dautray and J.-L. Lions. *Mathematical Analysis and Numerical Methods for Science and Technology, Volume 5, Evolution Problems I.* Springer-Verlag Berlin Heidelberg, 2000.

[3] A. Mayerhofer and K. Urban. *A Reduced Basis Method for Parameter Functions Using Wavelet Approximations*, pages 77–90. Springer International Publishing, Cham, 2017.