GAMM Workshop on Applied and Numerical Linear Algebra

University of Augsburg

October 5-6, 2023

The GAMM Activity Group on Applied and Numerical Linear Algebra (ANLA) aims at fostering collaboration in its field through the organization of scientific conferences and workshops. The Activity Group aims to provide a platform of communication for all involved researchers in Germany, Europe, and world-wide, and maintains close links with the SIAM Special Activity Group on Applied Linear Algebra and ILAS (International Linear Algebra Society).

This is the annual workshop of the GAMM ANLA Activity Group. It focusses on recent advances in numerical linear algebra methods and their use in applied mathematics, physics, engineering and data science. We welcome contributions on topics including but not limited to:

- eigenvalue problems
- matrix functions
- linear systems
- least squares problems
- tensor methods
- inverse problems
- optimization.

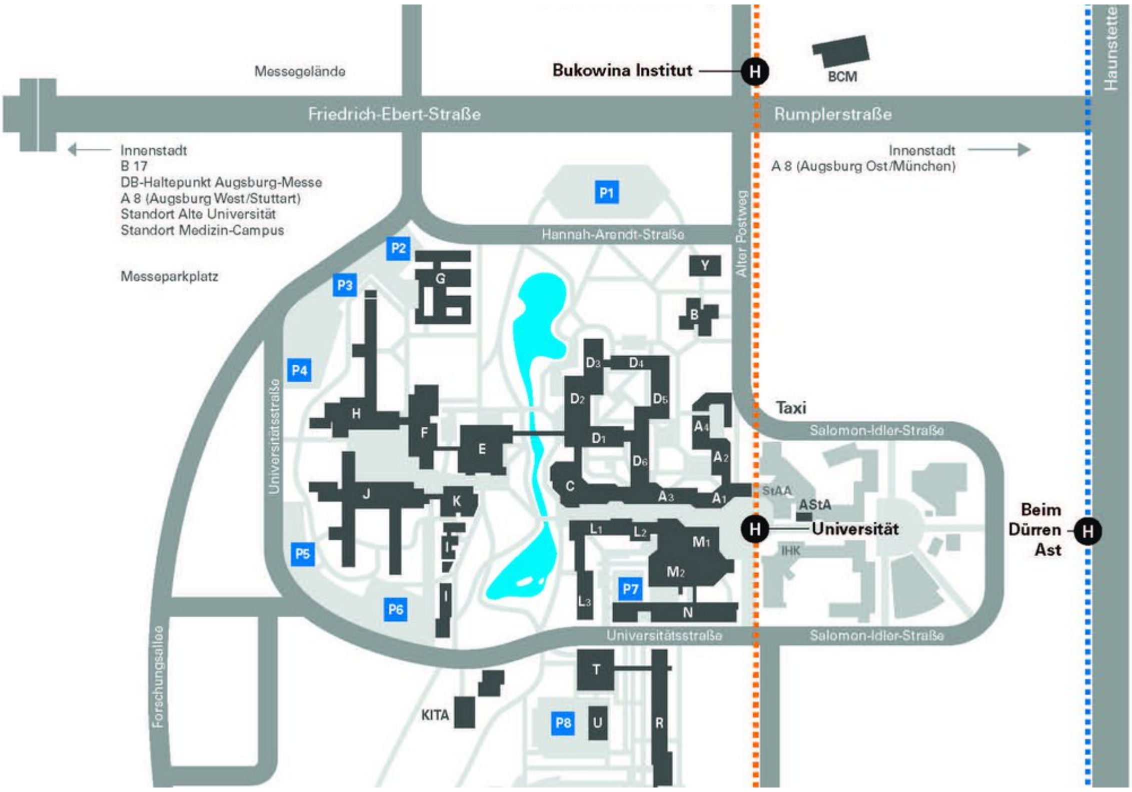
Organizing committee

Tatjana Stykel
André Uschmajew

Conference venue

The workshop takes place on the main campus of the University of Augsburg.

Address: Building C, Room HS IV
Universitätsstraße 10, 86159 Augsburg



Business meeting

The GAMM ANLA Business Meeting takes place on October 5, 2023 at 5:15 pm in Bulding L1, Room 1005.

Conference dinner

The conference dinner takes place on October 5, 2023 at 7:00 pm in *Riegele Wirtshaus*.

Address: Frölichstraße 26, 86150 Augsburg

Program

Thursday, October 5

9:00 – 9:25	**Welcome/Registration**	Building C, 2nd floor
9:25 – 9:30	**Opening**	Building C, Room HS IV
9:30 – 10:20	PL: **Karl Meerbergen** (KU Leuven) Rational approximation and linearization of matrix valued functions: algorithms and applications	
10:20 – 10:45	CT: **Ranjan Kumar Das** (MPI Magdeburg) Structured linearizations for Hermitian matrix polynomials preserving sign-characteristics	
10:45 – 11:15	**Coffee break**	Building C, 2nd floor
11:15 – 11:40	CT: **Ivana Kuzmanović Ivičić** (University of Osijek) Perturbation bounds for stable gyroscopic systems in motion about unstable equilibrium position	
11:40 – 12:05	CT: **Elias Jarlebring** (KTH Stockholm) Linearizability of eigenvector nonlinearities	
12:05 – 12:30	CT: **Thomas Mach** (University of Potsdam) Solving the parametric eigenvalue problem by Taylor series and Chebyshev expansion	
12:30 – 14:00	**Lunch**	
14:00 – 14:50	PL: **Ralf Zimmermann** (University of Southern Denmark) On classical and symplectic Stiefel and Grassmann manifolds and their applications in Riemannian interpolation, optimization, and model reduction	
14:50 – 15:15	CT: **Tatjana Stykel** (University of Augsburg) Computing symplectic eigenpairs of symmetric positive-semidefinite matrices via symplectic trace minimization	
15:15 – 15:45	**Coffee break**	Building C, 2nd floor
15:45 – 16:10	CT: **Thomas Bendokat** (MPI Magdeburg) Manifold structure of symmetric quasi-definite matrices	
16:10 – 16:35	CT: **Volker Mehrmann** (TU Berlin) Numerical methods for linear systems where the coefficient has semidefinite symmetric part	
16:35 – 17:00	CT: **Ieva Daužickaitė** (Charles University) Stability of mixed precision FGMRES	
17:15 – 18:00	**GAMM ANLA Business Meeting**	Building L1, Room 1005/zoom
19:00	**Conference dinner**	

Program

Friday, October 6

09:30 – 10:20	PL: **Virginie Ehrlacher** (École des Ponts ParisTech & INRIA) Sparse semidefinite programming for multimarginal quantum optimal transport problems
10:20 – 10:45	CT: **Daniel Kressner** (EPFL) Low-rank tree tensor network representation of Hamiltonians with long-range pairwise interaction
10:45 – 11:15	**Coffee break** Building C, 2nd floor
11:15 – 11:40	CT: **Josie König** (University of Potsdam) Balancing meets Bayesian inference
11:40 – 12:05	CT: **Jan Papež** (Czech Academy of Sciences) Algebraic error in AFEM
12:05 – 12:30	CT: **Yongseok Jang** (The French Aerospace Lab ONERA) Advanced GMRES methods with randomized orthogonalization
12:30 – 12:35	**Closing**

Sparse semidefinite programming for multimarginal quantum optimal transport problems

Virginie Ehrlacher, Luca Nenna

École des Ponts ParisTech & INRIA

Quantum optimal transport problems arise in various applications including quantum chemistry and quantum computing. For instance, the so-called Lieb functional, which is a key quantity for the computation of the electronic structure of molecules, can be expressed as a particular instance of multimarginal quantum optimal transport. Naive discretization methods for this type pf problems lead to very high-dimensonal semi-definite programming problems, the dimension of which scales exponentially with the number of electrons. In this talk, I will present some recent results about a new discretization approach for this type of problems which lead to sparse semidefinite programming problems which paves the road towards numerical algorithms in order to circumvent the curse of dimensionality. Recent results about the mathematical analysis of these algorithms will be presented, together with preliminary encouraging numerical results on some illustrative test cases.

Rational approximation and linearization of matrix valued functions: algorithms and applications

Karl Meerbergen

KU Leuven

The last twenty years, the computation of invariant pairs of nonlinear eigenvalue problems has gained attention. A nonlinear eigenvalue problem is an eigenvalue problem of a pencil that is not linear but nonlinear in the eigenvalue. Rational approximation such as AAA (Adaptive Antoulas Anderson) transform the nonlinear matrix valued function into a rational matrix. This rational matrix is further transformed to a generalized eigenvalue problem. We also show other applications of this approach: the solution of linear systems with nonlinear frequency dependencies in the time domain and time domain vector fitting.

On classical and symplectic Stiefel and Grassmann manifolds and their applications in Riemannian interpolation, optimization, and model reduction

Ralf Zimmermann

University of Southern Denmark, Department of Mathematics and Computer Science

The set of orthonormal p-frames, i.e., the collection of all p-dimensional, ordered orthonormal bases of the real Euclidean n-space carries a differentiable structure and is known as the (compact) Stiefel manifold. Associated with the Stiefel manifold is the Grassmann manifold of p-dimensional subspaces that are spanned by such orthonormal frames. Stiefel and Grassmann manifolds feature in a large variety of Riemannian computing problems in science and engineering, including image processing, machine learning and model reduction.

In this talk, we present a collection of classical and new facts about the numerical treatment of Stiefel and Grassmann manifolds. A special focus will be on the efficient computation of the so-called Riemannian normal coordinates for these manifolds. The Riemannian normal coordinates are based on the shortest connections between two manifold locations and are thus fundamental to almost every data processing task. They also help in the derivation and assessment of retraction maps, which are first-order approximations of the normal coordinates and can be used as efficient substitutes in practical applications.

For even-dimensional vector spaces that are equipped with a symplectic bilinear form, symplectic bases can be considered. Symplectic structures feature most prominently in Hamiltonian mechanics, and, in turn, in structure-preserving model reduction for Hamiltonian systems. Following the construction in Euclidean spaces, the symplectic Stiefel and Grassmann manifolds can be introduced and exploited. We will discuss the computation of Riemannian normal coordinates for these manifolds as well, expose challenges and point to open problems.

Whenever suitable, we illustrate the theory with numerical examples, where we consider applications of Riemannian interpolation, optimization and model reduction.

Manifold structure of symmetric quasi-definite matrices

Thomas Bendokat, Peter Benner

Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Symmetric quasi-definite (SQD) matrices feature a block structure with a symmetric positive-definite block and a symmetric negative-definite block on the diagonal. They arise in applications such as interior point methods and determine indefinite inner products. The set of all SQD matrices forms a cone and is a manifold. We see how to set up this manifold as a quotient space by making use of Lie theory to get a Riemannian structure suitable for optimization tasks.

Structured Linearizations for Hermitian Matrix Polynomials Preserving Sign-characteristics

Ranjan Kumar Das

Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Structured matrix polynomials play a crucial role in various applications, necessitating the development of structure-preserving linearizations from a computational perspective. We focus on a specific subset of Fiedler-like linearizations to create Hermitian linearizations that retain the sign characteristic of Hermitian matrix polynomials. Additionally, we introduce the construction of banded pencils with low bandwidth, enhancing the efficiency of numerical computations involving these structured matrix polynomials.

Stability of mixed precision FGMRES

Erin Carson, Ieva Daužickaitė

Charles University, Prague

In this talk, we focus on the flexible generalised minimal residual method (FGMRES) for solving systems of linear equations. A mixed precision framework with split-preconditioning is considered. Here four potentially different precisions can be used for computations with the coefficient matrix, application of the left preconditioner, and application of the right preconditioner, and the working precision. We will present bounds on the backward and forward errors in split-preconditioned FGMRES and provide insight into how the various precisions should be chosen.

Perturbation bounds for stable gyroscopic systems in motion about unstable equilibrium position

Ivana Kuzmanović Ivičić, Suzana Miodragovic

University of Osijek

We consider relative perturbation bounds for stable linear gyroscopic systems

$$M\ddot{x}(t) + G\dot{x}(t) + Kx(t) = 0,$$

where $M, K \in \mathbb{R}^{n\times n}$ are symmetric, M is positive definite, K is negative definite and $G \in \mathbb{R}^{n\times n}$ is skew-symmetric such that $G > kM - k^{-1}K$ for some $k > 0$. This means that all of the eigenvalues of the system are pure imaginary and semi-simple.
For this kind of systems, we present an upper bound for the relative change in eigenvalues as well as the $\sin\Theta$ type bound for the corresponding eigenvectors under the perturbation of the system matrices. The performance of obtained bounds is illustrated by numerical experiments.

Advanced GMRES methods with randomized orthogonalization

Yongseok Jang, Laura Grigori, Emeric Martin, Cedric Content
The French Aerospace Lab ONERA

A randomized Gram–Schmidt algorithm is advantageous in terms of computational costs and numerical stability for high-dimensional spaces. Random sketching is applied to the generalized minimal residual method (GMRES) for orthogonalizing Krylov basis vectors. Although the Krylov basis is not strictly l^2 orthonormal, its random projection onto the low-dimensional space exhibits l^2 orthogonality. Improved numerical stability is observed, independent of the problemś dimension, even for extreme-scale problems. On the other hand, as the Harmonic Ritz values are commonly used in GMRES with deflated restarting (GMRES-DR) to improve convergence, we develop the randomized GMRES-DR. Furthermore, we consider another deflation strategy, for instance disregarding the singular vectors associated with the smallest singular values. We thus introduce a new algorithm of the randomized flexible GMRES with singular value decomposition (SVD) based deflated restarting. We carry out some numerical experiments in the context of compressible turbulent flow simulations. Our proposed approach exhibits a quite competitive numerical behaviour to existing methods while reducing computational costs. Lastly, a novel augmentation method based on small singular vectors for randomized GMRES is addressed.

Linearizability of eigenvector nonlinearities

Elias Jarlebring, Rob Claes, Karl Meerbergen, Parikshit Upadhyaya
KTH Stockholm

We present a method to linearize, without approximation, a specific class of eigenvalue problems with eigenvector nonlinearities (NEPv), where the nonlinearities are expressed by scalar functions that are defined by quotient of linear functions of the eigenvector. The exact linearization relies on an equivalent multiparameter problem (MEP) that contains the exact solutions of the NEPv. Based on the linearization we propose numerical schemes that exploit the structure of the linearization.

Balancing meets Bayesian inference

Josie König, Melina A. Freitag

University of Potsdam

Data assimilation describes the seamless integration of large amounts of data into computational models. During the process, Bayesian inverse problems have to be solved, which requires a high computational cost. For this reason, model order reduction (MOR) is necessary to obtain cost-effective surrogate models that closely approximate the true behavior. In system theory, MOR is a long-researched topic of great interest. We apply established system-theoretic MOR techniques to Bayesian inference, mainly focusing on balancing-related ideas.

Low-rank tree tensor network representation of Hamiltonians with long-range pairwise interaction

Gianluca Ceruti, Daniel Kressner, Dominik Sulz

École Polytechnique Fédérale de Lausanne

Finding compact representations of operators is a crucial task when simulating high-dimensional quantum spin systems. This talk introduces new low-rank tree tensor network representation of Hamiltonians with long-range interacting particles. The construction relies on a correspondence between the chosen tree structure for the tree tensor network and a corresponding hierarchical decomposition of the interaction matrix. The tree tensor network representation allows a compact and memory-reduced representation of the operator. Numerical experiments for different quantum spin systems validate the results and compare how different tree structures influence the compactness of the represented operator.

Solving the parametric eigenvalue problem by Taylor series and Chebyshev expansion

Thomas Mach, Melina A. Freitag, Jan Martin Nicolaus, Pavel Kriz

University of Potsdam

We discuss two approaches to solving the parametric (or stochastic) eigenvalue problem. One of them uses a Taylor expansion and the other a Chebyshev expansion. The parametric eigenvalue problem assumes that the matrix A depends on a parameter μ, where μ might be a random variable. Consequently, the eigenvalues and eigenvectors are also functions of μ. We compute a Taylor approximation of these functions about μ_0 by iteratively computing the Taylor coefficients. The complexity of this approach is $O(n^3)$ for all eigenpairs, if the derivatives of $A(\mu)$ at μ_0 are given. The Chebyshev expansion works similarly. We first find an initial approximation iteratively which we then refine with Newton's method. This second method is more expensive but provides a good approximation over the whole interval of the expansion instead around a single point.

We present numerical experiments confirming the complexity and demonstrating that the approaches are capable of tracking eigenvalues at intersection points. Further experiments shed light on the limitations of the Taylor expansion approach with respect to the distance from the expansion point μ_0.

Finally, we present a dynamical system depending on a parameter μ. We estimate μ based on a recorded trajectory of the system using a kernel density estimator.

Numerical methods for linear systems where the coefficient has semidefinite symmetric part

Murat Manuoglu, Volker Mehrmann

TU Berlin

Many linear systems have coefficient matrices with positive semidefinite symmetric part, in particular those arising from the discretization of dissipative Hamiltonian systems and those arsing optimality systems of optimization problems. We discuss a new class of robust iterative solvers for this class of problems that is based preconditioning and the null-space method. We illustrate the new method by several examples from fluid dynamics.

Algebraic error in AFEM

Jan Papež
Czech Academy of Sciences

Adaptive finite element method (AFEM) for solving numerical PDEs is a well-established technique that generates a sequence of locally refined meshes together with a sequence of associated algebraic systems. Standardly, the approximation computed on the previous mesh is interpolated to the new one as an initial guess for an iterative solver. Then, however, the algebraic error (which is represented not only as a vector but also as a function in the solution domain) can be dominated by smooth components yielding a slow convergence of the solver.

Computing symplectic eigenpairs of symmetric positive-semidefinite matrices via symplectic trace minimization

Pierre-Antoine Absil, Bin Gao, Nguyen Thanh Son, Tatjana Stykel*
*University of Augsburg

We address the problem of computing the smallest symplectic eigenvalues and the corresponding symplectic eigenvector pairs of symmetric positive-semidefinite matrices in the sense of Williamson's theorem. This eigenvalue problem can be formulated as a trace minimization problem on the symplectic Stiefel manifold. We first investigate various theoretical aspects of this optimization problem such as characterizing the sets of critical points, saddle points, and global minimizers. Based on constructing Riemannian structures on the symplectic Stiefel manifold, we then present a numerical procedure for computing symplectic eigenpairs in the framework of Riemannian optimization. Numerical examples demonstrate the properties of the proposed algorithm.

List of Participants

Antonio Bellon	University of Augsburg	Germany
Thomas Bendokat	MPI Magdeburg	Germany
Ranjan Kumar Das	MPI Magdeburg	Germany
Ieva Daužickaitė	Charles University	Czech Republic
Matthias Deiml	University of Augsburg	Germany
Virginie Ehrlacher	École des Ponts ParisTech & INRIA	France
Sebastian Esche	TU Chemnitz	Germany
Melina Freitag	University of Potsdam	Germany
José Carlos Garay	University of Augsburg	Germany
Yongseok Jang	The French Aerospace Lab ONERA	France
Elias Jarlebring	KTH Stockholm	Sweden
Lukas Klingbiel	University of Göttingen	Germany
Josie König	University of Potsdam	Germany
Daniel Kressner	EPFL	Switzerland
Ivana Kuzmanović Ivičić	University of Osijek	Croatia
Yizhou Liang	University of Augsburg	Germany
Thomas Mach	University of Potsdam	Germany
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Ralf Zimmermann	University of Southern Denmark	Denmark