KUNGL. VETENSKAPS-AKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

KTH VETENSKAP OCH KONST

5th Workshop on Scientific Computing in Sweden

SwedComp 2024

Stockholm, October 23-24, 2024

Organizing committee:
Elias Jarlebring
Jennifer Ryan
Anders Szepessy
Anna-Karin Tornberg

Venue:
Kungl. Vetenskapsakademien
Lilla Frescativägen 4A
Stockholm

Metro: Universitetet

Workshop page including a programme and book of abstracts
https://www.kth.se/math/naost/na/swedcomp2024

Workshop Dinner at Vasa museum sponsored by

COMSOL

Program, titles, and abstracts

Program

Wednesday		Thursday	
11:00–11:10	Opening		
11:10–11:30	Kristin Kirchner	09:00–09:20	Roman Iakymchuk
11:40–12:00	Jan Nordström	09:20–09:40	Anna Broms
12:00–12:20	Andreas Langer	09:40–10:00	Marvin Jans
12:20–12:30	Photo session	10:00–10:10	Leg stretch
12:30–14:00	Lunch	10:10–10:40	Poster blitz
14:00–14:20	Valentina Schüller	10:40–12:10	Poster session w coffee
14:20–14:40	Khanh Nguyen	12:15–13:40	Lunch
14:40–15:00	Igor Tominec	13:40–14:00	Davoud Mirzaei
15:00–16:00	Coffee / guided tour	14:00–14:20	Jonatan Werpers
16:00–16:30	Poster blitz	14:20–14:40	Axel Målqvist
16:30–18:00	Poster session & Mingle	14:40	Closing
18:15	Bus to dinner		

All talks and sessions take place at:

Kungliga vetenskapsakademien
Lilla Frescativägen 4A, Stockholm
Metro: Universitetet

The conference dinner takes place at

Vasa Museum, Galärvarvsvägen 14
A bus will leave from KVA at 18:15 on Day 1.

Poster session Wednesday (day 1): Shihao Liu, Pritpal Matharu, Anders Szepessy, Tony Stillfjord, Niklas Kotarsky, Jaime Manriquez, Teodor Åberg, Per Pettersson,

Poster session Thursday (day 2): Kasper Bågmark, Fredrik Laurén, Ylva Ljungberg Rydin, Malin Mosquera, Xin Huang, David Krantz, Gustaf Lorentzon, Vilhelm Peterson Lithell, Niclas Jansson, Mattias Sandberg

Titles and abstracts of talks

Kristin Kirchner (KTH & TU Delft)

Spatiotemporal statistical modelling with stochastic PDEs

Abstract: Most environmental data sets contain measurements collected over space and time. It is the purpose of spatiotemporal statistical models to adequately describe the underlying uncertain spatially explicit phenomena evolving over time. In this talk I will present a new class of spatiotemporal statistical models which is based on stochastic partial differential equations (SPDEs) involving fractional powers of parabolic operators. In particular, I will discuss the efficient simulation of the spatiotemporal solution processes, which is closely related to the approximation of nonlocal space-time differential operators. Furthermore, I will address the motivation for employing this class of SPDEs in statistical applications and give an outlook on the computational benefits for statistical inference from spatiotemporal data.

Jan Nordström (Linköping University)

An Energy Stable Nonlinear Incompressible Multi-Phase Flow Formulation

Abstract: We show that a reformulation of the governing equations for incompressible multi-phase flow in the volume of fluid setting leads to a well defined energy rate. Weak nonlinear inflow-outflow and solid wall boundary conditions complement the development and lead to an energy estimate in terms of external data. The new formulation combined with summation-by-parts operators lead to provably nonlinear energy stability.

Andreas Langer (Lund University)

DeepTV: A Neural Network Approach for Total Variation Minimization

Abstract: In the context of unsupervised learning, neural network approaches have been demonstrated to work quite well to solve partial differential equations in practice. Thereby, approaches like physics-informed neural networks and the Deep Ritz method have become popular. In this talk, we present a related approach to solve an infinite-dimensional total variation minimization problem using neural networks. We theoretically analyze the newly obtained neural network problem and connect it to the original total variation minimization problem. In fact, we can show that minimizers of the neural network discretized problem converge to a minimizer of the infinite-dimensional total variation minimization problem. We present numerical experiments supporting our theoretical findings and demonstrating the applicability of this approach to image restoration tasks.

Valentina Schüller (Lund University)

Convergence Properties of Iteratively Coupled Surface-Subsurface Models

Abstract: Water management projects such as stream bed re-naturalization affect the water table, which is relevant, e.g., for flood prediction. These physical processes can be modeled using coupled surface-subsurface flow models. They solve some form of the Richards and shallow water equations. A typical setup couples these two nonlinear partial differential equations in a partitioned approach via boundary conditions. Full interaction between the subsolvers is ensured by an iterative coupling procedure. This can be accelerated using relaxation.

We have applied linear analysis techniques to study an idealized, linear, 1D-0D version of a surface-subsurface model. These result in explicit expressions for the convergence factor and an optimal relaxation parameter, depending on material and discretization parameters. We test our analysis results numerically for fully nonlinear 2D-1D experiments based on existing benchmark problems. As we will show in this talk, the linear analysis can explain fast convergence of iterations observed in practice for different materials and test cases, even though we are not able to capture various nonlinear effects.

Khanh Nguyen (Karlstad University)

Boundary-effect dominated design optimization of a Newtonian cooling heat sink

Abstract: We consider the problem of thermally optimizing a heat sink design. A computationally attractive alternative to modelling the governing physics, a coupled thermal–fluid system, is to use the Poisson equation with a so-called Newtonian cooling boundary condition. However, as has been shown in the literature [1, 2], using material distribution topology optimization to design a heat sink using this model usually provides a poor design.

In this study, we tackle that problem by adding the weighted thermal compliance stemming from standard Poisson equation to the objective function of the topology optimization. Furthermore, instead of using solid-void interfacial elements, we simulate Newtonian cooling on only solid-void interfacial sides of elements.

Numerical experiments show that the proposed approach does not only to improve the heatsink design and its thermal compliance, but it also enhances the computational performance (convergence rate). A direct comparison with the standard approach using several case studies demonstrates the method's effectiveness.

Authors: Khanh Nguyen and Eddie Wadbro

References:
[1] T.E.Bruns, Topology optimization of convection-dominated, steady-state heat transfer problems, International Journal of Heat and Mass Transfer, vol. 50, no. 15, pp. 2859–2873, 2007.
[2] J. Alexandersen, Topology optimization for convection problems, Technical University of Denmark, 2011. B.Eng. thesis

Igor Tominec (Stockholm University)

Well-posedness of the Stokes problem under modified pressure Dirichlet boundary conditions

Abstract: We show that the Stokes problem is well-posed when both velocity and pressure vanish on the domain boundary. This result is achieved by extending Nečas' inequality to square-integrable functions that vanish in a small band covering the boundary. It is found that the associated a priori pressure estimate depends inversely on the volume of the band. Numerical experiments confirm these findings. Based on these results, guidelines are provided for applying vanishing pressure boundary conditions in model coupling and domain decomposition methods.

Roman Iakymchuk (Uppsala Universitet)

Enabling mixed-precision and accuracy computation with the help of tools and numerical techniques

Abstract: Mixed-precision computing has the potential to significantly reduce the cost of exascale computations, but determining when and how to implement it in programs can be challenging. In this talk, we propose a methodology for enabling mixed-precision with the help of computer arithmetic tools and enhancing the accuracy with numerical techniques. We verify the proposed methodology on few benchmarks and mini-applications, including LULESH and Nekbone. We evaluate the derived mixed-precision programs in terms of accuracy, time-to-solution, and energy-to-solution. Notably, the introduction of mixed-precision reduces time-to-solution by up to 41% and energy-to-solution by up to 47% in parallel settings.

Anna Broms (KTH Royal Institute of Technology)

An accurate method of fundamental solutions for large and dense particle systems in Stokes flow

Abstract: The Stokes mobility and resistance problems for rigid particles in viscous fluids have broad applications in both natural processes and industrial contexts and are important in the study of transport or diffusion processes, rheology and nonlinear shear thickening. Hydrodynamic interactions between particles are challenging to determine, as they are simultaneously long-ranged and expensive to resolve for dense suspensions. The latter is caused by near-singular lubrication forces resulting from close-to-touching bodies in relative motion. With the aim of controlling the accuracy for dense suspensions with a computationally cheap method, we present a new technique for the two problems that combines the method of fundamental solutions (MFS) with the method of images. For rigid spheres, we propose to represent the flow using fundamental solutions (Stokeslets) located on interior spheres, augmented by lines of image sources adapted to each near-contact to resolve lubrication. Source strengths are found by a least-squares solve at contact-adapted boundary collocation nodes. Via one-body preconditioning, the resulting well-conditioned schemes are competing with state-of-the art solvers tailored for spherical particles in Stokes flow, yet are compatible also with other smooth particle shapes, and scale linearly in the number of objects. For instance, a problem of 10,000 ellipsoids is solved to 5-digit accuracy on a workstation in less than two hours.

Marvin Jans (Lund University)

A fully discretized domain decomposition approach for semi-linear SPDEs

Abstract: We consider a fully discretized numerical scheme for parabolic stochastic partial differential equations with additive or multiplicative noise. Our method is based on a non-iterative domain decomposition approach. Such methods can help parallelize the code and therefore lead to a more efficient implementation. The domain decomposition is integrated through an operator splitting approach, where one operator acts on one part of the domain. More precisely, we combine the implicit Euler method with the Douglas-Rachford splitting scheme. For an efficient space discretization of the underlying equation, we chose the discontinuous Galerkin method. For this fully discretized scheme, we provide a strong space-time convergence result. In the presentation, the numerical method will be explained, together with a short outline of the convergence proof. We conclude the presentation with numerical experiments validating our results.

Davoud Mirzaei (Uppsala Universitet)

A central RBF reconstruction for solving conservation laws

Abstract: Efficient numerical methods for hyperbolic PDEs must avoid oscillations near discontinuities, accurately capture shocks, and achieve high-order convergence. Such methods typically rely on artificial viscosity or high-order reconstruction techniques. This talk focuses on a high-order non-oscillatory reconstruction in a finite volume framework. In this category, essentially non-oscillatory (ENO) and weighted ENO (WENO) reconstructions have been widely developed and applied over the past three decades. These reconstructions involve determining a set of stencils around a control volume, computing a reconstruction on each stencil, and selecting the smoothest (or a weighted) reconstruction for the control volume. In this talk, we present an alternative approach and introduce a non-oscillatory high-order central reconstruction based on radial basis function (RBF) approximations. This method employs a single central stencil combined with a weighted smoothed reconstruction (WSR) technique to suppress non-physical oscillations near shocks or sharp fronts. We demonstrate the effectiveness of this approach in solving scalar and systems of conservation laws.

Jonatan Werpers (Swedish Defence Research Agency (FOI))

Summation-by-parts finite-difference operators for singular coordinate transforms

Abstract: We present a general scheme for using existing summation-by-parts (SBP) finite-difference (FD) operators with singular coordinate transformations. The scheme preserves the accuracy and SBP properties of the original operators and permits simple implementation into existing codes.

The scheme allows taking advantage of the many previously constructed SBP-FD operators and developments when solving problems involving coordinate singularities. This greatly simplifies the design of the numerical method by avoiding re-constructing operators for the given coordinate system.

The operators are modified by viewing them in a weak form and eliminating the degrees of freedom associated with the coordinate singularities. By then returning to a strong form formulation an operator for the reduced grid is achieved which can be handled as any other SBP-FD operator.

Using the scheme we derive a stable and high-order accurate finite-difference method for underwater acoustic wave propagation in an axisymmetric domain. The method handles range and depth-dependent material properties, including discontinuous jumps. The accuracy and stability properties of the method are proven and corroborated using numerical experiments.

Axel Målqvist (Chalmers University of Technology and University of Gothenburg)

Iterative solution of Timoshenko beam network models

Abstract: We consider fibre based materials, modelled as spatial networks of connected one dimensional beams. In order to simulate the elastic properties of such materials we use the Timoshenko beam model with rigid joints. The resulting systems of equations are notoriously ill-conditioned. We therefore introduce a subspace decomposition technique and derive an efficient and reliable preconditioner for the arising linear system of equations. The target application is simulation of the mechanical behaviour of paperboard (tensile and bending strength). The work has been done in collaboration with Fraunhofer Chalmers Centre.

Poster presentations

Kasper Bågmark (Chalmers)

Deep splitting methods for nonlinear filtering

Abstract: The problem of estimating the probability density of a continuous state given noisy measurements is called the filtering problem. In the case when the system of states and observations is nonlinear the problem cannot be solved analytically (except in a few special cases). Classical methods, namely particle filters, suffer under the curse of dimensionality in the underlying dimension of the state space. Deep learning is a powerful tool in creating scalable approximations for similar problems. The proposed method combines a deep splitting method, previously used for PDEs and SPDEs, with an energy-based approach, in order to approximate the solution to the Zakai equation. This is a linear SPDE, whose solution is in fact an unnormalized filtering density. This results in a computationally fast filter that takes observations as input and that does not require re-training when new observations are received. The method is tested on four examples, two linear in one and twenty dimensions and two nonlinear in one dimension. The method shows promising performance when benchmarked against the Kalman filter and the bootstrap particle filter.

Xin Huang (KTH)

Convergence rates for random feature neural network approximation in molecular dynamics

Abstract: This presentation examines the convergence rates of random feature neural network approximations for potential functions in Hamiltonian systems, with a focus on molecular dynamics correlation observables. For networks with K nodes and J data points, an expected error bound of $O((K^{-1} + J^{-1/2})^{1/2})$ is derived, under regularity assumptions on the potential and observables. Our analysis features a novel approach for generalization error estimate, bypassing conventional techniques like Rademacher complexity. Numerical experiments validate the theoretical error bounds and illustrate the efficacy of these approximations in molecular dynamics settings.

Niclas Jansson (KTH)

A sharp immersed boundary method for high-fidelity spectral element flow simulations

Abstract: We present our work on developing an immersed boundary method suitable for high-fidelity turbulent flow simulations with complex geometries. The proposed method is based on a continuous forcing approach with a lagrangian representation of the immersed geometry. Using a one-sided inverse distance method for applying the forcing, the immersed boundary method can accurately represent zero-thickness bodies with a sharp interface on coarse meshes. A detailed description of the method is given, together with implementation details and validation results from the high-order spectral element flow solver Neko.

Niklas Kotarsky (Lund)

Continuous analysis of waveform relaxation for heterogeneous heat equations

Abstract: We consider dynamical coupled problems such as heat transfer and fluid structure interaction, or more specifically PDEs that interact through a lower dimensional interface. Our general goal is a partitioned method that is high order, allows for different and adaptive time steps in the separate models, makes efficient use of hardware resources, is robust, and contains fast inner solvers. In order to design and effectively use such methods, it is important to have error estimates.

We study and analyze here Dirichlet-Neumann waveform relaxation for two coupled 1D heterogeneous heat equations in the continuous setting, and prove new linear and super-linear error bounds. Our numerical experiments show that the linear error bound is sharp for large simulation times, and that the super-linear error bound can be used to qualitatively describe the convergence behavior for short simulation times. Our analysis also predicts which subdomain should use Dirichlet transmission conditions for fast convergence.

David Krantz (KTH)

Adaptive quadrature for layer potentials over axisymmetric surfaces using error estimation

Abstract: Layer potentials represent solutions to partial differential equations in an integral equation formulation. When numerically evaluating layer potentials at target points close to the domain boundary, specialized quadrature techniques are required for accuracy because of rapid variations in the integrand. To efficiently achieve a specified error tolerance, we introduce an adaptive quadrature method with automatic parameter adjustment, facilitated by error estimation. This method is tailored for axisymmetric surfaces, employing a trapezoidal rule in the azimuthal angle and a Gauss-Legendre quadrature rule in the polar angle. Notably, while each surface must be axisymmetric, the integrand does not need to be, allowing for applications with complex geometries featuring multiple axisymmetric bodies.

The proposed quadrature method utilizes so-called interpolatory semi-analytical quadrature in conjunction with a singularity swap technique in the azimuthal angle. In the polar angle, such a technique

is used as needed, depending on the integral kernel, combined with an adaptive subdivision of the integration interval.

Error estimates for both numerical integration and interpolation are derived using complex analysis, and are used to determine the adaptive panel subdivision given the evaluation point and the desired accuracy. Numerical examples are presented to demonstrate the method's efficacy.

Fredrik Laurén (FOI)

Currect work at FOI on the Parabolic Wave equation

*A*bstract: Radar and radio communication are two application that operate on long distance s. For these applications, the use of a full Maxwell's equations solver is too expensive due to its extensive demand in computational power. Typically, the user only has access to limited amount of computer resources. As a cure, the parabolic wave equation has been extensively used in modelling radar – and radio wave propagation and is today one of the dominant tools for troposphere propagation. In this presentation, the parabolic wave equation is presented and typical solution strategies are briefly explained. There are a number of unsolved problems (such as handling uncertainties of the input data, the effect of reducing the problem to a 2D formulation, and introducing a rough sea surface are just a few examples) that will be discussed. Rather than presenting solutions, this talk will highlight several problems and future research questions that are well-suited for a numerical analyst.

Shihao Liu (KTH)

A new type of simplified inverse Lax-Wendroff boundary treatment for hyperbolic conservation laws

Abstract: We design a new kind of high order inverse Lax-Wendroff (ILW) boundary treatment for solving hyperbolic conservation laws with finite difference method on a Cartesian mesh. This new ILW method decomposes the construction of ghost point values near inflow boundary into two steps: interpolation and extrapolation. At first, we impose values of some artificial auxiliary points through a polynomial interpolating the interior points near the boundary. Then, we will construct a Hermite extrapolation based on those auxiliary point values and the spatial derivatives at boundary obtained via the ILW procedure. This polynomial will give us the approximation to the ghost point value. By an appropriate selection of those artificial auxiliary points, high-order accuracy and stable results can be achieved. Moreover, theoretical analysis indicates that comparing with the original ILW method, especially for higher order accuracy, the new proposed one would require fewer terms using the relatively complicated ILW procedure and thus improve computational efficiency on the premise of maintaining accuracy and stability. We perform numerical experiments on several benchmarks, including one- and two-dimensional scalar equations and systems. The robustness and efficiency of the proposed scheme is numerically verified.

Ylva Ljungberg Rydin (FOI)

Modellering - Vägen till förståelse inom undervattensforskning

Abstract: The poster will provide an overview of the research in scientific computing at the department of underwater research at FOI.

Gustaf Lorentzon (KTH)

Efficient Computation of Matrix Polynomials

Abstract: Evaluating a matrix polynomial is crucial in many methods for computing matrix functions, such as the matrix exponential function, exp(A). In this work, we study how these polynomials can be

evaluated efficiently. When computing matrix polynomials of very large matrices, the cost of matrix addition is negligible compared to matrix-matrix multiplication. Thus, our focus is on developing methods for computing matrix polynomials with as few matrix-matrix multiplications as possible.

We describe a general framework for polynomial evaluation using tables with scalar parameters. These tables parameterize the space of all polynomials that are computable for a given number of matrix-matrix multiplications. In this work, we develop transformations for these tables, which change how the polynomial is evaluated without affecting the result. These transformations can be used to reduce the number of input parameters without reducing the parameterized space. This simplifies the analysis of both new and existing methods, without losing any generality.

Using this simplified form, we characterize the space of computable polynomials for a given number of matrix-matrix multiplications, with a particular focus on 3 and 4 multiplications. These characterizations can be used to develop optimal evaluation algorithms—that is, evaluation algorithms that use as few matrix-matrix multiplications as is theoretically possible. The methods are illustrated on relevant problems.

Joint work with E. Jarlebring.

Jaime Manriquez (Lund)

An HDG method for Stokes-Darcy coupling on dissimilar meshes

Abstract: Nowadays, the development of higher-order schemes and non-body-fitted methods have become of interest in the community of numerical methods for partial differential equations (PDEs). A popular high-order method is the Hybridizable Discontinuous Galerkin (HDG) method, which presents the flexibility of DG methods with respect to more general grids (e.g. containing hanging nodes), but with the advantage of reducing the global number of degrees of freedom via hybridization of the intra-element variables. The Transfer Path Method (TPM), based on a Taylor expansion around the boundary, was developed as an unfitted method for the handling of non-conformities between the domain of a PDE and its discretization, transferring boundary data through a line integral (the transfer path) between the exact boundary and the discretized one.

Recently the TPM has been applied to the case where a domain is divided into separate subdomains independently discretized where the non-conformity is present at the interface (where a transmission condition holds) between the subdomains instead of the external boundary (where boundary data is known). The work presented here shows the analysis and results of an HDG method for a Stokes-Darcy coupling problem with dissimilar meshes coupled using the TPM technique.

Pritpal Matharu (KTH)

Quadrature Methods via Line Interpolation and Approximation Functions for Particles in Microscale Flows

Abstract: For axisymmetric particles in microscale flows, such as Stokes flows, boundary integral methods can be utilized for numerical evaluation of flow velocity on and outside particle surfaces. Precomputation yields a highly efficient and accurate quadrature by expansion (QBX) method for singular integrals when evaluating on-surface. For evaluation close to the particle surface, nearly singular integrals must be computed and may result in large numerical errors arising, even when using special quadrature methods. Instead a line interpolation method aided by quadrature error estimates is introduced, within a framework that can be extended for use in general kernels and in fast methods. Moreover, adaptive quadrature methods can be leveraged in a suitable region to assist interpolation for points very close to particle surfaces. In this presentation, we will discuss approximation functions used for line interpolation and the numerical remedies required to be useful in practice and combined with special quadrature methods for realistic flow problems.

Malin Mosquera (Gothenburg)

Numerical approximation of mixed partial differential equations

Abstract: We consider a mixed dimensional partial differential equation posed on a domain with a large number of interfaces running through. In this research, a fitted finite element approximation is implemented and previously solved using Schur complement and the preconditioned conjugate gradient method. The PCG method used a preconditioner based on subspace decomposition. We are now examining solving the system with the super localised orthogonal decomposition method.

Vilhelm Peterson Lithell (KTH)

From eigenvector nonlinearities to eigenvalue nonlinearities

Abstract: We study eigenvalue problems in which there is a nonlinear dependence on the eigenvector, abbreviated NEPv. In this sense, these problems generalize the familiar linear eigenvalue problem. Specifically, the nonlinearities appear as a sum of products of scalar functions of the eigenvector and rank-one matrices. The target problems may potentially contain many such nonlinear terms. Our attention is focused on exploiting this and similar structures that appear for instance in the Gross-Pitaevskii equation. To this end we present a method for reformulating the class of problems of this form into equivalent problems with eigenvalue nonlinearities (NEP), enabling us to use efficient methods for these problems as a means of obtaining solutions to the NEPv. In particular, these methods can efficiently compute several eigenvalues. We show how the transformation from NEPv to NEP can be constructed theoretically, and indicate how it can be handled in practice. Numerical experiments demonstrate that our method allows us to compute several eigenvalues of the NEPv to high accuracy, and the performance is compared with existing methods.

Based on ongoing work joint with Elias Jarlebring (KTH).

Per Pettersson (NORCE)

Multi-agent injection strategies in subsurface CO2 storage

Abstract: Efficient large-scale CO2 storage has been identified by the Intergovernmental Panel on Climate Change as a necessary means to mitigate global warming. This requires extensive use of subsurface reservoirs where independent agents perform CO2 injection that will be affected by other agents by means of pressure buildup in geologically connected sites. We propose a novel framework for optimizing large-scale CO2 injection strategies combining multi-agent models with multi-objective optimization, and reservoir simulation. We investigate whether agents, i.e., well operators, should form coalitions for collaboration to maximize the outcome of their storage activities.

Coalition structure generation for the games describing the activities performed by subsurface injection agents (well operators) is an NP-complete problem, and the value of every possible coalition structure can only be obtained as the numerical solution to a multi-objective optimization problem. Furthermore, each optimization problem requires repeated evaluation of a complex numerical model of a large-scale subsurface domain. We present remedies to these challenges and present numerical results for a prospective storage site in Barents Sea where injections are constrained by maximum sustainable pressure buidlup and assumed supply of CO2. We discuss the implications of the numerical results on the preferred collaboration between injectors.

Mattias Sandberg (KTH)

Numerical molecular dynamics approximations of quantum observables

Abstract: While the Schrödinger equation in quantum mechanics has many desirable properties, e.g. well established theoretical understanding and absence of empirical parameters, its main problem is

the great computational complexity needed for a direct quantum mechanical simulation. Therefore computationally cheaper molecular dynamics is typically used for simulations. We consider molecular dynamics simulations of systems at constant temperature using the so-called canonical ensemble. A computational bottleneck is the sampling from the Gibbs density of the electron operator, which due to the fermion sign problem has a computational complexity that scales exponentially with the number of electrons. In this poster I present an algorithm that approximates the mean-field constant temperature Hamiltonian by path integrals for fermions. The algorithm is based on the determinant of a matrix with components based on Brownian bridges connecting permuted electron coordinates which reduces the computational complexity associated with the fermion sign problem. This poster presents work by Xin Huang, Petr Plechac, Mattias Sandberg, and Anders Szepessy.

Tony Stillfjord Lund

Computing Cholesky-factors of finite-horizon Gramians

Abstract: The solution to a differential Lyapunov equation can be expressed in closed form as a matrix-valued integral, the so-called finite-horizon Gramian. Such Gramians also have applications in many other areas, such as Gauss-Markov regression. The Gramian is positive semi-definite, and often it is more useful to have a Cholesky factorization of it rather than the Gramian itself. This work considers a new efficient numerical method for computing such Cholesky factors of finite-horizon Gramians without first computing the full Gramian. In contrast to other methods applicable to this task, this method is a generalization of the scaling-and-squaring approach for approximating the matrix exponential. It exploits a similar doubling formula for the Gramian, and thereby keeps the required computational effort modest. Most importantly, we have performed a rigorous backward error analysis that guarantees that the approximation is accurate to the round-off error level in double precision if the method parameters are chosen appropriately. The poster describes the algorithm, states the main error results and shows some experimental results produced via our efficient and freely available Julia code.

Anders Szepessy (KTH)

Resampling random Fourier features

Abstract: The machine learning random Fourier feature method for data in high dimension is computationally and theoretically attractive since the optimization is based on a convex standard least squares problem and independent sampling of Fourier frequencies. The challenge is to sample the Fourier frequencies well. If you come to the poster I will show you results how to sample optimally, in some sense, without determining the Fourier coefficients which would be too costly.

Teodor Åberg (Lund)

Convergence analysis of Lie and Strang splitting applied to operator-valued differential Riccati equations

Abstract: Differential Riccati equations (DREs) are matrix-valued or operator-valued equations with quadratic nonlinearities that arise in many areas. Most importantly, in control theory, where their solutions provide the optimal feedback control laws for linear quadratic regulators on finite time intervals. There are numerous numerical methods for DREs, but most of these lack proper (temporal) convergence analyses. The few existing analyses consider the matrix-valued case, and rely on properties that may not necessarily hold in the operator case. This is problematic when the matrix-valued DRE arises from a spatially discretized operator-valued DRE, corresponding to the control of a partial differential equation. In this case, refining the spatial discretization increases the problem dimension, and might cause the temporal errors to grow uncontrollably. h In view of this, we provide rigorous convergence analyses of two numerical time-stepping methods, the Lie and Strang splitting schemes, when applied to operator-valued DREs. We show that they achieve the standard orders of convergence under different types of (low) regularity assumptions. Essentially, either the initial condition or

the operator giving rise to the nonlinearity should be smoothing to a certain degree, but not necessarily both. We illustrate these theoretical results with several numerical experiments on DREs arising from the control of partial differential equations.

List of participants

- Ahlkrona, Josefin, Stockholm University
- Ahmad, Mudassar, Mälardalen University
- Almquist, Martin, Uppsala Universitet
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