36th Northern German Colloquium on Applied Analysis and Numerical Mathematics

Jacobs University

April 24–25, 2015

Friday, April 24, 2015

12:00-13:00	Lunch in College Nordmetall
13:00-13:10	Welcome, IRC Seminar Room
13:10-13:35	Jens Rademacher (Universität Bremen) Spectra, bifurcations and dynamics of semi-localized patterns
13:35-14:00	Annibale Magni (Universität Münster) Variational analysis of a reduced Allen–Cahn action functional
14:00-14:25	Hannes Uecker (Universität Oldenburg) Spatial patterns in distributed optimal control problems
14:25-14:50	Alessandro Alla (Universität Hamburg) Coupling MPC and DP methods for optimal control problems
14:50-15:15	Tobias Preußer (Jacobs University and Fraunhofer MEVIS) Treating uncertain data in PDE based image processing with SPDEs
15:15-16:15	Coffee break
16:15-16:40	Hao Wu (FU Berlin) Observable operator description and analysis of metastable systems
16:40-17:05	Torge Schmidt (TU Hamburg-Harburg) Approximation of spectra and pseudospectra of operators on a Hilbert space
17:05–17:30	Wolfgang Erb (Universität zu Lübeck) Bivariate Lagrange interpolation at the node points of Lissajous curves
17:30-17:55	Sabine Le Borne (TU Hamburg-Harburg) Numerical techniques for aggregation integrals in population balance systems
17:55-18:20	Ulrich Eckhardt (Universität Hamburg) Projektion auf ein Simplex
19:00	Meet in front of the Campus Center for walk to restaurant
19:30	Conference Dinner Restaurant Nautico, Zum Alten Speicher 13, 28759 Bremen

Saturday, April 25, 2015

7:30-8:30	Breakfast in College Nordmetall
8:30-8:55	Felix Krahmer (TU München) Compressive sensing with redundant dictionaries and structured measurements
8:55–9:20	Stefan Kunis (Universität Osnabrück) Prony's method, moment problems, and super-resolution in higher dimensions
9:20-9:45	Rafael Reisenhofer (Universität Bremen) Complex shearlet transforms and applications to edge and line detection
9:45-10:10	Feliks Nüske (FU Berlin) Variational tensor approach for approximating the rare-event kinetics of macromolecular systems
10:10-10:35	Tatiana Levitina (TU Braunschweig) Discrete orthogonality and Kramer's sampling theorem
10:35 - 11:35	Coffee break
11:35-12:00	Nikolaos Roidos (Leibniz University Hannover) The porous medium equation on manifolds with conical singularities
12:00-12:25	Ingenuin Gasser (Universität Hamburg) A 1-D model for pressure retarded osmosis
12:25-12:50	Malte Braack (CAU Kiel) Stability and a priori analysis of discrete Navier–Stokes solutions with outflow condition
12:50-13:15	Armin Iske (Universität Hamburg) Optimally sparse approximation of signals by adaptive linear splines over anisotropic triangulations
13:15	Lunch in College Nordmetall

Poster presentations

Claudio Bierig (Universität Oldenburg)

 $\label{eq:expectation} \textit{Estimation of arbitrary order central statistical moments by the multilevel Monte Carlo method$

Patricio Farrell (WIAS) Simulating semiconductor devices: generalisations of the Scharfetter–Gummel scheme to non-Boltzmann statistics

Alexandru Mihai (Jacobs University) Stenotic channel flow using the lattice Boltzmann method

Franziska Pott (Universität Bremen)A regularizing Newton-like method for ozone retrieval from occultation measurementsWeiqi Zhou (Jacobs University)

Triangular truncation on Hermitian operators

Abstracts

Alessandro Alla (Universität Hamburg)

Talk: Coupling MPC and DP methods for optimal control problems

We consider the approximation of an infinite horizon optimal control problem which combines a first step based on Model Predictive Control (MPC) in order to have a quick guess of the optimal trajectory and a second step where we solve the Bellman equation in a neighborhood of the reference trajectory. The direct global solution approach via the Bellman equation can be rather expensive since we have to set the problem in a domain containing all the possible initial conditions x for the dynamics. Moreover, we have to impose (and choose) the appropriate boundary conditions for the Bellman equation. The main feature of MPC methods is to compute an approximate feedback control for the dynamics starting at a given initial condition x by solving a sequence of finite horizon optimal control problems. Therefore, it seems natural to first solve the problem for a given initial condition via MPC and then compute the value function in a neighborhood of that trajectory in order to reduce the global size of the computational problem. The second step is also necessary to allow for a more stable solution since we use the informations around the reference trajectory and not only those on the reference trajectory. We will present the main features of these new technique, and illustrate some numerical tests in order to show the effectiveness of this coupling.

Joint work with G. Fabrini and M. Falcone.

Claudio Bierig (Universität Oldenburg)

Poster: Estimation of arbitrary order central statistical moments by the multilevel Monte Carlo method

Due to permanent growth of computer power in the recent decades, exact numerical simulations for partial differential equations became possible – provided that the input data is known exactly. In practical applications, however, the exact data entering the computations are based on a mathematical model being itself only an approximation for the actually occurring process. Hence, there is no point in increasing numerical accuracy beyond the modelling error or the error in the measurements. One way to overcome this difficulty is to treat the lack of knowledge or the measurement error using probabilistic description, which might be viewed as a more realistic and powerful model for the underlying process. In this case, the input data can be modelled as random fields leading to stochastic partial differential equations, whose solutions become a random field as well. Our goal is to approximate the Expectation Value and higher order central moments of an output functional of the solution or the solution itself.

Malte Braack (CAU Kiel)

Talk: Stability and a priori analysis of discrete Navier-Stokes solutions with outflow condition

Existing a priori estimates for the discretized Navier–Stokes equations require Dirichlet conditions for the velocities on the entire boundary of the domain. An extension to flow problems with do-nothing outflow condition, as e.g. channel flows, is not possible due to the absence of a stability property of the continuous solution. However, a remedy consists in an appropriate modification of the classical do-nothing condition, the so-called directional do-nothing condition. In this talk we present the basic idea and derive an a priori estimate for the discrete solution stabilized with local projection stabilization of the convective term. Numerical examples demonstrate the benefits and enhanced stability of the method.

Ulrich Eckhardt (Universität Hamburg)

Talk: Projection auf ein Simplex

Im Jahre 1989 veröffentlichten Maculan und de Paula Jr. ein überraschendes Resultat, ein O(d)-Verfahren zur Ermittlung der metrischen Pojektion eines Punktes auf ein d-Simplex.

Es werden Bedingungen angegeben, unter welchen diese Aufgabe in polynomialer Zeit gelöst werden kann.

Wolfgang Erb (Universität zu Lübeck)

Talk: Bivariate Lagrange interpolation at the node points of Lissajous curves

Motivated by an application in Magnetic Particle Imaging, we study bivariate Lagrange interpolation at the node points of Lissajous curves. The resulting theory is a generalization of the polynomial interpolation theory developed for a node set known as Padua points. We will show that the node points of Lissajous curves allow unique interpolation in appropriately defined polynomial spaces and can be used for quadrature rules in the bivariate setting. An explicit formula for the Lagrange polynomials allows to compute the interpolating polynomial with a simple and fast algorithmic scheme. Compared to the already established schemes of the Padua and Xu points, the numerical results for the proposed scheme show similar approximation errors and a similar growth of the Lebesgue constant.

Patricio Farrell (WIAS)

Poster: Simulating semiconductor devices: generalisations of the Scharfetter–Gummel scheme to non-Boltzmann statistics

The Scharfetter–Gummel scheme was invented in the 1960s to numerically simulate the behaviour of semiconductor devices. We discuss how it can be adapted to more complicated distribution functions (in particular to non-Boltzmann statistics). Our main goal is to discretely preserve important properties from the continuous system such as existence and uniqueness of the solution, consistency with the thermodynamical equilibrium and unconditional stability. We also show how these numerical methods can be efficiently implemented for 2D and 3D applications.

Ingenuin Gasser (Universität Hamburg)

Talk: A 1-D model for pressure retarded osmosis

We present a model to describe so-called osmotic power plants. In such power plants the salinity gradient from the difference in the salt concentration between seawater and river water is used to produce electrical energy. Our model refers to certain proposed realisations. Finally, numerical simulations give an idea on the expected energyproduction.

Armin Iske (Universität Hamburg)

Talk: Optimally sparse approximation of signals by adaptive linear splines over anisotropic triangulations

Anisotropic triangulations provide efficient methods for sparse representations of signals. In previous work, we have proposed a locally adaptive greedy algorithm for sparse approximations of images and videos, termed adaptive thinning. Adaptive thinning relies on linear splines over anisotropic Delaunay triangulations (for images) and Delaunay tetrahedralizations (for videos). In this talk, we address both theoretical and practical aspects concerning the construction of signal approximation by linear splines over anisotropic triangulations (and tetrahedralizations). Our discussion leads us to asymptotically optimal N-term approximations on relevant classes of target functions, such as horizon functions across Hölder smooth boundaries and piecewise regular functions from Sobolev spaces of fractional order. The good performance of our adaptive thinning algorithm will finally be demonstrated by numerical examples and comparisons.

Felix Krahmer (TU München)

Talk: Compressive sensing with redundant dictionaries and structured measurements

Consider the problem of recovering an unknown signal from undersampled measurements, given the knowledge that the signal has a sparse representation in a specified dictionary D. This problem is now understood to be well-posed and efficiently solvable under suitable assumptions on the measurements and dictionary, if the number of measurements scales roughly with the sparsity level. One sufficient condition for such is the D-restricted isometry property (D-RIP), which asks that the sampling matrix approximately preserve the norm of all signals which are sufficiently sparse in D. While many classes of random matrices are known to satisfy such conditions, such matrices are not representative of the structural constraints imposed by practical sensing systems. We close this gap in the theory by demonstrating that one can subsample a fixed orthogonal matrix in such a way that the D-RIP will hold, provided this basis is sufficiently incoherent with the sparsifying dictionary D. We also extend this analysis to allow for weighted sparse expansions. Consequently, we arrive at compressive sensing recovery guarantees for structured measurements and redundant dictionaries.

This is joint work with Deanna Needell and Rachel Ward.

Stefan Kunis (Universität Osnabrück)

Talk: Prony's method, moment problems, and super-resolution in higher dimensions

Prony's method is a prototypical eigenvalue analysis based method for the reconstruction of a finitely supported complex measure on the unit circle from its moments up to a certain degree. In this talk, we give a generalization of this method to the multivariate case and prove simple conditions under which the problem admits a unique solution. Provided the order of the moments is bounded from below by the number of points on which the measure is supported as well as by some small constant divided by the separation distance of these points, stable reconstruction is guaranteed. In its simplest form, the reconstruction method consists of setting up a certain multilevel Toeplitz matrix of the moments, compute the coefficient vectors spanning its kernel, and compute by some method of choice the common zero set of the multivariate polynomials whose coefficients are given in the second step. All theoretical results are illustrated by numerical experiments.

Sabine Le Borne (TU Hamburg-Harburg)

Talk: Numerical techniques for aggregation integrals in population balance systems

The behavior of particulate flow is athematically modeled by population balance systems. Within such a system, particles are characterized through certain properties, e.g. mass or volume, and their distribution is quantified by a number density function. The various terms in the system can model phenomena including particle transport, nucleation, growth, aggregation or breakage.

Among these terms, the aggregation leads to an integro-differential equation, and its numerical treatment often dominates the overall simulation time since direct approaches lead to quadratic work complexities in the number of property variables.

In this talk, we show that the complexity can be reduced to an almost linear order through techniques such as separable approximations, fast Fourier transformations and fast wavelet transforms.

The novel methods will be illustrated through numerous numerical tests, showing their advantage compared to some standard methods from the literature.

Tatiana Levitina (TU Braunschweig)

Talk: Discrete orthogonality and Kramer's sampling theorem

Kramer's sampling theorem generalizes the statement of the famous Whittaker-Kotel'nikov-Shannon theorem and enables one to recover a function f(t) from a countable set of its samples $f_n = f(t_n), n \in \mathbb{N}$, provided that this function belongs to the range of an integral operator $\hat{k}, f(t) = \hat{k}[g](t) = \int_I g(\xi)k(t,\xi)d\xi, g \in \mathcal{L}_2(I)$, whose kernel $k(t, \cdot) \colon \mathbb{R} \times I \to \mathbb{R}$, satisfies the following requirements:

- For any $t \in \mathbb{R}$, $k(t, \cdot) \in \mathcal{L}_2(I)$, so that $K(t, s) = \int_I k(t, \xi) \overline{k(s, \xi)} d\xi \in Rg(\hat{k})$;
- Functions $k(t_n, \cdot), n \in \mathbb{N}$, form a complete orthonormal set on $\mathcal{L}_2(I)$.

As is well-known, the range of the operator \hat{k} , equipped with the scalar product $\langle f, h \rangle = \int_{I} \hat{k}^{-1}[f] \overline{\hat{k}^{-1}[h]} d\xi$, is a reproducing kernel Hilbert space with the reproducing kernel $K(t,s)^{1}$.

If in addition the operator $\hat{k}_I = \hat{q}_I \circ \hat{k} \colon \mathcal{L}_2(I) \to \mathcal{L}_2(I)$, with \hat{q}_I being a time-limiting opertor, is normal, i.e. $\hat{k}_I \circ \hat{k}_I^* = \hat{k}_I^* \circ \hat{k}_I$, then another sampling formula is valid based on the eigenfunctions φ_l of \hat{k}_I and their images $\Phi_l = \hat{k}\varphi_l$, $l = 0, 1, 2, ...^{23}$.

In this case the properties of Φ_l are very similar to those of finite Fourier transform eigenfunctions, in particular they exhibit double orthogonality (both over the finite interval I and over \mathbb{R}), double completeness (both in $\mathcal{L}_2(I)$ and in $Rg(\hat{k})$), etc. As an instant consequence of the new sampling formula, two discrete orthogonality relations hold,

$$\sum_{l} \Phi_{l}(t_{n}) \Phi_{l}(t_{m}) = \delta_{nm}, \text{ and } \sum_{n} \Phi_{l}(t_{n}) \Phi_{k}(t_{n}) = \delta_{lk}.$$
 (1)

One can prove that the former relation rephrases the pairwise orthogonality over I of functions $k(t_n,\xi)$, $n \in \mathbb{N}$, since $k(t,\xi) = \sum_l \Phi_l(t)\varphi_l(\xi)$, while the latter one expresses their completeness in $\mathcal{L}_2(I)$. Thus, the converse statement is also true:

Lemma 1 Let φ_n be the normalized eigenfunctions of the normal operator k_I , and let $\Phi_l = \hat{k}\varphi_l$. If there exists a sequence of points $\{t_n\}$, $n \in \mathbb{N}$, such that the discrete orthogonality relations (1) hold, then the sequence $k(t_n, t)$ is an orthonormal basis in $\mathcal{L}_2(I)$ and the Kramer sampling formula holds with $K(t, s) = \sum_l \Phi_l(t)\Phi_l(s)$.

Evidently, the sequence $\{t_n\}$ can be obtained from the condition $K(t_n, t_m) = \delta_{nm}$. The extension to higher dimensions is straightforward.

This is a joint work with Tahar Moumni (Department of Mathematics, Faculty of Science of Bizerte, University of Carthage, Zarzouna, Tunisia).

Annibale Magni (Universität Münster)

Talk: Variational analysis of a reduced Allen–Cahn action functional

We consider the sharp interface limit of the Allen–Cahn action functional, which can be understood as a formal action functional for a stochastically perturbed mean curvature flow. For given initial and final conditions we investigate the corresponding action minimization problem. After reformulating the problem in a generalized setting, we prove compactness as well as lower-semicontinuity properties of the action functional.

Alexandru Mihai (Jacobs University)

Poster: Stenotic channel flow using the lattice Boltzmann method

The lattice Boltzmann method provides an accessible avenue to analyze and model complex fluid dynamics without the need of higher level computing. We begin to analyze the

¹S. Saitoh, Proc. Amer. Math. Soc. 89, 74–78, 1983.

²G.G. Walter and X. Shen, Sampl. Theory Signal Image Proc. 2, 25–52, 2003.

³A. I. Zayed, Proc. Amer. Math. Soc. **135**, 2193–2203, 2007.

flow through a constricted channel in two dimensions using the LBGK collision model. There are currently no know analytic solutions for the flow through such a geometry, we aim to find the transition period of Reynolds numbers such that neither laminar nor turbulent flows occur. Initial results show that this transition period occurs for Reynolds numbers of approximately 1000 to 2000. Additional results for three dimensional flow through a stenotic cylinder will also be presented as a part of an ongoing project using the open source library OpenLB. The goal is to compare simulated results to experimental velocity profiles found using 4D Flow MRI.

Feliks Nüske (FU Berlin)

Talk: Variational tensor approach for approximating the rare-event kinetics of macromolecular systems

Biological macromolecules, such as proteins or nucleic acids, usually exhibit major structural re-arrangements which occur on timescales much longer than the fastest oscillations within the system. These re-arrangements are often responsible for changes in the biological function of the molecule. Essential information about the slow structural changes is contained in the eigenvalues and eigenfunctions of the dynamical operator of the system. A recent variational formulation allows to optimally approximate these eigenvalues and eigenfunctions when a basis set for the eigenfunctions is given. Here, we propose that a suitable choice of basis functions is given by products of one-coordinate basis functions, and that a sparse tensor product approach (based on the tensor-train format) can be employed in order to avoid a combinatorial explosion of products, i.e. of basis-set size. Our results suggest that the high-dimensional eigenfunctions can be well approximated using relatively small basis set sizes.

Tobias Preußer (Fraunhofer MEVIS and Jacobs University)

Talk: Treating uncertain data in PDE based image processing with SPDEs

Image data used in medical image processing is in general the result of a physical measurement, e.gå computed tomography (CT) measures the X-ray absorption, ultrasound imaging measures the acoustic scattering, etc. In natural sciences it is good scientific practice to provide measurement results with error estimates, however this is typically omitted in radiological image acquisition. When such error information is available it is natural to model the pixel values of the image as random variables, i.e. pixels do not have a fixed gray or color value. Instead, pixels have a probability density distribution that contains the information about the acquisition uncertainties. We refer to these images as stochastic images and we consider them to be elements of the tensor product space between a classical image space and a random space. Applying variational methods on stochastic images leads to stochastic partial differential equations (stochastic PDEs, SPDEs), i.e. PDEs with stochastic coefficients and/or right hand side. In the talk we will discuss the notion of stochastic images and SPDE approaches to various tasks from computer vision will be discussed. The resulting models enable us to propagate uncertainty and errors in the input data to the final result of the computer vision task. In medical imaging this can allow to make decisions in treatment and diagnoses that take

into account measurement uncertainty, e.g. in the monitoring of tumor progression during chemotherapy.

Franziska Pott (Universität Bremen)

Poster: A regularizing Newton-like method for ozone retrieval from occultation measurements

During the last decades a large public interest in physics and chemistry of the Earth's atmosphere arised due to alarming results and observations in scientific assessment reports. A great depletion of stratospheric ozone, global warming and increasing air pollution in the troposphere are only some of the worrying issues. It is necessary to improve the understanding and knowledge of chemical and physical processes, feedback processes in the atmosphere and the impact of human activities on global climate. A global observation system consisting of satellite instrument and ground-based networks has been developed to provide measurements for determining spatial and temporal changes in atmospheric constituents.

Jens Rademacher (Universität Bremen)

Talk: Spectra, bifurcations and dynamics of semi-localized patterns

Semi-localized patterns occur frequently in systems with spatial space separation, in particular reaction-diffusion systems with strongly different diffusion rates. This talk concerns some recent results on the spectral theory of such patterns as well as bifurcations and dynamics.

Rafael Reisenhofer (Universität Bremen)

Talk: Complex shearlet transforms and applications to edge and line detection

The complex shearlet transform is a complex-valued generalization of the shearlet transform⁴ in which anisotropically (i.e. in a directionally-dependent fashion) scaled and sheared wavelet-like basis functions provide sparse approximations of signals in two and higher dimensions. While shearlet-based transforms were in fact shown to provide optimally sparse approximations⁵ of elements within a certain class of natural images, complex-valued shearlet transforms are conceptually closer to the classical Fourier transform in the sense that a complex shearlet $\psi^c = \psi + i\mathcal{H}\psi$ consists of a real-valued shearlet ψ and its Hilbert transform $\mathcal{H}\psi$, where ψ is typically chosen to be symmetric, forcing \mathcal{H} to be odd-symmetric. A structure, which resembles the complex exponential $e^{ix} = \cos(x) + i\sin(x)$, where the real part consists of the even-symmetric cosine, the imaginary part consists of the odd-symmetric sine and sine and cosine just differ by a 90 degree phase shift.

⁴Guo, Kutyniok and Labate, Sparse multidimensional representations using anisotropic dilation and shear operators, 2005.

⁵Guo and Labate, Optimally sparse multidimensional representation using shearlets, 2007.

For edge detection, we exploit the fact that, given the right normalization, both the real and the imaginary part of a complex-valued shearlet transform exhibit a specific scale-independent behavior at the location of an edge. This observation leads to a computationally simple edge measure which is by construction contrast invariant, surprisingly stable in the presence of noise and capable of approximating tangent orientations as well as detecting both sharp and smooth transitions. Furthermore, by reversing the roles of the real and the imaginary parts of a complex-valued shearlet transform in the definition of said measure, lines can be detected instead of edges.

In addition, preliminary results of ongoing collaborations with the Institute of Environmental Physics and the Division of Engineering Thermodynamics of the University of Bremen will be presented, where the complex shearlet-based edge measure is used to determine the location and curvature of flame fronts in high speed recordings of flames and to locate transitions from water to tidal flats in synthetic aperture radar images of the Elbe river.

Nikolaos Roidos (Leibniz University Hannover)

Talk: The porous medium equation on manifolds with conical singularities

We consider the porous medium equation on manifolds with conical singularities. We show existence, uniqueness and maximal L^p -regularity of a short time solution. In particular, we obtain information on the short time asymptotics of the solution near the conical point. Our method is based on bounded imaginary powers results for cone differential operators on Mellin–Sobolev spaces and *R*-sectoriality perturbation techniques.

Torge Schmidt (TU Hamburg-Harburg)

Talk: Approximation of spectra and pseudospectra of operators on a Hilbert space

The study of spectral properties of linear operators on an infinite-dimensional Hilbert space is of great interest. This task is especially difficult when the operator is nonselfadjoint or even non-normal. Standard approaches like spectral approximation by finite sections generally fail in that case.

In this talk we present an algorithm which rigorously computes upper and lower bounds for the spectrum and pseudospectrum of such operators using finite-dimensional approximations. One of our main topics is to implement this algorithm efficiently. In addition we will demonstrate and evaluate methods for the computation of the pseudospectrum of finite-dimensional operators based on continuation techniques.

Hannes Uecker (Universität Oldenburg)

Talk: Spatial patterns in distributed optimal control problems

We present a framework to numerically treat spatially distributed optimal control problems with an infinite time horizon, illustrating the approach by some examples. The basic idea is to consider the associated canonical systems in two steps. First we perform a bifurcation analysis of the steady state canonical system, yielding branches of patterned canonical steady states. In a second step we compute time dependent canonical system paths to steady states having the so called saddle point property. It turns out that often patterned canonical steady states are optimal.

Hao Wu (FU Berlin)

Talk: Observable operator description and analysis of metastable systems

High-dimensional metastable processes are ubiquitous in physical systems. Examples include computer simulations of proteins, polymer (un)folding with single-molecule force probe experiments, or channel signalling with patch-clamp voltage measurements. A recurring and hard problem is the task of estimation effective dynamical models from low-dimensional projections of such processes. This is both difficult for computer simulation, where good reaction coordinate(s) are often unknown or difficult to compute, and even more so for single-molecule experiments, where good reaction coordinates may be experimentally unobservable. Here we develop an approach to modeling and estimating compact models of the observed (projected) Markov process without the widely used assumption of memoryless discrete jumping. It is found that the dynamics can be described exactly by small-sized observable operator models (OOMs) in the case of strong metastability, even if the dynamics are observed with nonequilibrium initial distribution and poor reaction coordinates. This provides a way to estimate the kinetics of complex dynamical systems in an unbiased way, yielding a general and important result for the physics of complex dynamical systems.

Weiqi Zhou (Jacobs University)

Poster: Triangular truncation on Hermitian operators

We present an explicit formula describing how triangular truncation acts on the eigen structure of Hermitian operators

Using which we develop new approach to estimate its operator norm on the Schatten class, to obtain the average norm of the truncation operators and to construct a few novel and illustrative examples

These abstract results are further applicable to the theory of the iterative methods, to link the spectral properties to convergence rate, and to justify new iteration schemes.