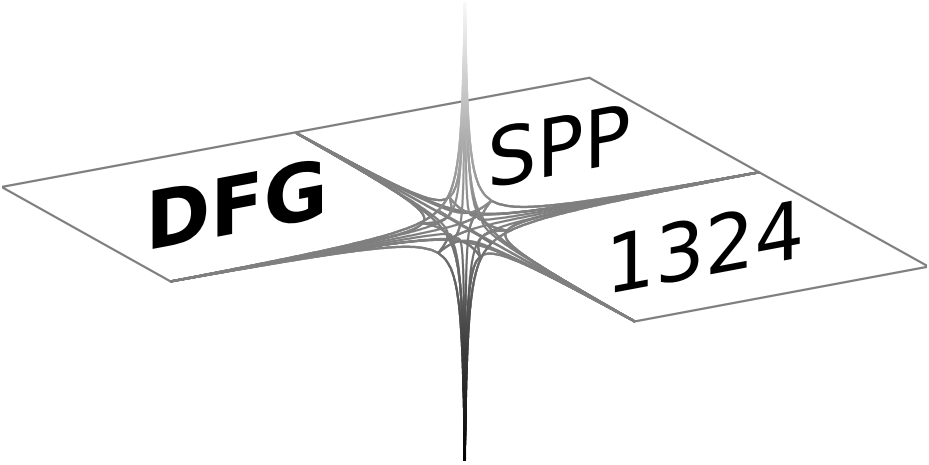
Extraktion quantifizierbarer Information aus komplexen Systemen

SPP-JT09

1st Annual Meeting of SPP 1324

Berlin, November 5-6, 2009



Program — 5th November 2009

Morning Session

8:30 – 9:15	*Registration*	
9:15 – 9:30	Stephan Dahlke *Opening*	
9:30 – 10:00	Christian Lubich *Variational approximations in quantum dynamics and the MCTDH method*	
10:00 – 10:30	Thorsten Rohwedder *Minimization Tasks in Electronic Structure Calculations and Minimization with Sums of Elementary Tensors*	
10:30 – 11:00	*Coffee break*	
11:00 – 11:30	Harry Yserentant *Regularity, Complexity, and Approximability of Electronic Wave Functions*	
11:30 – 12:00	Wang-Q Lim, Gerrit Welper *Directional Multiresolution Schemes for Transport Dominated Problems: Shearlet Constructions and Petrov-Galerkin Discretizations*	
12:00 – 12:30	Tobias Jahnke *On hybrid models for stochastic reaction kinetics*	
12:30 – 14:00	*Lunch*	

Program — 5th November 2009

Afternoon Session

14:00 – 14:30	Felix Lindner *Adaptive Wavelet Methods for Stochastic Partial Differential Equations*
14:30 – 15:00	Antje Mugler, Elisabeth Ullmann *Stochastic Galerkin Methods – Fundamentals and Algorithms*
15:00 – 15:30	Daniel Rudolf *Explicit error bounds for reversible Markov chain Monte Carlo*
15:30 – 16:00	Irene Klompmaker *Reinforcement Learning in a Continuous State Space*
16:00 – 16:30	*Coffee break*
16:30 – 17:00	Lars Grasedyck *Hierarchical and Black-Box Approximation of Tensors*
17:00 – 17:30	Sadegh Jokar *Kronecker Products and Compressed Sensing*
17:30 – 18:00	Markus Hansen *m-term approximation in Tensor product function spaces*

Program — 6th November 2009

9:00 – 9:30	Lutz Kämmerer *High dimensional sparse fast Fourier transforms*
9:30 – 10:00	Steffen Dereich *Constructive Quantization and Multilevel Algorithms for Quadrature of SDEs*
10:00 – 10:30	Armin Iske *Adaptive Approximation Algorithms for Sparse Data Representation*
10:30 – 11:00	Ulrich Friedrich *Adaptive Wavelet Methods for Inverse Parabolic Problems: Tensor Product Wavelet Bases on General Domains and new Existence and Uniqueness Results for the Forward Problem*
11:00 – 11:30	*Coffee break*
11:30 – 12:00	Dirk Lorenz, Gerd Teschke, Evelyn Herrholz *Compressive strategies for ill-posed problems*
12:00 – 12:30	Andreas Rupp *Valuation of Structured Financial Products*
12:30 – 13:00	Jessica Steiner *Validating Numerical Solutions of Backward SDEs Arising from Finance*
13:00 –	*Conclusion*

Location

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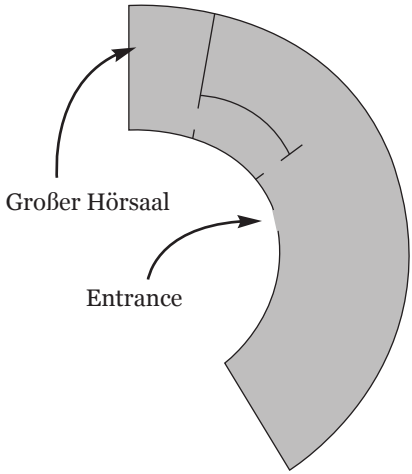

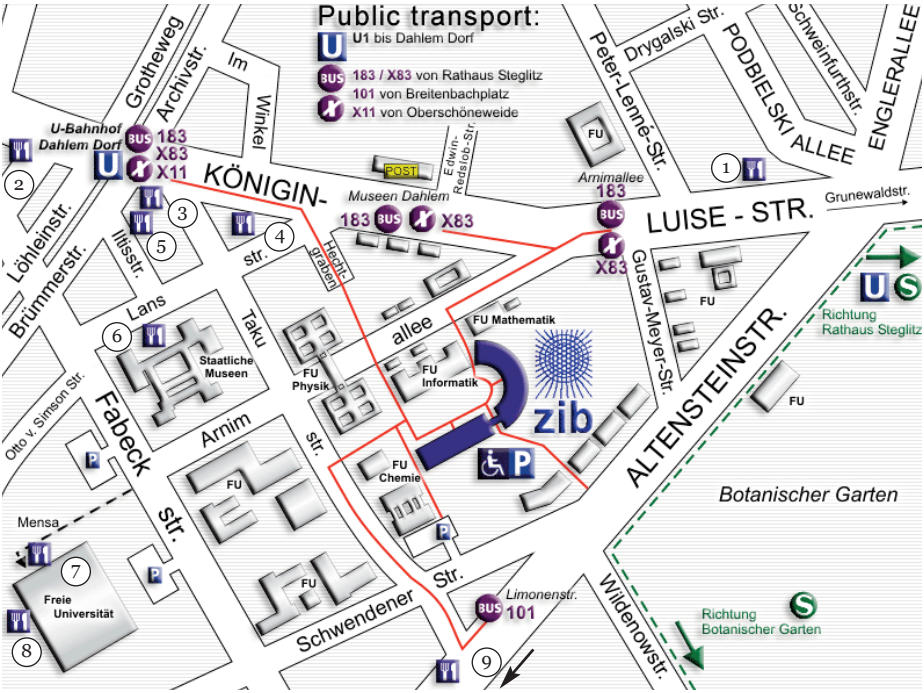

Location

Lunch

If you want to eat for lunch in the FU Mensa, you will need the MensaCard for paying at the cash desk. You can buy this card while the registration or the breaks for 10 €. This includes 8,45 € credit and 1,55 € pawn. After your last lunch you can get the pawn back at the cash desk of the FU Mensa.

Restaurants

1. **Restaurant Garibaldi**, Königin-Luise-Straße 11, Tel. 8324044
2. **Alter Krug**, Königin-Luise-Str. 52, Tel. 843 19 540
3. **Luise**, Königin-Luise-Str. 40, Tel. 841 88 80
4. **Asia Snack Dahlem**, Königin-Luise-Str. 38
5. **Ristorante Piaggio**, Königin-Luise-Str. 44, Tel. 832 022 66
6. **Cafeteria im Museum**, Lansstr. 8
7. **FU Mensa II**, Otto-von-Simson-Str. 26
8. **Pizzeria Galileo**, Otto-von-Simson-Str. 26, Tel. 831 23 77
9. **Fabecks,** Altensteinstr. 42 / Ecke Fabeckstr. , Tel. 26 07 97 67

WLAN

The ZIB will have a non-secure WLAN, named *Gast im ZIB*. ATTENTION! This means that the hole traffic could logged by a third person. At some places, for example the lector hall, it is possible to use the EDUROAM-Net from the FU, if you have an eduroam account of your home institution.

Abstracts

Constructive Quantization and Multilevel Algorithms for Quadrature of SDEs

Steffen Dereich (TU Berlin)

In this talk, I summarize the progress and the current state of the abovementioned project. In particular, we will discuss recent findings for multilevel Monte Carlo algorithms for Levy-driven SDEs.

Compressive strategies for ill-posed problems

Dirk Lorenz (TU Braunschweig), Gerd Teschke (Hochschule Neubrandenburg), Evelyn Herrholz (Hochschule Neubrandenburg)

In the short project presentation we discuss first ideas on a framework for solving inverse problems capitalizing compressive sampling strategies. Typically, in inverse problems the usual assumptions for compressive sampling are nor fulfilled and have to adapted. The actual approach relies on a specific combination of regularization and compression resulting in a particular design of the sampling functions. The applicability of this proceeding is verfied by first numerical experiments. In addition to this, we present verifiable conditions for exact recovery with orthogonal matching pursuit which also work for these problems and present an example from digital holography.

Adaptive Wavelet Methods for Inverse Parabolic Problems: Tensor Product Wavelet Bases on General Domains and new Existence and Uniqueness Results for the Forward Problem

Ulrich Friedrich (Philipps-Universität Marburg)

In the first part of the talk the work program of our project is lined out. This is motivated by the problem of identifying the parameters in a nonlinear parabolic equation modeling gene expression levels in the embryogenesis of drosophila blastodermis (fruit fly). A strategy to adaptively solve this ill-posed problem by iterated soft shrinkage and the associated forward problem is presented. In the second part of the talk, a basis construction for complex domains avoiding the curse of dimensionality based on the extension of local bases is given. Moreover existence and uniqueness results for the forward problem are presented.

Abstracts

Hierarchical and Black-Box Approximation of Tensors

Lars Grasedyck (Max-Planck-Institut f. Math. i.d.N.)

The talk covers the advances in black-box tensor approximation as well as the new reliable tensor representation and arithmetics in the hierarchical rank model. The results for the black-box approximation of tensors are in the classical tensor rank model where a priori estimates of truncation errors are missing. In the new hierarchical model we present a priori
error bounds in terms of the best approximation. The hierarchical rank k model contains all tensors of rank k (even border rank k) and is thus a much richer class.

m-term approximation in Tensor product function spaces

Markus Hansen (Friedrich-Schiller-Universitaet Jena)

We consider the problem of m-term approximation with respect to tensor product function spaces, which can be characterized by tensor product wavelet systems. In particular, we deal with Sobolev and Besov spaces of dominating mixed smoothness.
m-term approximation is a type of nonlinear approximation much discussed in recent years. Furthermore, we shall compare the approximation rates with those for (linear) approximation from sparse grids.

Adaptive Approximation Algorithms for Sparse Data Representation

Armin Iske (University of Hamburg)

This talk reports on recent progress concerning ongoing joint work with Gerlind Plonka-Hoch, Mijail Guillemard, and Stefanie Tenorth. Topics include the Easy Path Wavelet Transform (EPWT), analysis of high-dimensional signals by manifold learning, and sparse representation of video data.

Kronecker Products and Compressed Sensing

Sadegh Jokar (TU Berlin)

The Kronecker product of matrices plays a central role in mathematics and in applications found in engineering and theoretical physics. In this talk, we discuss dierent sparsity measures such as restricted isometry property (RIP), null space property (NSP), mutual incoherence, spark and their connections and how these measures behave in the case where the matrix is the Kronecker product of two matrices.

Abstracts

On hybrid models for stochastic reaction kinetics

Tobias Jahnke (Universität Karlsruhe (TH))

Many processes in systems biology can be modelled as reaction systems in which $d \in \mathbb{N}$ different species interact via $r \in \mathbb{N}$ reaction channels. In most applications the time evolution of such a system can be accurately described in terms of classical *deterministic reaction kinetics*: The reaction system is translated into a system of d ordinary differential equations (the reaction-rate equations), and the solution $y(t) \in \mathbb{R}^d$ indicates how the concentration or amount of each of the d species changes in time. The traditional model is simple and computationally cheap, but fails in situations where the influence of stochastic noise cannot be ignored, and where the amount of certain species is so small that it must be described in terms of integer particle numbers instead of real-valued, continuous concentrations. This is the case in gene regulatory networks, viral kinetics with few infectious individuals, and many other biological systems.

High dimensional sparse fast Fourier transforms

Lutz Kämmerer (TU Chemnitz)

Functions with bounded mixed derivatives allow for an effective approximation by trigonometric polynomials with Fourier coefficients supported on the hyperbolic cross. Interpolating on sparse grid nodes, such an approximation can be computed by means of the hyperbolic cross fast Fourier transform (HCFFT) efficiently.
In this talk, we discuss a generalisation of the HCFFT to arbitrary sampling nodes. Moreover, we show that the interpolation on the sparse grid is mildly ill conditioned and give examples of stable spatial discretisations.

Reinforcement Learning in a Continuous State Space

Irene Klompmaker (TU Berlin)

Reinforcement learning methods are methods for solving optimal control problems for which only a partial amount of initial data are available to the system that learns. To solve such optimal control problems, Dynamic Programming (DP) methods like for example Value Iteration, are used to determine the optimal value function and therefore the optimal control policy.
In the case of a continuous state space, appropriate discretization methods are needed. Especially in regard of making progress for higher dimensional problems, we examine the use of sparse grids in this context.
So in this talk, we will present an approach using adaptive sparse grids to ap-

proximate the value function via Dynamic Programming. By means of some low dimensional examples from deterministic and stochastic optimal control, we will point out some difficulties concerning the convergence of the approximation scheme.

Directional Multiresolution Schemes for Transport Dominated Problems: Shearlet Constructions and Petrov-Galerkin Discretizations

Lim Wang-Q (University of Osnabrueck), Gerrit Welper (RWTH Aachen)

Many important problem classes are governed by anisotropic features such as singularities concentrated on lower dimensional embedded manifolds. Therefore, analyzing the intrinsic geometrical features of the underlying object is essentially in many applications.
In the first part of this talk, presented by Wang-Q Lim, we will present constructions of compactly supported directional systems. We also show that they can be effectively used to extract anisotropic structures from given data.
The second part of the talk, presented by Gerrit Welper, is concerned with preparing for the use of such L_2 stable shearlet-frames for solving unsymmetric partial differential equations whose solutions exhibit strong anisotropic features. Here we shall confine the discussion to the model problem of linear convection. Specifically, we will present a a well posed variational formulation for the convection problem where the solution space is L_2 in order to be able to make use of the shearlet frames. The key point is to identify a proper test space. On one hand this leads to finite dimensional stable discretizations. On the other hand, we shall show how to construct a frame for that test space. This will be used to formulate adaptive solution strategies similar to those developed earlier for elliptic problems.

Adaptive Wavelet Methods for Stochastic Partial Differential Equations

Felix Lindner (TU Dresden)

In the first part of the talk the main goal of our project will be explained, which is the development of adaptive wavelet schemes for stochastic partial differential equations of parabolic type on piecewise smooth domains. In the second part, a first result concerning the weak order of a (not adaptive) numerical scheme for the stochastic heat equation driven by impulsive noise will presented. Finally, the last part of the talk will deal with adaptive wavelet tree approximation.

Abstracts

Variational Approximations in Quantum Dynamics and the MCTDH Method

Christian Lubich (University Tübingen)

The talk describes model reduction in the multi-particle time-dependent Schrödinger equation via the Dirac-Frenkel variational approximation principle and then turns to the multi-configuration time-dependent Hartree method (MCTDH) as an important, practically very successful example. This approach can be viewed as a dynamical low-rank approximation. The MCTDH nonlinear equations of motion and their numerical integration are discussed. The talk closes with an analysis of the modelling error in the MCTDH method, showing the mechanisms that may lead to convergence or failure.

Stochastic Galerkin Methods – Fundamentals and Algorithms

Antje Mugler (Westsächsische Hochschule Zwickau), Elisabeth Ullmann (TU Bergakademie Freiberg)

We briefly review the goals of our project of investigating and clarifying the mathematical underpinnings of stochastic Galerkin methods, currently one of the key approaches for approximating the solution of PDEs with random data, as well as developing efficient computational solution methods. We will split our presentation between the two subprojects. The first, presented by Antje Mugler, will discuss the approximation of input and solution random fields using multivariate polynomials. The second, presented by Elisabeth Ullmann, will give a progress report on linear solvers for stochastic Galerkin discretizations.

Minimization Tasks in Electronic Structure Calculations and Minimization with Sums of Elementary Tensors

Thorsten Rohwedder (TU Berlin)

In the first part of this talk, we give an introduction to the direct minimization tasks associated with Hartree-Fock and Density Functional Theory methods used in electronic structure calculations. In this context, we present some results from [Schneider, Rohwedder, Blauert, Neelov, 2008] concerned with the convergence of the eigenfunctions (i.e. the minimizer) and the energies (i.e. the quantity to be minimized) of the given functionals.

In the second part, we show how in a more general framework of functional minimization, the minimizer of a given functional J, given on a high-dimensional

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space $\mathcal{V}=\bigotimes_{i=1}^{n} V$ may be approximated by sums of elementary tensors of fixed rank r by iterating directly in the space $V^{r\cdot d}$, without truncation operations being involved [Espig, Hackbusch, Rohwedder, Schneider, 2009]. A transfer of the presented method to Tucker format is proposed.

Explicit error bounds for reversible Markov chain Monte Carlo

Daniel Rudolf (Friedrich Schiller University Jena)

Markov chain Monte Carlo methods for approximating the expectation play a crucial role in numerous applications. The problem is to compute the expectation with respect to some distribution. A straight generation of the desired distribution is in general not possible. Thus it is reasonable to use Markov chain sampling with a burn-in. An explicit error bound with respect to different norms of the function will be presented. By the estimation the well known asymptotical limit of the error is attained, i.e. there is no gap between the estimate and the asymptotical behavior.

Valuation of Structured Financial Products

Andreas Rupp (Universität Ulm)

The market of structured financial products has grown tremendously in the past decade. Especially the repackaging of mortgage loans, so called collateralized debt obligations, has partially led to the current financial crisis. Due to the complex structure of such a financial product, specifically due to the dependence structure of the single assets within a collateralized debt obligation, its modeling and pricing is not a trivial task.
In this talk, we will discuss basic properties of collateralized debt obligations and a reduced form contagion model for such products. Furthermore, we will discuss how (adaptive) wavelet methods can be used to price the tranches of a collateralized debt obligation.

An Error Criterion for Numerical Solutions of Backward SDEs

Jessica Steiner (Universität des Saarlandes)

Many option pricing and portfolio selection problems in mathematical finance can be reformulated in terms of backward SDEs (BSDEs). As the corresponding BSDE can rarely be solved in closed form, simulation of BSDEs is of prime im-

portance. However, the quality of the simulated solution depends on the interplay of different error sources, such as the discretization error, the simulation error, and e. g. the choice of basis functions (if the conditional expectations are estimated by least squares Monte Carlo). In this talk we suggest an error criterion which can be calculated explicitly in terms of the simulated solutions. Under suitable conditions it can be shown that this observable error criterion converges to zero at the same rate as the simulated solution converges to the unknown true solution. Finally, we illustrate how this error criterion can be applied to judge the quality of simulated solutions for some non-linear option pricing problems.

Regularity, Complexity, and Approximability of Electronic Wave Functions

Harry Yserentant (TU Berlin)

This talk considers the electronic Schrödinger equation of quantum theory that describes the motion of N electrons under Coulomb interaction forces in a field of clamped nuclei. Solutions of this equation depend on $3N$ variables, three spatial dimensions for each electron. Approximating the solutions is thus inordinately challenging, and it is conventionally believed that a reduction to simplified models, such as those of the Hartree-Fock method or density functional theory, is the only tenable approach. We indicate why this conventional wisdom need not be ironclad: the regularity of the solutions, which increases with the number of electrons, the decay behavior of their mixed derivatives, and the antisymmetry enforced by the Pauli principle contribute properties that allow these functions to be approximated with an order of complexity which comes arbitrarily close to that for a system of only two electrons. Some very recent results on the approximation by wavelets and on the decomposition into angular momentum eigenfunction are described.