Veranstaltungen im Sommersemester 2016

Das siebenundzwanzigste Treffen des Rhein-Main Arbeitskreises findet

Freitag, den 1. Juli 2016, 15:00 Uhr

an der

Johannes-Gutenberg-Universität Mainz, Fachbereich Physik, Mathematik und Informatik,
Staudinger Weg 9,
55128 Mainz

im **Raum 05-514** statt.

Programm

15:00 Uhr: Prof. Dr. Reinhold Schneider (TU Berlin)
Convergence rates of basis sets in Density Functional Theory and Hartree-Fock for electronic structure calculation.
The numerical solution of the stationary electronic Schroedinger equation is a fundamental task in the numerical simulation of atomic and molecular behaviour, with widespread applications in chemistry, molecular biology, solid state physics and material sciences. In Hartree Fock, resp. Density Functional Theory (DFT) the highdimensional linear Schroedinger equation is replaced by a system of nonlinear but low dimensional Hartree Fock resp. Kohn Sham equations. This allows the treatment of relativley large systems. We will discuss the numerical treatment of DFT as a constrained optimization problem. We are considering LAPW, numerical atomic orbitals and Gaussian basis functions and hp-finite elements for all electron calculations. We have shown that, under mild assumptions, these functions are converging almost exponentially, i.e. with any algebraic convergence rate. These results may explain the success of these functions in chemical and physical applications.
This is joint work together with M. Bachmayr (RWTH Aachen) and H. Chen (U Warwick).

15:45 Uhr: Tee/Kaffee

16:15 Uhr: Esther Hans (Johannes Gutenberg-Universität Mainz)
Globally convergent multilevel B-semismooth Newton methods for l1-Tikhonov regularization.
Tikhonov regularization with l1 coefficient penalties is widely used for the regularization of ill-posed problems if the underlying solution is sparse with respect to some given basis. Due to their local convergence speed, semismooth Newton methods are competitive for the minimization of the resulting nonsmooth Tikhonov functional. In the first part of the talk, we are concerned with the globalization of existing locally superlinearly convergent semismooth Newton methods. Here, we present a damped generalized Newton method based on the B(ouligand)-derivative of the specific nonlinearity.

The second part of the talk treats an acceleration scheme combining the resulting globally convergent generalized Newton method with algebraic multilevel methods, recently introduced by Treister, Turek and Yavneh. The results are based on joint work with Thorsten Raasch.

17:00 Uhr: Dr. Mario Hefter (TU Kaiserslautern)

Optimal strong approximation of the one-dimensional squared Bessel process.

We consider a stochastic differential equation (SDE) describing a one-dimensional squared Bessel process and study strong (pathwise) approximation of the solution at the final time point t=1. This SDE is a particular instance of a Cox-Ingersoll-Ross (CIR) process where the boundary point zero is accessible. We consider numerical methods that have access to values of the driving Brownian motion at a finite number of time points. We show that the polynomial convergence rate of the n-th minimal errors for the class of adaptive algorithms as well as for the class of algorithms that rely on equidistant grids are equal to infinity and 1/2, respectively. As a consequence, we obtain that the parameters appearing in the CIR process affect the convergence rate of strong approximation. A key step in the proofs consists of identifying the pathwise solution of the SDE and link this problem to global optimization under the Wiener measure. This is joint work with James M. Calvin and Andre Herzwurm.

anschließend: Nachsitzung