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MATHEMATIKKOLLOQUIUM

Das Institut für Mathematik lädt zu folgendem Vortrag ein:

Dynamical Tensor Approximation and Quantum Dynamics

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For the low rank approximation of time-dependent data matrices or tensors, and of solutions to matrix or tensor differential equations, for example resulting from space semi-discretization of partial differential equations, an increment based computational approach is proposed and analyzed. In this variational method, the derivative is projected onto the tangent space of the manifold of low rank tensors at the current approximation. This yields nonlinear ordinary differential equations that are well-suited for numerical integration. The error analysis compares the result with a pointwise best approximation. It is proven that the approach gives locally quasi-optimal low rank approximations and that under additional assumptions the error grows only linearly also over "long" time intervals. Numerical experiments illustrate the theoretical results. As an extension of this variational approximation to an infinite dimensional setting, we describe and analyze an approach to the approximate solution of the time-dependent electronic Schrödinger equation. To make the high-dimensional, linear Schrödinger equation tractable for numerical computation, we use the multiconfiguration time-dependent Hartree-Fock method (MCTDHF). This approximation on a nonlinear, solution-dependent manifold is defined by the Dirac-Frenkel variational principle and implies equations of motion which correspond to coupled nonlinear, single-particle Schrödinger equations. For the numerical integration of the MCTDHF equations we analyze the convergence of time semidiscretization based on symmetric additive (Strang) splitting of the vector field. It is proven that the convergence is of first order in H^1 and of second order in L^2 if the exact solution is in H^2. As a prerequisite, we prove that for initial data in the Sobolev space H^2, there exists a unique strong solution of the MCTDHF equations in H^2 for all times where the density matrix appearing in the definition of the equations stays invertible. The computationally most demanding part of the numerical solution of the MCTDHF equations is the evaluation of the high-dimensional "meanfield integrals". To reduce the computational effort we propose to use an approximation by "hierarchical matrices". We give theoretical error bounds for this approximation in the context of MCTDHF and demonstrate its advantages by numerical experiments with a well established MCTDHF code.

Zeit: Donnerstag, den 29. Oktober 2009 um 17^{15} Uhr

Ort: Technikerstr. 13b, Hörsaaltrakt Baufakultät, HSB 9

Mechthild Thalhammer

Gäste sind herzlich willkommen!