

## Einladung zum Oberseminar Wissenschaftliches Rechnen

Julius-Maximilians-Universität Würzburg Lehrstuhl für Wissenschaftliches Rechnen IX

## Gabriele Ciaramella

Lehrstuhl für Wissenschaftliches Rechnen, Universität Würzburg

## Newton methods for optimal control of closed quantum spin systems

Many applications in nanotechnologies deal with the problem of steering a quantum dynamical system from an initial state to a given target state. In particular, this class of problems appears in nuclear magnetic resonance (NMR) spectroscopy, magnetic resonance imaging (MRI) and quantum computing, where the governing model is the Liouville-von Neumann (LvN) equation, which describes the time evolution of the density operator that characterizes quantum spin systems. Mathematically, this problem can be regarded as an optimal control problem and as an exact-controllability problem.

An efficient and robust computational framework for solving quantum spin optimal control and exact-controllability problems governed by the LvN equation is presented. The computational framework is based on a matrix-free semi smooth Krylov-Newton scheme for solving optimal control problems. This Newton scheme is embedded in a continuation procedure for solving exact-controllability problems. Theoretical results are presented and validated by numerical experiments, which demonstrate the computational ability of the proposed framework.

Ort: Raum 30.02.003 (2.Stock) (Mathegeb. 30 West) Zeit: Dienstag, 17.06.2013, um 11.00 Uhr

Zu diesem Vortrag laden wir Sie herzlich ein.

gez. Prof. Dr. Alfio Borzi