Einladung zum Oberseminar Wissenschaftliches Rechnen

Julius-Maximilians-Universität Würzburg
Lehrstuhl für Wissenschaftliches Rechnen IX

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Towards the optimal control of TDDFT models

To bypass the enormous difficulties of solving the Schrödinger equation of a many-electron system, an equivalent description given by the time-dependent density functional theory (TDDFT) has been proposed. The TDDFT approach allows accurate simulation of interacting multi-electron systems and has been successfully applied to many quantum models. While the TDDFT simulation of quantum systems is well established, much less is known concerning the optimal control of systems governed by the TDDFT model.

The purpose of this talk is to introduce the concept of TDDFT and to investigate the extension of optimal control techniques to solve the problem of driving a TDDFT system to reach a desired target configuration in a Hilbert space. For this purpose, in this talk adjoint methods are considered, thereby the forward and adjoint equations are solved using operator splitting pseudo-spectral techniques. The resulting reduced gradient is used to implement fast numerical solvers to the TDDFT optimal control problem.

Ort: Raum 30.02.003 (2. Stock) (Mathegeb. 30 West) Zeit: Mittwoch, 17. Juni 2015, 10.00 Uhr

Zu diesem Vortrag laden wir Sie herzlich ein.

gez. Prof. Dr. Alfio Borzi
gez. Prof. Dr. Roland Griesmaier