Sonderforschungsbereich 1060

The Mathematics of Emergent Effects

Einladung zu einem Vortrag im SFB-Seminar

Prof. Dr. Eric Cances

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spricht zum Thema

Numerical methods for electronic structure calculation

Zeit: Dienstag, den 20. Mai 2014, 14.15 Uhr

Ort: Lipschitz-Saal 1.016, Endenicher Allee 60

Kaffee/Tee: anschl. im Plückerraum 1.015

gez. **Michael Griebel**

Abstract: Electronic structure calculation has become an essential tool in chemistry, condensed matter physics, molecular biology, materials science, and nanosciences. It is also an inexhaustible source of exciting mathematical and numerical issues.
In this talk, I will focus on two standard electronic structure models, namely the N-body Schrödinger equation, and the Kohn-Sham formulation of the Density Functional Theory (DFT). The former model is a (very) high-dimensional linear elliptic eigenvalue problem. It is out of reach of standard numerical methods, but its solutions can be numerically approximated either by stochastic methods, or by sparse tensor product techniques. The Kohn-Sham model is a constrained optimization problem, whose Euler-Lagrange equations have the form of a coupled system of nonlinear elliptic eigenvalue problems. Recent progress has been made in the analysis of these mathematical models and of the associated numerical methods, which paves the road to high-fidelity numerical simulations (with a posteriori error bounds) of the electronic structure of large molecular systems.