Graduate Course Autumn 2007

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From Classical to Quantum Molecular Dynamics:

Intermediate Models and Numerical Analysis

Thursday, 10-12, HG G 43, ETH Zürich Zentrum (starting Sep 27, 2007)

Abstract. Quantum dynamics of molecules poses a variety of numerical challenges:

- high-dimensional partial differential equations,
- highly oscillatory solutions,
- geometric structures (e.g., symplecticity) to be preserved in discretizations.

The course addresses such problems from the viewpoint of numerical analysis, illustrating them to a large extent on intermediate models between the Schrödinger equation of full quantum dynamics and the Newtonian equations of classical molecular dynamics.
The fruitful interplay between computational quantum dynamics and numerical analysis is emphasized: numerical algorithms originally developed for quantum dynamics can thus sometimes find a much wider scope of application areas, and numerical analysis can contribute theoretical insight and novel algorithms to computational quantum dynamics.

Target audience: master and graduate students of mathematics and computational sciences