Mini-Workshop
Topics in Numerical Quantum Dynamics
Uppsala University, October 19 2012
14.00-16.30
ITC room 2446

Background: During the last decades, new experimental techniques have enabled studies of the dynamics of chemical reactions. This has triggered intense research also in theoretical quantum dynamics, where a time-resolved description of chemical reactions is derived by solving the time-dependent Schrödinger equation (TDSE) for wave functions evolving on coupled potential energy surfaces. Numerical methods for the TDSE have been developed, analyzed and used by numerous researchers in both numerical analysis and chemistry/physics, and during the years many specialized papers of high quality have been produced. Also, researchers have presented large-scale parallel implementations of some of the schemes, producing results of interest in chemistry. The aim of this mini-workshop is to present a range of recent results describing numerical techniques for important sub-problems involved when solving quantum dynamics problems and engage in a discussion on future development of the field.

Speakers and Titles (20 minutes presentations + discussion):

Prof. Christian Lubich, Mathematics, University of Tübingen, Germany
On the MCTDH method

Prof. Regina de Vivie-Riedle, Chemistry, Ludwig-Maximilians-Universität München, Germany
Time windows for intramolecular electronic coherence and control

Dr. Vasile Gradinaru, Seminar for Applied Mathematics, ETH, Switzerland
On the convergence of the semiclassical time-splitting

Dr. Hans Karlsson, Quantum Chemistry, Uppsala University, Sweden
Time-resolved photoelectron spectroscopy on NaI : A computational point of view.

Emil Kieri (PhD student), Scientific Computing, Uppsala University, Sweden
An adaptive pseudospectral method for wave packet dynamics

Some refreshments will be served during the workshop

Welcome!

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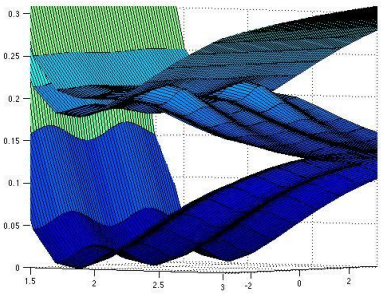

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