Mini-Workshop Numerical Methods for Quantum Dynamics Uppsala University, February 11, 2016 14.00-16.30 ITC room 2345

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 time-resolved descriptions of dynamic events such as chemical reactions are deduced from mathematical modelling and numerical simulations. Both the models and methods have been developed, analyzed and used by numerous researchers in both numerical analysis and chemistry/physics, and over the years many specialized papers of high quality have been produced. The main aim of this mini-workshop is to present recent results describing models and numerical techniques for solving quantum dynamics problems and engage in a discussion on future development of the field.

Speakers and titles (25 minutes presentations including questions and discussion):

Elisabeth Larsson, Division of Scientific Computing, Uppsala University

A Galerkin radial basis function method applied to the Schrödinger equation

Anders Szepessy, Department of Mathematics, Royal Institute of Technology, Stockholm

Quantum observables for the macroscopic conservation laws approximated by molecular dynamics

Tobias Jahnke, Institut für Angewandte und Numerische Mathematik, Karlsruher Institut für Technologie

A numerical method for a nonlinear Schrödinger equation with dispersion management

Caroline Lasser, Zentrum Mathematik, Technische Universität München A frozen Gaussian approximation for molecular quantum dynamics

Hans Karlsson, Quantum Chemistry, Uppsala University

Quantum dynamics of time-resolved photoelectron spectroscopy of Nal

Some refreshments will be served during the workshop

Welcome!

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