

“Modeling, Numerics and Simulations with Nonlinear Schrödinger and Boltzmann equations”

Abstract :

Within the general goals of the “University Priority Research Area” (“UniversitätsSchwerPunkt” USP) “Computational Science / Scientific Computing”, the PDE group at the faculty of mathematics wants to boost its activities in this direction and strengthen “interdisciplinary” collaboration within the natural sciences : The main goal of this project is the development of mathematical models and computational methods and their application to computer simulations in collaboration with partners in quantum physics, quantum chemistry and quantum electronics that use the kind of PDEs of this project.

The similarities in mathematical structures of models in different application areas allow to develop new methods in a general setting. The 2 “main themes”, Nonlinear Schrödinger equations and (quantum) Boltzmann equations are somewhat linked by “kinetic formulations” of PDEs and in particular by the Wigner transform that maps between the physical space of NLS (and macroscopic models like (quantum) fluid dynamics) and the “phase space” of kinetic equations. The topics of the work program of this project are focused on modeling and, in particular, developing of state-of-the-art numerical methods for the time-dependent PDEs that occur. For the sake of simulation of realistic applications also aspects of efficient implementation of the algorithms shall be dealt with, including the development of optimized codes for parallel machines, in particular the new “Schrödinger III” cluster that is partly already financed for the purpose of the USP.

The innovation of numerical simulation tools will be done in parallel with innovative modeling approaches, where e.g. also aspects of “stochastic PDEs” will be considered.