Berlin Leipzig Seminar
Analysis/probability theory
Second Meeting Winter Term 2008/09

Organized by the DFG Research Group *Analysis and Stochastics in Complex Physical Systems*

DATE: Friday, 12 December 2008

VENUE: Technical University Berlin, Institute for Mathematics, Str. des 17. Juni 136, 10623 Berlin, Room MA313/314

PROGRAMME:

9:40–10:30: **Mark Peletier (University of Technology Eindhoven)**

Unification of diffusion and reaction: derivation of the law of mass action

Abstract: Over the last ten years it has become understood how many diffusion equations can be equipped with a gradient-flow structure, based on the entropy as the driving force and the Wasserstein distance as the opposing 'brake'. In this talk I shall describe recent efforts to also bring reactions into this structure, by describing the reaction process as a Brownian motion in a chemical-energy landscape.

10:40–11:30: **Utpal Manna (MPI Leipzig)**

An Application of Stochastic Stackelberg Differential Games in Conflict Management

Abstract: There is broad agreement that global climate change may have substantial impacts on water resources. As multiple countries share a river, the likelihood of a water resource conflict stemming from climate change is higher in a transboundary setting. In this talk, using the framework of a stochastic Stackelberg differential game, we will explore the scope of cooperative bargain between an upstream and a downstream country over the level of transboundary water sharing by negotiating some non-water related issues of mutual interest to both the countries, given uncertainty in the river flow due to climate change. [Joint work with A. Bhaduri (University of Bonn), J. Liebe (University of Bonn), E. Barbier (University of Wyoming)].

11:40–12:30: **Reinhold Schneider (Technical University Berlin)**

Analysis of the projected Coupled Cluster Method in Electronic Structure Calculation

Abstract: The electronic Schrödinger equation plays a fundamental role in molecular physics. It describes the stationary nonrelativistic behaviour of a quantum mechanical N-electron system in the electric field generated by the nuclei. The *(Projected) Coupled Cluster Method* has been developed for the numerical computation of the ground state energy and wave function. It provides a powerful tool for high accuracy electronic structure calculations. The talk aims to provide a rigorous analytical treatment and convergence analysis of this method. If the discrete Hartree-Fock solution is sufficiently good, the quasi-optimal convergence of the projected coupled cluster solution to the full CI (*Configuration Interaction*) solution is shown. Under reasonable assumptions also the convergence to the exact wave function can be shown in the Sobolev H^1-norm. The error of the ground state energy computation is estimated by an Aubin-Nitsche-type approach. Although the Projected Coupled Cluster method is nonvariational it shares advantages with the Galerkin or CI method. In addition it provides size consistency, which is considered as a fundamental property in many particle quantum mechanics.

Everybody is welcome to attend. Wolfgang König, University of Leipzig