

# Berlin Center for Studies of Complex Chemical Systems

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Humboldt-Universität, Max-Delbrück-Centrum für Molekulare Medizin, Otto-von-Guericke-Universität Magdeburg, Physikalisch-Technische Bundesanstalt, Technische Universität Berlin, Universität Potsdam.

Seminar

## Complex Nonlinear Processes in Chemistry and Biology

*Honorary Chairman: G. Ertl.*

*Organizers: M. Bär, C. Beta, H. Engel, M. Falcke, M. J. B. Hauser, J. Kurths, A. S. Mikhailov, P. Plath, L. Schimansky-Geier, and H. Stark.*

Friday, 18th January, 2013, 16:00 s.t.

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Prof. Dr. Kay Hamacher

*Technical University Darmstadt*

### Global Optimization by Stochastic Tunneling And Self-Adapting Steering Techniques

Global optimization remains one of the great challenges in scientific computing. One particular successful approach is the usage of tunneling functions to cross barriers and transition states more easily thus allowing for a fast scan of the Potential Energy Surface under investigation. In this talk I discuss the general idea of stochastic tunneling (STUN) and a novel performance measurement procedure for such approaches. Furthermore, I propose an adaptive algorithm that is steered by this performance measure. This algorithm is based on a scale-free measure and thus applicable to general stochastic optimization schemes. Therefore, I show the transferability of this "meta-algorithm" to other optimization procedure such as extremal optimization or energy landscape paving.