



NIC Seminar

- Topic:** **Optimizing the round trip rates in replica exchange simulations**
- Speaker:** Robert Denschlag, BioMolecular Optics,
Ludwig-Maximilians-Universität München
- Contents:** To gain most benefit of replica exchange (RE) simulations the round trip rates of the replicas should be as high as possible. The talk will be dealing with two possibilities to achieve high round trip rates in RE simulations with explicit solvent. One approach is the choice of an optimal temperature ladder. However, it turns out that what is optimal depends on the applied exchange scheme. Thus, different exchange schemes will be presented and discussed. A second approach is to keep the number of replicas as small as possible. Here, I will present a Hamilton RE method which is blind with respect to the solvent-solvent interaction and, thus, strongly reduces the number of replicas necessary to cover a specific temperature range.
- Time:** Wednesday, 25 February 2009, 14:00
- Venue:** Besprechungsraum 2, room 146, Jülich Supercomputing Centre

Anyone interested is cordially invited to participate.

sgd Dr. Sabine Höfler-Thierfeldt