Speaker: Prof. Dr. Peter Güntert, Goethe University, Institute of Physical Chemistry and FIAS; Graduate School of Science, Tokyo Metropolitan University

Title: What can computation do for NMR with proteins?

Nuclear magnetic resonance spectroscopy (NMR) is one of the most important analytical techniques for biological macromolecules. Computational methods are indispensable for evaluating and interpreting structural and dynamical data from NMR and related techniques. Our computational research in this field is implemented in the software package CYANA that is used in most bio-NMR laboratories in the world. The talk will give an overview of the methods and present new results and applications.

NMR protein structures are calculated on the basis of experimental NMR data using simulated annealing by fast molecular dynamics simulation in torsion angle space. Distance measurements are obtained by automatically analyzing NOESY spectra, or corresponding solid-state NMR experiments.

NMR resonance assignment constitutes the first and often very time-consuming step to a protein structure. The new FLYA algorithm for the assignment of backbone and side-chain chemical shifts will be presented that has the reliability and flexibility to replace manual assignment procedures for most NMR studies of proteins. The algorithm enables, in combination with the assignment of NOE distance restraints, the fully automated structure determination of proteins starting from raw NMR spectra, in favorable cases even without any “through-bond” spectra.

Recent applications of the methodology include the structure determination of a protein in living cells, the de novo NMR structure determination of the seven transmembrane helix protein proteorhodopsin, the automated assignment and structure determination of amyloid fibrils by solid-state NMR, and the spatial elucidation of motion in proteins by ensemble-based structure calculation using exact NOEs.