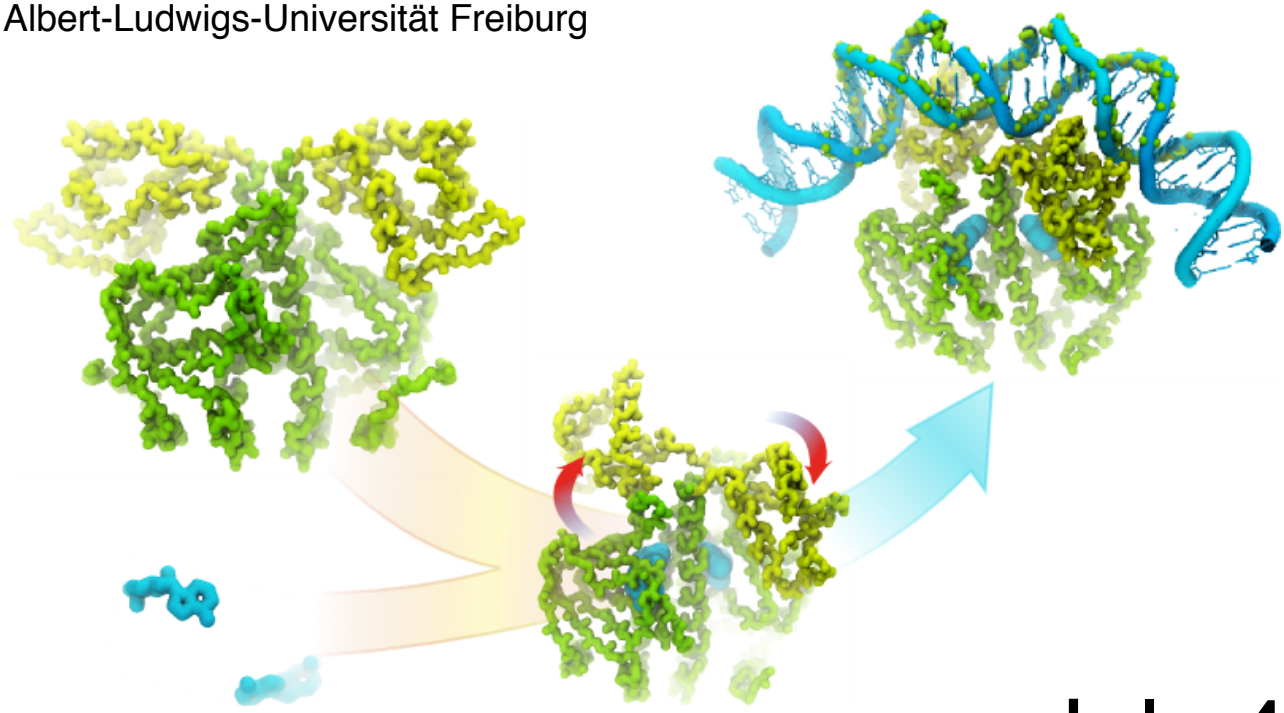
Physikalisches Institut

Albert-Ludwigs-Universität Freiburg



July 4

Structure determination from sparse NMR data with Rosetta

Oliver Lange

TUM, Munich

We use chemical shift data, backbone RDC data and sparse NOESY data to in cases where structure determination with conventional NMR methodology is difficult,determine protein structures such as membrane proteins, larger proteins (> 15kDa molecular weight) and low- or transiently populated alternative conformational states. To efficiently exploit the synergy between the low-resolution information in sparse NMR data and the high-resolution information in the Rosetta all-atom energy function we have developed RASREC, a genetic algorithm that recombines structural features in a resolution adapted manner. The methodology is applied to de-novo determination of protein structures up to 40kDa and to structurally characterize a low-populated conformational state of the L99A mutant of T4L.

Molecular Dynamics Seminars 2012

Seminar Room of Gustav Mie Haus, Ground Floor, 16:15

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