# CFEL SCIENCE

# SEMINAR

**27th February 2012 - 14:00 h**
building 49 - seminar room (108)
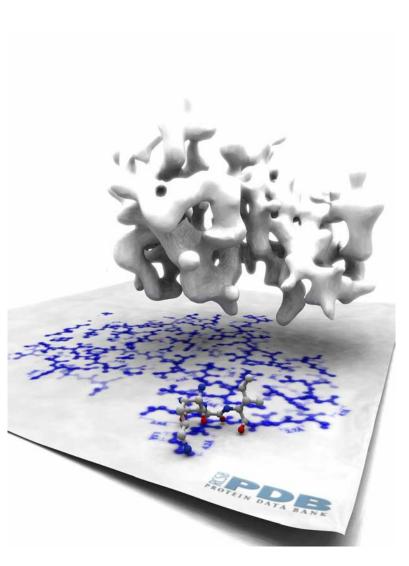
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## Protein Structure and Dynamics from Low-Resolution Data

Structure determination of large proteins and protein assemblies is a major challenge in molecular biology. Experiments, such as X-ray crystallography or single-particle Cryo-EM, on such complex systems often yield only low resolution (> 4Å) data, which are not sufficient to fully determine atomistic structures.

The refinement of approximate initial models is typically significantly harder than at high resolution. The Deformable Elastic Network (DEN) approach is presented that makes use of additional prior information on homologous structures which guides the refinement and dramatically improves the obtained structures. Furthermore, this approach can also be applied in combinations with molecular dynamics simulations to refine homology models in the absence of experimental information.

Single-particle Cryo-EM yields images of individual proteins in potentially different conformations and therefore yields a wealth of information on structural dynamics. This information is however very difficult to extract since each image is extremely noisy. The common approaches to reconstruct three-dimensional density maps average out any structural heterogeneity and the information on the dynamics is lost. We show how principal protein motions can be reconstructed from the variation contained in the single particle images.



Host: Thomas White - Coherent Imaging Division