BIOMATERIALS

Forces in Biomolecular Systems SFB 863

# Integrative Dynamical Biology


## Carlo Camilloni

### TU München, Chemie Department



Abstract:

Modelling the behaviour of heterogeneous systems like biomolecules is a challenging task. Common, complementary approaches include experimental techniques like X-RAY, NMR, SAXS, CRYO-EM, FRET and Force Microscopy and computational techniques like quantum, classical and coarse grain simulations. While from the first it is possible to model atomistic structures only when the system dynamic is limited, the latter are perfectly suited to model the atomistic behaviour on the accessible time scale. Unfortunately in addition to the limitation of the time scale accessible to simulatons, they are also affected by strong limitation in the quality of their Hamiltonians.

My work is focused in bridging the gap between structural experimental techniques and molecular simulations. In particular I will first show how it is possible to use the Maximum Entropy Principle and Enhanced Sampling Techniques to bridge this gap by including experimental knowledge in molecular simulations.

Furthermore I will introduce a completely general Bayesian framework that allows not only to include experimental data but to model heterogeneous and noisy data from multiple sources at the same time. This latter method, couple with Metadynamics, can pave the way to model even larger and more complex systems.


## Friday, November 20th, 2015, 13:00

## Room PH 127


Contact: Martin Zacharias, martin.zacharias@mytum.de, phone: ++49 89 289 12335