CECAM/Psi-k Conference on
Multi-scale Modeling from First Principles

Cap Roig, Playa de Aro, Spain, Sep. 8–13, 2013

Session on
Biological Systems and Neural Network Methods

Introduction

Matthias Rupp, University of Basel, Switzerland

Biological systems applications

Talks

Raymond Kapral: Molecular machines and self-propelled nanomotors
Mesoscopic multi-scale simulations of protein conformational dynamics

Paolo Carloni: Membrane biophysics investigated by multi-scale methods
Molecular simulation of membranes and membrane proteins

Challenges

- System size — environment; proteins; cells
- Time scales — folding; reactions
- Quantum phenomena — electron transfer; proton transfer; excitations
- Complexity of systems — diversity; set-up; observations (variables)

Parametrization of force fields? Systematic coarse-graining?
Talk to more than two communities?

Neural network methods

Talks

Jörg Behler: Extending length and time scales of atomistic simulations
Neural network potentials: scope, limitations, examples

Christoph Dellago: Studying nucleation processes with computer simulations
Neural network potentials: force calculation and structure recognition

Challenges

- Require many reference calculations — on-the-fly learning; active learning
- Limited number of elements — materials; biological systems
- Representation of system — open question; alchemical changes
- Comparison with other methods — parametric vs. non-parametric

Domain of applicability? Propagation of uncertainties?