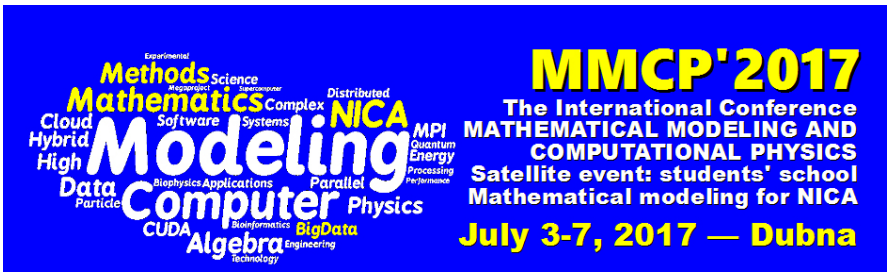

Contribution ID: **208** Type: **not specified**

Multiscale simulations of neuronal receptors

Monday, 3 July 2017 09:30 (30 minutes)

Molecular dynamics simulations of proteins may differ by the granularity of the underlying force fields (from quantum to coarse grain). At times, it is very useful to combine different descriptions in a hybrid description. Here I will present recent hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) –and MM/coarse grain (CG) based investigations of targets for pharmaceutical intervention. The predictive power and limitations of these multi-scale methods will be illustrated. The talk will close with a brief survey of multi-scale simulations within the recently formed consortium of the Human Brain Project, one of the two flagships grant funded by the EU.
The HPC-Leap, BioExel, Human Brain Project EU grants, along with the German agencies DFG and BMBF agencies are acknowledged for funding part of this research.

Primary author: Prof. CARLONI, Paolo (Forschungszentrum Jülich GmbH)

Presenter: Prof. CARLONI, Paolo (Forschungszentrum Jülich GmbH)

Session Classification: Plenary