

Multiscale hybrid modeling of biomembranes

Initiative: Modellierung und Simulation komplexer Systeme (beendet)

Ausschreibung: Biomoleküle-Zellen

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Heterogeneous membranes play a crucial role for many cellular processes and in biorelated nanotechnology. This project builds upon existing methodology and aims at the development of a genuine multiscale method, which is capable of including prior knowledge and allows to study the structure and dynamics of complex membrane systems on different scales. A "horizontal coupling" strategy is envisaged, that merges different levels of representation (originating from molecular field, phenomenological and coarse-grained particle descriptions) and different kinetic descriptions (diffusive Langevin and hydrodynamic Lattice-Boltzmann field) in a consistent way. This project encompasses a modular approach and validation of all elementary steps, i.e. for membranes of increasing complexity, using experiments (in Bayreuth and Leiden) and literature data. The new approach will ultimately be applied for a system of high scientific impact: to unravel the mechanisms in SNARE-mediated membrane fusion.

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