DY 11: Invited Talk

Time: Monday 15:00–15:30 Location: HÜL 186

Invited Talk DY 11.1 Mon 15:00 HÜL 186

A hydrodynamic view on the diffusion in membranes and dense solutions of proteins — •Gerhard Hummer[1,2], Sören von Bülow[1], Martin Vögele[1,3], Lisa Pietrek[1], Marc Siggel[1], Max Linke[1], Jürgen Köfinger[1], and Lukas Stelzl[1] — [1]Department of Theoretical Biophysics, Max Planck Institute of Biophysics, 60438 Frankfurt am Main, Germany — [2]Institute for Biophysics, Goethe University Frankfurt, 60438 Frankfurt am Main, Germany — [3]Computer Science Department, Stanford University, Stanford, CA 94305-9025, USA

Molecular dynamics simulations of the diffusion of proteins and other macromolecules in dense solutions and in lipid membranes revealed unexpected complexities. In systems mimicking the interior of a living cell, with densely packed proteins, the translational and rotational diffusion of proteins slow down dramatically at high protein concentrations, and the Stokes-Einstein relation appears to break down. In membranes, the apparent diffusion coefficient appears to grow without bound as the box size is increased. We resolve these issues by showing, first, that transient clustering of proteins explains quantitatively the increase in the apparent Stokes radius and the rise in the viscosity. Second, we show that the divergence of membrane diffusion is the result of the unusual hydrodynamics under periodic boundary conditions. Hydrodynamics also plays a central role in rotational diffusion, both in the bulk and within membranes. Accounting for hydrodynamics, we obtain diffusion coefficients that can be interpreted meaningfully and compared to experiment.