Research in the Department of Theory & Bio-Systems

So einfach wie möglich, aber nicht einfacher
Albert Einstein

The researchers and doctoral students of the Department of Theory and Bio-Systems form one experimental and six theoretical research teams. Each of these teams consists of the team leader and several students. The team leaders are:

- *Rumiana Dimova* (experiment, membranes and vesicles).
- *Thomas Gruhn* (theory, membranes and vesicles);
- *Jan Kierfeld* (theory, polymers and filaments);
- *Stefan Klumpp* (theory, transport by molecular motors; until 2005);
- *Volker Knecht* (theory; proteins and membranes; since 2006).
- *Christian Seidel* (theory, polymers and polyelectrolytes);
- *Julian Shillcock* (theory, supramolecular modelling; until 2005);
- *Thomas Weikl* (theory, proteins and membranes).

The Theory and Bio-Systems Department is responsible for and coordinates the International Max Planck Research School on "Biomimetic Systems", the European Early Stage Training Network about the same topic, in which three departments of the MPI participate, and the European Research Network on "Active Biomimetic Systems". The management of these networks is done by *Angelo Valleriani*.

In the following three subsections, the research within the Theory and Bio-Systems Department is described in terms of the underlying systems which exhibit a hierarchy of structural levels, the intriguing phenomena found in these systems, and the methods used to study them.

Systems

Our research is focused on bio-systems, which represents an abbreviation for "biomimetic and biological systems". If one looks at these systems bottom-up, i.e., from small to large length scales, one encounters a hierarchy of such systems including

- polymers and proteins,
- molecular motors,
- rods and filaments,
- membranes and vesicles, and
- networks in bio-systems.

When these systems are approached top-down, i.e., from larger to smaller scales, one encounters the problem of restricted geometries or confining walls and interfaces. In general, interfaces may be used to suspend and organize smaller bio-systems in order to make them accessible to systematic studies.

Phenomena

During the last two years, specific phenomena addressed in the area of polymers and proteins included the conformation of peptides at interfaces, the process of protein folding, and dense brushes of polyelectrolytes. As far as motor proteins or molecular motors are concerned, we studied the chemomechanical coupling of single motors and the cooperative transport by several such motors, see **Fig. 1**.

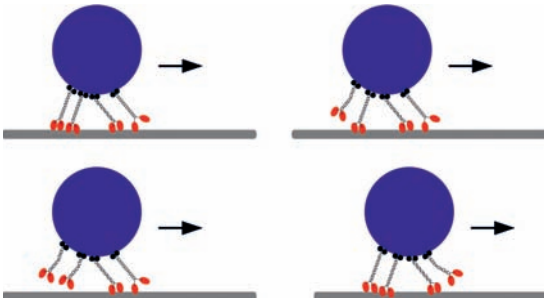


Fig. 1: Cooperative transport of cargo by several molecular motors

The cooperative behavior of rods and filaments provides many unusual phenomena such as the active polymerization of filaments, the ordering of filaments on substrate surfaces covered with immobilized molecular motors, see **Fig. 2**, and ordered mesophases of rods with adhesive endgroups.

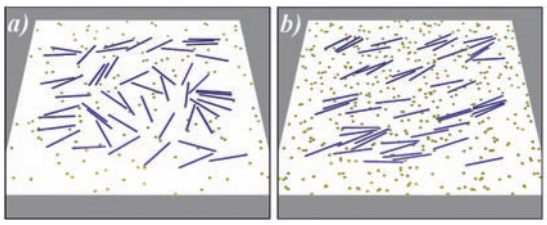
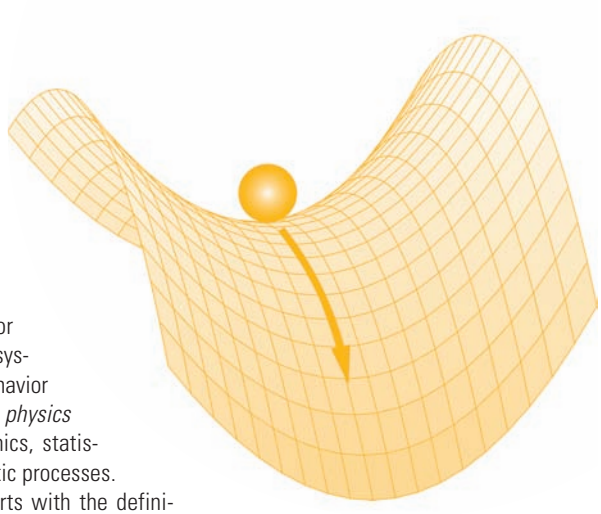


Fig. 2: (a) Disordered and (b) Ordered nematic states of rod-like filaments (blue) on a substrate surface with immobilized molecular motors (yellow spots). The transition from (a) to (b) is induced by an increase in the motor density.

In the research field of membranes and vesicles, we have improved our theoretical models for membrane fusion and membrane adhesion. A timely topic is the adhesion of membranes via specific molecular bonds, see **Fig.3**. In addition, the direct imaging of intramembrane domains and vesicle fusion has been further developed, see **Fig. 4**.



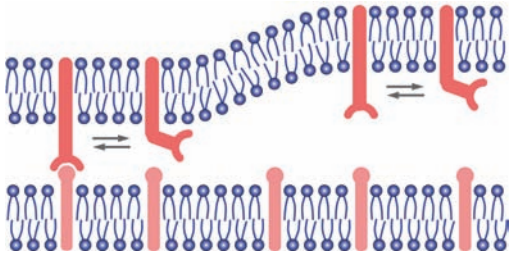


Fig. 3: Adhesion of two membranes via active receptors or stickers that can attain both an adhesive and a non-adhesive state.

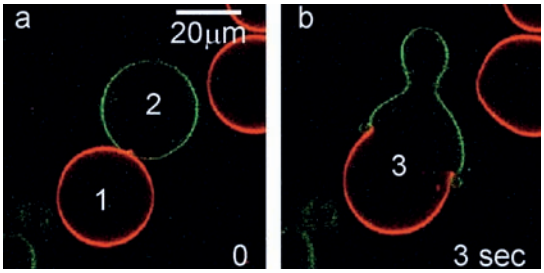


Fig. 4: Fusion of giant vesicles as observed by fluorescence microscopy. The two colors (red and green) correspond to two different membrane compositions that form stable domains after the fusion process has been completed.

Bio-systems are quite complex and exhibit many levels of self-organization. One rather general framework for these systems is provided by network models. During the last two years, we have worked on networks of motor cycles, activity pattern on scale-free networks, and network models for biological evolution.

All systems and phenomena that have been mentioned in this overview will be covered in more detail on the following pages.

Methods

The conceptual framework for the understanding of these systems and their cooperative behavior is provided by *statistical physics* which includes thermodynamics, statistical mechanics, and stochastic processes.

Our theoretical work starts with the definition of a certain model which (i) is amenable to systematic theoretical analysis and (ii) captures the essential features of the real system and its behavior. New models which have been introduced in our department include: semi-flexible harmonic chains for filaments; coarse-grained molecular models for bilayer membranes; lattice models for membranes with adhesion molecules; geometric models for membranes with lateral domains; lattice models for transport by molecular motors; Markov models for cooperative motor transport as well as network models for motor cycles.

These theoretical models are then studied using the analytical tools of theoretical physics and a variety of numerical algorithms. The analytical tools include dimensional analysis, scaling arguments, molecular field or self-consistent theories, perturbation theories, and field-theoretic methods such as renormalization. The numerical methods include the application of mathematical software packages such as Mathematica or Maple as well as special algorithms such as, e.g., the Surface Evolver for the calculation of constant mean curvature surfaces.

Several types of computer simulations are applied and further developed: Molecular Dynamics, Dissipative Particle Dynamics, and Monte Carlo methods. Molecular Dynamics is used for particle based models of supra-molecular assemblies; Dissipative Particle Dynamics, which is a relatively new simulation algorithm, is useful in order to extend the Molecular Dynamics Studies towards larger systems and longer time scales; Monte Carlo methods are used in order to simulate even larger mesoscopic systems such as filaments and membranes up to a linear size of hundreds of nanometers.

The experimental work is carried out in our membrane lab which is equipped with calorimetry, optical microscopy, micropipettes, and optical tweezers. This lab is also responsible for the advanced confocal microscope that is available to all four departments of the MPI.

Additional information about research in the Theory Department is available at *www.mpikg.mpg.de/th/*

Reinhard Lipowsky
Director of the Department of Theory & Bio-Systems