Research in the Department of Theory & Bio-Systems

There's plenty of room at the bottom
Richard Feynman

The researchers and graduate students of the Department of Theory and Bio-Systems form one experimental and several 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; until 2007);
- *Jan Kierfeld* (theory, polymers and filaments; until 2007);
- *Volker Knecht* (theory; proteins and membranes).
- *Christian Seidel* (theory, polymers and poly-electrolytes);
- *Thomas Weikl* (theory, proteins and membranes).

The Theory and Bio-Systems Department is responsible for the International Max Planck Research School on 'Biomimetic Systems'. Until the end of 2008, the department also coordinated the European Early Stage Training Network about the same topic and the European Research Network on `Active Biomimetic Systems'. The graduate programs are managed by *Angelo Valleriani*.

In the following three subsections, the research within the Theory and Bio-Systems Department is described in terms of the underlying molecular systems, the cooperative 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 of cargo particles by several such motors. When these motors belong to two different species, they perform a stochastic tug-of-war as shown in **Fig. 1**.

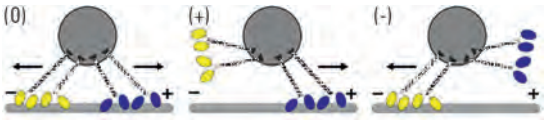

Fig. 1: Tug-of-war between 2 plus (blue) and 2 minus (yellow) motors pulling on the same cargo particle (gray). For configuration (0), the motors block each other so that the cargo does not move. For configuration (+) and (-), the cargo exhibits fast plus and minus motion, respectively.

One particularly intriguing aspect of filaments is the coupling of filament growth to active processes. One example is provided by actin polymerization coupled to ATP hydrolysis. In order to elucidate this process, we introduced a new theoretical model for cooperative ATP cleavage and Pi release as shown in **Fig. 2**.

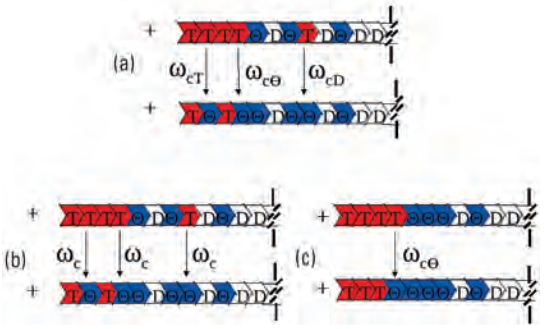

Fig. 2: Actin filaments consisting of three different types of protomers denoted T, Θ and D: (a) Cooperative ATP cleavage depending on the local neighborhood of the T protomer within the filament; (b) Random ATP cleavage and (c) Vectorial ATP cleavage.

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 multicomponent membranes to solid substrates as shown in **Fig. 3.** In addition, the deformation of lipid vesicles by alternating electric fields has been studied experimentally as a function of ion conductivities and field frequency, see **Fig. 4**.

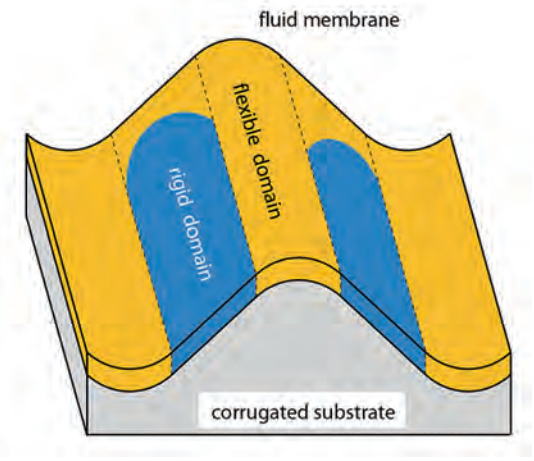

Fig. 3: Fluid membrane on a corrugated, solid substrate with two types of domains (blue and yellow) that differ in their bending rigidity. The blue domains are more rigid than the yellow one and tend to avoid the curved membrane parts provided the line tension of the domain boundaries is sufficiently small.

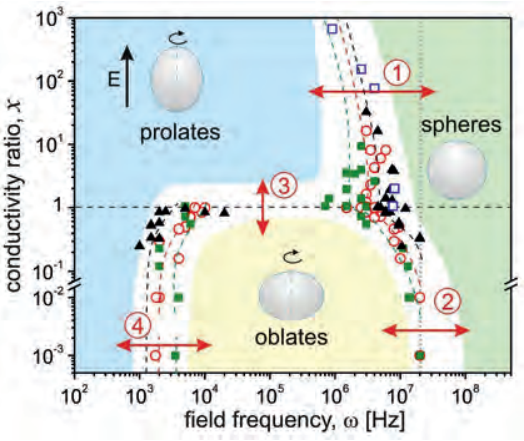

Fig. 4: Morphological diagram for lipid vesicles in alternating electric fields as function of field frequency and conductivity ratio.

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 simple neural networks.

Most of the 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.

The theory of 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. In general, the challenge is to find a theoretical representation that depends only on experimentally accessible parameters.

The 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 for calculus and algebra 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, Brownian Dynamics, and Monte Carlo methods. Molecular Dynamics is used for particle based models of supramolecular assemblies; Dissipative Particle Dynamics is useful in order to extend the Molecular Dynamics studies towards larger systems and longer time scales; Brownian Dynamics and 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.

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 departments of the MPI.

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

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of Theory & Bio-Systems