Argonne *Self-Organization in Active Biological Systems* 2007
Program

Friday, April 27

Reception: 7:00pm – 9:00pm
Argonne Guest House

Saturday – Monday talks will be held at Advanced Photon Source (APS), Building 401/402, rooms E1100 and E1200
APS is a short walk from the Guest House

Cancelations:
Albert Libchaber's talk has been canceled and some talks have been moved. Please let us know if the new schedule may cause a problem.

Saturday, April 28

Morning talks: 8:30am – 12:20pm

8:30am – 8:40am: Igor Aronson, Argonne
Opening remarks

8:40am – 9:20am: Lev Tsimring, *UCSD*
  Flows and ordering of growing populations of rod-like cells

9:20am – 10:00am: Jacques Prost, *ESPCI/Inst. Curie*
 TBA

10:00am – 10:20am: Break

10:20am – 11:00am: Gijsje Koenderink, *FOM Inst. AMOLF*
  Active self-organization and dynamics of reconstituted cytoskeletal protein networks driven by myosin motors

11:00am – 11:40am: Jean-Francois Joanny, *Inst. Curie*
        Cortical actin and cell oscillations

11:40am – 2:20pm: Lunch

<u>Afternoon talks: 2:20pm – 6:00pm</u>

2:20pm – 3:00pm: Leonid Berlyand, *Penn State*
  Discrete Network Approximation in Particle Suspensions and Biosuspensions

3:00pm – 3:40pm: Boris Shklovskii, *U. Minnesota*
  Entropy driven insulator-metal transition in ion channels and nanopores.

3:40pm – 4:00pm: Christine Sample, *Northwestern*
  Nonlinear Dynamics of a Double Bilipid Membrane

4:00pm – 4:20pm: Break

4:20pm – 4:40pm: Andrey Sokolov, *Argonne*
  Large scale flows and density instabilities in ensembles of swimming bacteria

5:00pm – 6:00pm: Materials' Science Lab tour

<u>Sunday, April 29</u>

<u>Morning talks: 8:30am – 12:10pm</u>

8:30am – 9:10am: Hugues Chate, *CEA*
    Universal features of minimal models for collective motion

9:10am – 9:50am: Raymond Goldstein, *Cambridge*
 Physical Aspects of Evolutionary Transitions to Multicellularity

9:50am – 10:10am: Break

10:10am – 10:50am: Carsten Beta, *Max-Planck Institute*
    Addressing directional sensing in quantitative single cell experiments

10:50am – 11:30am: Walter Zimmermann, *U. Bayreuth*
    TBA

11:30am – 12:10pm: Mike Graham, *U. Wisconsin*
    Simulation of suspensions of hydrodynamically interacting self-propelled particles

12:10pm – 2:40pm: Lunch

<u>Afternoon talks: 2:40pm – 6:00pm</u>

2:40pm – 3:20pm: Eric Clement, *ESPCI*
  From vibrated granular packing to transport in bacterial bath

3:20pm – 4:00pm: Michael Shelly, *Courant Inst.*
 Instabilities and dynamics in suspensions of self-locomoting rods – Part 1

4:00pm – 4:20pm: David Saintillan, *Courant Inst.*
 *Instabilities and dynamics in suspensions of self-locomoting rods –
 Part 2*

<center>**4:20am – 4:40am:** Break</center>

4:40pm – 5:20pm: John Kessler, *U. Arizona*
 Dynamics of concentrated swimming micro-organisms

5:20pm – 5:40pm: Luis Cisneros, *U. Arizona*
  TBA

5:40pm – 6:00pm: Falko Ziebert, *Argonne*
 Rheological and Structural Properties of Active Filaments Solutions

---

Monday, April 30

<u>Morning talks: 8:30am – 1:00pm</u>

8:30am – 9:10am: Karsten Kruse, *U. des Saarlandes*
Self-organization in systems of treadmilling filaments

9:10am – 9:50am: Jan Kierfeld, *Max Planck Inst.*
Enhanced ordering of interacting filaments by molecular motors

<center>**9:50am – 10:30am:** Break</center>

10:30am – 11:10am: Eli Ben-Naim, *Los Alamos*
 Alignment of Rods and Partition of Integers

11:10am – 11:50am: Hans Kaper, *Argonne/NSF*
 Persistence of Turing Patterns

11:50am – 12:10pm: Dmitry Karpeev, Argonne
 Interaction of Flexible Filaments and Molecular Motors

<u>Lunch & Adjournment: 12:30pm –</u>

Abstracts

Flows and ordering of growing populations of rod-like cells

L. S. Tsimring, S. Cookson, D. Volfson, J. Hasty

We examine the structural changes that a colony of bacteria experiences during growth and expansion. We will focus on rod-like strain of Escherichia coli lacking flagellae which serve as a model organism in many microbiological studies. Our experiments in an open microfluidic chamber show that rod-like bacteria quickly establish nematic order with the director field oriented along the direction of the expansion flow. We propose a theoretical description of this ordering transition using equations of nematodynamics incorporating the effects of cell growth and division, and we also compare the theory and experiments with numerical simulations of cell self-organization using a soft particle molecular dynamics algorithm.

Active self-organization and dynamics of reconstituted cytoskeletal protein networks driven by myosin motors

Gijsje Koenderink
FOM Institute AMOLF
Biological Soft Matter Group Kruislaan 407 Amsterdam,
1009 DB Tel 020-6081233 E-mail: gkoenderink@amolf.nl

Living cells are active materials in which non-equilibrium driving forces lead to shape changes, contractility and migration, and active transport of cargo. Active generation of mechanical forces is mediated by a dynamic cytoskeletal protein network dominated by filamentous actin. To elucidate the underlying principles of the mechanics of this highly complex network, we reconstitute simplified model systems from purified cytoskeletal proteins. In this seminar I will show that reconstituted networks of actin, myosin II and cross-linkers can exhibit both active stiffening and contractility. Addition of processive thick filaments of myosin II can stiffen networks of actin cross-linked with filamin A by two orders of magnitude. The motor activity generates internal stress, restructuring the network and driving it into a non-linear regime with a greatly increased stiffness. The effects of myosin activity on filamin A-actin network elasticity quantitatively parallel those of externally applied stress on such networks, thus providing a calibration of motor activity. Addition of processive thick filaments of myosin II can also lead to macroscopic contraction of networks of actin cross-linked with alpha-actinin. By systematically varying the myosin and alpha-actinin concentrations, we obtain a state diagram for contractility showing that contractility occurs only above a threshold motor density and in a narrow window of cross-linker concentrations.

The contraction velocity of active gels is proportional to the number of myosin motors in the network, and is similar to actin gliding velocities measured in motility assays. Contracting gels pull on and deform their surface, allowing us to estimate a contractile force of about 1 microNewton.

Dynamics of concentrated swimming micro-organisms

John O. Kessler
Physics Department, University of Arizona, Tucson AZ

Approximately close packed populations of the cylindrical self-propelled bacteria Bacillus subtilis intermittently form domains of aligned, co-directionally swimming organisms. The velocities of these phalanxes are often "high" compared to the speed of individual swimmers. Although the Reynolds number is <1, this collective dynamic phase, the "Zooming BioNematic" (ZBN), appears turbulent. A modified version of Particle Imaging Velocimetry (PIV) was used to quantify spatial and temporal correlations of velocity and vorticity, associated with the spontaneous appearance and decay of localized phalanxes, coherently advancing domains. Widely extended meanders that exhibit smooth and continuous variations in angular order were discovered and investigated. These new data, together with analysis of local energy balance and the trajectories of individual cells provide ingredients for a rational bio-fluid-dynamical theory of the ZBN.

Universal features of minimal models for collective motion

Hugues Chate

I will review the emerging properties of Vicsek-like minimal
microscopic models for collective motion in two and three dimensions.
1) collective motion without cohesion nor surrounding fluid
2) collective and cohesive motion without fluid
3) first attempts at modeling large populations in a viscous fluid

---

Entropy driven insulator-metal transition in ion channels and nanopores.

Boris I. Shklovskii
Department of Physics, University of Minnesota.

We consider ion transport of a protein ion channel in a lipid membrane or a water filled nanopore in silicon film. The large ratio of dielectric constants of water filling

the channel (81) and of the surrounding lipid (2) or silicon oxide (4), an ion placed inside the channel has its electric lines confined in the channel. This leads to a large electrostatic self-energy barrier and to exponentially large Ohmic resistance of the channel. Nevertheless biological channels are well transparent for ions. In order to address this paradox, we study reduction of the electrostatic barrier by a finite concentration of salt in water and/or by immobile charges on the internal channel walls. We show that both types of charges lead to the insulator-metal crossover (elimination of the barrier) with their increasing concentrations. The evolution of biological protein channels used the large biological concentration of monovalent salt and more importantly made some of them charged from inside to reduce electrostatic barrier for a given sign of ions.

Alignment of Rods and Partition of Integers

Eli Ben-Naim
Los Alamos National Laboratory

This talk will describe an exact solution for the theory of the phase transition from a nematic, ordered phase to an isotropic, disordered phase that occurs in a system of interacting rods, that are subjected to random forcing. Physically, such transitions are found in vibrated granular rods or chains, and the underlying alignment process can be found in biological systems such as molecular motors and microtubules. The steady-state solution for the nonlinear and nonlocal theory is obtained by expressing the Fourier transform of the orientation distribution as a function of the order parameter, which in turn, is obtained in terms of the driving strength. This solution is obtained using iterated partitions of the integer numbers.

Self-organization in systems of treadmilling filaments

Karsten Kruse
U. des Saarlandes

The cytoskeleton is an important substructure of living cells, playing essential roles in cell division, cell locomotion, and the internal organization of subcellular components. Physically, the cytoskeleton is an active polar gel, i.e., a system of polar filamentous polymers, which is intrinsically out of thermodynamic equilibrium. Active processes are notably involved in the nucleation of new filaments and in changing their length. They can lead to filament polymerization at one end and depolymerization at the other, a phenomenon called treadmilling which is essential for many subcellular processes. Here, we study the dynamics of a system of treadmilling filaments in the presence of agents affecting the addition and removal of filament subunits by using a mesoscopic meanfield description. We find that

the system can self-organize into asters and moving filament blobs. We discuss possible implications of our findings for subcellular processes.

Interactions of Semiflexible Filaments and Molecular Motors

<u>Dmitry Karpeev</u>, Igor Aranson, Hans Kaper, *Argonne*
Lev Tsimring, *UCSD*

We analyze numerical simulations of the interaction of a pair of biofilaments mediated by a molecular motor. The filaments are modeled as flexible rods, and the results are applicable to microtubules, which are relatively stiff, as well as to much softer filaments, such as actin. The results provide insight into the effects of flexibility on cytoskeleton formation and the rheology of semiflexible filament networks. The simulations are based on a nonlinear elasticity equation. The results show that flexibility enhances the tendency of the filaments to align. The enhancement in turn favors the formation of large-scale structures in multifilament systems. Simulations for soft filaments show that the action of the motor can result in the formation of multiple loops of the filaments as a result of buckling, which can affect the structure of a cross-linked network and thereby its rheology.

Large scale flows and density instabilities in ensembles of swimming bacteria

<u>Andrey Sokolov</u>, Igor Aranson, *Argonne*

We study experimentally self-organization of concentrated ensembles of swimming bacteria Bacillus Subtilis. Experiments are performed in a very thin (of the order of 1 bacterium diameter) fluid film spanned between four supporting fibers. Small amplitude electric field is used to adjust dynamically the density of bacteria inside the experimental cell. Our experiments revealed only gradual increase of the large scale flow correlation length with the increase in number density of bacteria, and no sharp transition. The variations of density of bacteria as a function of thickness of the film was explored.

Rheological and Structural Properties of Active Filaments Solutions

<u>Falko Ziebert</u>, Igor Aranson, *Argonne*

We study semiflexible filaments, like F-actin, interacting via molecular motors by means of molecular dynamics/Langevin simulations.

By applying oscillatory shear we get the elastic and loss moduli as a function of motor activity and by an empiric collapse we extract an active (rheological) temperature, increasing with increasing motor activity. However, structurally the effect of motors is not like a temperature, as investigated by the study of the orientational correlation function. The correlation length is increasing with time in the presence of motors. At short times there is indication of polarity sorting while at late stages strong bundling of the filaments occurs.

Physical Aspects of Evolutionary Transitions to Multicellularity

Raymond E. Goldstein
Department of Applied Mathematics and Theoretical Physics
University of Cambridge

An important issue in evolutionary biology is the emergence of multicellular organisms from unicellular individuals. The accompanying differentiation from motile totipotent unicellular organisms to multicellular ones having cells specialized into reproductive (germ) and vegetative (soma) functions, such as motility, implies both costs and benefits, the analysis of which involves the physics of buoyancy, diffusion, and mixing. In this talk, I discuss recent results on this transition in a model lineage: the volvocine green algae. Particle Imaging Velocimetry of fluid flows generated by these organisms show that they exist in the regime of very large Peclet numbers, where the scaling of nutrient uptake rates with organism size is highly nontrivial. In concert with metabolic studies of deflagellated colonies, investigations of phenotypic plasticity under nutrient-deprived conditions, and theoretical studies of transport in the high-Peclet number regime, we find that flagella-generated fluid flows enhance the nutrient uptake rate per cell, and thereby provide a driving force for evolutionary transitions to multicellularity. Thus, there is a link between motility, mixing, and multicellularity.

Simulation of suspensions of hydrodynamically interacting self-propelled particles

Michael D. Graham
University of Wisconsin-Madison

Simulations of large populations of hydrodynamically interacting swimming particles are performed at low Reynolds number in periodic and confined (slit and monolayer) geometries. Each swimmer is modeled as a rod containing beads with a

propulsion force

exerted on one end bead (with an equal and opposite force exerted on the fluid) and excluded volume potentials at the beads. At small concentrations, the swimmers behave analogously to a dilute gas in which the hydrodynamic interactions perturb the

ballistic trajectories into diffusive motion. Simple scaling arguments can explain the swimmer behavior and to some extent the behavior of passive tracer particles. The origins of deviations from simple scaling, due to correlations between swimmer trajectories, are described. As the concentration increases, the hydrodynamic interactions lead to large-scale collective motion.

Persistence of Turing Patterns

Hans Kaper, *Argonne/NSF*

We establish sufficient conditions for the existence of an attractor for spatiotemporal Turing patterns in activator-inhibitor systems of reaction-diffusion equations. The attractor consists of two steady-state points in the case of diffusion in one spatial dimension, and eight steady-state points in the case of diffusion in two spatial dimensions. We use the Schnakenberg and Gierer-Meinhardt equations to illustrate the results. (Joint work with S. Wang and M. Yari, Indiana University.)

Bacterial Response to Temperature Gradients **(canceled)**

Prof. Libchaber and Hanna Salman, *Rockefeller University*

Bacteria sense and respond to changes in their environment.
Using chemical and heat sensing receptors, they sample their surroundings and adjust their swimming pattern to reach their destination. Chemotaxis is now well understood but thermotaxis is still unclear. Unlike the response to chemical gradients, where bacteria swim towards higher concentration of attractants or lower concentration of repellents, in a temperature gradient they swim towards an optimal temperature.

We will describe various experiments to study the response and adaptation of bacteria. In particular, we will show that beyond a critical concentration, the bacteria behavior is altered caused by inter-cellular signaling.

Instabilities and dynamics in suspensions of self-locomoting rods – Part 1

<u>Michael Shelley</u>, *Courant Institute, New York University*

Suspensions of swimming micro-organisms are characterized by complex dynamics involving strong fluctuations and large-scale correlated motions. In this work, we use numerical simulations to investigate aspects of the dynamics and microstructure in suspensions of interacting self-locomoting rods at low Reynolds number. We propose a detailed model that accounts for hydrodynamic interactions based on slender-body theory and encompasses both biological and non-biological locomotion mechanisms. In agreement with previous theoretical predictions, we demonstrate that aligned suspensions of swimming particles are unstable as a result of hydrodynamic fluctuations in the suspending fluid, and we characterize the wavelength selection of this instability in both ordered and random suspensions.

Instabilities and dynamics in suspensions of self-locomoting rods – Part 2

<u>David Saintillan</u>, *Courant Institute, New York University*

Using the methods developed in Part 1, we investigate the dynamics in collections of self-locomoting rods in bulk suspensions and in thin liquid films. In the bulk, hydrodynamic interactions result in chaotic flow fields, which, as we show, are locally dominated by regions of nearly uniaxial flow extension or compression. In spite of these chaotic dynamics, we demonstrate that a local nematic ordering persists in the suspensions over short length scales and has a significant impact on the mean swimming speed. Consequences of the large-scale orientational disorder for particle dispersion are discussed and explained in the context of generalized Taylor dispersion theory. Dynamics in thin liquid films are also presented, and are shown to be characterized by a strong particle migration towards the liquid/gas interfaces.

Enhanced ordering of interacting filaments by molecular motors

<u>Jan Kierfeld</u>, *Max Planck Inst., Germany*

We study the cooperative dynamics of cytoskeletal filaments in motility assays, in which mutually repulsive filaments glide over a planar substrate surface driven by motor proteins whose

tails are anchored to the surface. Simulating the coupled dynamics of filaments, motor heads, and motor stalks, we find an active ordering of filaments, i.e., a non-equilibrium phase transition to a nematic phase with orientational filament order upon increasing the filament density or the motor density. We develop a quantitative theory for the location of the phase boundary as a function of motor density. The active nematic ordering is governed by an effective filament length containing the effects from the motor-driven motion of filaments. At high detachment forces of motors, we also observe filament clusters arising from blocking effects. Inactive motors or cross-links on the substrate increase the blocking effects and thus enhance the filament clustering.

Nonlinear Dynamics of a Double Bilipid Membrane

Christine Sample, *Northwestern U., USA*

The nonlinear dynamics of a biological double-membrane that consists of two coupled lipid bilayers, typical of some intra-cellular organelles such as mitochondria, is studied. A phenomenological free-energy functional is formulated in which the curvatures of the two parts of the double membrane and the distance between them are coupled to the lipid chemical composition. The derived nonlinear evolution equations for the double-membrane dynamics are studied analytically and numerically. The linear stability analysis is performed and the domains of parameters are found in which the double membrane is stable. For the parameter values corresponding to an unstable membrane numerical simulations are performed that reveal various types of complex dynamics, including the formation of stationary patterns.

Addressing directional sensing in quantitative single cell experiments

Carsten Beta, *Max Planck Inst., Germany*

Directional sensing – the ability of a cell to detect chemical gradients with high precision – has been intensively studied in recent years by the use of fluorescent fusion proteins. A number of models have been proposed to describe the initial symmetry breaking in the sub-cellular pattern of signaling proteins. Further progress in this field will rely on experimental techniques to examine the

theoretical predictions. This requires quantitative control of chemical stimuli on the length scale of individual cells, with a temporal resolution that matches the time scales of the intracellular signaling events. We combine microfluidic techniques with the photo-chemical release of caged signaling agents to expose single cells to well-defined stimuli with high spatial and temporal resolution. Gradients of well-controlled shape can be generated on micrometer length scales and sub-second switching times between different concentration profiles can be readily achieved. We apply this approach to quantify intracellular translocation of fluorescently labeled proteins in chemotactic Dictyostelium cells responding to complex stimuli of cAMP.

Discrete Network Approximation in Particle Suspensions and Biosuspensions

Leonid Berlyand, *Penn State University, USA*

We present a novel approach for calculation of effective properties of high contrast disordred composites and illustrate it by considering highly packed suspensions of rigid particles (joint works with Y. Gorb & A. Novikov and with A. Panchenko) .

The main idea of this variational approach is the approximation of the original continuum problem, which is described by PDEs with rough coefficients, to a discrete network. This approximation makes the dependence of physical parameters transparent and it is obtained with a controlled error estimate.

We next discuss an extension of this approach to bacterial suspensions (joint work in progress with V. Gyrya, based on recent experimental work at Argonne).

List of Attendees

Aranson, Igor	*Argonne, USA*
Ben-Naim, Eli	*Los Alamos, USA*
Berlyand, Leonid	*Penn State, USA*
Beta, Carsten	*Max-Planck Inst., Germany*
Chate, Hugues	*CEA, France*
Cisneros, Luis	*U. Arizona, USA*
Clement, Eric	*ESPCI, France*
Goldstein, Ray	*Cambridge U., UK*
Golovin, Sasha	*Northwestern U., USA*
Graham, Mike	*U. Wisconsin, USA*
Joanny, Jean-Francois	*Inst. Curie, France*
Kaper, Hans	*Argonne, USA*
Karpeev, Dmitry	*Argonne, USA*
Kessler, John	*U. Arizona, USA*
Kierfeld, Jan	*Max Planck Inst., Germany*
Koelling, Dale	*U.S. Dept. of Energy, USA*
Koenderink, Gijsje	*FOM Inst. AMOLF, Netherlands*
Kruse, Karsten	*U. des Saarlandes, Germany*
Libchaber, Albert	*Rockefeller U., USA*
Prost, Jacques	*ESPCI/Inst. Curie, France*
Saintillan, David	*Courant Inst., USA*
Sample, Christine	*Northwestern U., USA*
Shelly, Michael	*Courant Inst., USA*
Shklovskii, Boris	*U. Minnesota, USA*
Sokolov, Andrey	*Argonne, USA*
Swaminathan, Sumanth	*Northwestern U., USA*
Tsimring, Lev	*UCSD, USA*
Ziebert, Falko	*Argonne, USA*
Zimmermann, Walter	*U. Bayreuth, Germany*