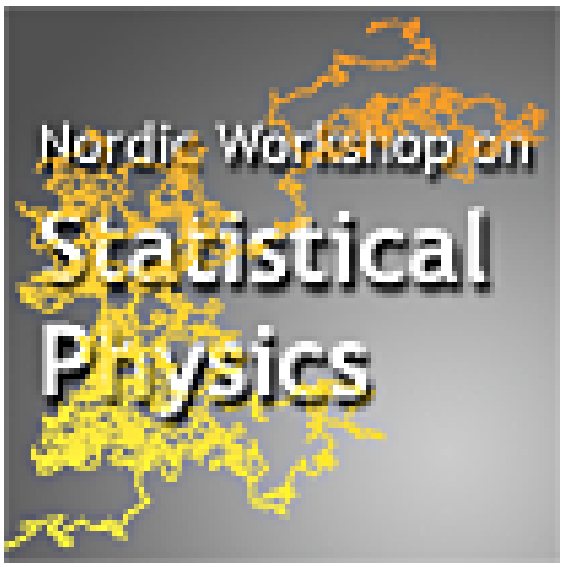
1st Nordic Workshop on Statistical Physics: Biological, Complex and Non-equilibrium Systems



Report of Contributions

https://indico.fysik.su.se/e/1838

Contribution ID: **250** Type: **not specified**

Opening

Wednesday, March 17, 2010 10:00 AM (15 minutes)

Contribution ID: **251** Type: **not specified**

DNA Analysis in Nanostructured Devices

Wednesday, March 17, 2010 10:15 AM (45 minutes)

We use standard staining protocols and epifluorescence microscopy to gain information on the local AT/GC ratio along large DNA molecules stretched in nanoscale channels[1]. Our development opens up a novel route to mapping of large-scale genomic variations as well as fast identification of rare or single cells.

With rising temperature, dark patches appear along the DNA corresponding to AT-rich regions that lose in intensity due to local melting of the double-stranded helix thereby resulting in a “barcode” pattern along the DNA (Figure 1) much like G-banding but with significantly improved resolution, currently on the order of 1-10kbp.

Compared to standard techniques, such as paired-end sequencing and array comparative genomic hybridization (CGH), our technology may offer a simpler and quicker way to identify structural variations such as deletions, translocations, insertions and copy number variations on scales ranging from 1kbp and up[2] on the single-molecule level. Furthermore, the resulting “barcode” may be used for identification of organisms, such as difficult-to-grow fungi, bacteria and viruses.

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[2] Stankiewicz, P. and J.R. Lupski, Genome architecture, rearrangements and genomic disorders. Trends in Genetics, 2002. 18(2): p. 74--82.

Presenter: TEGENFELDT, Jonas

Contribution ID: **252** Type: **not specified**

Polymer Escape from Metastable Kramers Potential: Path Integral Hyperdynamics Study

Wednesday, March 17, 2010 11:30 AM (45 minutes)

We study the dynamics of flexible, semiflexible and self-avoiding polymer chains under the Kramers metastable potential. Due to thermal noise the polymers, initially in the metastable well, can cross the potential barrier, but these events are rare at low temperatures.
To speed up the slow rate processes in computer simulations we employ the hyperdynamics method using the path-integral representation of the relevant Langevin dynamics [1]. In this study, we extend the method for many-particle systems with internal degrees of freedom, such as the polymer chain. We study the regime where the well size is comparable to chain length. We find that the flexible, semi-flexible and self-avoiding chains exhibit qualitatively different behavior. For the flexible chain, the crossing rate decreases monotonically with the polymer length (L), while for the semi-flexbile chain the rate saturates at a level that depends on the chain stiffness. For the self-avoiding chain, on the other hand, the rate varies non-monotonically with L. For L less than Lm, the rate decreases as L increases, while for L > Lm, the rate increases approximately linearly with L. We attribute this behavior to the coil-to-stretch transition of the chain, which lowers the effective free energy barrier and enhances the crossing rate. This effect can be instrumental in efficient separation of biopolymers.

[1] L. Y. Chen and N. J. M Horing, J. Chem. Phys. 126, 224103 (2007).

Presenter: IKONEN, Timo

Contribution ID: **253** Type: **not specified**

A Stochastic Model of Anomalous Heat Transport

Wednesday, March 17, 2010 12:15 PM (45 minutes)

Abstract: We investigate the non-equilibrium dynamics of a chain of harmonic oscillators in contact with two stochastic Langevin heat baths at different temperatures and undergoing random collisions between neighbours that exchange their momenta with a constant rate γ. By means of an appropriate continuum limit, we solve the equations for the covariance matrix to leading order in the stationary state, and derive exact expressions for the temperature profile and for the leading contribution of the energy current, which scales as $1/\sqrt{\gamma N}$. At finite times, we solve adiabatically the equation describing the time evolution of the temperature profile $T(y,t)$, obtaining that in the bulk of the system, $T(y)$ evolves according to the energy continuity equation, but with a space-time scaling that is described by a fractional diffusion equation.

Presenter: MEJIA-MONASTERIO, Carlos

Contribution ID: **254** Type: **not specified**

Interacting Random Walkers in One-Dimansional Systems

Wednesday, March 17, 2010 2:30 PM (45 minutes)

The problem of a single random walker has received a lot of attention in the science community during the last century. There is now an increasing amount of interest in the problem of INTERACTING random walkers (due to the strong connection of this problem to the fields of, for instance, biophysics, nanofluidics, and cell biology). In particular, much attention has been on the behavior of the non-equilibrium problem of interacting walkers in (quasi)one dimensional systems, so called single-file diffusion. The quantities of main interest in such a system is the mean square displacement (MSD) of a (fluorescently) tagged particle. It has been found previously (theoretically and experimentally) that the MSD for a tagged particle in a single file system scales as tˆ(1/2) for long times (in the thermodynamic limit), rather than t as for unconstrained diffusion.

In the talk three new single-file results will be presented:

1) The problem of hardcore interacting particles in a FINITE system
(box) is solved analytically using a Bethe-ansatz, see Ref [1]. Analysis of our exact solution reveals three time regimes, where the tˆ(1/2)-behaviour appears as an intermediate regime.

2) We recently introduced a procedure, which we refer as to as Harmonization, which maps the diffusive motion of any type of 1d short-range single-file system onto that of chain of harmonically coupled beads; the effective spring constant in the system is connected to the details of the potential between particles. The Harmonization procedure reproduces all known long-time results in the single-file field with some back-of-the envelope calculations and allow us to analytically solve the long-time behavior of more complicated single-file systems. For instance, the tagged particle motion in a harmonic potential, in a time-varying force field and correlation functions between particles are calculated.

3) Finally, single-file diffusion in a system where the particles have different diffusion constants is considered. By combining the Harmonization procedure with effective medium theory we derive analytic results for the MSD, and find that for certain types of distributions for the diffusion constants, the dynamics becomes ultra-slow; the MSD scales as tˆdelta, with delta<1/2, [3].

[1] L. Lizana and T. Ambjornsson, Single-file diffusion in a box, Phys. Rev. Lett. 100, 200601 (2008); Phys. Rev. E 80,

051103 (2009).

[2] T. Ambjornsson, L. Lizana, A. Taloni, E. Barkai and M.A. Lomholt, Foundation of fractional Langevin equations: Harmonization of a many-body problem, submitted, E-print: arXiv:0909.0881.

[3]. M. A. Lomholt, L. Lizana and T. Ambjornsson, in preparation.

Presenter: AMBJÖRNSSON, Tobias

Contribution ID: **255** Type: **not specified**

Lipid-Protein Membranes out of Equilibrium

Wednesday, March 17, 2010 3:15 PM (45 minutes)

Biological membranes are typically not in thermal equilibrium. Experiments on lipid-protein model membranes have revealed that protein activity influences the mechanical properties of the membrane. A possible explanation for this alteration is given by a theoretical model in which the active proteins act as force-dipoles on the surrounding medium. A prediction of this model is that the protein activity will modify the tension of the membrane. However, one has to be careful when one looks at the consequences of this tension modification for the fluctuation spectrum of the membrane shape.

Presenter: LOMHOLT, Michael

Contribution ID: **256** Type: **not specified**

Aging Dynamics is Trivial in Logarithmic Time

Wednesday, March 17, 2010 4:30 PM (45 minutes)

The dynamics of complex systems collectively known as glassy shares important phenomenological traits. I.e., a transition is generally observed from a time-homogeneous dynamical regime to an aging regime where physical changes occur intermittently and, on average, at a decreasing rate. It has been suggested that a global change of the independent time variable to its logarithm may render the aging dynamics homogeneous and thus trivialize it. In the talk this behavior is shown for experimental data from colloidal systems: the mean square displacement grows linearly in time at low densities but linearly in the logarithm of time at high densities. The intermittent nature of spatial fluctuations and the persistency of particle pairs is also discussed.

A phenomenological one-parameter family of models is introduced which relies on the growth and collapse of strongly correlated clusters (“dynamic heterogeneities”). The full spectrum of colloidal behaviors is reperoduced by the model. In the limit where large clusters dominate the dynamics, intermittency induced by record-size events occurs with rate $\propto 1/t$, implying a homogeneous, log-Poissonian process that qualitatively reproduces the experimental results. The crucial importance of record-size fluctuations for colloidal dynamics is emphasized.

Presenter: SIBANI, Paolo

Contribution ID: **257** Type: **not specified**

Aggregation of Variables in Linear Systems

Wednesday, March 17, 2010 5:15 PM (45 minutes)

I will present some new ideas for how to coarse grain linear dynamical systems through aggregation of variables. Both spectral methods and a very recent technique based on identification of ground states in a corresponding Potts glass model will be discussed. The methods are demonstrated by application to coarse graining of cellular automata and identification of the genetic code and higher level amino acid groups from DNA mutation statistics.

Presenter: JACOBI, Martin N.

Contribution ID: **259** Type: **not specified**

Lipids in Membranes Speak the Language of Curvature

Thursday, March 18, 2010 9:00 AM (45 minutes)

The physical properties of the lamellar lipid-bilayer component of biological membranes is controlled by a host of thermodynamic forces leading to overall tensionless bilayers with a conspicuous lateral pressure profile and build-in curvature-stress instabilities that may be released locally or globally in terms morphological changes. In particular, the average molecular shape and the propensity of the different lipid and protein species for forming non-lamellar and curved structures are a source of structural transitions and control of biological function. I will discuss the effects of different lipids, sterols, and proteins on membrane structure and show how one can take advantage of the curvature-stress modulations brought about by specific molecular agents, such as fatty acids, lysolipids, and other amphiphilic solutes, to construct intelligent drug-delivery systems that function by enzymatic triggering of curvature.

Presenter: MOURITSEN, Ole

Contribution ID: **260** Type: **not specified**

Complex Dynamics in Lipid Membranes

Thursday, March 18, 2010 9:45 AM (45 minutes)

A biological lipid membrane may be viewed as a two dimensional (liquid crystal) fluid that is immersed in a three dimensional water solution. The system is further complicated by that the membrane is non flat, undergo time dependent undulations and have a thickness that fluctuates in time and space. This gives rise to complicated correlation functions in time and space. Experimentally some of these functions can be probed by inelastic scattering of neutrons or light and more recently by neutron spin echo experiments. Field dependent NMR -relaxation experiments give also important information.
We report here about molecular dynamics simulations that indicate that many of these correlation functions are stretched exponentials rather than ordinary exponentials and discuss different ways to interpret.

Presenters: BRANDT, Erik; EDHOLM, Olle

Contribution ID: **261** Type: **not specified**

Diffusion Within Living Cells

Thursday, March 18, 2010 11:00 AM (45 minutes)

Using optical tweezers combined with image analysis we investigate motility of single proteins in membranes and of organelles inside living cellular organisms, one key issue being that the organisms are kept alive and healthy. Studies of two different biological systems will be presented: By specifically attaching a bead to a single protein, the lambda-receptor, which is a porin in the outer membrane of E. coli bacteria, we revealed its nanoscale diffusional motion and proposed a model that allows for extraction of the characteristic physical parameters including the diffusion constant. Surprisingly, the observed mobility is caused not only by thermal motion but in addition by an active motion associated with the metabolism of the organism. Connected to this, we show that antibiotics and antimicrobial peptides have a pronounced effect on single protein motility. The second biological system presented will be an S. pombe yeast cell, where the diffusion patterns of naturally occurring lipid granules have been uncovered using optical trapping and single particle tracking; the granules perform anomalous diffusion, with subdiffusion being most predominant at short time-lags, and the biological functions giving motility footprints at longer time-lags. The diffusional properties inside living yeast cells change during the cell cycle, and a novel maximal excursion method shows that the physical origin of the observed motility is probably fractional Brownian motion.

Presenter: ODDERSHEDE, Lene

Contribution ID: **262** Type: **not specified**

Diffusion Controlled Reactions and Living Cell Biochemistry

Thursday, March 18, 2010 11:45 AM (45 minutes)

The talk will discuss how Statistical Physics tools can be used to understand biochemistry of the living cell. Structures found in the living cell are rather special and to achieve such task techniques used in the field of Statistical Physics need to be slightly modified. A critical reflection is needed on which techniques to use and for what purpose. As an example the theory of diffusion controlled reactions will be reviewed with a purpose of using it for understanding spatio-temporal organization of the living cell.

It will be argued that formalism of diffusion controlled reactions is a suitable framework for describing living cell and the scope and the limitations of such approach will be discussed. Informal discussion will be given around problems (and possible traps) one meets when trying to compute properties of biochemical reactions in the cell interior. For example, mean field calculations are routinely used to model cell biochemistry and there usage is rarely questioned. The validity of mean field equations will be critically reviewed. Some situations when these equations do not work will be mentioned (low dimension, fluctuation dominated kinetics).

The generic features of spatio temporal organization of the living cell biochemistry will be discussed with particular emphasis on geometrical (spatial) features, ranging from shape of reactants towards spatial organization of intracellular reaction volumes. There is a great need for developing analysis tools that could help us understand intracellular organization and geometry and it will be argued that the theory of diffusion controlled reactions can be useful in the context. As an example, the brief overview of Geometry-Reaction InterPlay framework (GRIP) will be given.

KEYWORDS: fluctuation dominated kinetics, diffusion controlled reactions, reaction-geometry interplay, reactions in restricted geometries, shape of reactants, shape of reaction volume, topology of pathway graph

Presenter: KONKOLI, Zoran

Contribution ID: **263** Type: **not specified**

Mesoscopic Non-Equilibrium Thermodynamics

Friday, March 19, 2010 11:00 AM (45 minutes)

Classical thermodynamics is a theory for a collection of molecules in equilibrium. What happens if the number of molecules in the system becomes smaller and smaller, and the system boundaries reflect conditions further and further away from equilibrium? Can we still use thermodynamics? This lecture aims to explain that the field of non-equilibrium thermodynamics can be extended to describe in a systematic manner even molecular behaviour far from equilibrium conditions. We start introducing the concept of internal variables, derive the law of mass action, and end illustrating the theory by applications to RNA stretching experiments and active transport by the Ca-ATPase. We discuss that a thermodynamic theory is needed, also for molecules.

References

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J.M. Rubi, D. Bedeaux and S. Kjelstrup, Thermodynamics for small molecule stretching experiments, J. Phys. Chem. B, 110 (2006) 12733-12737
D. Bedeaux and S. Kjelstrup, The measurable heat flux that accompanies active transport by the
Ca- ATPase. Phys. Chem. Chem. Phys. 48 (2008) 7304-7317.

Presenter: BEDEAUX, Dick

Contribution ID: **264** Type: **not specified**

ALBANOVA COLLOQUIUM - Stochastic Thermodynamics: Theory and Experiments

Thursday, March 18, 2010 3:15 PM (1 hour)

Stochastic thermodynamics provides a framework for describing small systems embedded in a heat bath and externally driven to non-equilibrium. Examples are colloidal particles in time-dependent optical traps, single biomolecules manipulated by optical tweezers or AFM tips, and motor proteins driven by ATP excess. A first-law like energy balance allows to identify applied work and dissipated heat on the level of a single stochastic trajectory. Total entropy production includes not only this heat but also changes in entropy associated with the state of the small system. Within such a framework, exact results like an integral fluctuation theorem for total entropy production valid for any initial state, any time-dependent driving and any length of trajectories can be proven [1]. These theoretical predictions have been illustrated and tested with experiments on a colloidal particle pushed by a periodically modulated laser towards a surface [2]. Key elements of this framework like a stochastic entropy can also be applied to athermal systems as experiments on an optically driven defect center in diamond show [3,4]. For mechanically driven non-equilibrium steady states, the violation of the fluctuation-dissipation theorem can be quantified as an additive term directly related to broken detailed balance (rather than a multiplicative effective temperature) [5,6]. Integrated over time, a generalized Einstein relation appears which we have recently verified experimentally [7]. Finally, optimal protocols are derived which (i) minimize the work required to switch from one equilibrium state to another in finite time [8] and (ii) maximize the power of stochastic heat engines operating between two heat baths [9].

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Phys. Rev. Lett. 96: 070603/1-4, 2006.

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[6] U. Seifert and T. Speck, EPL, in press, 2010.

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Presenter: SEIFERT, Udo

Contribution ID: **265** Type: **not specified**

Fluctuation Theorems and Single Molecule Experiments

Thursday, March 18, 2010 5:00 PM (45 minutes)

The manipulation of individual macromolecules made possible by experimental techniques such as optical tweezers or atomic force microscopy gives a unique insight into the non-equilibrum thermodynamics of small systems. Besides a general introduction about the theoretical and experimental framework, this talk is focused on two topics: the proper way of measuring the work applied to the system in a single-molecule experiment, and a powerful generalization of Crooks fluctuation theorem that allows the exploration of misfolded and metastable states.

Presenter: MOSSA, Alessandro

Contribution ID: **266** Type: **not specified**

Equilibrium and Non-Equilibrium Physics of Nucleosome Positioning

Friday, March 19, 2010 9:00 AM (45 minutes)

Presenter: GERLAND, Ulrich

Contribution ID: **267** Type: **not specified**

Dynamics, Clustering and Collisions of Inertial Particles in Mixing Flows

Friday, March 19, 2010 9:45 AM (45 minutes)

We study the dynamics of small particles suspended in mixing flows (e.g. microscopic water droplets in turbulent rain clouds). We describe how the particles move, cluster together, and collide. Our results enable us, for example, to address the question of how long it takes to rain from a vigorously turbulent rain cloud. The talk is based on the manuscripts appended below.

Mehlig & Wilkinson, Phys. Rev. Lett. 92 (2004) 250602 Duncan, Mehlig, Ostlund & Wilkinson, Phys. Rev. Lett. 95 (2005) 165503 Arvedson, Mehlig, Wilkinson & Nakamura, Phys. Rev. Lett. 96 (2006) 030601 Wilkinson, Mehlig & Bezuglyy, Phys. Rev. Lett. 97 (2006) 048501 Gustavsson, Mehlig, Wilkinson & Uski, Phys. Rev. Lett. 101 (2008) 174503

Presenter: MEHLIG, Bernhard

Contribution ID: **268** Type: **not specified**

Metabolic Networks, Information, Null Model, and Evolution

Friday, March 19, 2010 11:45 AM (45 minutes)

The metabolism in an organism is reduced to a network of substances. The resulting degree-distribution is power law like with an exponent about 2.2.
In order to understand this, we use information theory to obtain a null-model defined by assigning equal probabilities to what is assumed to be the fundamental network possibilities. A stochastic variant of variational calculus is used to obtain the corresponding degree distribution for the null-model. The striking agreement implies that the null model catches the overall feature of the metabolic network. Using the network structure measures like clustering and assortativity, a small difference is identified as the only sign of any possible evolutionary pressure. However, this difference is only manifested in a slight difference in the degree distribution and seemingly not in any particular network design.

Presenter: MINNHAGEN, Petter

Contribution ID: **270** Type: **not specified**

Genetic Regulation in Time and Space

Thursday, March 18, 2010 2:00 PM (45 minutes)

Genetic circuits have been studied quite intensively in recent years. In particular, we have focussed on oscillatory patterns related to negative feed-back loops inside single cells in eucaryotic systems [1,2]. In many cases, however, it is of interest to study how cells communicate with each other when cells are arranged in certain spatial structures, like biofilms and tissues. We have attacked this problem by means of a repressor-lattice where single repressilators (closed feed-back loops) are placed on a hexagonal lattice [3]. Such systems can be build without any internal frustration and can in most cases exhibit stable, oscillating states. Commensurability effects however play a role and may lead to internal frustration causing breaking of symmetries and solutions of many different phases. Eventually, also chaotic solutions may be present [3]. We discuss both situations of directed and bi-directed interactions on the repressor-lattice.

[1] S. Pigolotti, S. Krishna and M.H. Jensen, "Oscillation patterns in negative feedback loops", Proc.Nat.Acad.Sci. 104, 6533-6537 (2007).

[2] S. Pigolotti, S. Krishna and M.H. Jensen, "Symbolic dynamics of biological feedback networks", Phys. Rev. Lett. 102, 088710 (2009).

[3] M.H. Jensen, S. Krishna and S. Pigolotti, "The Repressor-Lattice: Feedback, Commensurability, and Dynamical Frustration, Phys. Rev. Lett. 103, 118101 (2009).

Presenter: JENSEN, Mogens Høgh

Contribution ID: **271** Type: **not specified**

The Inverse Ising Problem: A Survey and some Empirical Results

Friday, March 19, 2010 2:00 PM (45 minutes)

The "Inverse Ising Problem" refers to finding the parameters (the J_ij's and the h_i's) in an Ising model given the first and second moments (the magnitizations m_i and the correclation functions c_ij).

This is of great interest in machine learning and data analysis whenever the data set and the number of variables is large, but the values taken by the variables can be taken to be "high" and "low". The maximum entropy distributions with given first and second moments then has the Ising form where the h_i's and J_ij's are Lagrange parameters.

The last years have seen an explosion in interest in approximate but fast methods borrowed from statistical mechanics to learn such "maxentropy" models from correlation data. Some motivations have been e.g. inferring casual structures underlying observed gene expression, or inferring functional connectivities between neurons from multi-neuronal recordings, where measurements from hundreds of neurons are available today, and millions have been envisaged.

Although methods borrowed from non-equilibrium may be more promising in applications, I will describe results using equilibrium statistical mechanics, and the testing ground will be mainly the Sherrington-Kirkpatrick spin glass.

The methods discussed are simple mean-field, TAP, and the "Susceptibility Propagation" introduced by Mezard. One main message is that all these are sensitive to the accuracy of the correlation data themselves. There is hence a three-way trade-off between computability, inference accuracy (given perfect data), and sensitivity to undersampling of the correlations.

This is work done or in progess with John Hertz, Yasser Roudi, Mikko Alava, Hamed Mahmoudi, Aymeric Fouquier d'Herouel, Jarkko Salojärvi, Zeng Hong-Li and Charles Ollion.

Similar results to ours on Susceptibility Propagation have been obtained by Enzo Marinari (paper available on arXiv.org).

Presenter: Prof. AURELL, Erik (KTH)

Contribution ID: **272** Type: **not specified**

The Inverse Ising Model: Why and How

Friday, March 19, 2010 2:45 PM (45 minutes)

Ising models form a natural framework for modeling the distribution of multi-neuron spike patterns: Of all models that correctly describe the firing rates and pairwise firing correlations, the Ising model is the one of maximum entropy. The problem at hand here is an inverse one to that we usually encounter. Normally, one has a model with given couplings (Jij) and the task is to compute averages and correlation functions of the variables of the model. Here we are given the averages and correlations and the task is to find the couplings.

In the simplest approach to this problem, one considers only the measured firing rates and equal-time pairwise firing correlations and tries to find the Ising model that has these statistics. In our work we have explored and compared a number of methods for doing this, using data from a realistic model network of spiking neurons. Several of these methods work remarkably well.

This success is tempered, however, by our second set of findings. Using an information-theoretic measure of the overall quality of fit, we find that, while the Ising model is a good description of the distribution of spike patterns for small populations of neurons (˜ 10), it does worse and worse for larger and larger populations (for reasons that are not yet understood).

Finally, I will describe some recent work, which extends the Ising approach to describe non-equal-time firing correlations.

Presenter: HERTZ, John (Nordita)

Contribution ID: **273** Type: **not specified**

Discussion and Closing

Friday, March 19, 2010 3:30 PM (1h 30m)