Polymer Translocation through Nanopores

September, 16 2012 - September 18, 2012
Schloss Waldhausen, Im Wald 1, 55257 Budenheim, Mainz, Germany

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PROGRAM

Day 1 - September, 16th 2012
18:00 to 21:00 - Welcome Reception, Restaurant “Turm”,
Im Wald 3, Mainz-Budenheim (about 5 min. walk from Schloss Waldthausen)
18:00 to 20:00 – Registration

Day 2 - September, 17th 2012
Morning Session

• 08:45 to 09:00 - Welcome
• 09:00 to 09:35 - Murugappan Muthukumar
  Theory of macromolecular transport through protein channels and nanopores
• 09:40 to 10:15 - Aniket Bhattacharya
  Emerging Physical Picture of DNA Dynamics Through a Nanopore
• 10:20 to 10:50 - Coffee Break
• 10:50 to 11:25 - Gerard Barkema
  Translocation simulations with elastic lattice polymers
• 11:30 to 12:05 - Alexander Grosberg
  Voltage drop on pore access resistance and its role in DNA capture and translocation
• 12:10 to 12:45 - Aleksei Aksimentiev
  The microscopic origin of ionic current blockades in nanopores
• 12:50 to 14:00 - Lunch Break

Afternoon Session

• 14:00 to 14:35 - Takahiro Sakaue
  On the distribution of translocation time
• 14:40 to 15:15 - Tapio Ala-Nissila
  Unifying model of driven polymer translocation
• 15:20 to 15:55 - Ralf Metzler
  Driven translocation: equilibrium versus non-equilibrium
• 16:00 to 16:40 - Kaifu Luo
  Dynamics of polymer translocation under an applied external field
• 17:00 to 18:30 - Poster Session
• 19:00 to 22:00 – Dinner
Day 3 - September, 18th 2012

Morning Session

- 09:00 to 09:35 - Anatoly Kolomeisky
  How Interactions Control Transport through Channels
- 09:40 to 10:15 - Johan Dubbeldam
  Driven and undriven translocation of a polymer: impact of fluctuations on dynamical scaling
- 10:20 to 10:50 - Coffee Break
- 10:50 to 11:25 - Dieter Heermann
  Polymer translocation through a nanopore – the effect of solvent conditions
- 11:30 to 12:05 - Debabrata Panja
  Anomalous dynamics of polymer translocation
- 12:10 to 12:45 - Peter Reimann
  Modeling DNA-translocation through solid-state and alpha-hemolysin nanopores: two case studies
- 12:50 to 14:00 - Lunch Break

Afternoon Session

- 14:00 to 14:35 - Gary Slater
  Undriven Polymer Translocation : the role of pore size and solvent viscosity
- 14:40 to 15:15 - Maria Fyta
  Biopolymer translocation through pores: scaling, dynamics, statistics through a multiscale approach
- 15:20 to 15:55 – Wokyung Sung
  The effects of chain flexibility and dichotomic driving on polymer translocation
- 16:00 to 16:35 - Riku Linna
  Event distributions of polymer translocation
- 16:40 to 17:00 - Closing word
Lectures
Theory of macromolecular transport through protein channels and nanopores

Murugappan Muthukumar

University of Massachusetts, Amherst, USA

An understanding of the ubiquitous phenomenon of translocation of electrically charged macromolecules through narrow channels requires an adequate description of polyelectrolyte dynamics, electrolyte dynamics, and hydrodynamics, and the confinement effects from the charge-decorated pores. The biophysics of polyelectrolyte translocation process will be discussed using concepts from polyelectrolyte physics and electrophysiology, against a background of single-molecule experiments. Specifically, the capture and threading of DNA/RNA and proteins through alpha-hemolysin channels and solid-state nanopores under an external electric field, DNA ejection in bacteriophages, and translocon in mitochondria will be discussed.
Emerging Physical Picture of DNA Dynamics Through a Nanopore
Aniket Bhattacharya

Department of Physics, University of Central Florida, Orlando, FL 32816-2385, USA

Translocation of a polymer chain through a nano-pore depends on several factors. Even for the idealized case of a narrow pore and an infinitely thin wall, it has been established how pore friction and finite chain length affect the translocation dynamics[1]. For translocation under a bias present within the pore, a fully flexible translocating chain is out-of-equilibrium and conformations at the cis and trans sides are very different[2,3]. Recently we have demonstrated these out-of-equilibrium effects by analyzing conformations of sub-chains as a function of the distance from the pore[3]. The emerging physical picture in terms of an effective Flory exponent for each subchain is consistent with the tension propagation picture first introduced by Sakaue [4]. In this talk I will first discuss various non-equilibrium aspects for a fully flexible translocating chain. I will then discuss how semi-flexibility affects these results[5].

References
Translocation simulations with elastic lattice polymers

Gerard Barkema

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We present computer simulation results for translocation, as obtained with elastic lattice polymers. In our simulations, the polymer dynamics occurs via Langevin dynamics without hydrodynamic effects. The simulations confirm the theoretical prediction of Panja et al. [JPCM 19, 432202 (2007)] that as a function of polymer length $N$, the dwell time (i.e., time between the polymer entering the pore on one side and leaving it on the other side of the membrane) scales as $\tau_d \sim N^{2+\mu}$ for unbiased translocation; as $\tau_d \sim N^2$, for pulled translocation; and as $\tau_d \sim N^{(1+2\mu)/(1+\mu)}$ for weak field-driven translocation.
Voltage drop on pore access resistance and its role in DNA capture and translocation

Alexander Grosberg

New York University, Department of Physics, USA

While electric field is undoubtedly strongest inside the pore, the field outside the pore also exists. Importantly, it is long ranged and not subject to Debye screening. These two facts have far reaching consequences. In the talk and accompanying poster, we will explore the delicate interplay between electric and hydrodynamics forces as DNA approaches the pore, inserts its end into the pore, and then crawls.
The microscopic origin of ionic current blockades in nanopores

Aleksei Aksimentiev

University of Illinois at Urbana-Champaign, USA

The possibility of DNA sequence detection by measuring the blockade ionic current in nanopores has been the driving force for the spectacular development of the nanopore research field. Nevertheless, fifteen years after the first measurements, the molecular mechanism(s) of ion current modulation by the sequence of DNA nucleotides remains elusive. Here, we report the results of extensive all-atom molecular dynamics and Brownian dynamics simulations of three nanopore systems: a biological nanopore MspA, a solid-state nanopore and a graphene nanopore, aimed at elucidating the microscopic mechanism of the ion current modulation. In the case of solid-state and graphene nanopores, we determined the effect of sequence convolution on the ionic current value by simulating the ionic current blockades produced by all 64 permutations of the DNA nucleotide triplets. In the case of MspA, we determined the effect of the sequence, the global orientation, and the conformation of a DNA strand on the distribution of the ion current blockades. Based on the results of our simulations, we suggest possible routes for increasing the resolution of DNA sequence detection by measuring the nanopore ionic current and the inherit limitations of the method.
On the distribution of translocation time
Takahiro Sakaue, Takuya Saito

Department of Physics, Kyushu University 33, Fukuoka 812-8581, Japan

In typical experiments of polymer translocation, one records many of translocation events, the passage time of which differs on each occasion. One thus obtains a distribution of translocation times, from which various statistical quantities can be deduced. Among others, the most important is the average whose scaling structure with respect to the chain length as well as the magnitude of the driving force has been extensively investigated in literature.

In the meeting, I would like to present our recent attempt to understand the origin and nature of the stochasticity in driven translocation process based on the tension propagation scenario. In particular, we argue that (i) the main source of the stochasticity arises from the random initial condition characterized by the polymer configuration at the beginning of the translocation, and (ii) the standard deviation of the translocation time distribution obeys the same scaling law as that for the average translocation time. Therefore, the stochastic effect quantified as the ratio of standard deviation to average remains even in the long chain limit.

References
“Process time distribution of driven polymer transport”
We present a Brownian dynamics model of driven polymer translocation, in which non-equilibrium memory effects arising from tension propagation (TP) along the cis side subchain are incorporated as a time-dependent friction. To solve the effective friction, we develop a finite chain length TP formalism, based on the idea suggested by Sakaue [Sakaue, PRE 76, 021803 (2007)]. We validate the model by numerical comparisons with high-accuracy molecular dynamics simulations, showing excellent agreement in a wide range of parameters. Our results show that the dynamics of driven translocation is dominated by the non-equilibrium TP along the cis side subchain. Furthermore, by solving the model for chain lengths up to $10^{10}$ monomers, we show that the chain lengths probed by experiments and simulations are typically orders of magnitude below the asymptotic scaling limit. This explains both the considerable scatter in the observed scaling of translocation time w.r.t. chain length, and some of the shortcomings of other present theories. Our study shows that for a quantitative theory of polymer translocation, explicit consideration of finite chain length and frictional effects is required.
Driven Translocation: Equilibrium versus Non-equilibrium

Ralf Metzler

[1] Inst for Physics & Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany AND [2] Finland Distinguished Professor, Physics Dept, Tampere University of Technology, Korkeakoulunkatu 3, FIN-33101 Tampere, Finland

Classical translocation through a narrow pore is investigated by 3D Langevin dynamics simulations, finding a significant distinction between slow and fast dynamics. Thus under low driving forces the scaling of the translocation time with chain length is characterised by the critical exponent $1+\nu$, where $\nu$ is the Flory exponent. In contrast for large driving force the obtained exponent is around 1.37. The shift away from the value $1+\nu$ for fast translocation is interpreted in terms of non-equilibrium effects of the chain configuration.
Dynamics of polymer translocation under an applied external field

Kaifu Luo

CAS Key Laboratory of Soft Matter Chemistry Department of Polymer Science and Engineering
University of Science and Technology of China Hefei 230026, Anhui Province, China

Polymer translocation is of considerable importance to many biological processes. I will talk polymer translocation under an applied external field, including
(1) Translocation dynamics of a polymer chain into a long narrow channel driven by longitudinal flow [1];
(2) Polymer translocation through a long nanochannel: Interplay between the channel length and the chain length [2];
(3) Polymer translocation into confined systems, such as a slit [3], a fluidic channel [4], cavities with different geometries [5].

References

The motion of molecules across channels and pores is critically important for understanding mechanisms of many biological, chemical and physical processes. Here we investigate the role of interactions in the molecular transport through pores by analyzing exactly solvable discrete stochastic models. According to this approach the channel transport is viewed as a set of chemical transitions between discrete states that provides a full dynamic description of the translocation process. It is shown that the strength and spatial distribution of molecule/channel interactions can strongly modify the particle currents. Our analysis indicates that the most optimal transport is achieved when the binding sites are near the entrance or exit of the pore depending on the sign of interaction potential. Our theoretical predictions allow to explain single-molecule experiments on translocation of different polypeptides. We also hypothesize that intermolecular interactions during the channel transport might also significantly influence the translocation dynamics. Our explicit calculations show that the increase in the flux can be observed for some optimal interaction strengths. The mechanisms of these phenomena are discussed from microscopic point of view.
Driven and undriven translocation of a polymer: impact of fluctuations on dynamical scaling

Johan Dubbeldam [1], Vakhtang Rostiashvili [2], Andrey Milchev [2], Thomas Vilgis [2]

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[2] Max-Planck Institute for Polymer Research, Mainz, Germany

We suggest a theoretical description of the force-induced translocation dynamics of a polymer chain through a nanopore. Consideration is based on the tensile blob picture of a driven chain and the notion of a propagating front of tensile force along the chain backbone, suggested by Sakaue (Phys. Rev. E 81, 041808 (2010)). The driving force is associated with a chemical potential gradient that acts on each chain segment inside the pore. Depending on its strength, different regimes of polymer motion (named after the typical chain conformation, ``trumpet'', ``stem-trumpet'', ``stem'') occur. Assuming that the local driving and drag forces are equal (i.e., in a quasi-static approximation), we derive an equation of motion for the tensile front position. We show that the scaling law for the average translocation time versus chain length changes as the driving force $f$ grows. As a result the corresponding scaling exponent increases with $f$. This and other predictions are tested by Molecular Dynamics (MD) simulation. Data from our computer experiment indicate indeed that the translocation scaling exponent increases with the pulling force $f$ albeit the observed exponent stays systematically smaller than the theoretically predicted value [1]. In order to study the role of fluctuations (which are ignored in the quasi-static approximation), we assumed that the translocation coordinate $s(t)$ is a random process governed by the so-called velocity Langevin (V-Langevin) equation [2]. With this in mind we have derived the corresponding Fokker-Planck equation (FPE) for the translocation coordinate probability distribution function $W(s,t)$ which has a nonlinear drift term and time-dependent (running) diffusion coefficient $D(t)$. Our direct MD-simulation performed in 3D shows that the driven translocation follows a super-diffusion with a running diffusion coefficient $D(t)$. This finding being used in the numerical solution of FPE demonstrates an important conclusion: under relatively small driving forces fluctuations can facilitate the translocation dynamics. Moreover, the effective translocation exponent becomes smaller. In the undriven case the translocation is slightly sub-diffusive and can be treated within the framework of fractional Brownian motion (fBm) [3]. In particular, this means that $W(s,t)$ is Gaussian but with a time-dependent variance which grows sub-diffusively. These results are supported by extensive MD-simulation.

Polymer translocation through a nanopore – the effect of solvent conditions

Dieter Heermann, Felix Kapahnke, Ulrich Schmid, Matthias Weiss

University of Heidelberg, Germany

We have studied the translocation of a polymer through a nanopore by means of dissipative particle dynamics (DPD). Unlike Langevin approaches, DPD explicitly takes into account the interactions of solvent and polymer. We find that unforced translocation follows a scaling $\tau \sim N^{\eta}$ with $\eta \approx 2.32$ irrespective of the solvent conditions. This exponent is a consequence of the one-dimensional diffusion through the pore and an entropic activation barrier for the polymer near to the membrane. Biased translocation between a good-solvent and a bad-solvent reservoir (tuned via the repulsion between solvent and polymer) yields a preferential translocation towards the good solvent, with an exponent $\eta \approx 1$ for strongly varying solvent conditions.

Imposing attractive monomer-monomer interactions to vary the solvent quality (like in Langevin approaches), resulted in a translocation towards the bad-solvent side. Our results hence demonstrate that mimicking bad solvent conditions via artificial monomer-monomer attraction may yield artificial results.
Anomalous dynamics of polymer translocation

Debabrata Panja

Universiteit van Amsterdam, The Netherlands

Standard examples of anomalous polymer dynamics are single polymeric systems such as phantom Rouse, self-avoiding Rouse, Zimm (both in good and theta solvents), reptation, and many-polymeric systems such as polymer melts. In all these examples the trajectory description of tagged monomers in polymeric systems is robustly formulated by the Generalized Langevin Equation (GLE); the basis of which stems from the polymers’ (viscoelastic) relaxation response to local strains, mediated by chain connectivity [1,2]. The anomalous dynamics of unbiased [3] and weak field-driven translocation [4], and translocation by a pulling force [5] follows exactly the same principle, which allows one to identify the scalings of the pore-blockade times with polymer length. The same scaling exponents are also seen for polymer adsorption [6], and polymer desorption by a pulling force.

References

Modeling DNA-translocation through solid-state and alpha-hemolysin nanopores: two case studies

Peter Reimann

Bielefeld University, Germany

The first part addresses the translocation dynamics of a single protein molecule attached to a double-stranded DNA that is threaded through a solid-state nanopore by optical tweezers and an electric field. A simple theoretical model is introduced which explains all experimental findings very well. In the second part we reconsider the model of Lubensky and Nelson for the electrically driven translocation of polynucleotides through an alpha-hemolysin pore. We show that the model correctly describes two further important properties of the experimentally observed translocation time distributions, namely their spread (width) and their exponential decay.
Undriven Polymer Translocation: the role of pore size and solvent viscosity

Gary Slater, Hendrick W. de Haan

*University of Ottawa, Canada*

In principle, the undriven translocation of a polymer of length $N$ through a monomer-size nanopore looks like a rather simple problem. Early models by Sung and Park (1996) and by Muthukumar (1999) predicted that the translocation time should scale like $\tau \sim N^\alpha$, with the exponent $\alpha = 2$ or $3$ depending on whether the monomer translocation process was controlled by the friction in the pore or the drag on the monomers outside the pore. Computer simulations have produced a number of values for $\alpha$, mostly around $\alpha = 1 + 2u \approx 11/5 = 2.2$, as predicted by Chuang, Kantor and Kardar (2001). We have studied the influence of hydrodynamics, solvent viscosity and pore size on this exponent. Our conclusions are clear: there is no universal exponent that relates $\tau$ and $N$, even in the limit of single-file translocation. Instead, one obtains exponents in the range of 2 to 3, depending on the situation. The dynamics of unbiased translocation is controlled by friction in the nanopore, the time required to relax the polymer subchains, and finally the correlations between consecutive monomer jumps. This absence of a universal exponent may explain why different computer simulations produced different values for $\alpha$. 
Biopolymer translocation through pores: scaling, dynamics, statistics through a multiscale approach

Maria Fyta

Physik Department (T37) Technische Universitaet Muenchen James Franck Strasse 85748 Garching Germany

Our recently developed novel multiscale approach which concurrently couples a mesoscopic fluid solvent with molecular motion has been efficiently applied to the problem of biopolymer translocation through nanopores. We present results from numerical simulations of short and long (up to $10^4$) biopolymers translocating through narrow and wide pores. The statistical scaling behavior of the translocation process matches unexpectedly well to the experimental observations. Our results provide valuable insight into the cooperative aspects of biopolymer and hydrodynamic motion. In the case of wide pores, capable of hosting multiple polymer strands, there is clear evidence of folding quantization. The translocation proceeds through multi-folded configurations, characterized by a well-defined integer number of folds. In this case, the translocation time acquires a dependence on the average value of the folding number, leading to a deviation from the single-exponent power-law characterizing the single-file translocation through narrow pores. We also discuss some recent results when electrokinetic effects are implemented in the methodology.
The effects of chain flexibility and dichotomic driving on polymer translocation

Wokyung Sung

Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea

The polymer translocation through membranes and the polymer crossing over activation barriers in general, are ubiquitous in cell biology and biotechnological applications. Because they are interconnected flexible systems, polymers in translocation incur entropic barriers but can thermally surmount them with unusual sensitivity to background biases. In the presence of a non-equilibrium fluctuation characteristic of living environments, modeled as a dichotomic noise, the translocation can speed up much when resonant activation occurs. As a related issue, I will also discuss the problem of polymer surmounting a potential barrier, where the chain flexibility enhances the crossing. Furthermore, when the chain flexibility leads to conformational changes, the crossing rate can be even more dramatically increased. This conformational flexibility and variability enhance the stochastic resonance, where the chain crossing dynamics at an optimal temperature and chain length is maximally coherent and resonant to a minute periodic force. Utilizing the self-organizing behaviors mentioned above, we may learn about bio-molecular machinery of living as well as clever means of manipulating it.
I will outline our findings on the strong out-of-equilibrium characteristics of polymer translocation and the effect of hydrodynamic interactions. These findings suggest that the varying scaling exponents found for the process might be resulting from the event distributions changing with e.g. the applied pore potential. To address the posed question I will present event distributions for the polymer translocation obtained by extensive Langevin dynamics simulations. Such distributions have not been reported previously and they provide new understanding of the stochastic characteristics of the process. We extract at a high length scale resolution distributions of polymer segments that continuously traverse through a nanoscale pore. The obtained log-normal distributions together with the characteristics of polymer translocation show that it is describable as a multiplicative stochastic process. In spite of its clear out-of-equilibrium nature the forced translocation is surprisingly similar to the unforced case. We find forms for the distributions almost unaltered with a common cut-off length. We show that the individual short-segment and short-time movements inside the pore dominate and give the scaling relations $\tau \sim \alpha N^\alpha$ and $\tau \sim f^{-\eta}$ for the polymer translocation.
Posters
Introducing Péclet number as a parameter for finding translocation regime in the chaperone-driven polymer translocation

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Biopolymer translocation through narrow pores is a fundamental process in cell metabolism and biotechnology. Although there are many experimental and theoretical works on the electric field driven biopolymer translocation in which the related experiments are conducted in vitro, there are few works on the models proposed for the process in vivo. Our focus here is on an important model proposed for the translocation in vivo which is based on binding proteins called chaperone. By binding on the biopolymer asymmetrically, chaperones biased the translocation process through the Trans side. We investigate chaperone driven translocation of a stiff biopolymer, both theoretically and by a metropolis Monte Carlo simulation. We’ll show that by changing the length, binding energy and chaperone concentration the translocation regime will be changed from a completely diffusive to a ballistic drift dominated regime. Moreover it is being argued that the translocation regime can be determined effectively by considering a dimensionless parameter called Péclet number. It is a number used for comparing diffusion and drift in a special movement process. Especially the translocation time versus length scaling exponent is determined by calculating the Péclet number.
Investigation of tracer diffusion in crowded cylindrical channel

Rajarshi Chakrabarti, Stefan Kesselheim, Peter Kosovan and Christian Holm

Institute for Computational Physics, University of Stuttgart, Germany

Based on a coarse-grained model, we carry out molecular dynamics simulations to analyze the diffusion of a small tracer particle inside a cylindrical channel whose inner wall is covered with randomly grafted short polymeric chains. We observe an interesting transient sub-diffusive behavior along the cylindrical axis at high attraction between the tracer and the chains, however, the long time diffusion is always normal. This process is found to be enhanced for the case that we immobilize the grafted chains, i.e. the sub-diffusive behavior sets in at an earlier time and spans over a longer time period before becoming diffusive. Even if the grafted chains are replaced with a frozen sea of repulsive, non-connected particles in the background, the transient sub-diffusion is observed. The intermediate sub-diffusive behavior only disappears when the grafted chains are replaced with a mobile background sea of mutually repulsive particles. Overall, the long time diffusion coefficient of the tracer along the cylinder axis decreases with the increase in system volume fraction, strength of attraction between the tracer and the background and also on freezing the background. We believe that the simple model presented here could be useful for a qualitative understanding of the process of macromolecular diffusion inside the nuclear pore complex.
Protein translocation on DNA molecules: mechanisms of facilitated diffusion

Andrey Cherstvy

Institute of Solid State Research, Forschungszentrum Julich, Germany

Search and recognition of targets on DNA by DNA-binding proteins is a biologically vital process. Some proteins find their DNA target sequences with the rates that are 100-1000 times faster than predicted by Smoluchowski for a pure diffusion in 3D space. A dimensionality reduction from 3D in the buffer to 1D on the DNA is the basic mechanism of facilitated protein diffusion. We present a theoretical model that describes some physical-chemical aspects of protein target search in DNA coil. We consider the search process as a repetitive sequence of cycles of 3D diffusion in solution and 1D protein sliding along the DNA. The parameters of such non-equilibrium model is protein binding energy to DNA, the concentrations of free and bound proteins, the density of DNA coil, as well as some fine features of protein binding-unbinding kinetics. The model gives rise to a new “correlation” term in the total search time, missing in previous theoretical studies. It comes from accurate description of diffusion process in a stochastic DNA-protein interaction potential [1]. We show that the search time attains a minimum for intermediate strengths of protein-DNA interactions and for intermediate protein concentrations. The possible facilitation degree is close to the experimentally observed one. These non-monotonic trends are quantitatively supported by recent computer simulations for the same system [2]. A faster-than-diffusion search is achieved by a parallel scanning of DNA by many bound proteins. After reaching such hot spot on DNA, a recognition and specific binding of proteins to the double helix takes place. Finally, we unravel some electrostatic features of this DNA-protein recognition process stemming from peculiar charge patterns on DNA and protein surfaces [3].

References

Polymer Translocation through a Nanopore in the Presence of Obstacles: an Example of Translocation driven by Asymmetry

Hendrick de Haan, Gary W. Slater

University of Ottawa, Canada

In principle, the undriven translocation of a polymer of length $N$ through a monomer-size nanopore looks like a rather simple problem. Early models by Sung and Park (1996) and by Muthukumar (1999) predicted that the translocation time should scale like $\tau \sim N^{\alpha}$, with the exponent $\alpha=2$ or 3 depending on whether the monomer translocation process was controlled by the friction in the pore or the drag on the monomers outside the pore. Computer simulations have produced a number of values for $\alpha$, mostly around $\alpha = 1+2u \sim 11/5 = 2.2$, as predicted by Chuang, Kantor and Kardar (2001).

We have studied the influence of hydrodynamics, solvent viscosity and pore size on this exponent. Our conclusions are clear: there is no universal exponent that relates $\alpha$ and $N$, even in the limit of single-file translocation. Instead, one obtains exponents in the range of 2 to 3, depending on the situation. The dynamics of unbiased translocation is controlled by friction in the nanopore, the time required to relax the polymer subchains, and finally the correlations between consecutive monomer jumps. This absence of a universal exponent may explain why different computer simulations produced different values for $\alpha$. 
Responsive Concave and Convex Cylindrical Brushes

Sergei Egorov

University of Virginia, Department of Chemistry, Charlottesville, USA

We present a self-consistent field theoretical study of the microstructure of concave cylindrical brushes as a function of the cylinder radius, grafting density, grafted chain length, and the solvent quality. We show that the results for the radial monomer density profile and the distribution of the free ends are in good agreement with the corresponding molecular dynamics results.

In addition, we consider conformational behavior of a free macromolecule in a cylindrical brush. The central result is the observed non-monotonous variation of the size of a free chain in a brush-coated tube when the tube radius is systematically changed. An interpretation of this behavior is given by considering the overlap between the free polymer and the grafted chains as a function of the tube radius.

In the second part of the talk, we present a self-consistent field theoretical study of phase separation in binary polymer brushes physisorbed on cylindrical surfaces. In agreement with earlier simulation and experimental work, we find that macrophase separation occurs for two immiscible polymers of the same length, while chain length mismatch between two polymer types promotes microphase separation, with ring-shaped alternating stripes forming perpendicular to the cylinder axis. We observe that the width of the stripes increases with increasing immiscibility, increasing substrate curvature, decreasing mismatch in the chain length, and decreasing amount of adsorbed polymer. We rationalize these observations by analyzing entropic and energetic contributions to the Helmholtz free energy of the system.
Effects of dielectric mismatch and chain flexibility on the translocation barriers of charged macromolecules through solid state nano pores

Christian Holm, Stefan Kesselheim, Marcello Sega

Institute for Computational Physics, University of Stuttgart, Germany

We investigate the impact of dielectric boundary forces on the translocation process of stiff charged macromolecules through solid-state nanopores by means of coarse grained molecular dynamics simulations [1]. We find that the low dielectric permittivity of typical pore materials (compared to the surrounding water) is able to create a high free energy barrier of more than 10 $k_B T$ under low salt conditions for pore radii comparable to the Debye length. Interestingly the translocation barrier is significantly enhanced for flexible charged macromolecules. To achieve a comparable description of free energy profile we introduce a new reaction coordinate that can describe in a consistent way the whole translocation process for flexible and stiff macromolecules, and investigate the barrier for idealized model systems of a rigid double-stranded DNA and a flexible single-stranded DNA.
Drag forces on the DNAs counterions: What is the origin of current reduction?

Stefan Kesselheim, Christian Holm

Institute for Computational Physics, University of Stuttgart, Germany

We investigate different sources of drag forces on the ions in direct vicinity of a DNA molecule passing through a nanopore. Coarse grained reasoning leads to a hydrodynamic reduction of the mobility while atomistic simulations point to a picture where interactions with the DNA molecule are important. We present a quantitative discussion that bridges from the mesoscale to the atomistic scale where we elucidate that it is not at all clear, that DNA molecules in nanopores reduce currents.
Optimization of translocation time through tailoring of interaction potential landscape

Vladimir Palyulin [1], Ralf Metzler[1,2]

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Tailoring of copolymer sequences provides a way to control the pore-polymer interactions during the translocation process. If the polymer is long enough it can be viewed in the first approximation as a continuous potential landscape for 1D translocation equation. We have compared translocation times corresponding to different potentials. If polymer degrees of freedom are neglected, then the interaction potential corresponds to the copolymer sequence directly. What is an energy landscape which leads to the minimum of the mean first passage time between two points x_1 and x_2, whose energies are E_1 and E_2 (E_1 > E_2)? Naively, one might suggest that the solution is a linear potential drop between the two points. However, in our analysis we show that for an energy landscape consisting of two linear parts, a potential barrier with height E_b>E_1 leads to a decrease of the mean first passage time.

In copolymer sequence language that means smaller passage times for some inverse tapered copolymers than for linear gradient ones. The results were obtained by the solution of subdiffusive Fokker-Plank equation and continuous time random walk simulations.
Translocating Polymer as a Heat Pump Captured into a Nanopore by Electric Field

Payam Rowghanian, Alexander Grosberg

Department of Physics, New York University,

We study the threading and capture of a long and flexible polymer molecule through a nanopore. For a polymer driven electrically inside the pore, we formulate the threading dynamics by modifying a previously developed trumpet model and accounting for the dramatic deformations of the polymer during its passage. Introducing the concept of “iso-flux trumpet”, we show that the trailing part is properly characterized by a flux scale which determines the translocation rate and time. Although the speed of the process is determined by the friction which is dominated by the trailing part moving through the solvent, only a small portion of the energy provided by the electric field to the polymer is dissipated by the friction far from the pore, and it is mostly dissipated by the irreversible stretching and contracting of the polymer squeezed into the small pore. Due to the presence of the membrane, the polymer segment inside the pore is pulled by the strongly stretched pieces of the Polymer on both sides of the pore. Although the two strong pulling forces almost balance each other, they cause a net heat transfer during translocation from the trans to the cis side of the membrane. Currently, the theory is being improved by accounting for the nonzero field outside the pore and considering the coupling between the electric and hydrodynamic fields. The interaction of the DNA molecule with the electro-hydrodynamic field outside the pore is such that if the entropic barrier for entering the pore is large, the capture rate increases with the DNA length. Moreover, the field outside the pore significantly deforms the initial state of the polymer from which the threading process starts.
Pressure-driven flow through a channel with symmetric striped-pattern

Jiajia Zhou [1], Aleksey V. Belyaev [2, 3], Friederike Schmid [1], Olga I. Vinogradova [2, 3, 4]

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The influence of periodic patterned surfaces on the flow properties in Newtonian fluids through a planar channel is investigated by dissipative particle dynamics (DPD) simulations. The patterns are formed by alternating areas with no-slip and partial slip boundary conditions. We consider a situation where the patterns are symmetric. A number of relevant parameters are studied systematically, such as the flow direction, the pattern periodicity, and the channel height. Effective slip lengths are calculated for various parameters, and the simulation results are compared with predictions from continuous theory.