Diffusing polymers in microdomains and extracting geometrical information from chromosome capture data

Amitai, Assaf
(École normale supérieure - Paris, Group of Applied Mathematics and Computational Biology, IBENS, Paris, France)

The encounter between chromosomal sites inside the nucleus can regulate gene expression, exchange of genetic material and repair of DNA breaks. In addition, by forming a loop, the DNA molecule can bring a transcription factor to its promoter site, thus gene expression can be activated by binding far away along the chain. Recent chromosome capture techniques revealed encounter frequencies of chromosomal loci in vivo. This data correspond to the probability to form loops in the crowded nuclear environment. Is it possible to extract the size and structure of chromosomal territories (confined domain) from this data?

To answer this question, we developed a modeling approach that allows us to estimate the mean time for two monomers located on a polymer to meet (the mean first encounter time MFETC). We obtain an expression for the MFETC as a function of key parameters such as the radius of the confined domain and the distance along the DNA strand between the two loci. Using this formula, we extracted the size and structure of the territories explored by loci and we apply it to chromosome II in Yeast. This approach can be used to extract features from chromosome capture data about the nuclear organization, such as crowding, long range confinement and local interactions. These features could be compared to live cell imaging microscopy.

References
- A. Amitai, I. Kupka and D. Holcman, “Kinetics and encounter rates of diffusing polymers in confined microdomains”, J. Stat. Phys, In Press (2013).
- A. Amitai and D. Holcman, “Diffusing Polymers in Confined Microdomains and Estimation of Chromosome Territory Sizes from Chromosome Capture Data”, Phys. Rev. Lett. 110, 248105 (2013).
- A. Amitai, I. Kupka and D. Holcman, “Computation of the Mean First-Encounter Time between the Ends of a Polymer Chain”, Phys. Rev. Lett. 109, 108302 (2012).

Tribology of colloidal systems

Bechinger, Clemens
(Universität Stuttgart, 2. Physikalisches Institut, Physics, Stuttgart, Germany)

Tribology of colloidal systems

Clemens Bechinger

Universität Stuttgart, 2. Physikalisches Institut, Stuttgart

Friction between solids is responsible for many phenomena like earthquakes, wear or crack propagation. Unlike macroscopic objects which only touch locally due to their surface roughness, spatially extended contacts form between atomically flat surfaces. They are described by the Frenkel-Kontorova model which considers a monolayer of interacting particles on a periodic substrate potential. In addition to the well-known slip-stick motion such models also predict the formation of kinks and antikinks which largely reduce the friction between the monolayer and the substrate. Here, we report the direct observation of kinks and antikinks in a two-dimensional charge-stabilized colloidal crystal which is driven across different types of ordered substrates created by interfering laser beams. We show that the tribological properties only depend on the number and density of such excitations which propagate through the monolayer along the direction of the applied force. In addition, we also present first results, on how the friction depends on the strength of the pair interaction. In agreement with theoretical predictions, we find

that the friction vanishes upon exceeding a critical value of the pair interaction potential. Finally, we also discuss, how a higher degree of order in a colloidal system can be obtained by driving it across a periodic potential landscape.

[1] T. Bohlein, J. Mikhael, and C. Bechinger, Observation of kinks and antikinks in colloidal monolayers driven across ordered surfaces, Nature Materials 11, 126 (2012).

[2] T. Bohlein, and C. Bechinger, Experimental observation of directional locking and dynamical ordering of colloidal monolayers driven across quasiperiodic surfaces, Phys. Rev. Lett. 109, 058301 (2012).

Geometry-induced superdiffusion in driven crowded systems

Benichou, Olivier
(CNRS-UPMC, LPTMC, Paris, France)

Determining the response of a medium whilst in the presence of a tracer particle (TP) driven by an external force is a ubiquitous problem. It is for example at the heart of active micro-rheology, which has become a powerful experimental tool for the analysis of different systems in physics, chemistry, and biology . At the theoretical level, it has been the subject of many studies, most of which focus on analysing the velocity of the TP. Behavior beyond this force-velocity relation has been addressed in recent Molecular Dynamics simulations of active microrheology of glass-forming liquids and revealed superdiffusive fluctuations associated with the position of the TP. Such anomalous response, whose mechanism remains elusive, has been shown to occur only in systems close to their glass transition, suggesting that this could be one of its hallmarks. I will show that the presence of superdiffusion is in actual fact much more general, provided that the system is crowded and geometrically confined. I will rely on an analytical solution of a minimal model consisting of a driven TP in a dense, crowded medium in which the motion of particles is mediated by the diffusion of packing defects, called vacancies. This model represents a combination of two paradigmatic models of non-equilibrium statistical mechanics; asymmetric (for the TP) and symmetric (for the host particles in the system) simple exclusion processes. Through examining such non glassy systems, our analysis predicts a long-lived superdiffusion which ultimately crosses over to giant diffusive behavior. We find that this trait is present in confined geometries, for example long capillaries and stripes, and emerges as a characteristic response of crowded environments to an external force.

Anomalous dynamics of DNA hairpin folding

Carlon, Enrico
(KU Leuven, Theoretical Physics, Physics and Astronomy, Leuven, Belgium)

By means of computer simulations of a coarse-grained DNA model we show that the DNA hairpin zippering dynamics is anomalous, i.e. the characteristic time scales non-linearly with N, the hairpin length. We find that tau~N^alpha with alpha>1, in sharp contrast with the prediction of the zipper model for which tau~N. We show that the anomalous dynamics originates from an increase in friction during zippering due to the tension built in the closing strands. From a simple polymer model we get alpha=1+nu=1.59 with nu the Flory exponent, a result which is in agreement with the simulation data.

Diffusion of Interacting Particles in Discrete Geometries

Cleuren, Bart
(Hasselt University, Physics, Hasselt, Belgium)

We evaluate the self-diffusion and transport diffusion of interacting particles in a discrete geometry consisting of a linear chain of cavities, with interactions within a cavity described by a free-energy function. Exact analytical expressions are obtained in the absence of correlations, showing that the self-diffusion can exceed the transport diffusion if the free-energy function is concave. The effect of correlations is elucidated by comparison with numerical results. Quantitative agreement is obtained with recent experimental data for diffusion in a nanoporous zeolitic imidazolate framework material, ZIF-8.

Diffusion in narrow asymmetric channels on curved manifolds

Dagdug, Leonardo
(Universidad Autonoma Metropolitana-Iztapalapa, Physics, Mexico City, Mexico)

The transport of molecules and small particles spatially constrained within pores, channels, or other quasi-onedimensional systems has gained increasing attention over the last decade; as such systems are ubiquitous in both nature and technology. This problem is important in biology, chemistry, and nanotechnology, having straightforward applications in channels such as pores in zeolites, carbon nanotubes, synthetic nanopores, serpentine channels in microfluidic devices, artificially produced pores in thin solid films, channels in biological systems, and protein and solid-state nanopores as single-molecule sensors for the detection and structural analysis of individual molecules such as DNA and RNA.

Along with progress in experimental techniques, the problem of particle transport on Euclidian spaces through confined structures containing narrow openings, bottlenecks, and obstacles has led to recent theoretical efforts to study diffusion dynamics appearing in those geometries. Previous studies by Jacobs and Zwanzig ignited a revival of research on this topic. The so-called Fick-Jacobs (FJ) approach dramatically simplifies the problem if one assumes that solute distribution in any transverse direction of the channel is uniform as at equilibrium. This fast equilibrium assumption allows one to reduce a two-dimensional problem with a complex boundary to the one-dimensional problem of diffusion along the longitudinal direction of a channel in the presence of an entropy barrier. Significant progress in understanding such reduction has been made in recent years. For wide channels, one can map particle motion onto an effective one-dimensional description in terms of diffusion along the centerline of the channel, in the presence of the entropy potential.

It is well known that confinement in higher dimensions gives rise to an effective entropic potential in reduced dimensions. The associated approximate description relies on the generalized FJ equation for the probability density in the channel which is formally equivalent to a Smoluchowski equation, where the potential is replaced by the entropic barrier and the diffusion coefficient becomes space dependent D(x). This equation with a position-independent diffusion coefficient is known as the FJ equation. In this talk we shall show, using the projection method proposed by Kalinay and Percus, how can be obtained a robust effective diffusion coefficient in two dimensions that can be used to study wide channels with a non-straight midline and varying width and how these can be extended up to channels embedded on symmetric manifolds. We study some specific 2D asymmetric channel configurations to test the applicability.

Diffusion of DNA in nanochannels

Dorfman, Kevin
(University of Minnesota, Chemical Engineering and Materials Science, Minneapolis, MN, USA)

Nanochannels are emerging as a new technology for obtaining large-scale genomic information where the DNA is stretched and fluorescent genomic information is optically “read” from the linearized DNA. These applications motivated renewed interest in the basic physics of confined polymers, where DNA plays the role of a model polymer. While the scaling laws for strong (Odijk) and weak (de Gennes) confinement were established decades ago, recent experiments have illuminated the complex physics arising between these limiting cases for semi-flexible chains such as DNA. I will present our recent

results on DNA transport, which take advantage of a model that accurately reproduces the free solution properties of DNA. Using a combination of Monte Carlo models and hydrodynamics calculations, in conjunction with experiments in our lab and elsewhere, we have identified intriguiging hydrodynamic results arising from the interplay between the semi-flexible nature of the chain and the hydrodynamic interactions.

Effects of crowding and pore friction on the translocation time

Dubbeldam, Johan
(Delft University of Technology, Delft Institute of Applied Mathematics (DIAM), Applied Mathematics, Delft, Netherlands)

It is well known that the the translocation time tau scales with the chain length N as $tausimeq N^{alpha}$, where $alpha$ is a parameter that depends on the driving force. Moreover, it has been known from numerical simulations and theoretical arguments that $alpha=1+nu$, where nu is the Flory exponent, for very long chains.
In this paper I will derive a expressions for the translocation times based on scaling arguments. It is shown that large pore friction may lead to a smaller value of $alpha$, and crowding effects can generally be neglected.

Molecular diffusion and hydrophobic binding kinetics in water: insights from explicit-water simulations

Dzubiella, Joachim
(Humboldt-Universität zu Berlin, Department für Physik, Berlin, Germany)

Using explicit-water molecular dynamics computer simulations we study the binding kinetics and diffusivity of molecules in simple hydrophobic model systems. In particular, we firstly present results for curvature effects on water diffusion and escape times in the first hydration layer of spherical hydrophobic solutes. The results indicate a dynamic crossover regime at curvatures close to the well-known hydrophobic crossover length scale. Secondly, we study the binding kinetics of a small hydrophobic molecule associating with a shape-complementary binding pocket. Due to slow collective water flucutations in the binding pocket, interesting local stochastic coupling effects occur which partially control the kinetics of the binding process in this system. The presented findings may be useful to understand better the dynamics of biochemical processes on a molecular level.

One dimensional Brownian motion of an adiabatic piston in a hard rod gas

Fouladvand, Ebrahim
(Zanjan University & IPM, Institute for studies in Theyoritical physics and mathmatics (IPM), Physics, Tehran, Iran, Islamic Republic of)

We have investigated the motion characteristics of a movable piston immersed in a one dimensional gas of hard rods by event-oriented molecular dynamics in the absence of thermal noise. Periodic and reflecting boundary conditions are explored. It is shown that the piston undergoes systematic oscillations with decaying amplitudes in short times before it comes to global thermodynamic equilibrium. Moreover, the diffusion of the piston is explored and analytical expressions for its equilibrium mean-squared displacement is obtained.
It is shown that MSD of the piston does not differ much from the normal rods despite its mass and length are significantly larger. The main difference of our model to the preceding ones is that our fluid particles are not point-like but are rods. This problem was originally introduced by Tonks and the fluid is known as Tonks gas in the literature. In this talk we focus our attention to the motion and diffusion properties of a tracer particle (the piston) under a fully deterministic hard core potential among rods and the piston. The

tracer mass and length notably differ from other normal rods. The piston motion mimics the motion of a Brownian particle immersed in a gas of smaller rods. From the theoretical perspective, we also hope that our investigations shed more light on collective phenomena that arise in 1D fluids.

Narrow Escape Theory and Applications

Holcman, David
(IBENS, Ecole Normale Superieure Paris, Applied Mathematics and Computational Biology, France, France)

The Narrow escape is the mean first passage time for a stochastic particle to find a small target in a confined domain. I will review here the Narrow Escape Theory starting with asymptotic computations, modeling and numerical simulations.
I will then continue with applications in cellular biology and high throughput data analysis.

Rectifying Particle Transport via Entropic Barriers and Hydrodynamics

Hänggi, Peter
(Universität Augsburg, Dept. of Physics, Theoretical Physics I, Augsburg, Germany)

Diffusive transport of particles or, more generally, small objects, is a ubiquitous feature of physical and chemical reaction systems. In configurations containing confining walls or constrictions, transport is controlled by both, the fluctuation statistics of the jittering objects and the phase space available to their dynamics. Consequently, the study of transport at the macro- and nano-scales must address both Brownian motion and entropic effects [1].
In presence of a fluid flow across the microfludic channel where a solute of Brownian particles is subject to both, an external bias and a pressure-driven flow a new phenomenon emerges [2]; namely, the identically vanishing of the average particle flow which is accompanied by a colossal suppression of diffusion. This entropy-induced phenomenon, which we termed hydrodynamically enforced entropic trapping, offers the unique opportunity to separate particles of the same size in a tunable manner [3].
The presented work has been accomplished with the colleagues cited in the references given below.
References
[1] P. S. Burada, P. H¨anggi, F. Marchesoni, G. Schmid, and P. Talkner: Diffusion in Confined Geometries,
ChemPhysChem 10, 45-54 (2009).
[2] S. Martens, A. Straube, G. Schmid, L. Schimansky-Geier, and P. H¨anggi: Hydrodynamically enforced entropic trapping of Brownian particles, Phys. Rev. Lett. 110, 010601 (2013).
[3] S. Martens, G. Schmid, A. V. Straube, L. Schimansky-Geier, and P. H¨anggi: How entropy and hydrodynamics cooperate in rectifying particle transport, Eur. Phys. J. - ST (Special Topics) 222, 2453–2463 (2013).

Effective transport equations in quasi 1D systems.

Kalinay, Pavol
(Slovak Academy of Sciences, Institute of Physics, Bratislava, Slovakia)

The effective description of quasi one dimensional (1D) transport is demonstrated on a simple system: a particle diffusing in a 2D channel of varying width. Various approximations are presented: Starting from the simplest Fick-Jacobs equation, corresponding to the concept of the entropic potential, we end up with the effective equations based on the method of homogenization.

Next, the considerations presented are extended to more complex systems; a particle driven by an external force along the channel, or deflected by a transverse field. We show that the Fokker-Planck (Klein-

Kramers) equation projected onto the real space by a similar algorithm gives the Smoluchowski equation corrected by the mass dependent effective diffusion coefficient, reflecting also inertial effects in the overdamped regime.

Finally, validity and applicability of various effective equations for stationary and nonstationary processes are discussed.

Barriers to transport induced by multiplicative noise

Kantz, Holger
(Max Planck Instititute for the Physics of Complex Systems, Dresden, Germany)

Optimizing Diffusive Transport through a Synthetic Membrane Channel

Keyser, Ulrich
(University of Cambridge, Cavendish Laboratory, Biological and Soft Systems, Cambridge, United Kingdom)

We developed a simple but versatile experimental model system that allows to study diffusion-driven transport through microfluidic channels with exact control over the potential landscape [1] with the aim to understand transport through protein channels. Our system is based on the combination of holographic optical tweezers and particle tracking with sub-pixel and millisecond temporal resolution [2]. Our experiment enables us to follow the trajectories of all particles in the channels, bulk and entrance regions yielding exact measurements of the diffusion constants with sub-particle resolution [2]. We used our system to prove that a binding potential spanning the microfluidic channel enhances the diffusive current by a factor of up to four [1] in qualitative agreement with analytical models [3]. The system offers the great advantage that rare event like the successful translocation of particles can be measured rather than simulated allowing unprecedented view to the processes governing particle translocation through channels..

[1] S. Pagliara, C. Schwall, and U. F. Keyser. Optimizing Diffusive Transport Through a Synthetic Membrane Channel. Advanced Materials, 25(6):844-849, 2013.
[2] S. Dettmer, K. Misiunas, S. Pagliara, U. F. Keyser. Hindered diffusion coefficients of spherical particles confined by microchannels. Submitted, 2013.
[3] A. M. Berezhkovskii , S. M. Bezrukov. Optimizing transport of metabolites through large channels: Molecular sieves with and without binding. Biophys. J., 88 (3):L17-19, 2005.

Rocking Subdiffusive Ratchets: Origin, Optimization and Efficiency

Kharchenko, Vasyl
(National Academy of Science of Ukraine, Institute of Applied Physics, Theoretical department, Sumy, Ukraine)

We study subdiffusive Brownian ratchets periodically rocked by an external zero-mean force in viscoelastic media within the framework of a non-Markovian generalized Langevin equation approach and associated multidimensional Markovian embedding dynamics. Viscoelastic deformations of the medium caused
by the transport particle are modeled by a set of auxiliary Brownian quasiparticles elastically coupled to the transport particle and characterized by a hierarchy of relaxation times which obey a fractal scaling. The most
slowly relaxing deformations which cannot immediately followto the moving particle imprint long-range memory about its previous positions and cause subdiffusion and anomalous transport on a sufficiently long time scale.
This anomalous behavior is combined with normal diffusion and transport on an initial time scale of motion. Anomalously slow directed transport in a periodic ratchet potential with broken space inversion symmetry emerges due to a violation of the thermal detailed balance by a zero-mean periodic driving and

is optimized with frequency of driving, its amplitude, and temperature. Such optimized anomalous transport can be low dispersive and characterized by a large generalized Peclet number. Moreover, we show that subdiffusive
ratchets can sustain a substantial load and do useful work. The corresponding thermodynamic efficiency decays algebraically in time since the useful work done against a load scales sublinearly with time following to the transport particle position, but the energy pumped by an external force scales with time linearly. Nevertheless, it can be transiently appreciably high and compare well with the thermodynamical efficiency of the normal diffusion ratchets on sufficiently long temporal and spatial scales.

How to break a bond -- theory of rapid force spectroscopy

Kroy, Klaus
(Universität Leipzig, Institut für Theoretische Physik, Fakultät für Physik und Geowissenschaften,)

Dynamic force spectroscopy, the examination of intermolecular binding affinities and kinetics through single-molecule manipulation techniques, is a valuable complement to more traditional means of structural investigation. In contrast to scattering techniques or classical microscopy, it allows the experimentalist to gauge the dynamic and plastic behavior of a given material by directly probing the underlying free energy landscape, on a molecular scale. However, in spite of the strong forces required to do so, established theories of force spectroscopy still build on a quasistatic version of Kramers' theory. Originally devised for the usually slow process of spontaneous unbinding, it is set to break down at high loading rates. We extend these theories to rapid force spectroscopy protocols by explicitly resolving the non-equilibrium internal bond dynamics. Our analytical predictions are exact for fast loading protocols and reduce to established quasistatic results in the limit of slow external loading. Their large range of applicability renders them an ideal companion to Bayesian methods of data analysis, yielding an accurate tool for analyzing and comparing force spectroscopy data from a wide range of experiments and simulations, even without precise a priori knowledge of the underlying energy landscape.

Analysis and approximation of a finite-range jump process

Lehoucq, Rich
(Sandia National Laboratoires, Computational Mathematics, Albuquerque, USA)

The classical Brownian motion model for diffusion is not well-suited for applications with discontinuous sample paths. For instance, the mean square displacement of a diffusing particle undergoing a jump process often grows faster than that for the case of Brownian motion, or grows at the same rate but is of finite variation or nite activity. Such jump processes are viable models for anomalous super-diffusion or nonstandard normal diffusion. In particular, such jump diffusions are expedient models when the process sample-path is discontinuous because nearly instantaneous price volatility, species migration or heat conduction is suggested by the length and time scales over which the data is collected.

My presentation is on recent work for the associated deterministic equation on bounded domains where the jump process is of finite-range, i.e, the jump-rate is bounded. We refer to the associated deterministic equation as a volume-constrained nonlocal diffusion equation. The volume constraint is the nonlocal analogue of a boundary condition necessary to demonstrate that the nonlocal diusion equation is well-posed and be consistent with the jump process. A critical aspect of the analysis is a variational formulation and a recently developed nonlocal vector calculus.

Brownian motion of redox molecules in nanochannels

Lemay, Serge
(University of Twente, MESA+ Institute for Nanotechnology, Enschede, Netherlands)

We have developed a new single-molecule technique based on the measurement of electrochemical currents generated by molecules undergoing Brownian motion between two electrodes embedded in a nanochannel. Individual molecules act as diffusive charge shuttles, picking up electrons from one

electrode and delivering them to the second electrode. The time response of this system is characterized by stochastic fluctuations associated with Brownian motion, including both rapid shot-like noise from the shuttling process as well as slower equilibrium particle number fluctuations. We employ cross-correlation analysis of the

number fluctuations to measure record-low flow rates of order 1 pL/min, and study the distribution of first-passage times for individual molecules in these nanochannels.

Brownian motion of artificial colloidal microswimmers

Löwen, Hartmut
(University of Dusseldorf, Insitute of Theoretical Physics II: Soft Matter, Physics, Dusseldorf, Germany)

Abstract: Brownian motion is one of the key concepts to describe the motion and the dynamics of colloidal particles in solution.
In this talk this concept
will be generalized to artificial colloidal microswimmers which are
self-propelled and swimming in a solution. The self-propulsion leads to
to new behaviour in the mean-square-displacements, in particular if
the rotational degrees of freedom are considered [1,2]
and the particle swims in circles [3,4,5]. Moreover, active Brownian
particles exhibit novel collective behaviour like swirling [6,7]
kinetic clustering [8,9,10], and the crystallization
transition is different from ordinary bulk freezing [11,12].
The essentials of these phenomena
will be briefly discussed in the talk.

[1] B. ten Hagen, S. van Teeffelen, H. Lowen, J. Phys.: Condensed Matter 23, 194119 (2011).

[2] D. J. Kraft, R. Wittkowski, B. ten Hagen, K. V. Edmond, D. J. Pine, H. Lowen, Brownian motion and the hydrodynamic friction matrix for colloidal particles of complex shape, Phys. Rev. E 2013, see also http://arxiv.org/abs/1305.1253

[3] S. van Teeffelen, H. Lowen,
Phys. Rev. E 78, 020101 (2008)

[4] R. Wittkowski, H. Lowen, Phys. Rev. E 85, 021406 (2012).

[5] F. Kummel, B. ten Hagen, R. Wittkowski, I. Buttinoni,
R. Eichhorn, G. Volpe, H. Lowen, C. Bechinger,
Physical Review Letters 110, 198302 (2013),

[6] H. H. Wensink, H. Lowen,
J. Phys.: Condensed Matter 24, 460130 (2012).

[7] H. H. Wensink, J. Dunkel, S. Heidenreich,
K. Drescher, R. E. Goldstein, H. Lowen, J. M. Yeomans,
PNAS 109, 14308 (2012).

[8] I. Buttinoni, J. Bialke, F. Kummel, H. Lowen, C. Bechinger, T. Speck,

Physical Review Letters 110, 238301 (2013).

[9] J. Bialke, H. Lowen, T. Speck,
EPL 103, 30008 (2013).

[10] P. Cremer, H. Lowen,
Scaling in cluster growth of coagulating active particles,
http://arxiv.org/abs/1308.1520

[11] J. Bialke, T. Speck, H. Lowen,
Physical Review Letters 108, 168301 (2012).

[12] A. M. Menzel, H. Lowen,
Physical Review Letters 110, 055702 (2013).

Active Brownian Particles in a Channel

Marchesoni, Fabio
(Universita' di Camerino, Dipartimento di Fisica, Camerino, Italy)

Directed Brownian transport in narrow channels [1] of various geometries is discussed in the presence of different external biases, including periodic drives, magnetic fields and other time correlated energy sources.
High rectification (or ratcheting) efficiency is obtained by employing active (or self-propelling) Brownian particles both in a dilute solution and in binary mixtures [2]. In the latter case a small fraction of active Brownian particles suffices to force collective transport of the entire mixture along the channel. Applications to chemotactic processes are also discussed.

[1] P. S. Burada, P. Hänggi, F. Marchesoni, G. Schmid, P. Talkner, ChemPhysChem {bf 10}, 45 (2009).

[2] P.K. Ghosh, V.R. Misko, F. Marchesoni, F. Nori, Phys. Rev. Lett. {bf 110}, 268301 (2013).

First steps to incorporate the impact of most general force fields and particle inertia into the Fick-Jacobs approach

Martens, Steffen
(Technische Universität Berlin, Department of Physics, Berlin, Germany)

In small systems on length scales of micrometers and nanometers spatial confinement causes entropic forces that in turn implies spectacular
consequences for the control for mass and charge transport.

In view of its importance, recent efforts in theory triggered activities which allow for an approximate description that involves a reduction of dimensionality - the Fick Jacobs approach; thus making detailed predictions tractable. Up to present days, mostly the focus was (1) on the role of conservative forces and its interplay with confinement whereby (2) the impact of inertial effects has been neglected.

Within our recent works cite{Martens13,Martens13-2}, we overcame this limitation and succeeded in considering also ``magnetic field" like, so termed non-conservative forces that derive from a vector potential. A relevant application is the fluid flow across microfluidic structures where a solute of overdamped Brownian particles is subject to both, an external bias and a pressure-driven flow. Then a new phenomenon emerges; namely, the intriguing finding of identically vanishing average particle flow which is accompanied by a colossal suppression of diffusion. This entropy-induced phenomenon, which we termed textit{hydrodynamically enforced entropic trapping} cite{Martens13}, offers the unique

opportunity to separate particles of the same size in a tunable manner cite{Martens13-2}.

Nevertheless that the ``generalized Fick-Jacobs formalism'' can provide a highly accurate description, its derivation entails a tacit requirement, namely, the existence of a
hierarchy of relaxation times. This hierarchy guarantees the separation of time scales and supports adiabatic elimination resulting in an effective, kinetic description for particle transport in the presence of finite damping. The possibility of such description is intimately connected with equipartition and vanishing correlation between the particle's velocity components. We demonstrate that this approach is accurate for moderate to strong damping and for weak forces cite{Martens12,Ghosh12}. For strong external forces, equipartition may break down due to reflections at the boundaries. This leads to a non-monotonic dependence of particle mobility on the force strength.

begin{thebibliography}{10}
bibitem{Martens13} S. Martens et al., textit{Phys. Rev. Lett.} textbf{110}, 010601 (2013).
bibitem{Martens13-2} S. Martens et al., textit{EPJ-ST} textbf{222}, 2453--2463 (2013).
bibitem{Martens12} S. Martens et al., textit{Comm: J. Chem. Phys.} textbf{136}, 111102 (2012).
bibitem{Ghosh12} P.~K.~Ghosh et al. textit{Eur. Phys. Lett.} textbf{98}, 50002 (2012).
end{thebibliography}

Ageing single file motion

Metzler, Ralf
(Uni Potsdam, Physics & Astronomy, Potsdam, Germany)

Single file motion of excluded volume, thermally driven particles occurs in a variety of biological and thechnological applications. Here I will address the situation when the single file moves in a strongly disordered environment. This may occur, for instance, in a narrow cylindrical channel when the particles of the single file are functionalised with sticky ends and the channel walls are complementarily functionalised. As shown experimentally, this may give rise to power-law distributed sticking times of the particle onto the channel wall. I will present a non-renewal, ageing generalisation of the continuous time random walk to describe the motion of a labelled particle in this single file. Remarkably, the motion of the tracer particle becomes logarithmically slow, instead of the power-law growth with 1/2 exponent of the regular Brownian single file. The motion is weakly non-ergodic. Moreover, an interesting intermediate state occurs.

Theory of polymer capture and translocation through nanopores

Muthukumar, Murugappan
(University of Massachusetts, Polymer Science and Engineering, Amherst, USA)

Using a combination of theory and simulations, we will address the phenomenon of polymer capture and translocation through nanopores. The effect of entropic barrier arising from polymer confinement will be specifically considered.

Model colloids in 2D channel geometry in equilibrium and in external fields

Nielaba, Peter
(University of Konstanz, Physics Department, Konstanz, Germany)

Structure formation and dynamical properties of model colloids in two
dimensional channel geometry are studied by Brownian Dynamics simulations.
Layering phenomena as well as subdiffusive properties in equilibrium
are analyzed as well as non-equilibrium structure formation
phenomena in external driving fields.
Good agreement with experimental results is found.

Channel-facilitated diffusion boosted by particle binding at the channel mouth

Pagliara, Stefano
(University of Cambridge, Cavendish Laboratory, physics, cambridge, United Kingdom)

Particle transport through membrane channels and pores that connect 3-dimensional (3D) compartmentalized environments, represents a crucial step in a variety of biological, physical and chemical processes.[1] Such channels often exhibit binding sites specific for the transported particles. Binding in the channel can be optimized to maximize particle transport exceeding the one in the corresponding nonbinding channel.[2] This has been extensively investigated experimentally,[3-6] confirmed by molecular dynamics simulations[7] and an experimental model system,[8] and independently rationalized by a continuum diffusion model based on the Smoluchowski equation,[9] a discrete stochastic model,[10] a generalized macroscopic Fick's diffusion law[11] and a general kinetic model.[12] On the contrary although binding sites are also found at the entry of bacterial membrane channels[13,14] and in the 3D environments in proximity of cellular pores,[15,16] the function and mechanism of these external sites remain mainly undisclosed. We address the effect of external binding sites on particle transport in an experimental model system[8] by investigating the diffusion of colloidal particles in an array of closely-confining micro-channels permeated by a variety of energy landscapes. These are generated simultaneously and independently by combining microfluidics and laser line traps obtained with holographic optical tweezers.[8,17] Specifically we test energy landscapes constituted by internalized binding sites positioned in the center of the channels as opposed to binding sites extending from the channel to the 3D bulk and compare their transport properties to the ones of a non-binding channel. We find that the internalized binding site, although increasing the channel occupation probability, does not have a strong influence on the particle transport. It produces a four fold enhancement compared to the diffusion through a non-binding channel. On the contrary the most efficient energy landscape is the one with binding sites extending into the 3D bulk reservoirs. Optimizing the binding strength allows for an enhancement of two orders of magnitude and 40 times in the number of particles entering and translocating the binding channel, respectively. Our findings highlight the crucial role of the energy configuration at the connection between the channel and the nearby bulk reservoirs. We suggest that membrane transport might benefit of binding sites not merely localized in the center of the protein pores but rather extending to the periplasmic/extracellular space in proximity of the pore. Finally our results suggest guidelines to design synthetic membranes with enhanced transport performances.

[1] T. Chou, D. Lohse Phys. Rev. Lett. 82, 3552 (1999)
[2] J.J. Kasianowicz, T.L. Nguyen, V.M. Stanford Proc. Natl. Acad. Sci. USA 103, 11431 (2006)
[3] M. Luckey, H. Nikaido Proc. Natl. Acad. Sci. USA 77, 167 (1980)
[4] J.E.W. Meyer, G.E. Schulz Protein Sci. 6, 1084 (1997)
[5] R. Benz, A. Schmid, T. Nakae, G.H. Vosscherperkeuter J. Bacteriol. 165, 978 (1986)
[6] L. Kullman, M. Winterhalter, S.M. Bezrukov Biophys. J. 82, 803 (2002)
[7] M.O. Jensen, S. Park , E. Tajkhorshid , K. Schulten Proc. Natl. Acad. Sci. USA 99, 6731 (2002)
[8] S. Pagliara, C. Schwall, U.F. Keyser Adv. Mater. 25, 844 (2013)
[9] A.M. Berezhkovskii, S.M. Bezrukov Biophys. J. 88, L17 (2005)
[10] A.B. Kolomeisky Phys. Rev. Lett. 98, 048105 (2007)
[11] W.R. Bauer, W. Nadler Proc. Natl. Acad. Sci. USA 103, 11446 (2006)
[12] A. Zilman Biophys. J. 96, 1235 (2009)
[13] C. Hilty, M. Winterhalter Phys. Rev. Lett. 86, 5624 (2001)
[14] K.R. Mahendran, E. Hajjar, T. Mach, M. Lovelle, A. Kumar, I. Sousa, E. Spiga, H. Weingart, P. Gameiro, M. Winterhalter, M. Ceccarelli J. Phys. Chem. B 114, 5170 (2010)
[15] I.G. Macara Microbiol. Mol. Biol. Rev. 65, 570 (2001)
[16] C. Strambio-De-Castillia, M. Niepel, M.P. Rout Nat. Rev. Mol. Cell Biol. 11, 490 (2010)
[17] S. Pagliara, C. Chimerel, R. Langford, D.G.A.L. Aarts, U.F. Keyser Lab Chip 11, 3365 (2011)

Collective molecular motor dynamics in confined geometries

Pagonabarraga, Ignacio
(University of Barcelona, Physics Faculty, Fundamental Physics, Barcelona, Spain)

I will disucss the relevance of confinement on the motion of passive and active diffusing particles. In particular, I will analyze how active diffusion, exemplified by molecular motors, give rise to qualitative new scnearios of coopeartive motion due to the presence of heterogeneous confinement.
I will analyz different means of cooperative motion and how the interplay between activity and entropic constraints lead to cooperative rectification. I will also discuss the peculiarities of the hydrodynamic coupling of moleular motors in these systems.

Diffusion in confining and fluctuating environments : From atomistic diffusion to cell migration.

Palmieri, Benoit
(McGill University, Weizmann Institute of Science, Physics (McGill)/Materials and Interfaces,)

Diffusion in confining and fluctuating environment has been studied using fully microscopic models and coarse-grained, continuous, models. In the first part of this talk, fully microscopic studies of noble gases diffusing inside crystalline channeled structures (zeolites [1] and quartz) will be reviewed [2–4]. One novelty of these recent studies is that they incorporate the energy exchange between the diffusing atoms and the environment with very high accuracy. This is achieved by describing the system dynamics from a set of generalized Langevin equations that accurately reproduce the crystal vibrational density of states. The results showed that, for diffusion in small channels having concomitantly large energy barriers, such as argon diffusing in quartz, the crystal vibrations significantly reduced the predicted diffusion coefficients. This reduction was even greater when the lattice vibrations were treated quantum-mechanically. It will be shown that this effect arises due to zero point motion which increases the amplitude of the lattice vibrations. Second, coarse-grained, continuous, points of view of diffusion processes in confining and fluctuating environments will be presented [5]. In this approach, the confining environment is modeled as a soft, thermally fluctuating tube (or continuum limit of a zeolite channel). The soft tube properties are chosen to describe the dynamics and flexibility of the environment and microscopic forces for bending and stretching bonds in the crystal lattice are replaced by elastic moduli and surface tension. The theory generalizes earlier work based on the Fick-Jacobs equation [6, 7] and the results showed that tube thermal fluctuations decrease the transport rates for all system parameters. On the one hand, the tube fluctuations can randomly “push” the diffusing guest along the tube axis (parallel to the net flux) and enhance its diffusivity. However, the results demonstrate that this effect is always less important than the one where the system wastes time trying to re-equilibrate in the direction perpendicular to the tube axis so that the overall diffusive transport is decreased. Finally, recent theoretical efforts to describe the Brownian motion of motile cells on a substrate will be discussed [8]. In a confluent monolayer, the motion of each cell is confined by the “channel” defined by the other cells. This behavior is related to one crucial step in the metastatic process where the soft cancer cells invade the vascular network by squeezing through narrow channels defined by stiff endothelial cells [9, 10].
The last part of this talk will present ongoing theoretical efforts to model the Brownian motion of cells in a monolayer as a dense system of highly deformable elastic bodies. The goal is to identify the minimum number of ingredients required to reproduce the enhanced motility of cancer cells in a confluent monolayer of normal cells (compared to the motion obserbed in a monolayer comprising soft cancer cells only).

Transport through ion channels

Percus, Jerome K.
(New York University, Courant Institute of Mathematical Sciences, Mathematics/Physics, New York, USA)

The dimensional reduction of 3-dimensional transport through a complex confining potential has been studied for ages, with the Fick-Jacobs approximation

for single particle diffusion as the first breakthrough. This approximation is extremely simple and correspondingly a bit naive. However, the general form that it suggests can be rewardingly the zeroth order of a well-defined approximation hierarchy under well-defined controlling conditions. In this presentation, long-time behavior is expressed as a functional of a basic FJ-type quantity, and application is made to transport through several classes of ion channel. Along the
way, the effects of charge, wall degrees of freedom, "gunky" environment, and the nature of input and output must be treated in a leading idealized fashion.

The Dynamics of Diffusive Capture Processes

Redner, Sidney
(Boston University Physics Department, Physics, Boston, USA)

Entropic separation and transport in confined systems

Reguera, David
(Universitat de Barcelona, Departament de Fisica Fonamental, Barcelona, Spain)

Confinement plays a very important role in many physical and biological systems. The diffusion of particles in zeolites and in microfluidic devices, the motion of biomolecules in the interior of a living cell or through ion channels, or the translocation of viral DNA into a cell, are examples where the evolution of the system is influenced by the tortuosity of a bounded region.

In this talk, I will discuss how these systems can be nicely described by introducing the concept of an entropic potential. We will see how the peculiar nature of the entropic barriers has important and counterintuitive consequences in the transport in these media. In particular, phenomena such as entropic stochastic resonance, diffusion enhancement, and rectification take place in these systems and can be controlled by a smart application of external forces. These mechanisms can be used to optimize transport in confined media and for the manipulation and control of single molecules. In particular, I will discuss how the interplay of entropy, noise, and asymmetry can be used in an efficient separation mechanism that induces motion of particles of different sizes in opposite directions. This entropic splitting effect can be optimized for practical purposes and could be implemented in narrow channels and microfluidic devices.

Working under confinement

Rubi, Miguel
(Universitat de Barcelona, Facultat de Física, Departament de Fisica Fonamental. ub, Barcelona, Spain)

How does confinement alter the transport properties of colloidal particles, the functionalities of molecular machines and in general the mechanisms of energy-transfer and energy-conversion at small scales? This question, fundamental for the modelling of soft-matter systems and biological systems, is attracting the interest of many researchers in the field. In a basic model proposed, the confinement effects are considered through an entropic potential. It has been shown that transport through entropic barriers or entropic transport exhibits peculiar characteristics very different from those observed when activation takes place through energetic barriers.
Here, we review recent progresses in the study of entropic transport and its applications to soft-matter and biological systems. We show that the confinement plays a very important role in the mechanisms of energy-conversion at the nanoscale, in particular in the functionality of molecular machines.

Anomalous Diffusion of Self-propelled Particles on Directed Random Networks

Shaebani, M. Reza
(Saarland University, Faculty of Natural Sciences and Technology, FR 7.1 Theoretical Physics, Saarbrücken, Germany)

We study the influence of structural characteristics of filamentous networks, or equivalently the stepping

strategy in continuous space, on the transport properties of a random walker. A general master equation formalism is developed to investigate the persistent motion of self-propelled particles, which enables us to identify the key parameters and disentangle their contributions to the transport process. An anomalous diffusive behavior emerges, depending on the choice of the persistency of the walker and the anisotropy and heterogeneity of the structure or stepping properties. We establish the existence of up to three different regimes of motion, and determine the phase diagrams of the behavior. We verify that the crossover times between different regimes as well as the long-term diffusion coefficient can be enhanced by a few orders of magnitude within the biologically relevant range of control parameters. The analytical predictions are in excellent agreement with simulation results.

Polymer translocation through a narrow pore with fluctuating driving forces

Shin, Jaeoh
(University of Potsdam, Institute of Physics and Astronomy, Potsdam, Germany)

We study the driven translocation of polymer through a pore in the presence of fluctuating forces using Langevin dynamics simulations. For the case of sticky pore, the translocation time shows a resonant minimum at an optimal rate of the fluctuating force. We identify that the resonant behavior is due to the free energy well in the last emptying process of the translocation. We also study effects of various system parameters such as chain length and driving force amplitudes. Our finding suggests that fluctuating driving forces may play an important role in polymer translocation in biological systems and may also be useful in practical applications.

The effect of interparticle interaction on the kinetics of geminate reactions of Brownian particles

Shushin, Anatoly
(Semenov Institute of Chemical Physics, Moscow, Russian Federation)

We analyze the effect of attractive interparticle interaction on the kinetics of diffusion-controlled geminate reactions of Brownian particles in spaces of different dimensionalities. The interaction potential is assumed to be of the shape of potential well.

In the limit of strong interparticle interaction, when the potential well is deep enough, the analytic expression for the reaction kinetics is obtained by rigorous solution of the corresponding Smoluchowski equation. The expression shows that the interaction results in formation of the quasistationary state within the well (cage), the time dependent population of which essentially determines the reaction kinetics.

The time dependence of the cage population (and thus the kinetics of reaction of interacting particles) is found to significantly depend on the dimensionality (D) of Brownian motion of particles. In 3D case the caging manifests itself in the exponential stage of the cage depopulation kinetics at relatively short times, which is subsequently changed by the inverse power type one (~t^{-3/2}) at long times. As for 1D and 2D cases, which are of special interest for the analysis of processes in the presence of geometric constrains and in low dimensional structures, the kinetics of the time-evolution of cage population in these cases is, in general, essentially non-exponential at all times. The ling time asymptotic behavior of the kinetics is also of inverse power type, but with the exponent depending on the reactivity. These low-dimensional kinetic features of reactions are described with simple and rigorous analytical expressions.

Rigorous formulas are also derived for the kinetics of interaction affected processes in the presence of an external field. For all dimensionalities the influence of the external field shows itself in the changeover of inverse power type asymptotic behavior of the kinetics to the exponential one.

Nanofluidics and triboly inside individual nanotubes

Siria, Alessandro
(CNRS, ILM, France)

New models of fluid transport are expected to emerge from the confinement of liquids at the nanoscale, with potential applications in ultrafiltration, desalination and energy conversion.

Nevertheless, advancing our fundamental understanding of fluid transport on the smallest scales requires mass and ion dynamics to be ultimately characterized across an individual channel to avoid averaging over many pores.

A major challenge for nanofluidics thus lies in building distinct and well-controlled nanochannels, amenable to the systematic exploration of their properties.

In this talk we will discuss on how Focused Ion Beam nanopores drilled in ultra-thin solid state membranes and hierarchical fluidic systems made of individual nanotubes allows to explore the fluid behavior at the limit of the classic description.

We will show how the fluid-solid interface governs the transport in nano channels and how tuning the surface properties may lead to new tools that can profit of exotic behavior of fluid at nanoscale

Models of subdiffusion induced by geometrical restrictions

Sokolov, Igor
(Humboldt-Universität zu Berlin, Institut für Physik, Berlin, Germany)

The particles' motion in many physical systems can be modeled by random walks. In inhomogeneous environments these do not necessarily lead to normal diffusion in the long time limit. Examples are given by subdiffusive behavior of random walks on comb structures, on random walk trajectories and in percolation systems close to criticality. Some multiparticle systems (like single-file diffusion or polymer motion) can be mapped on geometrically restricted diffusions in the state space. After discussing properties of specific models and trying to classify the possible scenarios of their behavior with respect to stationarity and ergodicity (or absence thereof), we turn to general properties of geometrically induced subdiffusion and show that quite general statements on the type of their behavior are possible.

Formation and transport of colloidal doublets in a modulated ratchet potential: theory and experiment

Straube, Arthur
(Humboldt-Universität zu Berlin, Department of Physics, Berlin, Germany)

We present a combined experimental and theoretical study describing the motion of paramagnetic colloidal particles driven above a stripe-patterned magnetic garnet film. An elliptically polarized rotating magnetic field modulates the stray field of the garnet film and generates a translating periodic potential which induces particle motion. Increasing the driving frequency, a single particle displays the sharp transition from a locked motion with a constant mean speed to a sliding dynamics characterized by a slower frequency-dependent mean speed. We focus on the sliding motion and show that by varying the ellipticity of the rotating magnetic field, we can induce attractive interactions between the colloidal walkers, leading to the formation of moving doublets. We suggest an analytically tractable theoretical model that explains the formation and motion of the doublets, which is in agreement with the experiment.

First-passage times of random walks in confinement

Voituriez, Raphael
(CNRS -- UPMC, LPTMC -- LJP, Paris, France)

How long does it take a "searcher" to reach a "target" for the first time? This first-passage time is a key quantity for evaluating the kinetics of various processes, and in particular chemical reactions involving "small" numbers of particles such as gene transcription, or at larger scales the time needed for animals to find food resources.

I will present recent results which enable the evaluation of the distribution of first-passage time for a wide range of random search processes evolving in a confined domain. This approach reveals a general dependence of the first-passage time distribution on the geometry of the problem, which can become a key parameter that controls the kinetics of the search process. I will show how these results apply to transport in disordered and fractal media, and highlight their implications in transcription kinetics and other search processes at larger scales.