

Book of Abstracts

Workshop on

**Polymers with spatial and mechanical
constraints**

Venice, July 7-9 2016

Workshop on Polymers with spatial and mechanical constraints

Venice, July 7-9 2016

Istituto Veneto di Scienze, Lettere ed Arti

Thursday, July 07, 2016

8:30 - 9:00

WELCOME

SESSION I

9:00 - 9:40

Cees Dekker Topological aspects of DNA, from single molecules to cells

9:40 - 10:20

Tapio Ala-Nissila Iso-Flux tension propagation theory and its application to driven polymer translocation

10:20 - 11:00

Ralf Metzler Crowding and confinement in lipid bilayers and polymer chains

11:00 - 11:30

COFFEE BREAK

11:30 - 12:10

Stu Whittington Adsorbed Self-Avoiding Walks subject to a force

12:10 - 12:50

Suckjoon Jun Why cell size matters for chromosome organization in bacteria

12:50 - 14:30

LUNCH BREAK

SESSION 2

14:30 - 15:10

Elena Angeli Polymeric nanochannels: a single structure for multiple applications

15:10 - 15:50

Takahiro Sakaue Topological constraint on the phase behavior of ring polymer blends

15:50 - 16:30

Gary Slater Polymer translocation: three different ways to apply constraints to the polymer chain

16:30 - 17:00

COFFEE BREAK

17:00 - 17:40

Max Di Ventra DNA, RNA and proteins in confined geometries: from precision medicine to new nanoscale phenomena

17:40 - 18:20

Patrick Doyle TBA

18:20 - 18:50

2-minutes presentations by poster presenters, followed by **POSTER SESSION**

Friday, July 08, 2016

SESSION 3

- 9:00 – 9:40 **Aleksandra Radenovic** **Controlled translocation of a DNA-Protein complexes through a glass nano-capillary**
- 9:40 - 10:20 **Erwin Frey** **Many-Body Effects and Breakdown of Reptation Theory in Entangled Semiflexible Polymer Solutions**
- 10:20 - 11:00 **Yitzhak Rabin** **Hairy Nanopores**
- 11:00 - 11:30 **COFFEE BREAK**
- 11:30 – 12:10 **Alexander Grosberg** **Polymer rings in the melt and their minimal surfaces**
- 12:10 - 12:50 **Tobias Ambjörnsson** **Statistical physics of nanochannel-based DNA barcodes with applications on plasmid characterization**
- 12:50 – 14:30 **LUNCH BREAK**

SESSION 4

- 14:30 - 15:10 **Walter Reisner** **Strongly Non-equilibrium Dynamics of Nanochannel Confined DNA**
- 15:10 – 15:50 **Mehran Kardar** **Polymer-mediated forces between scale-free objects**
- 15:50 – 16:30 **Yacov Kantor** **Ideal polymers near scale-free surfaces: Statics and dynamics**
- 16:30 – 17:00 **COFFEE BREAK**
- 17:00 – 17:40 **Peter Cifra** **Linear and ring DNA in nanochannels under stripe and slab confinement**
- 17:40 – 18:20 **Michele Caraglio** **Knots and knotted polymers under tension**
- 18:20 – 20:00 **POSTER SESSION**
- 20:00 **SOCIAL DINNER AT “RISTORANTE SAN TROVASO”**

Saturday, July 09, 2016

SESSION 5

9:00 – 9:40

Felix Ritort **The remarkable elastic properties of single stranded DNA**

9:40 – 10:20

Christos Likos **Coarse-graining of flexible and stiff ring polymers**

10:20 – 11:00

Enrico Carlon **The effect of twist-bend coupling on the torsional properties of double- stranded DNA**

11:00 – 11:30

COFFEE BREAK

11:30 – 12:10

Dmitrii Makarov **TBA**

12:10 – 12:50

Giovanni Dietler **Statistical Properties of DNA in 2 dimensions and in channels**

CLOSING REMARKS

Welcome

Dear colleagues,

It is our pleasure to welcome you at the "Istituto Veneto di Scienze Lettere ed Arti" for this workshop on

Polymers with spatial and mechanical constraints.

The workshop is primarily meant to provide a state-of-the-art perspective on recent theoretical and experimental advancements on nano-manipulation of polymers and biofilaments by passive and active means (e.g. spatial confinement, nanofluidics, nano-pore translocation and pulling by AFM and optical/magnetic tweezers) and the insight that can be gleaned regarding the spatial organization of these molecules.

We wish to thank again for making this workshop possible by attending it, giving a talk or presenting a poster and by contributing to the discussions.

We also acknowledge financial and logistic support from the Physics Department of the University of Padova, SISSA and IVSLA.

Cristian Micheletti, Enzo Orlandini and Attilio Stella

Contents

Welcome	v
Invited talks	1
Topological aspects of DNA, from single molecules to cells (<i>Cees Dekker</i>) .	2
Iso-Flux Tension Propagation Theory and It's Application to Driven Polymer Translocation (<i>Tapio Ala-Nissila</i>)	2
Crowding and confinement in lipid bilayers and polymer chains (<i>Ralf Metzler</i>)	3
Adsorbed Self-Avoiding Walks subject to a force (<i>Stu Whittington</i>)	3
Why cell size matters for chromosome organization in bacteria (<i>Suckjoon Jun</i>)	4
Polymeric nanochannels: a single structure for multiple applications (<i>Elena Angeli</i>)	4
Topological constraint on the phase behavior of ring polymer blends (<i>Takahiro Sakaue</i>)	5
Polymer translocation: three different ways to apply constraints to the polymer chain (<i>Gary Slater</i>)	5
DNA, RNA and proteins in confined geometries: from precision medicine to new nanoscale phenomena (<i>Massimiliano di Ventra</i>)	5
TBA (<i>Patrick Doyle</i>)	6
Controlled Translocation of a DNAProtein Complexes through a Glass Nanocapillary (<i>Aleksandra Radenovic</i>)	6
Many-Body Effects and Breakdown of Reptation Theory in Entangled Semiflexible Polymer Solutions (<i>Erwin Frey</i>)	7
Hairy Nanopores (<i>Yitzhak Rabin</i>)	7
Polymer rings in the melt and their minimal surfaces (<i>Alexander Grosberg</i>)	7
Statistical physics of nanochannel-based DNA barcodes with applications on plasmid characterization (<i>Tobias Ambjörnsson</i>)	8
Strongly Non-equilibrium Dynamics of Nanochannel Confined DNA (<i>Walter Reisner</i>)	8
Polymer-mediated forces between scale-free objects (<i>Mehran Kardar</i>) . . .	9
Ideal polymers near scale-free surfaces: Statics and dynamics (<i>Yacov Kantor</i>)	9
Linear and ring DNA in nanochannels under stripe and slab confinement (<i>Peter Cifra</i>)	10
Knots and knotted polymers under tension (<i>Michele Caraglio</i>)	11
The remarkable elastic properties of single stranded DNA (<i>Felix Ritort</i>) . .	12
Coarse-graining of flexible and stiff ring polymers (<i>Christos N. Likos</i>) . . .	12

The effect of twist-bend coupling on the torsional properties of double-stranded DNA (<i>Enrico Carlon</i>)	13
TBA (<i>Dmitrii Makarov</i>)	13
Statistical Properties of DNA in 2 dimensions and in channels (<i>Giovanni Dietler</i>)	13
Posters	15
Conformational behavior of end-grafted PEO chains as potential protection layer against protein adsorption (<i>Zuzana Benková</i>)	16
Knotted ring polymers in nanochannels (<i>Mattia Marendà</i>)	16
Coarse-grained simulations of DNA under torsional stress (<i>Christian Matek</i>)	17
Threading Dynamics of Ring Polymers in a Gel (<i>Davide Michieletto</i>) . . .	17
Density effects in entangled solutions of ring polymers (<i>Negar Nahali</i>) . . .	18
Dynamics of Active Polymers Under Confinement (<i>Dino Osmanovic</i>) . . .	18
Pore translocation of knotted chains (<i>Antonio Suma</i>)	18
Gas Permeability of polydimethylsiloxane (PDMS) membranes: thickness and surface effects (<i>Ugo Valbusa</i>)	19
Ring polymers under confinement: A comparison to their linear counterparts (<i>Lisa Weiss</i>)	20
List of Participants	21

Invited talks

Topological aspects of DNA, from single molecules to cells

Cees Dekker

Kavli Institute of Nanoscience Delft, Department of Bionanoscience,
Delft University of Technology, The Netherlands

Contents:

- Nanopore detection of DNA knots
- DNA sequence dependence of plectonemic supercoils
- DNA condensation by condensin
- Chromosomal structure of DNA in shape-relaxed *E. coli* cells

Text

Iso-Flux Tension Propagation Theory and It's Application to Driven Polymer Translocation

Tapio Ala-Nissila

Department of Applied Physics
Aalto University School of Science
Espoo, Finland

The translocation dynamics of polymers through nanopores driven by external fields is a far-from-equilibrium process, which is described by the tension propagation (TP) theory of Sakaue [1]. In particular, the Brownian Dynamics TP theory within the iso-flux (IFTP) assumption [2] allows a self-consistent derivation of analytic equations of motion for the dynamics, including an explicit form for the chain length dependence of the average translocation time [3]. In this talk I will review the IFTP theory and discuss its application to the case of a flickering pore and an oscillating external driving force [4], and translocation dynamics of semi-flexible polymer chains [5].

1. T. Sakaue, Phys. Rev. E 76, 021803 (2007).
 2. P. Rowghanian and A. Y. Grosberg, J. Phys. Chem. B 115, 14127 (2011).
 3. J. Sarabadani, T. Ikonen and T. Ala-Nissila, J. Chem. Phys. 141, 214907 (2014).
 4. J. Sarabadani, T. Ikonen and T. Ala-Nissila, J. Chem. Phys. 143, 074905 (2015).
 5. J. Sarabadani et al., unpublished (2016)
-

Crowding and confinement in lipid bilayers and polymer chains

Ralf Metzler

Department of Physics,
Tech. Univ. Munich, D-85748 Garching, Germany

Crowding and confinement play important roles in biological systems. Two examples will be presented in this talk.

In the first part I will discuss the anomalous and non-Gaussian diffusion of lipid chain molecules in a bilayer crowded with proteins. Indeed part of the non-Gaussian nature of the motion can be understood as confined motion of a subset of the lipids.

The second part will deal with the looping properties of polymer chains in solutions of crowders of different sizes. Both the looping statistics and the dynamics are influenced by the crowder ratio and size. Additional effects enter due to the competition of length scales when the polymer has a finite persistence and is allowed to move in a container of finite size.

References:

JH Jeon, M Javanainen, H Martinez-Seara, R Metzler, and I Vattulainen, Phys Rev X, at press

R Metzler, JH Jeon, and AG Cherstvy, Biochim Biophys Acta (2016)

J Shin, AG Cherstvy, and R Metzler, ACS Macro Lett 4, 202 (2015)

J Shin, AG Cherstvy, and R Metzler, Soft Matter 11, 472 (2015)

Adsorbed Self-Avoiding Walks subject to a force

Stu Whittington

University of Toronto

A self-avoiding walk on a lattice is the standard model of the configurational properties of linear polymers in dilute solution in a good solvent. The system can be modified to model polymer adsorption and it has recently been adapted to include a force pulling the adsorbed polymer off the surface. We shall present a collection of rigorous results about the model, focussing on the temperature dependence of the critical force for desorption. In three dimensions we can show rigorously that the force-temperature curve is reentrant. We shall also discuss some results about how the behaviour depends on the precise way in which the force is applied, and extensions to other architectures such as ring polymers.

Why cell size matters for chromosome organization in bacteria

Suckjoon Jun

Biological Science,
University of California, San Diego, USA.

Polymeric nanochannels: a single structure for multiple applications

Elena Angeli

Dipartimento di Fisica, Università di Genova
Genova, Italy

Polymeric nanofluidic devices are very versatile tools whose exploitation covers a wide spectrum of fields. In fact, slightly changing the characteristics of a basic structure like a nanochannel, it is possible to study a variety of different phenomena spanning from biopolymer conformation to nanoparticles translocation processes. We created various nanodevices combining, in a number of different configurations, a simple basic nanostructure: a nanochannel patterned by a focused ion beam on a silicon mold and replicated using polydimethylsiloxane. In particular, long straight nanochannels allow a detailed observation and analysis of biopolymers like long DNA chains in nanoconfinement conditions [1-2], while series of nanochannels interrupted by deep pits enable the study of the dynamics of DNA conformational changes [3]. Moreover, devices with short channels can be used for counting and sizing fluorescent nanoparticles one-by-one taking advantage of an electro-optical tracking method. This method is based on simultaneous acquisition of electrical traces, exploiting resistive pulse sensing techniques, and on recording nanoparticles optical tracks in the proximity of the nanochannel. This multimodal analysis approach greatly increases the reliability of this sensor compared to conventional monomodal (only electrical or optical) approaches. The versatility of these nanodevices makes them very valuable tools for several areas of Nanotechnology.

1. C.Manneschi et al., *Macromolecules* 46,4198 (2013).
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 3. E.Angeli et al., *Lab on chip* 11,2625 (2011)
 4. E.Angeli et al., *Nano Letters* 15(9), 5696 (2015)
-

Topological constraint on the phase behavior of ring polymer blends

Takahiro Sakaue

Department of Physics,
Kyushu University 33, Fukuoka, Japan.

The miscibility of polymer blends, a classical problem in polymer science, may be altered, if one or both of the component do not have chain ends. Based on the idea of "topological volume", we propose a mean-field theory to clarify how the topological constraints in ring polymers affect the phase behavior of the blends. While the large enhancement of the miscibility is expected for ring-linear polymer blends, the opposite trend toward demixing, albeit comparatively weak, is predicted for ring-ring polymer blends. Scaling formulas for the shift of critical point for both cases are derived. We discuss the valid range of the present theory, and the crossover to the linear polymer blends behaviors, which is expected for short chains. These analysis put forward a view that the topological constraints could be represented as an effective excluded-volume effects, in which the topological length plays a role of the screening factor.

Polymer translocation: three different ways to apply constraints to the polymer chain

Gary Slater

Department of Physics,
University of Ottawa, Ottawa, Canada

DNA, RNA and proteins in confined geometries: from precision medicine to new nanoscale phenomena

Massimiliano di Ventra

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La Jolla, CA 92093-0319 USA

Confining biological macromolecules - such as DNA, RNA and proteins - in channels of nanoscale dimensions offers unprecedented opportunities in precision medicine, namely in our ability to tailor drugs to the specific genome/transcriptome/proteome of each individual [1,2]. In addition, this research is opening up the possibility of exploring physical properties and new phenomena of liquids and polymers in confined geometries that were not even conceivable a decade ago. As an example of the first research direction, I will show a novel technique for de novo protein sequencing that involves translocating a polypeptide through a synthetic nanochannel and measuring the ionic current of each amino acid through an intersecting perpendicular nanochannel [3]. The distribution of ionic currents for each of the 20 proteinogenic amino acids encoded by eukaryotic genes is found to be statistically

distinct. I will then discuss phenomena that are analogous to those encountered in nanoscopic/mesoscopic physics, such as ionic Coulomb blockade [4], and ionic “quantized conductance” [5]. The first has been recently verified experimentally using MoS₂ 2-dimensional membranes [6], while the second leads to a universal mechanism for ion selectivity in graphene and other atomically thin pores [7].

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TBA

Patrick Doyle

MIT,
Cambridge, MA, USA.

Controlled Translocation of a DNA-Protein Complexes through a Glass Nanocapillary

Aleksandra Radenovic

Laboratory of Nanoscale Biology, Institute of Bioengineering,
School of Engineering Ecole Polytechnique Federale de Lausanne

Combination of glass nanocapillaries with optical tweezers allowed us to detect DNA-protein complexes in physiological conditions. In this system, a protein bound to DNA is characterized by a simultaneous change of the force and ionic current signals from the level observed for the bare DNA. Controlled displacement of the protein away from the nanocapillary opening revealed decay in the values of the force and ionic current. We suggest that such behavior is due to the dominant impact of the drag force. We have developed stochastic model that takes into account the specific geometry of a nanocapillary. In addition we have used this technique to localize different ligands along a DNA molecule and estimate their size based on the current signatures as well as their charge knowing the impact of the drag force.

Many-Body Effects and Breakdown of Reptation Theory in Entangled Semiflexible Polymer Solutions

Erwin Frey

Arnold Sommerfeld Center for Theoretical Physics, Universitat Munchen

Reptation theory has been highly successful in explaining the unusual material properties of entangled polymer solutions. It reduces the complex many-body dynamics to a single-polymer description where each polymer is envisaged to be confined to a tube through which it moves in a snake-like fashion. For flexible polymers, reptation theory has been amply confirmed by both experiments and simulations. In contrast, for semiflexible polymers experimental and numerical tests are either limited to the onset of reptation, or were performed for tracer polymers in a fixed, static matrix. I will discuss Brownian dynamics simulations and a complementary scaling approach for the dynamics of entangled solutions of semiflexible polymers, which show that reptation theory breaks down and that tube reorganisation becomes the stress relaxation mechanism instead. These simulations demonstrate that internal bending modes equilibrate before polymers disengage from the tube, such that terminal relaxation is due to many-body effects rather than curvilinear motion along a tube.

Hairy Nanopores

Yitzhak Rabin

Department of Physics,
Bar-Ilan University, Israel.

We study the morphology of polymer-coated nanopores as a function of their geometry, chain length, grafting density and solubility. We then consider the transport of small ions through polyelectrolyte-modified nanopores. Finally, we discuss electrostatic effects on the transport of charged nanoparticles through the nuclear pore complex.

Polymer rings in the melt and their minimal surfaces

Alexander Grosberg

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Statistical physics of nanochannel-based DNA barcodes with applications on plasmid characterization

Tobias Ambjörnsson

Department of Theoretical Physics,
Lund University, Sweden.

Strongly Non-equilibrium Dynamics of Nanochannel Confined DNA

Walter Reisner

Department of Physics,
Mc Gill University, Montreal, Canada

Nanoconfined DNA exhibits a wide-range of fascinating transient and steady-state non-equilibrium phenomena. Yet, while experiment, simulation and scaling analytics are converging on a comprehensive picture regarding the equilibrium behavior of nanochannel confined DNA, non-equilibrium behavior remains largely unexplored. In particular, while the DNA extension along the nanochannel is the key observable in equilibrium experiments, in the non-equilibrium case it is necessary to measure and model not just the extension but the molecule's full time-dependent one-dimensional concentration profile. Here, we apply controlled compressive forces to a nanochannel confined molecule via a nanodozer assay, whereby an optically trapped bead is slid down the channel at a constant speed. Upon contact with the molecule, a propagating concentration "shockwave" develops near the bead and the molecule is dynamically compressed. This experiment, a single-molecule implementation of a macroscopic cylinder-piston apparatus, can be used to observe the molecule response over a range of forcings and benchmark theoretical description of non-equilibrium behavior. We show that the dynamic concentration profiles, including both transient and steady-state response, can be modelled via a partial differential evolution equation combining nonlinear diffusion and convection. Lastly, we present preliminary results for dynamic compression of multiple confined molecules to explore regimes of segregation and mixing for multiple chains in confinement.

Polymer-mediated forces between scale-free objects

Mehran Kardar

MIT,
Cambridge, USA.

The free energy of a long polymer is modified if confined by barriers; resulting in a fluctuation-induced force between the confining objects. When the obstacles are scale invariant shapes (such as cones, wedges, lines or planes) the only relevant length scales are the polymer size R and characteristic separations, severely constraining the functional form of entropic forces. Specifically, we consider a polymer (single strand or star) attached to the tip of a cone, at a separation h from a surface (or another cone). At close proximity to a repulsive surface, such that $h \ll R$, separation is the only remaining relevant scale and the entropic force must take the form $F = AkT/h$. The amplitude A is universal, and can be related to exponents governing the anomalous scaling of polymer correlations in the presence of obstacles. We use analytical, numerical and epsilon-expansion techniques to compute the exponent for a polymer attached to the tip of the cone (with or without an additional plate or cone) for ideal and self-avoiding polymers. The entropic force is of the order of 0.1pN at $0.1\mu\text{m}$ for a single polymer, and can be increased for a star polymer. When absorbed to an attractive surface, there is an attractive force independent of separation, related to the (non-universal) free energy gain per unit length upon absorption. We argue that at the polymer absorption/desorption transition, the force is again universal, similar to the repulsive surface, $F = A'kT/h$, but with a new universal amplitude.

Work in collaboration with: Mohammad F. Maghrebi and Yacov Kantor

Ideal polymers near scale-free surfaces: Statics and dynamics

Yacov Kantor

Many equilibrium and dynamical properties of a single long polymer (in a dilute solution) are universal. E.g., the radius of gyration R of such polymer increases with the number of monomers N as $R \sim N^\nu$, while the relaxation time (in the absence of hydrodynamic interactions, i.e. in the free-draining regime) is proportional $N^{1+2\nu}$, where the *critical exponent* ν is independent of many microscopic details. Many of such simple features survive (with minor modifications) in the presence of scale-free (SF) surfaces. In particular, the entropic forces between SF surface and a polymer [1] have a simple dependence on the distance between them, which is completely characterized by the critical exponents. Ideal polymers for which the repulsion between monomers is disregarded, present a set of problems which sometimes can be solved analytically, thus providing clues for more realistic models. We can calculate exactly [2] the pressure exerted by an ideal polymer held by its end at some point A on a SF surface, and relate both the monomer density and the pressure to the potential of an electrostatic problem where a charge is held at the point A near a

conducting SF surface. In particular, we see that the pressure diverges near sharp points. (The last feature also appears in polymers in good solvents.) When an ideal polymer is moved towards or away from a surface at a finite rate, the forces cannot be extracted from equilibrium considerations. However, if the rates are not too large, we can use Jarzynski equality [3] to reconstruct the free energy difference ΔF between configurations far away from or close to SF surface from the *non-equilibrium measurements* of the distribution $P(W)$ of the work W performed while moving the polymer. We argue, that there is an N -dependent critical velocity v_c , such that for $v < v_c$ such reconstruction can be easily performed. We first analyze an exactly solvable model of dragging an ideal polymer in free space and show that $v_c \sim N^{1/2}$ for Newtonian dynamics, and $v_c \sim N^{3/2}$ for over-damped Langevin dynamics, and demonstrate (numerically) that the same v_c is valid when a polymer is dragged away from a surface. While the distribution $P(W)$ depends on N , for fixed (small) values of v/v_c some of its features are almost independent of N . For polymers in good solvents, in free-draining regime, $v_c \sim N^{(1+\nu)}$, with the exponent ν corresponding to polymers with excluded volume interactions.

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Work in collaboration with: Raz Halifa-Levi, Yosi Hammer and Mehran Kardar

Linear and ring DNA in nanochannels under stripe and slab confinement

Peter Cifra

Polymer Institute, Slovak Academy of Sciences,
Bratislava, Slovakia

We investigate suggested advantageous analysis in the linearization experiments with DNA macromolecules confined in a stripe-like channel using Monte Carlo simulations. The enhanced chain extension in a stripe that is due to significant excluded volume interactions between monomers in two dimensions weakens on transition to experimentally feasible slit-like channel. Based on the chain extension-confinement strength dependence and on the structure factor behavior for the chain in stripe we infer the excluded volume regime typical for two-dimensional systems. On transition to the slab geometry, the advantageous chain extension decreases and the Gaussian regime is observed for not very long semi-flexible chains. The evidence for pseudo-ideality in confined chains is based on indicators such as the chain extension curves, variation of the extension with the persistence length or the structure factor. The slab behavior is observed when the stripe (originally of monomer thickness) reaches the thickness larger than cca 10nm in the third dimension. This maximum height of

the slab to retain the advantage of the stripe is very low and this have implication for DNA linearization experiments. The presented analysis, however, has a broader relevance for confined polymers. Comparison of ring and linear macromolecule showed a stronger relative chain extension of ring relative to the linear chain what is in accord with enhanced self-avoidance in channel-confined ring. As for the linear chains we present details on transition between the stripe and slab geometry also for rings. Work in collaboration with: Zuzana Benková, Pavol Námer

Knots and knotted polymers under tension

Michele Caraglio

Department of Physics
University of Padova, Italy.

The behavior of tensioned knotted chains has been already investigated in different contexts. For instance, Farago et al. [1], by comparing the force-extension relations of unknotted and knotted chains, related the strong finite size correction observed in the knotted case to the typical size of knots and concluded that the latter are weakly localized in open chains. A further avenue is the stochastic motion of knots along elongated or confined chains [2-4] with implications for the knots' lifetimes [5-7].

Yet, how knotted chains respond to weak mechanical stretching, how this behavior differs from the unknotted case and how knots diffuse along the chain in these conditions are still open questions. Here we try to address them by applying a suitable theoretical and computational framework to flexible and semiflexible self-avoiding chains with different topology and subject to a wide range of forces and relying on direct measures of knot size.

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The remarkable elastic properties of single stranded DNA

Felix Ritort

Departament de Física Fonamental,
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Coarse-graining of flexible and stiff ring polymers

Christos N. Likos

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Ring polymers and the properties of both isolated molecules and concentrated solutions of the same have attracted a great deal of interest, since the interplay of polymer behavior and topological constraints gives rise to novel and intriguing structural and dynamical behavior [1- 3]. In this talk, I will be first reviewing recent results pertaining to coarse-graining approaches of isolated ring polymers, which highlight the role of topological constraints and of knottedness on the effective potential between rings [4] and bring forward the key differences they have in comparison to their linear counterparts [5]. Unlike linear chains, the effective potential picture breaks down in a dramatic, qualitative fashion at high concentrations, an effect due to ring shrinking. This property calls for a multiblob coarse-graining approach, which successfully addresses the issue and reproduces the correlations in concentrated solutions [6]. To reduce the shrinking, bending rigidity has been added to the rings [7], a property that brings forward a novel glassy state in which collective dynamics is arrested but self-dynamics is not [8]. Finally, I will be discussing findings of ongoing work on coarse-graining approaches of rigid rings modeled as "soft discs", and the associated cluster- and layer-formation in the bulk and under confinement [9].

* In collaboration with Ronald Blaak, Barbara Capone, Angel Moreno, Arturo Narros, and Peter Poier.

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The effect of twist-bend coupling on the torsional properties of double-stranded DNA

Enrico Carlon

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Single-molecule magnetic tweezers experiments performed in the past few years report a clear deviation of the effective torsional stiffness of DNA from the predictions of the twistable worm-like chain model. Here we show that this discrepancy can be resolved if a coupling term between bending and twisting is introduced. Although the existence of such an interaction was predicted more than two decades ago (Marko and Siggia, *Macromol.* 27, 981 (1994)), its effect on the static and dynamical properties of DNA has been largely unexplored. Our analysis yields a twist-bend coupling constant of $G=50\pm 10$ nm. We show that the introduction of twist-bend coupling requires a re-tuning of the other elastic parameters of DNA, in particular for the intrinsic bending stiffness.

TBA

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Statistical Properties of DNA in 2 dimensions and in channels

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Linear and circular DNA is deposited on very flat surfaces and its contour is determined by Atomic Force Microscopy. The statistical analysis of the contour of many DNA molecules permits to determine a) the critical exponents governing the end-to-end distance and the radius of gyration, b) the shape parameters (asphericity) and c) persistence length. The effect of confinement in 2 dimensions and in narrow channels on the statistical parameters of the DNA is discussed.

Posters

Conformational behavior of end-grafted PEO chains as potential protection layer against protein adsorption

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Recently, poly(ethylene oxide) (PEO) has received a great deal of attention in scientific community. It is a synthetic polymer of amphiphilic nature and exceptionally good solubility in water as well as many organic solvents. Thanks to its biocompatibility and nontoxicity it is widely employed in biomedical and biotechnical devices. Of special relevance is a system composed of PEO chains irreversibly grafted onto a solid surface as a barrier against protein adsorption. The efficiency of such a layer depends on the conformations of grafted PEO chains which in turn are governed by the grafting density, chain length, temperature, pH, ionic strength and the presence of water. The effects of the grafting density, chain length and the presence of water on the structural properties have been studied using the all-atomistic molecular dynamics simulations. A PEO chain in the presence of other densely grafted PEO chains is reminiscent of a cylindrically confined chain. The relations derived for the structural properties of grafted chains are based on the same analysis as relations for a cylindrically confined chain. However, these relations are based on the coarse-grained approach. The molecular simulations might serve as a bridge between the theory and experiment. The presented MD results are compared with the analytical predictions and available experimental data. The conditions for mushroom-brush transition are determined in terms of the chain length, grafted densities and presence or absence of water.

Work in collaboration with: M. Natália and D. S. Cordeiro, Department of Chemistry, University of Porto, Porto, Portugal

Knotted ring polymers in nanochannels

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Coarse-grained simulations of DNA under torsional stress

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Threading Dynamics of Ring Polymers in a Gel

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Ring polymers continue to present a challenge to the theoretical community as the polymers lack of ends represents a severe topological constraint on their conformations, especially when diffusing through a gel. In particular, threadings between rings have always been conjectured to play an important role in solutions of closed chains, from the work of Klein (Klein, *Macromolecules* **118** (1986)) to more recent ones (Halverson et al, *J. Chem. Phys.* **134** (2011)), but always proved very hard to detect and quantify. We performed large-scale Molecular Dynamics simulations of unknotted, unlinked rings either in a background gel or in a concentrated solution. In the former case we formulated an algorithm to unambiguously detect inter-ring threadings by exploiting the presence of the background architecture while in the latter we studied the response of the rings with respect to a “pinning” perturbation, in which a fraction of rings was frozen in space and time in their equilibrated configurations. We discovered that a *vanishing* fraction of pinned rings is enough to drive a kinetic arrest of the whole system in the limit of long rings, thereby suggesting the spontaneous vitrification at a critical ring length (DM, M. S. Turner, *Proc. Natl. Acad. Sci. USA*, **113**(19), pp 5195-520). These findings encourage the original conjecture that threadings between rings are important in their dynamics and that a “topological glass” might emerge in systems where the components display topologically complex interactions among them.

Work in collaboration with: Matthew S. Turner, Warwick Univ.

Density effects in entangled solutions of ring polymers

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We employ extensive Molecular Dynamics computer simulations in order to provide a detailed description concerning the equilibrium and dynamical properties of ring polymers in solutions of different densities [1].

The problem was motivated by the recent observation [2] that the physical behavior of ring polymers in solution is connected to the experimentally observed territorial segregation of interphase chromosomes in eukaryotic nuclei. Since there is rapidly growing evidence that folding of the chromatin fiber inside the interphase nucleus plays a crucial role in the regulation of gene expression, it is thus important to understand and characterize the unusual physical properties of ring polymer solutions. In this work we find that, at odds with their linear counterparts, rings tend to become more and more crumpled by increasing the concentration of the corresponding solution. As a consequence of it, small colloidal particles appear to diffuse faster in rings solutions than in linear chains solutions.

1. N. Nahali and A. Rosa, J. Phys.: Condens. Matter. 28, e065101 (2016).
2. A. Rosa and R. Everaers, Plos Comput. Biol. 4, e1000153 (2008).

Work in collaboration with Angelo Rosa, SISSA.

Dynamics of Active Polymers Under Confinement

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Pore translocation of knotted chains

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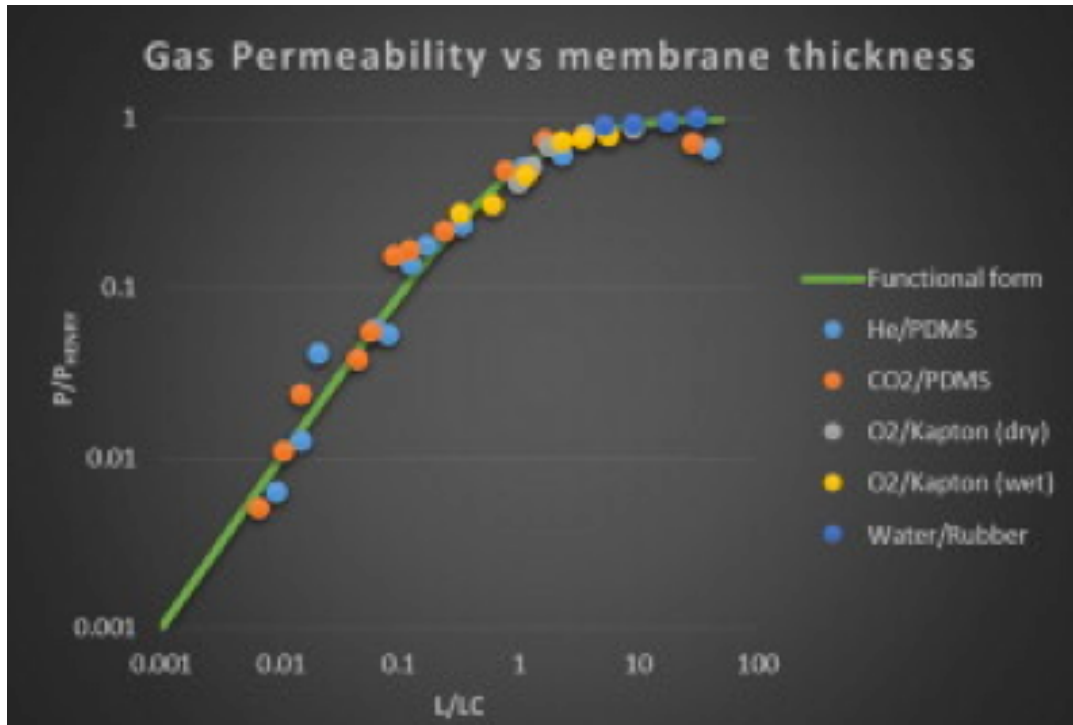


Figure 1:

Gas Permeability of polydimethylsiloxane (PDMS) membranes: thickness and surface effects

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The paper investigates the effect of membrane thickness on the gas permeability of a PDMS membrane. The data show that permeability becomes thickness dependent below some tens of micro-meters. A model, based on the non-equilibrium sorption-desorption process at the interface, fits quite well the experimental data. The model allows to determine the surface reactions rate constants for CO₂ and He on PDMS. The introduction of a specific characteristic thickness L_c provides a functional form, which describes very accurately the results of the present paper and other experiments on polymeric membranes as reported in Figure 1 below [1]. Gas permeability results also to be dependent from surface corrugation. Permeability measurements of membranes with corrugated surfaces with thickness below some tens of micro-meters will be reported and discussed.

[1] G.Firpo, E.Angeli, L.Repetto, U.Valbusa *J.Membrane Science* 481(2015) 1

Ring polymers under confinement: A comparison to their linear counterparts

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Ring polymers are an important class of biological macromolecules. Due to the lack of free ends they are expected to show distinct behaviour to their linear counterparts, as for example with respect to migration mechanisms. Furthermore, the knottedness of ring polymers is assumed to influence transport properties as well. This work aims to tackle the question of their static and dynamical properties under confinement. Since many biological ring polymers are in aqueous solution hydrodynamics are taken into account by a simulation method called Multi-Particle Collision Dynamics while the polymer itself is treated with Molecular Dynamics. Results will be shown regarding the diffusive behaviour of polymers in equilibrium, their mobility under flow in microfluidic channels and the influence of the macromolecular architecture.

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