Modelling malaria parasite motility in heterogeneous environments

Anna Battista, Friedrich Frischknecht, Ulrich S. Schwarz

Plasmodium sporozoites are the parasites responsible for malaria transmission from a mosquito to a vertebrate host. The movement of a sporozoite in the skin of the host appears to be irregular, whereas the same parasite describes a roughly circular trajectory on a flat substrate and a roughly helical trajectory in an unstructured 3D environment [1,2]. This observation, together with experiments focusing on the trajectories of parasites moving on substrates regularly patterned with micropillars [3], suggest that the movement of the parasite in the tissue is strongly determined by the nature of the surrounding environment. Nevertheless it is expected that the parasite has evolved a strategy to cope with irregularities in its environment, because malaria can develop only if it reaches a blood vessel within a few minutes after injection. We present a first theoretical model which predicts trajectories based, for the time being, mainly on geometrical considerations. In particular, we discuss different scenarios for the interaction with obstacles and how these change the circular/helical path in 2D/3D environments.

[1] S. Munter et al., Cell Host & Microbe Vol. 6, 2009
[2] R. Amino et al., Nature Medicine Vol. 12, 2006
[3] J.K. Hellmann et al., Plos Pathogens Vol. 7, 2011

Proton Transfer Reaction - Mass Spectrometry coupled to bioinformatics: physicists working in a multidisciplinary field

Luca Cappellin

Genomics, metabolomics are perhaps not so common words but nowadays they are fields of utmost importance. Physicists are providing their contributions. The possibility to couple modern mass spectrometric techniques with advanced methods of bioinformatics is a trend in this direction...

Spatial disorder in the Voter Model

Claudio Borile

When we try to study the organization and the properties of ecological systems, non-equilibrium statistical physics is a natural candidate to develop a unified framework for understanding the emergent properties of these kind of systems. Simple interacting particle systems, as the Voter Model (VM), have found a surprisingly good agreement with empirical data and proved to be a useful null-model that can be treated analytically. Despite the recent progress in this field, still a major issue in ecology and conservation ecology is to understand the effects of habitat fragmentation and heterogeneities on the biodiversity of an ecosystem. Motivated by this open problem, we study the effects of quenched spatial disorder on the long-time behavior of the VM and its nonlinear generalizations.

Optimization on networks: message-passing algorithms in a resource allocation model.

Caterina de Bacco

The rapid growth of communication and transport networks with the needs of high and efficient transmission and low energy consumptions asks for the development of theoretical and algorithmic tools able to investigate dynamical processes on networks and of networks. The aim is to develop strategies and algorithms for network control and optimization. A representative model of newtork resource allocation,where variables defined on the nodes evolve according to interaction with the variables on the neighboring nodes, will be introduced and analyzed. Techniques like the Cavity Method and its algorithmic counterpart, the message passing algorithm, will be employed to optimize the energy associated to the network using local iteration procedures. In particular a suitable cost function will be introduced in order to penalize link overlaps (i.e. traffic congestion).

Nanoparticles in non-isothermal systems

Gianmaria Falasco

Recent years have seen a rapidly growing interest in studying the dynamics of col- loids in presence of temperature inhomogeneities. On the one hand, in situations like optical particle trapping and tracking, the heating of suspended nanoparticles is an unintended but inevitable side effect. On the other hand there exist promis- ing applications, among which photothermal detection [1] and active propulsion via thermophoretic effects [2], where nanoparticles are deliberately kept at a higher temperature than the surrounding fluid. In both cases a deep understanding of the non-equilibrium phenomena which determine the dynamics is strongly required. In this talk I discuss a Markovian theory for the Brownian motion of a heated nanoparticle [3, 4], presenting which perspectives such theory offers in the description of colloids under more general non-isothermal conditions.

[1] R. Radunz, D. Rings, K. Kroy and F. Cichos, J. Phys. Chem. A 113, 1674 (2009).
[2] H. Jiang, N. Yoshinaga, M. Sano, Phys. Rev. Lett. 105, 268302 (2010).
[3] D. Rings, R. Schachoff, M. Selmke, F. Cichos and K. Kroy, Phys. Rev. Lett. 105 090604 (2010).
[4] D. Chakraborty, M. V. Gnann, D. Rings, J. Glaser, F. Otto, F. Cichos and K. Kroy Eur. Phys. Lett. 96 60009 (2011).

Scaling body size fluctuations

Andrea Giometto, Florian Altermatt, Francesco Carrara, Amos Maritan, Andrea Rinaldo

Size of an organism matters for its metabolic, growth, mortality and other vital rates. Scale-free community size spectra (i.e., size distributions regardless of species) are routinely observed in natural ecosystems and are the product of intra- and inter-species regulation of the relative abundance of organisms of different sizes. Intra- and inter-species distributions of body sizes are thus major determinants of ecosystem structure and function. We show experimentally that single-species mass distributions of unicellular eukaryotes covering different phyla exhibit both characteristic sizes and universal

features over four orders of magnitude in mass. Remarkably, we find that the mean size of a species is sufficient to fully characterize its size distribution and that the latter has a universal form across all species. We show that an analytical physiological model accounts for the observed universality, which can be synthesized in a log-normal form for the intra-species size distributions.

Growth or Reproduction? Emergence of a Strategy

Jacopo Grilli

A balance between the need to grow and procreate is rather common in ecological communities and in human societies. However its origin has not yet been elucidated. We propose a general model for a community of individuals, e.g. plants in a forest, competing for the same resources, present in a finite amount, where each competitor is characterized by a specific strategy for growth versus reproduction. The evolution drives the system toward a stationary state characterized by dynamically selected strategy, where the distribution of resource among individuals is a truncated power law which obeys finite size scaling, as observed in many different living systems.

Anomalous diffusion in confined geometries

Emanuele Locatelli

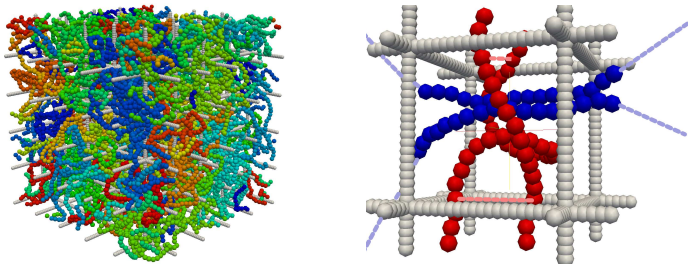
The diffusion of particles confined within a channel of radius comparable with their size (Single File Diffusion) is a paradigmatic example of anomalous diffusion with important applications in biology and nanotechnology. Due to the impossibility of mutual passage, the motion of the individual particles is correlated and Fick's law is no longer obeyed for sufficiently long times. By means of numerical simulations, we study the diffusion of the (central) particle in a single file, emphasizing the role of boundary and initial conditions on the anomalous regime. In addition to the study of the anomalous diffusion, we focused on the survival probability of the central particle, varying the position of symmetric absorbing boundaries. Although the tagged particle can be within an anomalous regime, we surprisingly find that the decay of the survival probability tail is still exponential. The exponential decay constant is equal to the mean first passage time as it happens for normal diffusive processes, even in the presence of overcrowding.

Ring polymers in gel: topology and dynamics

Davide Michieletto

Since the pioneering work of Edwards and de Gennes the dynamics of polymers in melt has been understood using the tube and the reptation models. However, ring polymers continue to present a challenge to the theoretical community as they behave differently from their linear counterpart [1]. In order to study inter-ring interactions, we simulate a concentrated solution of unknotted, unlinked rings diffusing within an ideal gel, made up of a three-dimensional cubic lattice of (static) polymer segments with lattice spacing equal to the chain's Kuhn length, see Fig. 1a. Each ring visits many unit cells, and

therefore more closely resembles a branched polymer than a crumpled globule [2]. The topology of closed loops allows inter-ring threadings, or penetrations. We exploit the ordered architecture of our gel to unambiguously identify inter-penetrating rings, see Fig. 1b, which we show to have a life-time that is at least comparable to that of the longest relaxation time of the chains and may be much longer for longer chains. We suggest that, in the limit of very long chains, a percolating cluster of threading rings may arise, which would then exhibit very slow (glassy) dynamics at the scale of centre of mass motion for each chain, while retaining substantially unhindered motion at the level of individual chain segments. Our primary result is that we found that the probability of a ring of being threaded seems to increase linearly with its length, a trend which strongly supports the existence of the above mentioned topological glass transition, although the transition itself would occur for chain contour lengths that are much larger than those reached in our simulations.



(a) (b)

Figure 1: (a) Snapshot of our system. (b) Snapshot of a two chains configuration where the blue one is threading through the red one inside of one cubic lattice cell, bounded on the edges by gel polymer. Light red and light blue dotted lines indicate the asymptotic closure construction that we employ in order to identify threading, using a standard topological measure of contour linking.

[1] M. Kapnistos, M. Lang, D. Vlassopoulos, W. Pyckhout-Hintzen, D. Richter, D. Cho, T. Chang, and M. Rubinstein, *Unexpected power-law stress relaxation of entangled ring polymers.*, Nature materials, vol. 7, pp. 997-1002, Dec. 2008.

[2] A. Grosberg and Y. Rabin, *Crumpled globule model of the three-dimensional structure of DNA*, Europhysics Letters, vol. 23, p. 373, 1993.

Simulations of flowing liquid crystals

Marco Neri Da Re

I am presenting numerical simulations, based on a hybrid Lattice Boltzmann algorithm , of a liquid crystal confined between two parallel walls. I studied Couette flow and Poiseuille flow of the LC under several boundary conditions, and calculated the director orientation and the velocity profiles.

How a spermatozoon swims

Guglielmo Saggiorato

Spermatozoon swims by a snake-like motion of its tail, the flagellum, a universal structure that can be found in spermatozoa, ciliated cells and some bacteria. The internal structure of the flagellum is formed from biopolymers and motor proteins whose function is the generation of bending moments all along its length, thus creating, for example, the snake-like motion of the sperm tail. It is still unclear how a sperm generates their tail's motion, indeed there can be no driving unit to prescribe the shape, instead, coordination must be achieved by many autonomous units distributed along its length. Our aim is to investigate how the internal mechanics affects the reaction of the flagellum to external flow fields, and how this affects the swimming and the collective swimming behaviour.

Topological and geometrical entanglement in polymers: some knotty problems.

Luca Tubiana

It is known that the presence of knots on polymers affects their salient physical properties, like polymers' size, gel-electrophoretic mobility, resistance to mechanical stretching, etc.. While a comprehensive understanding of this phenomenon is still lacking, it is often acknowledged that topology-dependent physical properties arise because of a sophisticated interplay of polymer geometry and topology. One of the most important player in this relationship is arguably the length of the knotted portion of the polymer chain, that is, whether the knot is tight or loose on the polymer. Here I will discuss the problems of such an apparently simple measure and show that in general there is no unique answer to what is the length of a knot on a chain. I will discuss some consequences of this fact.

Protein design with simplified scoring function

Stefano Zamuner

It is commonly accepted that the structure of a protein is fundamental for its biological function, but the question of how the amino acid sequence of a protein specifies its three-dimensional structure remains to be answered. We investigate the possibility of designing a sequence that will eventually fold in a specified structure by using a simple bayesian statistical approach.