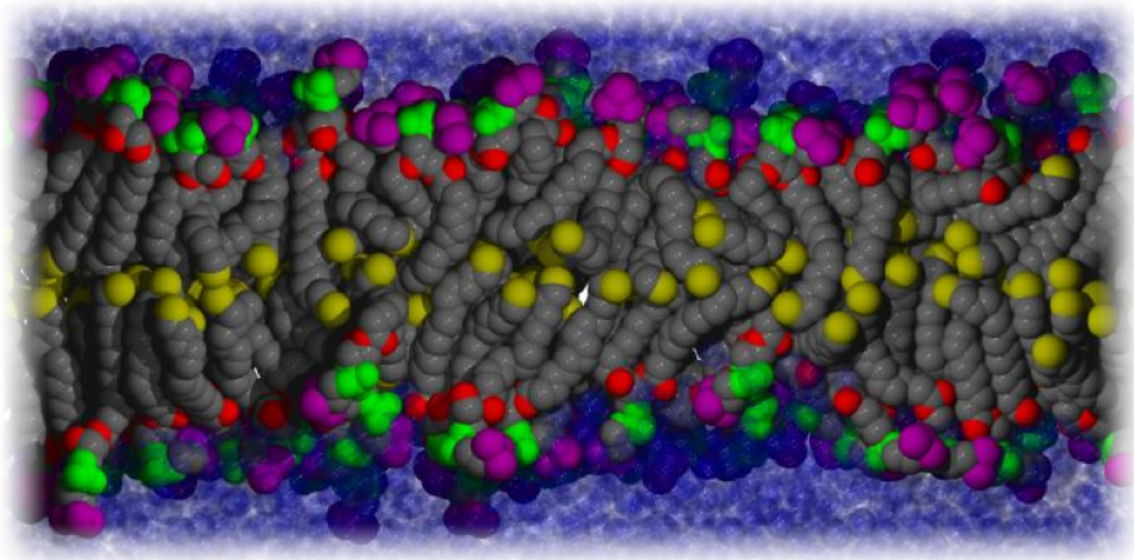


Focus Day (Monday February 21, 2011, 9:00 am to 6:45 pm)

# A Biophysics Day

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*Seminar Room, Department of Studies on Structures, Roma Tre  
Via Corrado Segre, 6 (3rd floor) 00146 Roma*

In the morning, from 9:00 am on, **Lena Rebecca Zastrow** and **Marco Ribezzi Crivellari** will defend their doctoral theses: ***A simplified 1D model for the chemo-mechanical coupling in sarcomere dynamics*** and ***A dual-trap optical tweezer setup for single-molecule manipulations: development and testing***, respectively.

In the afternoon, from 2:00 pm to 6:45 pm, a ***Mini-Workshop*** will take place (*see programme overleaf*). We are delighted to have as our guest speakers **Fabio Cecconi** from INFN-CNR Centre for Statistical Mechanics and Complexity (SMC) & Istituto dei Sistemi Complessi (ISC-CNR), Rome, **Fabrizio Cleri** from Institut d'Electronique, de Microélectronique et de Nanotechnologie, Université des Sciences et Technologies de Lille 1, Villeneuve d'Ascq, **Cristian Micheletti** from International School for Advanced Studies (SISSA-ISAS), Trieste, and **Massimo Reconditi** from Laboratorio di Fisiologia – Dipartimento di Biologia Evoluzionistica «Leo Pardi», Università di Firenze, Florence.

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# Mini-Workshop Programme

## Session 1 – 2:00 pm - 4:05 pm

*2:00 pm* A. DiCarlo: Opening

*2:05 pm* M. Reconditi: Structure-function relation in striated muscle

*3:05 pm* C. Micheletti: Coarse-grained simulations of DNA in confined geometries

## Session 2 – 4:40 pm - 6:45 pm

*4:40 pm* F. Cleri: Ion-switched biomolecular recognition as a self-assembly tool for nanotechnology

*5:40 pm* F. Cecconi: Transport of proteins across nanopores: a physicist's perspective

*6:40 pm* A. DiCarlo: Closure



## Abstracts

**Massimo Reconditi** (Laboratorio di Fisiologia – Dipartimento di Biologia Evoluzionistica «Leo Pardi», Università di Firenze)

### **Structure-function relation in striated muscle**

This presentation will focus on the progress achieved by time-resolved small angle X-ray scattering from muscle, an approach made possible by the highly ordered arrangement of both contractile proteins—myosin and actin—in the ca 2 $\mu$ m-long structural unit, the sarcomere, that repeats along the whole length of the muscle cell. The latest development of this technique allows Ångstrom-scale measurements of the axial movement of the motors that pull the actin filament towards the centre of the sarcomere, by exploiting the X-ray interference between the two arrays of myosin motors in the two halves of the sarcomere.

**Cristian Micheletti** (International School for Advanced Studies (SISSA-ISAS))

### **Coarse-grained simulations of DNA in confined geometries**

The packing of DNA inside bacteriophages arguably yields the simplest example of genome organization in living organisms. An indirect indication of how DNA is packaged is provided by the detected spectrum of knots formed by DNA that is circularized inside the P4 viral capsid. The

experimental results on the knot spectrum of the P4 DNA are compared to results of coarse-grained simulation of DNA knotting in confined volumes. We start by considering a standard coarse-grained model for DNA which is known to be capable of reproducing the salient physical aspects of free (unconstrained) DNA. Specifically, the model accounts for DNA bending stiffness and excluded-volume interactions. By subjecting the model DNA molecules to spatial confinement, it is found that confinement favours chiral knots over achiral ones, as found in the P4 experiments. However, no significant bias of torus over twist knots is found, contrary to what is found in P4 experiments. A good agreement with experiment is found, instead, upon introducing an additional interaction potential that accounts for the tendency of contacting DNA portions to order as in cholesteric liquid crystals. Accounting for this local potential allows us to reproduce the main experimental data on DNA organization in phages, including the cryo-EM observations and detailed features of the spectrum of DNA knots formed inside viral capsids. The DNA knots we observe are strongly delocalized and, intriguingly, this is shown not to interfere with genome ejection out of the phage.

**Fabrizio Cleri** (Institut d'Electronique, de Microélectronique et de Nanotechnologie (IEMN), Université des Sciences et Technologies de Lille 1)

### **Ion-switched biomolecular recognition as a self-assembly tool for nanotechnology**

The intrinsic recognition properties of biomolecules are at the focus of many innovative nanotechnologies. Such molecules as ligand–receptor pairs, complementary DNA or RNA strands, or glycoconjugate species display the two basic features of selectivity and adhesivity, which are the necessary prerequisites to drive the automatic self-assembly of building blocks. On the other hand, ionicity or pH changes represent one of the best switching mechanisms. In fact, ions can be added or removed from a solution with relative ease; their diffusion constants are usually quite large, allowing for relatively fast switching rates; moreover, in many cases the concentration threshold driving the switching is very sharp. In recent times, our team has focussed on phenomena of two types, both of which represent ideal examples of ion-switched biomolecular recognition and self-assembly: (1) carbohydrate–carbohydrate interactions, and (2) non-Watson-Crick base pairing. These phenomena share several very interesting features. Firstly, both kinds of processes are switched by ionicity changes ( $\text{Ca}^{2+}$  concentration for the first, pH or base-protonation for the second), are highly selective, rely on structurally simple motifs, and provide quite stable, yet

reversible bonding. Secondly, all of them have a great relevance in cell biology, but their biological function is still poorly understood, and a satisfactory explanation of the underlying microscopic mechanisms is still lacking. Finally, both processes are of the greatest interest in nanotechnology: hydrophilic carbohydrate interactions can be exploited to produce selective, powerful surface adhesives for specific self-assembly of nanoscale objects; non-W-C base pairs lead to stable, extended nanowire structures, known as i-motifs. The lecture will present results of ab-initio and empirical molecular dynamics carried out on such systems, emphasizing in particular the connections between bio-inspired systems and potential nanotechnology applications.

**Fabio Cecconi** (INFN-CNR Centre for Statistical Mechanics and Complexity (SMC) & Istituto dei Sistemi Complessi (ISC-CNR))

### **Transport of proteins across nanopores: a physicist's perspective**

Voltage driven translocation experiments constitute the ideal technique to investigate the physical principles of the transport of biopolymers across biological or solid-state nano-channels. We propose a computational model for these experiments to simulate the importation process into a cylindrical nanopore of a protein driven by a constant force field  $F$ . Our purpose is to characterize how the structural properties of the protein, described by a coarse-grained native-centric model, affect its translocation dynamics. Molecular dynamics results are then analyzed through a suitable drift-diffusion Smoluchowski equation. In this integrated statistical-physics approach, the kinetic characterization of protein translocation is achieved by monitoring the statistics of channel blockade events, the mobility and the translocation probability as a function of the pulling force acting in the pore. We find that the transport exhibits a critical threshold  $F_c$  depending on a free-energy barrier which the macromolecule has to overcome to cross the channel. This barrier results from the competition between the unfolding energy and the entropy associated with the confinement effects of the pore. We compute the free-energy profile in the protein centre of mass via umbrella sampling simulations. This information is then used to develop a one-dimensional phenomenological model in the reaction coordinate which explains and reproduces the behaviour of the observables during the translocation process.

