

# Workshop on Nanomechanics of Biomolecules

August 20-25 2006  
Center Stephano Franscini

## List of Posters

**Arnaud Amzallag**  
EPFL – FSB – IMB – LCVMM  
Lausanne, Switzerland

### **"3-D reconstruction and comparison of shapes of DNA minicircles observed by cryo-electron microscopy"**

We use cryo-electron microscopy to compare shapes of 158 bp long DNA minicircles that only differ in the sequence of 18 bp block containing either TATA box or CAP site. We present a sorting algorithm that autocorrelates the reconstructed 3-D shapes of analyzed DNA minicircles and groups them into distinct categories. We observe that the presence of TATA box sequence, that is believed to be easily bendable, does not significantly affect the shape of the analyzed minicircles.

**Marc Baaden**  
Laboratoire de Biochimie Théorique, CNRS UPR9080  
Institut de Biologie Physico-Chimique  
Paris, France

### **"Probing mechanical properties of molecular motors and fusion proteins"**

Exocytosis involves the transport of molecules stored within lipid vesicles from the inside of a cell to its environment. Several steps are required, one of which is transport along microtubules powered by kinesin molecular motors and subsequently fusion of the vesicles with the cell membrane mediated via SNARE (soluble N-ethylmaleimide sensitive factor attachment protein receptor) fusion proteins. The function of these proteins likely requires specific mechanical properties adapted to their task, which we aim to characterize. We present first exploratory results on the kinesin motors and on the four-helical SNARE complex using a theoretical approach and atomistic or bead-scale models.

**Nils Becker**  
Max Planck Institute for the Physics  
of Complex Systems  
Dresden, Germany

### **"Comparing Dinucleotide Elastic Potentials for DNA"**

**Andrey Cherstvy**  
Max Planck Institute for the Physics  
of Complex Systems  
Dresden, Germany

**"DNA-DNA and DNA-protein electrostatic interactions"**

**Davide Demurtas**  
UNIL LAU  
Lausanne, Switzerland

**"Characterization of 94 bp long DNA minicircles by cryo-Electron Microscopy"**

**Mohammadreza Ejtehad**  
Institute for research in Theoretical Physics and Mathematics (IPM)  
Tehran, Iran

**"Anisotropic Elastic Model of DNA Loops"**  
**and**  
**"Viral stability against the pressure fluctuations"**

**Hernan Garcia**  
California Institute of Technology  
Pasadena, USA

**"Transcriptional Regulation and Action at a Distance: Using cells as test tubes to probe DNA in vivo"**

DNA mechanics plays a central role in gene expression. Transcriptional control is realized through the interaction of the transcriptional machinery with DNA-bound transcription factors which can loop the DNA between two distant sites. DNA mechanics influences the gene expression readout of a wide variety of transcriptional networks.

We develop a statistical mechanical model to quantify the in vivo energy cost of different DNA conformations in bacteria, which allows us to extract mechanical properties of DNA and to compare completely different regulatory systems such as the lac operon and the arabinose operon. Based on this quantitative understanding of DNA looping in the lac operon we propose to use an artificial lac system as a tool to probe DNA mechanics in vivo. In particular, we use this system to determine if sequence dependent flexibility of nucleosomal positioning sequence is a measurable effect in bacteria in the complete absence of nucleosomes. This work demonstrates that a careful interplay between quantitative data and quantitative models leads to a consistent picture of transcriptional regulation which yields falsifiable predictions.

**Illya Horenko**  
Free University of Berlin  
Scientific Computing  
Berlin, Germany

**"Data-based dimension- and model- reduction: inverse modelling in molecular dynamics"**

**Prof. John E. Johnson**  
Department of Molecular Biology  
The Scripps Research Institute  
La Jolly,  
USA

**"A quorum of covalent crosslinks in HK<sub>97</sub> bacteriophage capsids spring-loads a conformational switch"**

**Filip Lankas**  
EPFL – FSB – IMB – LCVMM  
Lausanne, Switzerland

**"Atomistic molecular dynamics simulations of DNA minicircles"**

**Boris Marcone, Francesco Zonta**  
Padova University  
Department of Physics "Galileo Galilei"  
Padova, Italy

**"Knots in proteins"**

**Chantal Prevost**  
Laboratoire de Biochimie Théorique, CNRS UPR9080  
Institut de Biologie Physico-Chimique  
Paris, France

**"DNA deformations in homologous recombination"**

**Prashant K. Purohit**  
Dept. of Mechanical Engineering and Applied Mechanics  
University of Pennsylvania,  
Philadelphia, USA

**"Elasticity of DNA loops"**

**Eugene Starostin**  
Department of Civil and Environmental Engineering  
University College London  
London, UK

**"DNA Condensation: From Toroids To Hollow Spheroids"**

**Antonio Trovato**  
INFM - UDR PADOVA  
Padova, Italy

**"Computation of accessible surface area for self-avoiding tubes"**

**Prof. Ir. Gijs J.L. Wuite**  
Vrije Universiteit  
Division of Physics & Astronomy / FEW  
Amsterdam, The Netherlands

**"Unraveling the H-NS-mediated organization of bacterial chromatin using a dual DNA manipulation assay"**