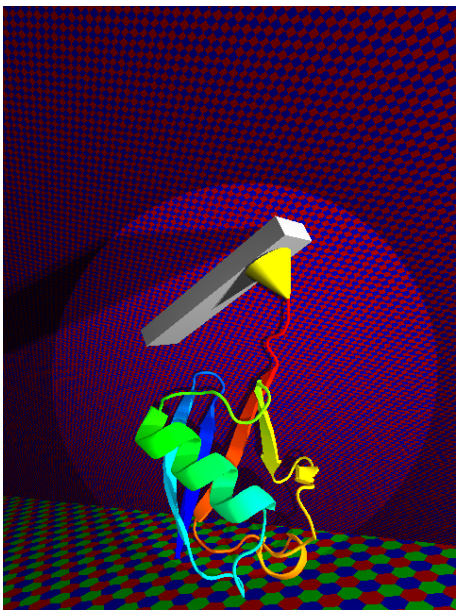

Final Report

Unraveling the structure of biomolecules: from nonequilibrium statistical mechanics to mechanical manipulation

Firenze, February 16-18, 2009

Institute for Complex Systems – Firenze

Organizing Committee:

Alberto Imparato (Aarhus)
Alessandro Torcini (Firenze)

Supported by:

European Science Foundation – SimBioMa program
Consiglio Nazionale delle Ricerche
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Contents

Summary

Leading scientists in the field of experimental manipulation of biopolimers, of computer simulations and of theory of out-of-equilibrium systems have been asked to prepare 40 minutes talks that were at same time as general as possible, and that could give the auditors an insight of the most updated research results. We had a morning and an afternoon session on February 16th and 17th, and an extended single session on the 18th. The overall number of given talks was 23.

In each of the three days of the meeting we had poster sessions, where master and PhD students, and junior post-doc had the possibility to show their work and discuss with senior reserachers experte in the field. During such sessions, given the fact that we arranged for three meeting rooms, many interesting discussions took places. In total, 66 people (including the organizers and the chairmen) participated to the workshop, 23 speakers, 20 active participants (i.e. presenting a poster) and 21 guests. We believe that the presence of so many students demonstrate a rising interest in the manipulation of biomolecules. The workshop was also an occasion for some students to get job proposals and/or to enter in contact with leading scientists in the field for continuing their academic career.

A complete description of the workshop with shedules, abstracts of the talks and of the posters as well as copy of the major part of the delivered talks in ppt or pdf format can be found in the official website of the workshop:

http://biostruct09.fi.isc.cnr.it/

Description of the scientific content

The working fields of the speakers can be roughly grouped into three main areas. The first group of scientists work on fluctuation relations. The second group work on computer simulations of biomolecules. The third group work on manipulation experiments on protein and nucleic acids.

From a theoretical point of view, the conference helped to understand the current development of theories characterizing the behaviour of small out-of-equilibrium systems. Indeed, manipulated biomolecules, represent a typical example of systems driven out of equilibrium, where the classical tools of equilibrium statistical mechanics fail to describe the thermodynamical properties of microscopic systems.

As far as computer simulations are concerned, the speakers working in this field have clearly suggested a number of possible experiments, which are so far not accessible in laboratories, due to technical constrains . In particular there has been an interesting discussion on what is the meaning of the free energy landscape as obtained from fluctuation relations and manipulation experiments.

Speakers working in the field of experimental manipulations, have shown the most updated results in this field. Many speakers gave talks on manipulations of proteins, but a number of them discussed the manipulation of RNA molecules. Their seminars and the following discussions clearly indicated which are the typical quantities that can be observed in such experiments, namely the unfolding and folding energy barriers, the unfolding lengths, the free energy landscapes, and the typical unfolding pathways. The speakers also discussed how such quantities depend on the manipulation conditions, i.e., force intensity and force direction, and how this dependence is relevant in living cells, to regulate cellular processes.

Results and impact on the future direction of the field

The workshop definitely helped in exchanging ideas and methods across people coming from different communities. The success of the workshop was evident from the very first day, during which many (young) participants expressed their appreciation for the workshop. In particular many experimental scientists expressed a deep interest for the results recently introduced in out-of-equilibrium statistical mechanics, that allow one to obtain the free energy landscape of a biopolymer through mechanical unfolding experiments. On the other hand, recent results of manipulation experiments have been shown, and it has appeared clear that the techniques to apply controlled forces to molecules are now well established, and for the future the frontier of this research appear to be the manipulation of biomolecules "in vivo". The speakers working on computer simulations of biomolecules have bridged the gap between the two communities, and proposed possible experiments, not yet performed in laboratory because of the technical constraints.

Note on Financial Support

Apart the costs and financial supports stated in the ESF Science Meeting - Final Report and reported directly on the ESF web page online, our workshop has been supported also by Department of Physics and Astronomy - Aarhus University - Denmark.

But this further support has not been included in the on line report, since we have not managed directly such fundings.

Essentially the Department of Physics and Astronomy of Aarhus University has printed the workshop posters and delivered them to many european institutions, moreover they also have printed the badges for the workshop participants and covered the travel expenses of one of the orgenizers: Dr Alberto Imparato.

All together the Department of Physics and Astronomy - Aarhus University - Denmark – has spent 19,233 DKK (roughly 2,578 euros) to support the workshop.

In details:

Postage DKK 1,246

Print of Posters DKK 11,258

Badges and Straps DKK 541

Packing Costs DKK 250

Travel of Alberto Imparato DKK 5,938

Total Support DKK 19,233

As a final remark we should mention that the Istituto Nazionale di Fisica Nucleare (INFN) has finally decided not to give any financial support to our workshop, they have just expressed their scientific approval for the workshop allowing for the use of their Logo in the poster and web page of the workshop itself.

Program

Monday, February 16th

Duration of talks includes 5 minutes for discussion.

08:10 – 08:45	**Registration**
08:45 – 09:00	**Welcome**
09:00 – 09:40	**Non-equilibrium measurements of free energy, thermodynamic length and the orientation of time's arrow** Gavin Crooks, Berkeley
09:00 – 09:40	**Nonequilibrium fluctuations in small systems investigated by mechanically unzipping single DNA molecules** Felix Ritort, Barcelona
10:20 – 10:40	**Coffee Break**
10:40 – 11:20	**Injected and dissipated power fluctuations in out of equilibrium systems** Sergio Ciliberto, Lyon
11:20 – 12:00	**Predicting the molecular (un)folding pathways of proteins by rare event simulations** Peter Bolhuis, Amsterdam
12:10	**Lunch**
13:00 – 14:00	**Posters**

Monday, February 16th

14:00 – 14:40	**Mechanical unfolding of biopolymers with an Ising-like model** Alessandro Pelizzola, Torino
14:40 – 15:20	**Role of handles in determining the folding landscape of RNA hairpins** Dave Thirumalai, College Park
15:20 – 16:00	**Renormalized Graph Dynamics of Model Proteins** Roberto Livi, Firenze
16.00 – 16:20	**Coffee Break**
16:20 – 17:00	**Sampling rare non-equilibrium trajectories** Christoph Dellago NOOO, Wien
17:00 – 17:40	**DNA unwinding by helicases** Maria Mañosas, Paris
18:00 – 20:00	**Posters**

Tuesday, February 17th

Duration of talks includes 5 minutes for discussion.

09:00 – 09:40	**Nanomechanics of scaffoldins, the most robust proteins thus far** Mariano Carrión-Vázquez , Madrid
09:40 – 10:20	**Reconstruction of the free energy landscape of model proteins via mechanical manipulation** Stefano Luccioli, Firenze
10:20 – 10:40	**Coffee Break**
10:40 – 11:20	**Multidimensional aspects of forced unfolding of proteins** Peter Olmsted, Leeds
11:20 – 12:00	**Determination of physical properties of an elastomeric polymer by AFM stretching experiments** Massimo Vassalli, Firenze
12:10	**Lunch**
13:00 – 14:00	**Posters**
14:00 – 14:40	**Structure-based models of proteins: stretching, dynamics of knots, hydrodynamic effects, and virus capsids** Marek Cieplak, Warszawa
14:40 – 15:20	**Entropy and the arrow of time** Christian van den Broeck, Diepenbeek
15:20 – 16:00	**Mechanical unfolding pathways of proteins investigated by all-atom Monte Carlo simulations** Anders Irbäck , Lund
16:00 – 16:20	**Coffee Break**
16:20 – 17:00	**Work and heat distribution in working molecular motors** Luca Peliti NOOO, Napoli
17:00 – 17:40	**Adding a dimension to DNA melting curves** Michel Peyrard , Lyon
17:45 – 18:45	**Posters**
20.00	**Social Dinner**

Wednesday, February 18th

Duration of talks includes 5 minutes for discussion.

09:30 – 10:10	**Energy Landscapes, pathways and dynamics of biomolecules** David J. Wales, Cambridge
10:10 – 10:50	**Single molecule mechanical unfolding of T4 lysozyme: The importance of topology in the cooperative unfolding of a protein** Ciro Cecconi, Modena
10:50 – 11:30	**Coffee Break**
11:30 – 12:10	**Orac: A molecular dynamics simulation program to explore free energy surfaces in biomolecular systems at the atomistic level** Piero Procacci, Firenze
12.10 – 12:50	**Saddles of the energy landscape and folding of model proteins** Luca Angelani NOOO, Roma
12:50 – 13:30	**Conformational Mechanics of Single Protein Molecules** Matthias Rief, München
13:30 – 13:45	**Closing**
14:00	**Lunch**

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