# Report on the Workshop on Nanomechanics of Biomolecules

**Center Stefano Franscini**
**Monte Verita, Ascona, Switzerland**

**November 20 – 25, 2006**

The objective of this one-week long workshop was to bring experts from around the world together for intensive discussions addressing interdisciplinary issues arising in the modelling of the nanomechanics of biomolecules. The talks presented a survey of state of the art in a number of diverse fields. The relatively small number of talks was designed so as to allow ample time for scientific discussion and to maximize the probability of new collaborations being formed.

Overall the conference was judged to be a great success according to the comments received from the participants. In particular many participants felt that the major strength of the meeting was the truly interdisciplinary character with a small overall attendance, and within a completely residential setting. This meant that practitioners coming from the fields of mathematics, mechanics, physics, chemistry and biology had the opportunity not only to listen to talks from scientists in the other fields, but also to follow up with informal discussions, and thus to obtain a meaningful entree into the literature and approaches of the other disciplines to the common problem of multi-scale modelling of biomolecules.

Some explicit remarks written by the attendees were:

A:
"One remark is that this was an especially valuable meeting for me because it brought together people who I would otherwise not have a chance to interact with or even meet. This includes:

-- people working in different disciplines (e.g., proteins instead of nucleic acids, or in cell biology) but whose scientific problems, questions, and methods have clear parallels to my own research area and may be directly applicable to my own work (and maybe even vice versa); and

-- people having expertise in theoretical or computational areas, who help me think about my own research in new ways, for example, by distinguishing hypothesized mechanisms or processes that cannot exist from those that can, or that are unlikely to occur from those that are likely. At the same time, I believe that discoveries from my own research suggest interesting and significant problems for research in theory and computation."

B:
“There has been a recent explosion of in vitro and in vivo measurements on cells and the macromolecules that make them function. Many of these measurements are of an increasingly quantitative character, resulting in the need for correspondingly quantitative models. This conference brought together a diverse group of biologists, chemists, physicists, mathematicians and engineers, with the purpose on examining some of these experiments and the kinds of models that can be used to think about them. One particularly exciting class of problems center on the interplay between the informational and physical characteristics of DNA.”

C:
“The arrangements were perfect, the venue was extraordinary and the science was superb. It was an eye opener for me and I am eager to maintain some of the contacts that I made.”

It is of course too early to see if the 2006 meeting will have given birth to meaningful scientific collaborations. However in some sense the current conference was a follow on to the 2001 conference "Atomistic to Continuum Models for Long Molecules and Thin Films" that was also held at the Center Stefano Franscini, with several members of the organizing committee in common. It may be of interest to note that one rather specific consequence of the prior meeting was the establishment of the Ascona B-DNA Consortium or ABC. That collaboration is a consortium of Laboratories around the world who have agreed to pool computational resources in order to be able to construct a database of Molecular Dynamics simulations that will provide a compatible source of predictions of B-form DNA structural parameters as a function of all possible tetramers within the sequence. After five years that collaboration is still ongoing, and has lead to multiple publications, and regular subsequent discussion meetings.

In addition to funds received directly from the Centro Stefano Franscini (ETH) itself, the conference was sponsored by the European Science Foundation - Programme SimBioMa, the DFG – Programme Matheon, and the School of Basic Sciences and the Institute of Mathematics B from the Swiss Federal Institute of Technology Lausanne. Further, we would like to thank the SNF Swiss National Science Foundation for the financial support.

There were a total of 43 attendees from 9 countries, with 18 talks and 17 posters. Full poster and talk titles and abstracts are available at the web page:

http://lcvmwww.epfl.ch/~lcvm/conferences/MonteVerita2006/