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Biocomplexity Faculty Search committee
c/o Prof. Rob de Ruyter van Steveninck
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Dear Prof. van Steveninck,

I write to you in support of Dr. Reza Ejtehadi's application for a position at your institution.

Reza has worked in my group at the Max-Planck-Institute for Polymer Research in Mainz for three years starting in the fall of 1999. He was involved with the development of coarse-grained models of DNA. Reza has mainly collaborated with myself and a PhD student, Boris Mergel. In addition he kept in touch with his former students in Iran.

A long-term goal of the work I started with Reza is to understand the dynamic response of DNA to mechanical forces as they are exerted by binding enzymes. The first step is to create a hierarchy of DNA models on different length scales which are linked by a systematic coarse-graining procedure. In a second step, we want to use this model for a systematic study of the dynamic response of DNA to forces which are large enough to alter the local structure.

My own prior experience was in simple, continuum elastic wormlike chain models, while Reza had worked on toy models of proteins. So we (i.e. mostly Reza) had to sit down and familiarize ourselves with the atomistic details of the various structures of DNA and to select the length scale where we wanted to start modeling the molecule. Weighing all the available information, we decided to develop a method where parts of the DNA such as the bases, sugars and phosphates are treated as rigid bodies with effective interactions.

While coarse-graining reduces the number of independent degrees of freedom, the interactions become more complicated. For example, chemical bonds reduce the relative motion of rigid entities such as sugar and base to rotations around non-centrosymmetric axis, a situation far from the behaviour of two point particles connected by a harmonic spring ("Rigid-body formalism for simulating Macromolecules", Reza Ejtehadi and R. Everaers, *Computer Physics Communications* **147**,

339-341 (2002)). Based on such general concepts, Reza developed a first version of an object-oriented C++ code which performs Monte Carlo simulations of rigid bodies allowing for a fairly wide choice of generalized connectivities.

Similarly, the non-bonded interactions between groups of atoms are substancially more complicated than those between point particles. For example, the van-der-Waals and excluded volume interactions between the disc like bases cannot be represented by a simple 6-12 Lennard-Jones potential. For this purpose, parts of the liquid crystals community employ the Gay-Berne potential, which is a heuristic generalization of the Lennard-Jones potential to anisotropic particles. While we started out with the Gay-Berne potential, it soon became clear that it has quite a few unphysical features and so I decided to develop an alternative ("Interaction potentials for soft and hard ellipsoids", Ralf Everaers and Mohammad R. Ejtehadi, *Phys. Rev. E*, **67**, 041710 (2003)). Reza's help with the numerics and, in particular, his experience with the Gay-Berne potential were crucial for the success of this project.

It must have been hard for Reza to leave before he could really earn the fruit of his labor. In the end, it was Boris Mergell who wrote the final version of the simulation code, ran all simulations and performed the data analysis for our DNA paper ("A generic model of DNA conformations and elasticity at the base-pair level", Boris Mergell, Mohammad R. Ejtehadi and Ralf Everaers, *Phys. Rev. E*, **68**, 021911 (2003)). In a second step he extended the methodology to chromatin ("Influence of the nucleosomal interactions on the structure and the elasticity of chromatin fibers", Boris Mergell, Ralf Everaers and Helmut Schiessel, submitted to *Phys. Rev. E*).

To conclude, I found Reza a personally pleasant collaborator, who is truely motivated by biophysical problems. I feel a bit guilty for having suppressed his scientific creativity and for having forced him to do much of the hard, tedious ground work. I hope that he will find an academic enviroment and the time to develop his strenghts more independently than he could in Mainz.

Yours sincerely,

Ralf Everaers