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Polymer physics with focus on proteins

Overall goal

Proteins can without any exaggeration be called "building bricks of life". The proper work of all living organisms depends on a proper work of the proteins they consist of. And this proper work depends in turn not only on their chemical structure, but on their three dimensional shape.

While much effort so far has been concentrated on investigating specific proteins to understand their particular properties, it is also of interest to study more general models to discover universal behavior.

For that reason we are working on an effective Hamiltonian which can describe thermodynamic properties of polymer chains, which should be considered as a first approach to model all polypeptides. This Hamiltonian can reproduce both secondary and tertiary structures of proteins. To investigate the properties of this system we perform classical Monte Carlo simulations, using our own software.

Since the topic is new there are many things that need to be done. Thus all projects are quite flexible and can be adjusted according to your interests, skills and preferences. However, basic programming skills are required.

Projects in classical physics

Investigate the phase diagrams of one or two polymer chains: how the thermodynamic properties depend on parameters of the potential and parameters of the model itself. See if we can reproduce aggregation of proteins, one phenomena that is responsible for some serious diseases. Investigate the behavior of heteropolymers.

Projects in quantum physics

Electronic transport properties of polymers. Try to find a good model to describe electronic transport in our system. Investigate phase diagram: how the quantum

observable (for example, conductivity) depends on parameters of the potential and parameters of the model. Check how “quantum” phases correlate with classical ones.

If you are interested in programming

You also can help to develop the code and learn some good programming practices which are useful far beyond the science itself.

The program is designed in a way to satisfy all requirements of modern software research engineering. The main code is written in C++11 and MPI. We use CMake, Google Test Environment, git and Doxygen. Now we are at the beginning of implementation of OpenCL to be able to take advantages of not only CPU but GPU as well. In addition to the main code there are several utilities written in Python for visualisation.

Contact

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