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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