**Weekly Report**

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**Minor groove width prediction of nucleosomal sequences from malaria parasite**

Using Tianyin’s high throughput prediction program, minor groove width of malaria parasite nucleosomal sequences (both non-shuffled and shuffled) was predicted (Figure 1).

**Figure 1** Predicted minor groove width of Plasmodium falciparum nucleosomal sequences on average. Non-shuffled (blue) sequences tend to have narrower minor groove width at two ends compared to those of shuffled sequences, which show a more uniformly distributed minor groove width.

**Visual inspection of nucleosome structures**

All nucleosome structures currently available in PDB were downloaded and a quick visual inspection was done. The observation that interactions between H3 tails and entering or exiting DNA were found in all the structures (which seems to be unique) leads to a hypothesis in which interactions between H3 and DNA are firstly formed during nucleosome formation (Figure 2).
This hypothesis can help explain the narrower minor groove width at two ends of P. falciparum
nucleosomal sequences shown in Figure 1. To test the hypothesis, sequence composition of DNA
at protein-DNA interfaces should be analyzed. It would be interesting to see if there is any
sequence bias in those interacting regions on DNA and if there is, how the strength of sequence
bias in those regions is distributed.

Figure 2 H3 tails (green and purple) protruding out of histone core from between two DNA duplex were found
in all the downloaded structures. On the other hand, similar behavior of H2 tails (yellow and light green) were
found in many structures but not in all of them.
**MD simulation on protein-DNA complex by GROMACS**

For the first time, the GROMACS program was executed in parallel on more than 24 cores which was the upper limit on the number of cores that could be used in one simulation. The current program can potentially run on unlimited number of cores and a run with 96 cores in parallel has been tested. This is an important step forward in the setup of MD simulation environment and is also unique in our program since no one (according to Luigi) has ever run such a big parallel program on the cluster.