Field of the Master: Computer science, Computational biology, Physics
Level: M1/M2
Required skills: computer programming, numerical simulations
Duration: 3 to 6 months
Period: any periods between January and July 2016

Title of the research project: Development of a fast GPU-based numerical method for simulating chromosomes

Names of the supervisors: Daniel Jost (daniel.jost@imag.fr) & Cédric Vaillant (cédric.vaillant@ens-lyon.fr) - Lab. TIMC-IMAG, CNRS, Université Grenoble Alpes & Lab. de Physique, CNRS, ENS Lyon

Context: Efficient molecular simulations of large systems have become a powerful tool to investigate complex biological processes. In our group, we are interested in modeling the nuclear organization and dynamics of chromosomes. Based on polymer physics, we are currently developing a lattice polymer model of chromosome that we simulate using kinetic Monte-Carlo simulations. However, with the recent advances in experimental methods that can now produce high-resolution data, there is a clear need to perform simulations at the full genomic scales in all species ranging from yeast (12 Mbp) to human (3 Gbp). Improving the actual numerical tools in order to significantly reduce computation time is thus a crucial prerequisite that will allow to refine our understanding of the complexity of "spatial" regulation of the genomes.

Objectives and expected results: For that purpose we aim to develop an efficient parallelized version of our current algorithm. The student will implement an original numerical scheme for polymer modeling that allows fast parallelization. Using this algorithm we expect a 500 fold decrease of equilibration times for a yeast genome (from 3mn to 0.3 s) and a 50000 fold decrease for the human genome (from few days to few seconds), compared to our current serial implementation of the model. Full parallelization will be implemented on CPU and GPU architectures. Efficiency tests will be performed to optimize the algorithm in terms of coding and architectures. By achieving such optimizations we will make a clear breakthrough in that booming field of genome 3D organization. Finally, the student will apply the model to different biological examples.