Master Internship

GPU acceleration of Markov chain Monte Carlo (MCMC) simulations applied to the energy minimization problem in spin network systems

The Ising model is one of the most popular statistical physics models due to its simplicity and at the same time its predictive power for physical systems undergoing a second order phase transition. In its most basic version, this model consists of a spin lattice with a nearest neighbour interaction. Despite its simplicity, there are no exact solutions for this model for a number of dimensions higher than 2. The only solution in this case is via numerical simulation, which is based on minimization of the system Hamiltonian using the Markov Chain Monte Carlo (MCMC) method.

It is obvious that the computation time as well as the memory usage for this kind of models increase exponentially with the size of the system. On the other hand, it is important to be able to study systems of the largest possible size for reasons linked to precision (minimization of edge effects, representative statistics) but also because large systems are suitable for introducing less localized interactions and effects (e.g. crystal imperfections).

The internship aims at taking advantage of the recent advances in computer architectures (GPU, multi-core architectures) in order to be able to increase the size of tractable systems. Starting from an existing MCMC code, different domain decomposition strategies will be applied for the distribution of the computation on a number of GPU nodes, while respecting the transition conditions from one domain to another. The results of the developed code will be compared to the reference data from the literature with a focus on the study of ferromagnetic material behaviour as a function of temperature and the magnetic field. This topic is viewed as an intermediate step towards a more long-term project on the development of a fully-fledged computational tool for the study of magnetic materials.

Candidates with a physics, engineering or computer science background and good programming skills with the Python language are eligible for this topic. Knowledge in GPU programming and/or parallel/multithreaded computational techniques can be beneficial. A general culture on statistical physics will be also helpful but not essential.

The internship will take place at CEA Saclay in interaction with the physics department of the National and Kapodistrian University of Athens. The candidate will benefit from the access to the infrastructure of the host department including our cluster facilities, the CEA central library and transport network as well as the canteens of the Saclay centre. The duration of the internshp is 6 months.

Contact person:

Anastassios Skarlatos, Email: anastasios.skarlatos@cea.fr