Stage Master 2 in high performance tensor computations arising from molecular simulations
Part of ERC Synergy project Extreme-scale Mathematically-based Computational Chemistry

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*Funded internship*, to start in March/April, for 5/6 months. Can be pursued with a PhD, in the context of ERC Synergy EMC2 project.

*Context:*
This project takes place in the context of ERC Synergy project EMC2, which is an interdisciplinary project that carries out innovative and cutting-edge research at the interface of chemistry, computer science, and mathematics. The final goal is to make possible the discovery of in silico new molecules and materials. Molecular simulation is an active field of research with applications ranging from theoretical chemistry and drug design to material science and nanotechnology. However, molecular simulation still has strong limitations. In particular, the simulation of very large molecular systems, or smaller systems in which electrons interact strongly with each other, remains out of reach today. Overcoming these limitations is difficult and provides mathematicians with a range of challenging and exciting problems to solve.
For more details see description at:

*Description of the project:*
Our focus will be on molecular simulations that lead to solving problems of large size and featuring high dimensions. The data in this case is represented by objects called tensors, or multilinear arrays. The goal of this research is to design novel tensor techniques to allow their effective compression, i.e. their representation by simpler objects in small dimensions, while preserving the information. The algorithm should be highly parallel to allow to deal with the large number of dimensions and large data sets, while preserving the required information for obtaining the solution of the problem.

The goal of this internship is to consider a specific tensor format and exploit the usage of randomized approaches popular in big data applications. In addition, we will evaluate the impact of the algorithm on methods from quantum chemistry to make it possible to efficiently calculate the electronic structures of systems with highly correlated electrons.