Stage Master 2 Randomized tensor computations for complex simulations
Part of ERC Synergy project EMC²
https://erc-emc2.eu/

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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 physics/chemistry, computer science, and mathematics. Molecular simulation is an active field of research with applications ranging from drug design to material science and nanotechnology. However, molecular simulation still has strong limitations. In particular, the simulation of very large molecular systems remains out of reach today. Overcoming these limitations is difficult and provides mathematicians with a range of challenging and exciting problems to solve.

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 internship is to consider a specific tensor format and exploit the usage of randomization techniques that allow to represent high dimensional vectors by their low dimensional random projections while preserving some geometry. This will be studied in the context of an eigenvalue problem for which low rank compression techniques are used. In collaboration with other members of the project, the methods will be studied on molecular systems of interest.