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Paris, 17 Jul 2014

The Fast Multipole Method in the context of Computational Chemistry

Subject: The Fast Multipole Method (FMM) is a widely used and very successful tool to compute the interaction of large *N*-body systems that scales linearly in *N* invented by Greengard and Rocklin [1]. On the other hand, the electrostatic interaction between atoms is modelled by multipoles residing on each atomic site in force-fields models that are widely used in molecular dynamics and in consequence, the framework of the original FMM that serves to compute point-charge interaction is no longer valid.

Objective: The objectives are the following:

- Learning C++ and the mathematical background of the FMM in an initial phase
- Using and mastering the existing FMM-library ScalFMM
- Adapting the library for the purpose needed in computational chemistry outlined above.

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[1] Greengard, L.; Rokhlin, V. A fast algorithm for particle simulations. J. Comput. Phys. 73 (1987), no. 2, 325--348.

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