Accelerating the Kernel-Independent Fast Multipole Method

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A thesis submitted in partial fulfillment of the requirements
for the degree Master of Science

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July 4, 2020

Declaration

I, Srinath Kailasa, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

Abstract

The Fast Multipole Method (FMM) is a numerical method to accelerate the solution of the 'n-body' problem, which appears in numerous contexts in science and engineering, for example in solving for gravitational or electrostatic potentials. It does so by approximating the Green's function of the system with analytic infinite series expansions (the origin of the 'multipole' in its name), and coalescing the effect of distinct distant sources together so as to reduce the number of computations. The analytic expansions of the original Fast Multipole Method depend on the Green's function of the system in question (Helmholtz, Laplace etc.), and in practice a new implementations must be written for a given system.

The Kernel-Independent Fast Multipole Method (KIFMM), first presented by Ying et al. [Lex04], is a similar approach that replaces the analytic series expansions with a continuous distribution of so called 'equivalent density' supported at discrete points on a box enclosing a set of particles. These equivalent densities are found by matching the potential they generate to those generated by the original sources at another surface in the far field. Usefully, this approach doesn't require multipole expansions of the Green's functions of a system, and therefore can be programmed in an agnostic way, hence the origin of it's name.

This thesis presents a Python implementation of the KIFMM, with investigations made into both mathematical and computational techniques for the acceleration of the algorithm. Python is chosen as it has emerged as a standard for scientific and data intensive computing in recent years, with a huge increase in usage and a well supported ecosystem of libraries and tools available for accelerating numerical codes. The wider context of this thesis is an ongoing collaboration with the ExaFMM Project [Rio11] to produce a Pythonic implementation of the KIFMM that can compete in terms of performance with a C++ equivalent. This thesis presents a systematic performance analysis of a naive implementation of the KIFMM algorithm, before proceeding to examine and implement acceleration techniques. The speed and accuracy of the implementation is tested for some simple Green's functions, and it concludes with a discussion on future avenues for investigation.

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4.1 Section 1

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Appendix

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Bibliography

[Lex04] Denis Zorin Lexing Ying George Biros. "A kernel-independent adaptive fast multipole algorithm in two and three dimensions". In: *Journal of Computational Physics* 196.2 (2004), pp. 591–626. DOI: http://dx.doi.org/10.1016/j.jcp.2003.11.021.

[Rio11] Lorena A. Barba Rio Yokota. *ExaFMM User's Manual*. 2011. URL: http://www.bu.edu/exafmm/files/2011/06/ExaFMM-UserManual1.pdf.