Towards Exascale Multiparticle Simulations

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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 past three decades have seen the emergence of so called ‘fast algorithms’ that are able to rapidly apply and invert the operator matrices arising from boundary integral forms of elliptic PDEs. Such equations are common in acoustic and electromagnetic scattering, with applications from X to Y. - However, a ‘data-sparse’ but dense system matrix arises in other problems too, for example in dense covariance matrices for Kalman filtering, and other compuational statistics problems. - The unification of software for the forward and inverse application of these operators in a single set of open-source libraries optimised for distributed computing environments is severely lacking, and is the central concern of this thesis. Where implementations exist they are fragmented, with a focus on a specific algorithm or problem area, with portions of code parallelised and compatible with distributed computing systems, with other portions being restricted to a single-node. Developing high-performance implementations of fast algorithms is challenging due to highly-technical nature of their underlying mathematics, making it difficult to differentiate between numerical and logical errors when debugging. This is further complicated by the diversity of software and hardware environments in which research code is expected to run - from desktop workstations to the latest supercomputing clusters. - In this subsidiary thesis, we present current work on implementing scalable software for the fast forward application of these integral operators, as well as our investigations into the optimal software engineering techniques for their implementation. - We present our work in the context of ongoing work to implement a unified framework for the rapid forward and inverse application of fast algorithms to the dense system matrices that arise in boundary integral formulations for wave scattering problems. - The first part of this thesis introduces the analytic Fast multipole method, and its semi-analytic and algebraic variants and their trade-offs. - We proceed to a discussion on of an attempted Python implementation of the semi-analytic KIFMM, and its shortfalls and subsequently introduce Rust - a relatively new, but emerging language for scientific and high-performance computing. - We present progress on a Rust based implementation of the fast multipole method, and discuss numerical results and remaining challenges as we hope to scale to exascale particle simulations. - We conclude with a look to the future, and sketch a plan for a unified forward/backward solver framework.

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This is a reference [1].

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Bibliography

[1] 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`.