PyExaFMM: Designing a highly-performant particle fast multipole solver in Python with Numba

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Abstract—**PyExaFMM is a pythonic kernel-independent particle fast multipole method [FMM] implementation, built on the success of the ExaFMM project, to answer the question of whether we could develop a highly-performant scientific code without resorting to a lower level language. The FMM is a good case study for understanding the maturity of Python for developing high-performance software, due its reliance on a complex heirarchical octree data structure. In this article we explore the software engineering and mathematical techniques used to extract performance for PyExaFMM, and we report that we are able to achieve runtimes within $\mathcal{O}(10)$ of the state of the art C++ implementation, with comparable accuracy for three dimensional electrostatic problems.**

■ **THE FAST MULTIPOLE METHOD** [FMM], originally developed by Greengard and Rokhlin [1], approximates the solution of the so called N body problem, in which one seeks to calculate the pairwise interactions between N objects. This problem arises in numerous contexts in physics and engineering, for example in the calculation of the resulting electrostatic potentials due to a set of charged particles. Considering the calculation of electrostatic potential as our model problem, the potential, $\phi(x_j)$, for a given charged particle at position x_j, or 'target', due to N particles at

positions x_i, or 'sources', where $i \in [1, ..., N]$, each with a charge q_i, can be written as,

$$\phi(x_j) = \sum_{i=1}^{N} K(x_i, x_j)q_i, \qquad (1)$$

here $K(\cdot, \cdot)$ is called the Green's function, or kernel function, which for electrostatic problems in three dimensions is,

$$K(x, y) = \frac{1}{4\epsilon_0 \pi |x - y|}, \qquad (2)$$

where ϵ_0 is the permittivity of free space. This kernel function is often referred to as the Laplace kernel.

Attempting to evaluate the sum in (1) directly for N target particles at positions x_j where $j \in [1, ..., N]$ due to N sources, results in algorithm of $\mathcal{O}(N^2)$ runtime complexity, however the FMM is able to approximate (1) with just $\mathcal{O}(N)$ runtime complexity, with proscribed error bounds.

The key idea behind the FMM is to encode the potential in the far field due to a cluster of particles with a representative analytic multipole expansion, which can be truncated to tune for desired accuracy. This truncation allows one to approximate the sum in (1) with fewer calculations. However, as the coefficients of a given multipole expansion are kernel-dependent in the sense that they will depend on the form of (2), software implementations have to be rewritten for each specific physical model.

Fast multipole methods for general kernels [CITATION] have been developed, however there are fewer implementations that rely only on numerical kernel evaluations, rather than analytic series expansions, examples include [CITATION]. The latter approaches are often referred to as kernel-independent fast multipole methods [KIFMM]. ...

PyExaFMM utilizes the approach first presented by Ying et. al [2]. This KIFMM represents the multipole expansions due to a cluster of charges as set of equivalent densities supported on a surface enclosing the cluster, with the fields generated by the charges matched with the equivalent field via a least-squares fitting in the far field. As originally developed in [2], this method generalizes the FMM to non-oscillatory second-order elliptic partial differential equations with constant coefficients, however further work has extended the method to include oscillatory problems [3].

At present numerous high-quality open source implementations exist to solve the analytic FMM for various kernels [CITATION], as well as the KIFMM [2] and [DARVE]. The desire for yet another FMM implementation lies in the disconnect between the computational skills of many users of FMM solvers, such as natural scientists and engineers, and the complex softwares developed by software specialists in compiled languages such as Fortran or C++. Despite often offering Python interfaces, it is still not feasible for many domain specialists to contribute to the software development of these existing libraries without a significant investment in acquiring new skills.

Python has emerged as a de-facto standard for the majority of computational scientists for both data analysis, and application development [CITATION], and in recent years high-performance libraries that aid in bypassing the limitations of the Python interpreter have emerged to make it a serious contender for use in developing software for high-performance computing [HPC]. The final vision being the ability to rapidly prototype an algorithm in Python, drop in high-quality libraries, and build a HPC application without necessarily being a software expert. PyExaFMM therefore represents a compromise between usability and performance, with the audience of the software in mind. Many HPC libraries in Python optimize operations on linear data structures, such as arrays. However, the FMM relies on a hierarchical tree, as such it represents a non-trivial algorithm to optimize with currently available tools. In developing PyExaFMM we aimed to demonstrate the possibility of building a HPC application purely in Python, while achieve comparable performance with state of the art compiled language implementations.

In this article we begin by providing an overview of the mathematical formulation behind the KIFMM in [2], before introducing Numba and discussing how it is used by PyExaFMM to accelerate computations, as well as program efficient data structures. We continue by discussing the mathematical and software based optimiza-

tions used by PyExaFMM for performance, and provide an overview of the software design used in order to implement optimizations effectively. We conclude with a discussion comparing the performance, in terms of accuracy, runtimes, and memory footprint, with the comparable state-of-the-art C++ implementation from the ExaFMM project, ExaFMM-T [4].

THE KERNEL-INDEPENDENT FAST MULTIPOLE METHOD

Algorithm
TECHNIQUES FOR ACHIEVING PERFORMANCE

What is Numba?

What is does, how is it useful? Where do we use it, and why there. How much difference can it make in an idealized routine. What doesn't work, why doesn't it work. Where to be careful. Programming to an (invisible) framework . . .

Where is numba used heavily? Tree construction routines on Morton coordinates. Multithreading of tree construction, as well as P2M evaluation. Experiment to demonstrate the speed of kernel evaluation, with caveat that data must be pre-organised.

Precomputing Operators

Transfer vectors, hashing, HDF5, loading into memory.

Compressing the M2L step with a randomised SVD

Introduce [2]. Numerical bounds on error out of scope, but show how experiments demonstrate that the FMM error dominates the SVD error.

Software Architecture

The key is separating routines to be accelerated, and organising data ready to run. The data organisation part (and it's slowness) should be demonstrated as a bottleneck using experiment.

PERFORMANCE COMPARISON WITH STATE OF THE ART

Description of main experiments, and how they are conducted. What are the main results? Are they expected from theory? What conclusions can be drawn about developing HPC codes entirely in Python, is it worth it?
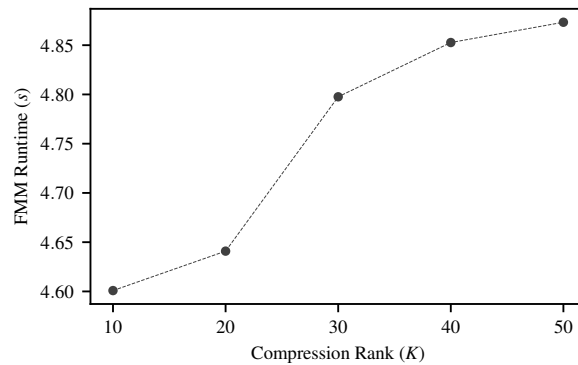
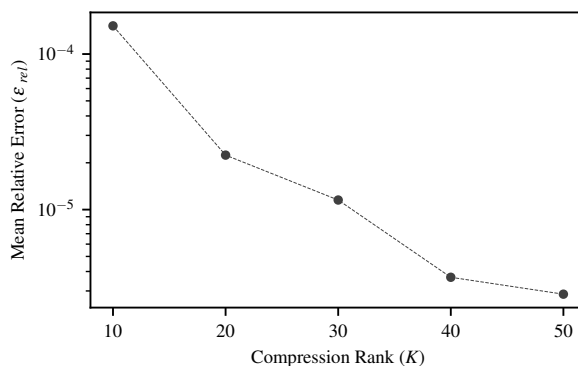

Figure 1. Compression Rank and runtime

Figure 2. Compression Rank and accuracy

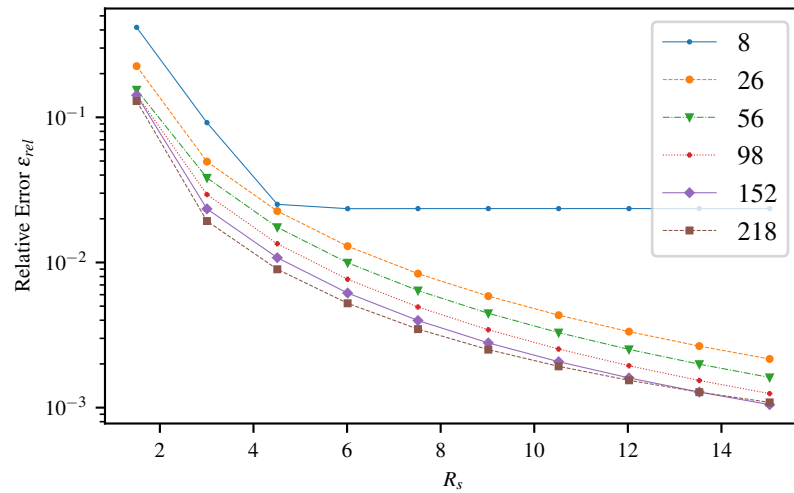**Figure 3.** Compression Rank and accuracy

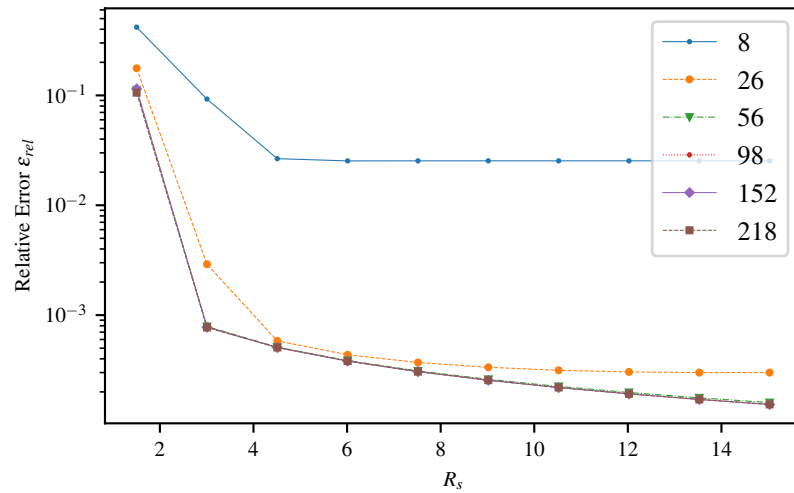**Figure 4.** ExaFMM Multipole Expansion Convergence

Figure 5. PyExaFMM Multipole Expansion Convergence

CONCLUSION

What have we learned, what will we be working on next?

ACKNOWLEDGMENT

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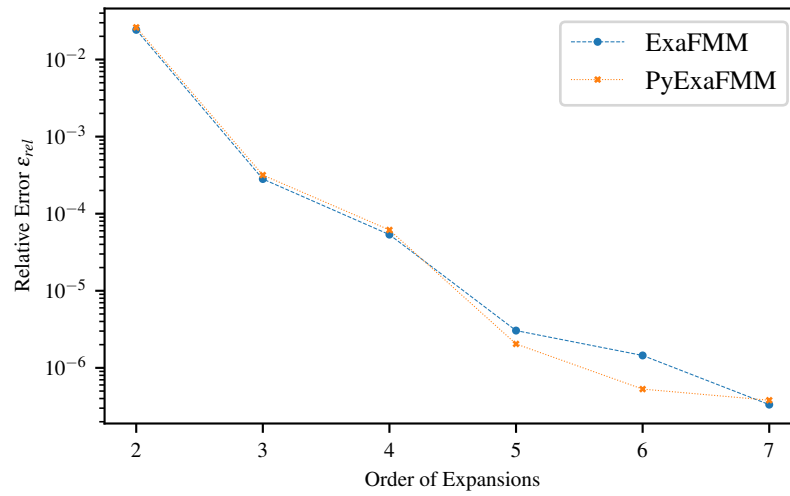
Figure 6. Potential Convergence Comparison

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