PyExaFMM: Designing a high-performance particle fast multipole solver in Python with Numba

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***Abstract*—The particle fast multipole method [FMM] is a good case study for understanding the efficacy of Python for developing high-performance software for non-trivial algorithms, due its reliance on a hierarchical tree data structure. In this paper we explore the mathematical and software design techniques used to extract performance for PyExaFMM, a Python based FMM solver accelerated with Numba, designed to be run on single-node multicore architectures. We report that we achieve runtimes within $\mathcal{O}(N)$ of the state of the art C++ implementation, with comparable accuracy and memory footprint for three dimensional problems in double precision.**

WE INTRODUCE PYEXAFMM[1]

- What's the context of PyExaFMM? - Compiled language implementations exist - Numba JIT compiler for Python can translate hot loops code to efficient machine code. - Python is well understood in SC community. - FMM is a benchmark for complex SC software built using Python alone. - This paper consists of: - Brief intro to FMM algorithm (¡1000 words) - Math methods, software design and parallelization strategies for achieving performance with Numba. (2500 words) - Benchmarks wrt comparable C++ module (1500 words)

[1] https://www.github.com/exafmm/pyexafmm

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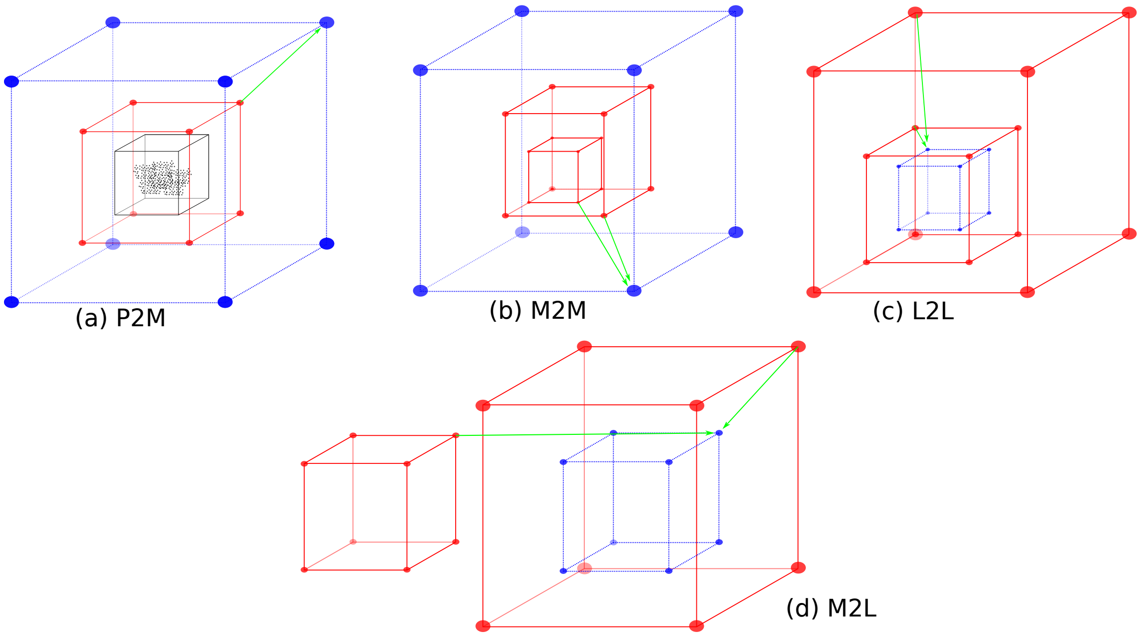

(a) P2M

(b) M2M

(c) L2L

(d) M2L

Figure 1. The operators of the KIFMM. Equivalent surfaces are shown in red, check surfaces in blue, and the charged points in black. Surfaces are plotted with 8 quadrature points, one at each vertex.

FAST MULTIPOLE METHODS

HIGH PERFORMANCE PYTHON WITH NUMBA

TECHNIQUES FOR ACHIEVING PERFORMANCE

Efficient Operators

PERFORMANCE

CONCLUSION

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REFERENCES

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