

PyExaFMM, an exercise in designing high-performance software with Python and Numba

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Abstract—Numba is a game changing compiler for high performance computing with Python. The machine code it produces runs outside of the single-threaded Python interpreter, and can therefore fully utilize the resources of modern CPUs. This means support for parallel multithreading and auto vectorization if available, just like in a compiled language such as C++ or Fortran. Here we document our attempt to use Numba to develop a fully multithreaded implementation of the Fast Multipole Method, an algorithm which relies on a non-linear data structure and contains a significant amount of data organization that would ordinarily be run through the Python interpreter. We explain how Numba influences the design and structure of software, as well as its major pitfalls. We find that Numba doesn't live up to its promise due to overhead from the unavoidable interaction between the Python interpreter and Numba compiled code, and that our software remains up to 30 times slower than ExaFMM-T, the leading C++ implementation of the same algorithm. However, the dramatic speedup in comparison to vanilla Python [INSERT BENCH HERE], means that Numba is demonstrably an excellent choice for projects in which the hackability, portability and simplicity that Python offers are a greater priorities than raw performance.

■ **PYTHON**¹, is designed for memory safety and developer productivity, not speed. Its main selling point being that it allows Computational Scientists to spend more time exploring the science, and less time being confused by strange software quirks, infuriating memory errors, and the nightmare of incompatible dependencies, all of which conspire to drain productivity when working with lower level languages.

The catch is that code is run through an interpreter and restricted to run on a single thread via a software construction called the Global Interpreter Lock [GIL]. However, libraries for high performance computational science have traditionally bypassed the issue of the GIL by using Python's C interface to call extensions built in C or other compiled languages which can be multithreaded and compiled to target special hardware features. Popular examples of this approach include Numpy and SciPy, which together have helped propel Python's popularity in computational science by providing high performance data structures for numerical data as well as interfaces for fast compiled implementations of algorithms for numerical linear algebra, and mathematical solvers for problems from differential equations to statistics and machine learning.

As the actual number-crunching itself happens outside of the interpreter, the GIL only becomes a bottleneck to performance if a program must repeatedly pass control between the interpreter and non-Python code. This is most often an issue when an optimized compiled language implementation of your desired algorithm doesn't exist in the Python Open Source, or if it requires a lot of data organization to form the input for an optimized Numpy or SciPy code, which must unavoidably take place within the interpreter. Previously, an unlucky developer would have been forced to write a compiled implementation themselves and connect it to their Python package, relegating Python's role to an interface. More problematically, not all Computational Scientists have the necessary software skills or research interest in developing and maintaining complex codebases that couple multiple languages.

This is the context in which Numba was

introduced [1]. It is a compiler that specifically targets and optimizes Python code written with Numpy's ndarray data structure. Its power comes from the ability to generate multithreaded architecture optimized compiled code while *only writing Python*. The promise of Numba is the ability to develop applications with speed that can rival C++ or Fortran, while retaining the simplicity and productivity of working in Python. We put this promise to the test by developing PyExaFMM², an implementation of the particle Kernel-Independent Fast Multipole Method [FMM] [2], in three dimensions. Efficient implementations of this algorithm are complicated by a recursively defined tree data structure and a series of operations which each require significant data organization and careful memory allocation. These features made PyExaFMM an excellent test case to see whether Numba could free us as Computational Scientists from the complexities of compiled languages.

We begin by introducing Numba, focussing on when and where its use is appropriate. After introducing the key concepts of the FMM in order to understand its data structure and the computations involved in its computation, we proceed to an overview of how we designed our software's data structures and API to optimally use Numba. We show how we optimized multithreaded functions for cache re-use, and proceed with a discussion on the main pitfalls we encountered with Numba. We conclude with two benchmarks. Firstly, we measure the impact that Numba has on vanilla Python implementations of the FMM's operators. Secondly, we demonstrate PyExaFMM's performance by comparing memory usage and runtime with ExaFMM-T [3], the leading C++ implementation of the same algorithm. We note that a strict like-for-like comparison between the two implementations isn't possible. The softwares take different approaches to the implementation of their operations and data structures. However, as the differences in the design of PyExaFMM are heavily influenced by Numba and Python, it remains useful as an illustration of what can be achieved with Python compared with a compiled language.

¹We use 'Python' to refer to CPython, the popular C language implementation of Python, which is dominant in computational science.

²<https://github.com/exafmm/pyexafmm>

NUMBA

- Scope and aim of Numba. What is it designed to do, and what isn't it designed to do. Where it can be impactful. (ndarrays, fusing loops, autovectorization and what this is via llvm)
- diagram of how Numba works, including how the api works i.e. python wrapper function, that dispatches python objects to compiled numba functions.
- Explain how Numba can target multiple types of target due its generic design.
- how numba functions interacts with python interpreter, and the explanation of boxing/unboxing and a metric for this cost vs function arguments.
- code snippet for numba in real life, and when/where it is not appropriate. Contextualization of the code snippet wrt to the diagram of how Numba works.
- overview of multithreading in scientific python and the current state of affairs and why this isn't appropriate for hpc apps in pure python, and multithreading api in numba, and make analogies with openmp where they exist. Thread oversubscription issues and their origin and how to avoid this.

THE FAST MULTIPOLE METHOD

- data structure - hierarchical, non-uniform leaves, results in 4 distinct interactions. (U, V, X, W). Explanation how this is represented linearly here in order to work with Numba. this can be illustrated with a picture. Can refer to a figure in another paper.
- Discretization needs to be illustrated, check surface and equivalent surfaces. Can refer to a figure in another paper.
- approximate potentials with equivalent expansions
- upward pass - post order traversal
- P2M - parallel. loop over leaves. check potential = $O(n_l \cdot n_{crit} \cdot n_c)$ equivalent charge = $O(n_l \cdot n_e \cdot n_c)$.
- M2M - serial. cannot parallelize over leaves, there are parallel writes to parent multipole expansion from siblings. Parallelizing over sibling leaves is hard due to linear representation of tree
- have to perform expensive neighbours searches to find siblings to perform group by. equivalent charge = $O(8^l \cdot n_e \cdot n_c)$ at a given level l .

- downward pass - pre-order traversal
- L2L. serial - interaction
- M2L
- S2L
- P2P

Pictures: - illustrate expansion orders for approximating in a single box?

- tree figure, and list of kernels that are computed at each stage, and exactly what the computations involve for kernel independent fmm. Offer complexity bounds on these calculations. Contextualize the computations required of each kernel. i.e. P2P is raw multithreading performance.
- Offer analysis of where it is suitable to parallelize.
- A short note on the decision for M2L via SVD for FMM experts.

DATA ORIENTED DESIGN

- Data oriented design. - How this is reflected in tree design - How this is reflected in kernel design - API design
- Software design diagram - Minimize the impact of running code in the interpreter.

MULTITHREADING IN NUMBA

- how kernels are multithreaded bearing in mind issues raise in Numba section, and data oriented design section. - Optimal design of multithreading approach relies on the actual constraints of the kernel in question, will need to get into specifics here of how each kernel was approached. - metric for portion of code that is run on single vs multiple threads, can actually time this at least roughly.

PITFALLS OF NUMBA

- Numba/Numpy API differences for numerical methods can be a pitfall (svd)
- it is not Python, and writing like python (OOP) will lead to failure, numba is a framework
- not everything that is supported is fast, e.g. hashing example, and how we got around this.
- it's really designed for numerical work alone, and that's where it shines.

BENCHMARKS

- contrast multithreading impact for each kernel

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- compare and contrast pyexafmm vs exafmm for a given accuracy, try and find optimum compression parameter.(?)

CONCLUSION

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