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

S. Kailasa
Department of Mathematics, University College London

T. Betcke
Department of Mathematics, University College London

T. Wang
Department of Mechanical and Aerospace Engineering, The George Washington University

L. A. Barba
Department of Mechanical and Aerospace Engineering, The George Washington University

***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: can we develop a highly-performant scientific code, without resorting to a lower level language? The FMM is a good case study to benchmark the maturity of Python in the development of non-trivial algorithms, due its reliance on a complex heirarchical octree data structure. In this paper we offer an overview the kernel-independent FMM algorithm and the techniques involved in developing performant implementations, before introducing Numba and it's role in developing PyExaFMM. We discuss the software development practices adopted to circumvent as much as possible the bottleneck to performance introduced by the Python interpreter, and offer benchmarks of the software's accuracy, speed, and memory footprint in comparison to the state of the art C++ implementation from the ExaFMM project. We report that we achieve runtimes within O(10) of the state of the art, with comparable accuracy.**

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$$A = \pi r^2. \tag{1}$$

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Avoid using lists. Instead, use full sentences and flowing paragraphs. If you absolutely must use a list, use them rarely and keep them short:

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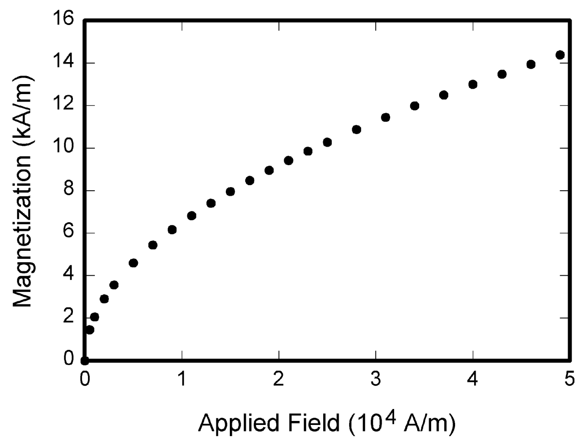

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If multiple appendices are required, they should labeled "Appendix A," "Appendix B," etc. They appear before the "Acknowledgment" or the "References" section.

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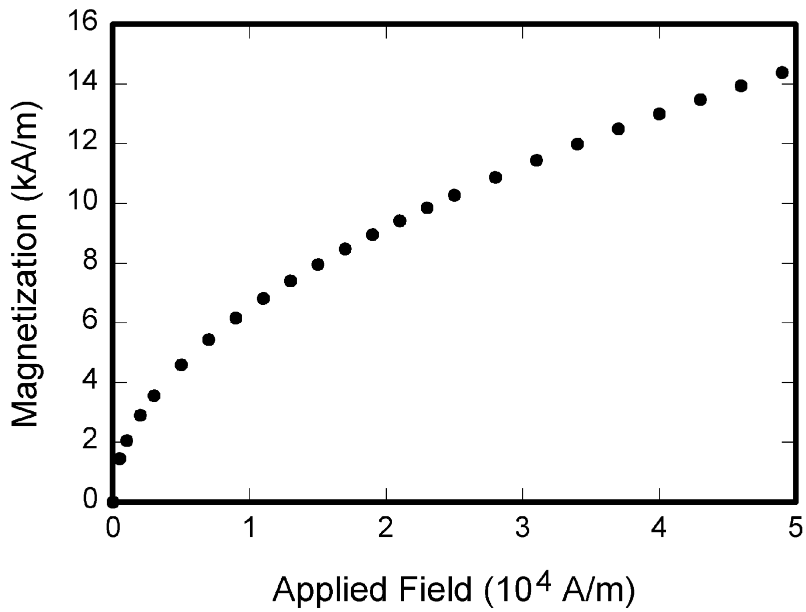
The "Acknowledgment" (no's) section appears immediately after the conclusion. If applicable, this is where you indicate funding for the work. The preferred spelling of the word "acknowledgment" in American English is without an "e" after the "g." Avoid expressions such as "One of us (S.B.A.) would like to thank . . . ." Instead, write "We thank . . .." Sponsor and financial support acknowledgments are included in the acknowledgment section. For example: This work was supported in part by the U.S. Department of Commerce under Grant BS123456 (sponsor and financial support acknowledgment goes here). Researchers that contributed information or assistance to the article should also be acknowledged in this section. Also, if corresponding authorship is noted in your paper it will be placed in the acknowledgment section. Note that the acknowledgment section is placed at the end of the paper before the reference section.



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CONCLUSION

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ACKNOWLEDGMENT

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Table 1. Units for magnetic properties.

Symbol	Quantity	Conversion from Gaussian and CGS EMU to SI[a]
Φ	Magnetic flux	1 Mx $\rightarrow 10^{-8}$ Wb $= 10^{-8}$ V $\cdot$ s
B	Magnetic flux density, magnetic induction	1 G $\rightarrow 10^{-4}$ T $= 10^{-4}$ Wb/m^2
H	Magnetic field strength	1 Oe $\rightarrow 10^{-3}/(4\pi)$ A/m
m	Magnetic moment	1 erg/G $=$ 1 emu $\rightarrow 10^{-3}$ A $\cdot$ m^2 $= 10^{-3}$ J/T
M	Magnetization	1 erg/(G $\cdot$ cm^3) $=$ 1 emu/cm^3 $\rightarrow 10^{-3}$ A/m
$4\pi M$	Magnetization	1 G $\rightarrow 10^{-3}/(4\pi)$ A/m
σ	Specific magnetization	1 erg/(G $\cdot$ g) $=$ 1 emu/g $\rightarrow$ 1 A $\cdot$ m^2/kg
j	Magnetic dipole moment	1 erg/G $=$ 1 emu $\rightarrow 4\pi \times 10^{-10}$ Wb $\cdot$ m
J	Magnetic polarization	1 erg/(G $\cdot$ cm^3) $=$ 1 emu/cm^3 $\rightarrow 4\pi \times 10^{-4}$ T
χ, κ	Susceptibility	$1 \rightarrow 4\pi$
χ_ρ	Mass susceptibility	1 cm^3/g $\rightarrow 4\pi \times 10^{-3}$ m^3/kg
μ	Permeability	$1 \rightarrow 4\pi \times 10^{-7}$ H/m $= 4\pi \times 10^{-7}$ Wb/(A $\cdot$ m)
μ_r	Relative permeability	$\mu \rightarrow \mu_r$
w, W	Energy density	1 erg/cm^3 $\rightarrow 10^{-1}$ J/m^3
N, D	Demagnetizing factor	$1 \rightarrow 1/(4\pi)$

Vertical lines are optional in tables. Statements that serve as captions for the entire table do not need footnote letters.
[a]Gaussian units are the same as cg emu for magnetostatics; Mx = maxwell, G = gauss, Oe = oersted; Wb = weber, V = volt, s = second, T = tesla, m = meter, A = ampere, J = joule, kg = kilogram, H = henry.

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Srinath Kailasa is a graduate student at University College London. He is currently pursuing a PhD in Computational Mathematics, having received an MPhys in Physics (2017) and an MSc Scientific Computing (2020) from the University of Durham, and University College London respectively. His research interests are in high-performance and scientific computing. Contact him at srinath.kailasa.18@ucl.ac.uk.

Timo Betcke is a Professor of Computational Mathematics at University College London. Contact him at t.betcke@ucl.ac.uk.

Tingyu Wang is a PhD student in Mechanical Engineering at the George Washington University. Contact him at twang66@email.gwu.edu.

Lorena. A. Barba is a Professor of Mechanical and Aerospace Engineering at the George Washington University. Contact her at labarba@email.gwu.edu.