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

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***Abstract*—We present PyExaFMM, 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, that remains competitive with the state of the art C++ implementation? The FMM is a good case study to benchmark the utility of Python's high-performance ecosystem to accelerate non-trivial algorithms, due its reliance on a complex heirarchical octree data structure. PyExaFMM is built on top of Numpy, Numba and CuPy. In this paper we offer an overview the FMM algorithm, before introducing Numba and CuPy'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.**

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

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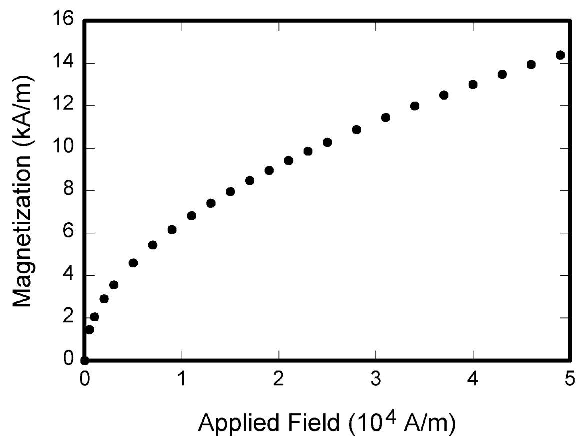

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If multiple appendices are required, they should labeled “Appendix A,” “Appendix B,” etc. They appear before the “Acknowledgment” or the “References” section.

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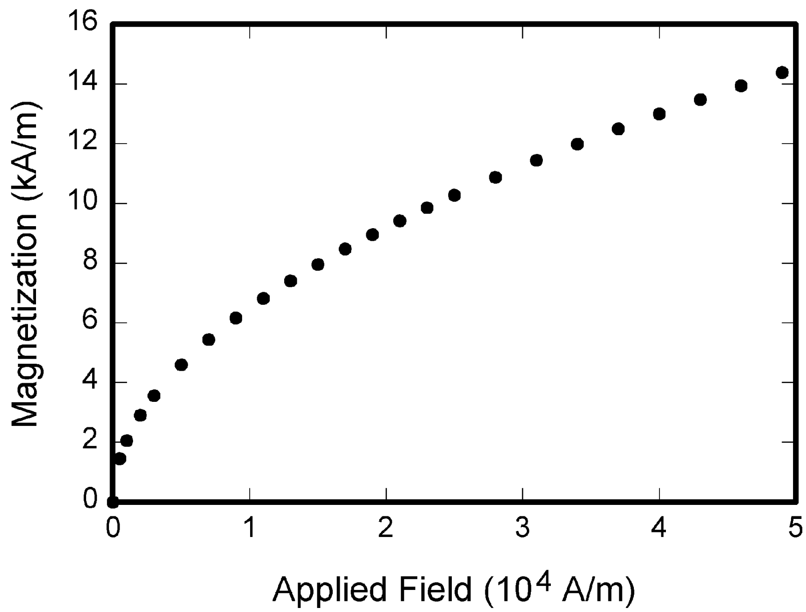

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CONCLUSION

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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 computing, specifically in the application of software engineering, parallel computing and heterogenous computing systems, to problems in computational electromagnetics. Contact him at srinath.kailasa.18@ucl.ac.uk.

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