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

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***Abstract*—We present PyExaFMM, a 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 is competitive with the state of the art C++ implementation? The FMM represents a good case study for understanding the utility of Python's high-performance ecosystem. Performant FMM implementations have to take special care to handle the complex hierarchical adaptive-octree datastructure on which it is dependent. As many of Python's numerical libraries are built to accelerate computations over simple arrays, making PyExaFMM performant is not as trivial as the availability of 'drop-in' tools may make it seem.**

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

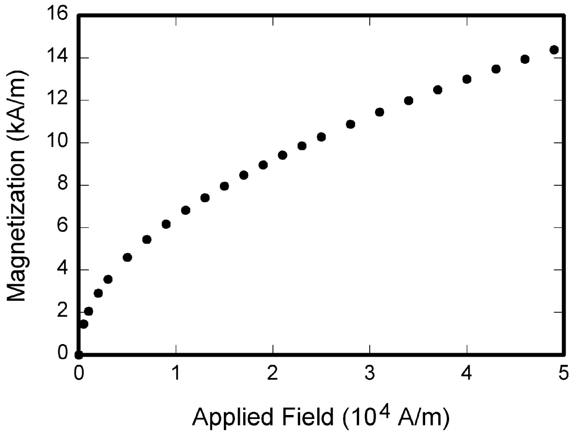

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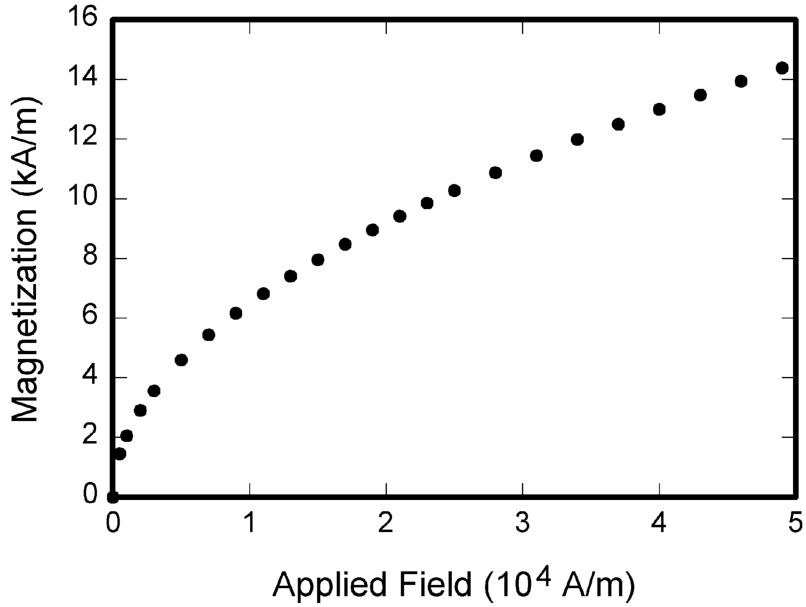
Table 1. Units for magnetic properties.

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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