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kifmm-rs: A Kernel-Independent Fast Multipole Method in Rust

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Summary

The Fast Multipole Method (FMM) is a core algorithm for scientific computing, commonly cited as one of the top algorithmic advances of the twentieth century (Cipra, 2000), as well as being included as a Berkeley 'Seven Dwarf' kernel (Asanovic et al., 2006). High performance implementations, that are easy to extend, and deploy to multiple hardware targets are uncommon due to the complexity of algorithm implementation. We present `kifmm-rs` a Rust based implementation of the kernel-independent FMM, with Python bindings, that allows for

$$\phi(x_i) = \sum_{j=1}^{N} K(x_i, y_j) q_j$$

Statement of need

`kifmm-rs` is an

- Rust package build for speed and flexibility
- API designed to be user friendly, and easy to bind
- Simple trait based design, allow for separation of concerns and interface
- Can
  - evaluate potentials, potential gradients, for a range of compatible kernels
  - heterogenous support for critical operations
  - multi-platform deployment with Rust
  - state of the art performance on a single node.
  - design flexible, can easily extend to multi-node problems in a future release.

Combination of - speed + design + extensibility to new functionality (related algorithms)

Past and ongoing research projects

- where does this software fit in?
- Older FMM efforts
- Embedded within new Bempp-rs

Single Node Performance

We benchmark our codes against other leading implementations ...

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Cipra, B. A. (2000). The best of the 20th century: Editors name top 10 algorithms. *SIAM News*, *33*(4), 1–2.