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## COMPUTATIONAL SOFTWARE

# PVFMM: A Parallel Kernel Independent FMM for Particle and Volume Potentials

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**Abstract.** We describe our implementation of a parallel fast multipole method for evaluating potentials for discrete and continuous source distributions. The first requires summation over the source points and the second requiring integration over a continuous source density. Both problems require $\mathcal{O}(N^2)$ complexity when computed directly; however, can be accelerated to $\mathcal{O}(N)$ time using FMM. In our PVFMM software library, we use kernel independent FMM and this allows us to compute potentials for a wide range of elliptic kernels. Our method is high order, adaptive and scalable. In this paper, we discuss several algorithmic improvements and performance optimizations including cache locality, vectorization, shared memory parallelism and use of coprocessors. Our distributed memory implementation uses space-filling curve for partitioning data and a hypercube communication scheme. We present convergence results for Laplace, Stokes and Helmholtz (low wavenumber) kernels for both particle and volume FMM. We measure efficiency of our method in terms of CPU cycles per unknown for different accuracies and different kernels. We also demonstrate scalability of our implementation up to several thousand processor cores on the Stampede platform at the Texas Advanced Computing Center.

**AMS subject classifications**: 31-04, 35J05, 65Y05, 65Y20

**Key words**: Fast multipole method, N-body problems, potential theory.

## Program summary

**Program title:** Parallel Volume Fast Multipole Method (PVFMM)

**Nature of problem:** solving constant coefficient elliptic PDEs and N-body problems

**Software licence:** GPL 3.0

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**CiCP scientific software URL:**

**Distribution format:** .gz

**Programming language(s):** C/C++

**Computer platform:** Any

**Operating system:** Unix-like operating systems

**Compilers:** icpc, g++

**RAM:** at least 1GB

**External routines/libraries:** MPI, OpenMP, BLAS, LAPACK, FFTW3

**Running time:**

**Restrictions:**

**Supplementary material and references:** Software homepage, `http://pvfmm.org`

**Additional Comments:**

# 1 Introduction

Many problems in physics and engineering require computing potentials for discrete or continuous source distributions. In this paper, we focus on potentials related to constant coefficient elliptic PDEs. Applications include computing gravitational interactions in astrophysics [12, 18, 24], fluid flows [7, 12, 17], electro-magnetic and acoustic scattering [3,22] and many others [6,10,11]. Particle N-body problems also arise from discretization of boundary integral representation [21, 28]. Volume potentials are required for solution of elliptic PDEs. Several applications discretize volume potential problems in to particle N-body problems with mollification of the kernel function [17]. However, these methods are low order. Our implementation uses a high order adaptive method of [15], which is designed for computing volume potentials. The method uses piecewise Chebyshev polynomials on an adaptive octree to represent the continuous source distribution and also the final potential. Our particle and volume FMM is based on the kernel independent formulation of [26] and this allows us to solve problems for a wide range of kernels corresponding to constant coefficient elliptic PDEs. In this paper, we present results for Laplace, Stokes and low-frequency Helmholtz (wavenumber $< 20$). We support free-space and periodic boundary conditions. Our method can also be used to solve variable coefficient elliptic PDEs by solving the integral formulation using iterative linear solvers. The details of that work can be found in [20].