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COMPUTATIONAL SOFTWARE

Simple FMM Libraries for Electrostatics, Slow Viscous Flow, and Frequency-Domain Wave Propagation

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Abstract. We have developed easy to use fast multipole method (FMM) libraries for the Laplace, low-frequency Helmholtz, and Stokes equations in two and three dimensions. The codes are based on a new method for applying translation operators and provide reasonable performance on either single core processors, or small multi-core systems using OpenMP.

AMS subject classifications: 52B10, 65D18, 68U05, 68U07

Key words: Fast multipole method, Laplace equation, Helmholtz equation, Stokes equation, layer potentials, projection-based point and shoot translation operators.

Program Summary

Program title: FMMLIB

Nature of problem: Fast multipole method

Software licence: GPL 2.0

CiCP scientific software URL:

Distribution format: tar.gz, .zip

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Programming language(s): Fortran, Matlab

Computer platform: Any

Operating system: Any

Compilers: GNU Fortran, Intel Fortran Compiler

RAM:

External routines/libraries: FFTPACK (included)

Running time:

Restrictions:

Supplementary material and references:

Additional Comments:

1 Introduction

The FMMLIB package provides fully adaptive implementations of the fast multipole method (FMM) for the Laplace, Helmholtz and Stokes equations. It is not highly optimized, intended rather to be accessible and modifiable with only modest effort. In particular, the translation operators used in the three-dimensional libraries are based on rotation and projection – a new, unified, and simple framework discussed briefly in Section 3.1. For optimal performance, plane wave-based translation operators should be used [3, 14]. This, however, would add significant complexity to the code, and would make the algorithm less transparent to the user and more difficult to modify. Instead, we provide a fully parallelized code which is reasonably well optimized for performance on small multi-core systems using OpenMP. Further acceleration could be obtained by precomputation and storage in matrix form of many of the modules in the library (formation of expansions from sources, evaluation of multipole and local expansions, etc.). In addition to increasing the memory costs, this would generally require a two-pass procedure and would, again, make the software itself less accessible.

The fast multipole method computes N-body interactions and evaluates layer potentials in $\mathcal{O}(N\log N)$ time for non-pathological particle distributions. Typically, $\mathcal{O}(N\log N)$ work with a small constant is needed to build the adaptive tree data structure on which the method relies and $\mathcal{O}(N)$ work with a larger constant is then required for the computation itself. In the case of the Helmholtz equation, we assume that the entire computational domain (the support of the scatterers) is a modest number of wavelengths in size. This is the "low frequency" regime from the point of view of either scattering theory or FMM implementation. The high-frequency version of the FMM is a more complex algorithm, and has not been incorporated into this software release. We do, however, provide a subroutine which is able to evaluate the scattered field at an arbitrary distance from the scatterers in terms of a single multipole expansion about the center of the computational domain.