Generalized Fast Multipole Method

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ABSTRACT

The fast multipole method (FMM) is a technique allowing the fast calculation of long-range interactions between \( N \) points in \( O(N) \) or \( O(N \ln N) \) steps with some prescribed error tolerance. The FMM has been applied with great success in the field of integral equations and boundary element methods by accelerating the solution of dense linear systems arising from such formulations. FMMs typically require analytical expansions of the pair-wise interaction kernel, for example using a spherical harmonic series for the Helmholtz kernel or Taylor expansions for the Laplace kernel. These analytic expressions are used to construct an FMM for that kernel.

In recent years, the range of applicability and the ease of use of FMMs has been extended by the introduction of black box [1] or kernel-independent techniques [2]. In these approaches, the user need only provide a subroutine that computes the interaction kernel to the FMM. This allows the method to be applied to any kernel with minimal change to the program. In this talk, we present a novel kernel-independent FMM. This new approach uses diagonal multipole-to-local operators, which results in a significant reduction of the computational cost in the most computationally intensive step of the method.

We present the development of this novel approach from Cauchy’s integral formula and the Laplace transform. We also provide an introduction to the numerical analysis, methods to choose the parameters in the FMM to satisfy a given error tolerance, and the concepts behind building a multilevel scheme to achieve optimal asymptotic computational requirements.

Numerical results are given for a number of benchmark calculations to demonstrate the accuracy as a function of the number of multipole coefficients, the computational cost of the steps in the method, and the convergence of the error. These results are compared and contrasted with the method of [1] where applicable.

References
