Massively Parallelized Interpolated Factored Green Function Method

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Abstract

We present the first parallel implementation of the novel "Interpolated Factored Green Function" (IFGF) method introduced recently for the accelerated evaluation of discrete integral operators arising in wave scattering and other areas (Bauinger and Bruno, Jour. Computat. Phys., 2021). On the basis of the hierarchical IFGF interpolation strategy, the proposed (hybrid MPI-OpenMP) parallel implementation results in a highly efficient data communication, and it exhibits in practice excellent parallel scaling up to large numbers of cores, which is demonstrated on the basis of numerical results for problems of up to 4,096 wavelengths in electrical size, and scaling tests spanning from 1 compute core to all 1,680 cores available in the HPC cluster used.

Keywords: Wave Scattering, Integral Equations, High Performance Computing

1 Parallel IFGF Method

We present a hybrid MPI-OpenMP parallel implementation of the novel "Interpolated Factored Green Function" (IFGF) method for the accelerated evaluation of discrete integral operators arising in wave scattering and other areas [1]. The proposed implementation demonstrates in practice excellent parallel scaling up to large numbers of cores essentially without any hard limitations on the number of cores concurrently employed in an efficient manner — even for small problems — while preserving the linearithmic complexity ($\mathcal{O}(N \log N)$ computing cost) inherent in the sequential IFGF algorithm. The IFGF method accelerates the evaluation of discrete integral operators by relying on a certain factorization of the Green function into two factors, a "centered factor" that is incorporated easily as a common factor in the calculation, and an "analytic factor" which enjoys a property of analyticity up to and including infinity — and which thus motivates the IFGF strategy, namely, evaluation of a given discrete integral operator by means of a hierarchical interpolation approach which relies on use of a large number of small and independent interpolation procedures. In particular, the IFGF approach does not utilize acceleration elements commonly used by other acceleration methods [2–7] such as the FFT (Fast Fourier Transform), spherical harmonics expansions, high-dimensional linear algebra factorizations, translation operators, equivalent sources, or parabolic scaling.

The parallelization of other accelerated Green function methods has been the subject of a significant literature [8–12]. In contrast to these approaches, the IFGF method admits an elegant and highly efficient parallelization strategy due to it's algorithmic simplicity. This parallel strategy is based on adequately partitioning the interpolations performed on each level of the underlying octree structure, which facilitates the spatial decomposition of the surface discretization points. As shown in [1], the number of interpolations performed on each level is large and approximately constant (as a function of the octree level), thus admitting a large number of independent tasks suitable for parallelization. The decomposition and distribution of the interpolation data is based on a total order in the set of spherical cone segments representing the interpolation domains, which is an extension of a domain decomposition based on a Morton curve to the box-cone data structure inherent in the IFGF approach. While the usage of space-filling curves for the representation of octree structures underlying the various acceleration methods is not a novel concept [13–15], it requires some adjustments to be applicable to the present box-cone structure of the IFGF method. In view of its strong reliance on the IFGF's box-cone structure, the proposed parallelization strategy is not applicable to other acceleration methods such as the Fast Multipole Method.

In addition to the IFGF method itself and the proposed parallelization strategy, this talk will include a variety of numerical results, which

illustrate the character of the proposed parallel method, are presented in this talk. They include results showing excellent weak and strong parallel scaling properties in all cases considered—for problems of up to 4,096 wavelengths in electrical size, and scaling tests spanning from 1 compute core to all 1,680 cores on 30 nodes available in the HPC cluster used.

2 Numerical Results

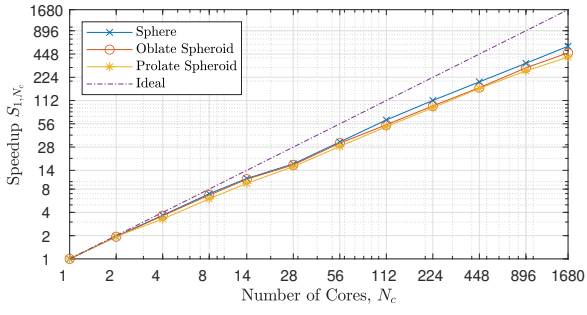

Figure 1: Measured speedup S_{1,N_c} (vertical axis) versus number of cores N_c (horizontal axis) in a strong scaling test transitioning from 1 core to 1,680 cores (= 30 compute nodes) for three geometries: a sphere of size 128 wavelengths (blue), an oblate spheroid of size 128 wavelengths (red), and prolate spheroid of size 256 wavelengths (yellow). The dash-dotted purple line indicates the theoretical perfect speedup.

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