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# A Kernel-Independent Treecode Based on Barycentric Lagrange Interpolation

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**Abstract.** A kernel-independent treecode (KITC) is presented for fast summation of particle interactions. The method employs barycentric Lagrange interpolation at Chebyshev points to approximate well-separated particle-cluster interactions. The KITC requires only kernel evaluations, is suitable for non-oscillatory kernels, and relies on the scale-invariance property of barycentric Lagrange interpolation. For a given level of accuracy, the treecode reduces the operation count for pairwise interactions from $\mathcal{O}(N^2)$ to $\mathcal{O}(N\log N)$, where $N$ is the number of particles in the system. The algorithm is demonstrated for systems of regularized Stokeslets and rotlets in 3D, and numerical results show the treecode performance in terms of error, CPU time, and memory consumption. The KITC is a relatively simple algorithm with low memory consumption, and this enables a straightforward OpenMP parallelization.

**AMS subject classifications**: 65D99, 76D07

**Key words**: Treecode, barycentric Lagrange interpolation, scale-invariance, Chebyshev points, regularized Stokeslets.

## 1 Introduction

Consider the problem of evaluating the sum

$$u(\mathbf{x}_i)=\sum_{j=1}^{N}k(\mathbf{x}_i,\mathbf{x}_j)f_j,\quad i=1,\cdots,N, \tag{1.1}$$

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where $u(\mathbf{x}_i)$ is a velocity (or potential or force) and $\{\mathbf{x}_i\} \subset \mathbb{R}^d$ is a set of particles with weights $\{f_i\}$. Depending on the application, the velocity and weights may be scalars or vectors, and the kernel may be a tensor. The kernel $k(\mathbf{x},\mathbf{y})$ describes the interaction between a target particle $\mathbf{x}$ and a source particle $\mathbf{y}$, and we are interested in non-oscillatory kernels that are smooth for $\mathbf{x} \neq \mathbf{y}$ and decay slowly for $|\mathbf{x}-\mathbf{y}| \to \infty$. It is understood that if the kernel is singular for $\mathbf{x} = \mathbf{y}$, then the sum omits the $i = j$ term.

These sums arise in particle simulations involving point masses, point charges, and point vortices, as well as in boundary element methods where the particles are quadrature points. Evaluating (1.1) by direct summation requires $\mathcal{O}(N^2)$ operations which is prohibitively expensive when $N$ is large, and several fast methods have been developed to reduce the cost. One can distinguish between two types of methods, *particle-mesh methods* in which the particles are projected onto a uniform mesh where the FFT or multigrid can be used (e.g. P3M [29], particle-mesh Ewald [16], spectral Ewald [2], multilevel summation [9, 27]), and *tree-based methods* in which the particles are partitioned into a hierarchy of clusters with a tree structure and the particle-particle interactions are replaced by particle-cluster or cluster-cluster approximations (e.g. treecode [4], fast multipole method (FMM) [24], panel clustering [26]).

**Tree-based methods.** The present work is concerned with tree-based methods that rely on degenerate kernel approximations of the form,

$$k(\mathbf{x},\mathbf{y}) \approx \sum_{k=0}^{n} \phi_k(\mathbf{x})\psi_k(\mathbf{y}). \tag{1.2}$$

Such approximations can be classified as *near-field/local* or *far-field/multipole* depending on their domain of validity in the variables $\mathbf{x},\mathbf{y}$. The treecode originally used a far-field monopole approximation for the Newtonian potential [4], while the FMM improved on this by employing higher-order multipole and local approximations, in particular using Laurent series for the 2D Laplace kernel and spherical harmonics for the 3D Laplace kernel [24, 25]. Later versions of the FMM used plane wave expansions for the 3D Laplace kernel [10] and spherical Bessel function expansions for the Yukawa potential [23]. Methods based on Cartesian Taylor expansions were also developed for some common kernels [13, 15, 30, 36, 38, 52, 57].

**Kernel-independent methods.** The tree-based methods cited above rely on analytic series expansions specific to each kernel and alternative approximation methods have been investigated. An early example in this direction was an FMM for Laplace kernels based on discretizing the Poisson integral formula [3], and this was followed by a pseudoparticle method that reproduces the multipole moments for these kernels [39]. Later work developed approximations suitable for a wide class of non-oscillatory kernels. One approach based on polynomial interpolation [32, section 11.4] has been applied in the context of multilevel approximation [21], hierarchical matrices [7], and the black-box FMM (bbFMM) [19]. An alternative method employed in the kernel-independent FMM (KIFMM) uses equivalent densities [60, 61], while other kernel-independent FMMs