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Introduction to ''A Fast Algorithm for Particle Simulations''

The paper by Leslie Greengard and Vladimir Rokhlin, ''A Fast Algorithm for Particle Simulations,'' that appeared 10 years ago in these pages marked the beginning of what is now a thriving cottage industry in creating fast hierarchical algorithms for a variety of applications. Their paper, describing the fast multipole algorithm (FMA), was not the first to propose exploiting the multipole approximation and a hierarchical decomposition of space to reduce the computational effort of solving the N-body problem. Appel in 1985 (cited within) and Barnes and Hut [1] in 1986 both proposed schemes in the context of the gravitational N-body problem which could be adapted to the electrostatic case as well. Indeed Pincus and Scheraga [2] described the possibility of such approximate representations of distant interactions many years earlier. Rokhlin had published a number of important ideas behind the FMA in the context of the boundary value problem for the Laplace equation in these same pages in 1985 (cited within).

Nonetheless, the Greengard–Rokhlin paper has had the most profound effect on subsequent developments, for several reasons. First, the highly regularized hierarchical ''interaction lists,'' describing which subregions of the simulation space interact at a given level of spatial decomposition, provided a good basis for rigorously bounding the errors and operation counts of the method. Second, the introduction of the ''local expansion'' and the related notion of box-to-box interactions at various levels of the spatial decomposition instead of the simpler (but more expensive in the aggregate) box-to-particle interactions of the earlier schemes led to a linear time implementation rather than the $N \log(N)$ cost of the earlier papers. Finally, though parallel implementations of all of these methods are certainly possible, Greengard and Bill Gropp pointed out early on the suitability of the FMA for parallel processing [3].

In practice, the FMA as described here is not the most efficient way to solve the N-body problem; various hybrids of the FMA and the earlier schemes proposed in the intervening years achieve better performance. The FMA gives all these later variants much enhanced credibility, however, as in most cases rigorous error bounds can be determined based on the FMA bounds; this overcomes the somewhat ad hoc feel of the earlier methods used alone.

The concepts of the FMA are not restricted to the $1/r$ potential of gravitation and electrostatics. Anderson [4] and Ding *et al.* [5, 6] pointed out that there is nothing magical about the multipole expansion and its related spherical harmonics; essentially any function which approximates the effect of the distant particle interaction via a truncatable converging series can be used. This in turn has led to work which continues to this day to extend an FMA-like framework to a wide variety of potential and other functions. We can look forward to continued progress toward a quite general framework for fast hierarchical function evaluation thanks largely to the insights of Greengard and Rokhlin in what follows.

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