Comparison of Solid Harmonics and Cartesian Taylor Expansions for the Fast Multipole Method for Laplacian Potentials

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Abstract

The Fast Multipole Method (FMM) and related Treecodes are important tools in N-body problems, as they allow to reduce the costly $\mathcal{O}(N^2)$ complexity of direct summations to $\mathcal{O}(N)$ and $\mathcal{O}(N \log N)$, respectively. Despite three decades of development, however, several questions, arising when implementing FMM, don't have a definite answer yet. In the present work we address the choice of expansions between Cartesian Taylor (CT) expansions [1,2,3], Spherical and Solid Harmonics (SH) [1,4,5].

For a multipole expansion up to order p, CT expansions require $\mathcal{O}(p^3)$ storage and have $\mathcal{O}(p^6)$ complexity, while SH require only $\mathcal{O}(p^2)$ storage and $\mathcal{O}(p^4)$ complexity. Despite lower requirements, however, previous comparisons ([1,3]) report lower computation time for CT than for SH, which could be attributed to the fact that the authors optimized the CT expansions via template meta-programming, but not the SH ones, with the argument that the expressions are more complex. To the best of our knowledge, the SH expansions were optimized to a comparable extent for the first time in [5].

We take a similar approach to [5] for optimizing SH - unrolling and vectorization - and revise the optimized FFT acceleration from [4] for higher orders. Detailed comparisons between CT and SH are presented, showing identical performance for the lowest possible orders and SH outperforming CT from there on by an ever larger margin, in agreement with theoretical expectations. Comparisons to state-of-the-art FMM libraries are also presented.

References

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