Flexibly imposing periodicity in kernel independent FMM: A Multipole-To-Local operator approach

WEN YAN, Center for Computational Biology, Simons Foundation, MICHAEL SHELLEY, Center for Computational Biology, Simons Foundation and Courant Institute of Mathematical Sciences, New York University — An important but missing component in the application of the kernel independent fast multipole method (KIFMM) is the capability for imposing singly, doubly, and triply periodic boundary conditions. In most popular packages such periodicities are imposed with the hierarchical repetition of periodic boxes, which may give an incorrect answer due to the conditional convergence of some kernel sums. Here we present an efficient method to properly impose periodic boundary conditions using a near-far splitting scheme. The near-field contribution is directly calculated with the KIFMM method, while the far-field contribution is calculated with a multipole-to-local operator which is independent of the source and target point distribution. This new method is designed to observe the same $O(N)$ complexity as KIFMM and to have small cost by reusing the data computed by KIFMM for the near-field. We present accuracy and timing test results for the Laplace kernel with single periodicity and the Stokes velocity kernel with double and triple periodicity. We further present applications of this method in the study of wall-bounded Stokes flow and the active stress of cytoplasmic suspensions.

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