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Fast Multipole Method for Coulomb Interaction Based on Traceless Totally Symmetric Tensor¹ HE HUANG, Old Dominion University, RUI LI, JIE CHEN, Jefferson Lab, LI-SHI LUO, Old Dominion University, HE ZHANG, Jefferson Lab — The fast multipole method (FMM) is widely used to calculate the Coulomb interaction between a huge amount of charged particles. The efficiency of FMM scales with O(N) for N particles with any arbitrary distribution. Hence it is apposite for problems with complicated charge distribution or geometry. Under the same FMM framework, there are different approaches, such as using spherical harmonic functions or Maxwell Cartesian tensors. Here we will present a version using traceless totally symmetric Maxwell Cartesian tensor. The previous Maxwell Cartesian tensor based FMM uses totally symmetric tensor. There are (n + 1)(n + 2)/2independent elements in a rank n totally symmetric tensor. However, there are only 2n + 1 independent elements in a rank n traceless totally symmetric tensor, due to which the efficiency of the traceless version is highly improved compared with the old version, especially when high accuracy is needed and high rank tensors are used.

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