

# $\mathcal{O}(N)$ methods for rapidly computing pairwise potentials in large system

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## Abstract

The need to compute pairwise potentials occurs in number situations. These range from computing potentials such as Coulombic/gravitational, Lennard-Jones, London, diffusion/Klien-Gordon, Yukawa (screened Coulomb), etc. Computing these potentials in large systems poses a severe bottleneck as the number of pairwise interactions increases. Indeed, if there are mutually interacting pairs, the cost of computing these potentials scales as  $\mathcal{O}(N^2)$ . Methods to overcome this computational bottleneck have been a topic of research for while. For instance, the fast multipole method (FMM) and their cousins—tree codes—have revolutionized the computation of electrostatic potentials ( $R^{-1}$ ). Here, the reduction in computational cost is achieved using a multipole-representation for the Greens function. In this talk, I will explore the generation of similar schemes using Cartesian Harmonics. In the proper framework, these harmonics provide several advantages; it is possible to (i) exploit symmetry, (ii) construct a methodology wherein the errors are independent of the height of the tree, and (iii) combine different potential functions together. This talk will first focus on construction of classical FMM using Cartesian harmonics, and then extend this for potentials of the form  $R^\nu$ ,  $R^{-1}e^{-kR}$ ,  $t^{-3/2}e^{-kR^2/t}$ , and  $R^{-1}e^{-jkR}$  and  $R^{-1}\partial(t-R/c)$  at low frequencies. Means to obtain a fast scheme for the latter two potentials at all frequencies will be highlighted as well. Several numerical results will be presented to demonstrate the accuracy and efficiency of the proposed scheme, as well as application to practical problems.