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An O(N) Method for Rapidly Computing Periodic Potentials Using Accelerated Cartesian Expansions

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The evaluation of long-range potentials in periodic, many-body systems arises as a necessary step in the numerical modeling of a multitude of interesting physical problems. Direct evaluation of these potentials requires O(N^2) operations and O(N^2) storage, where N is the number of interacting bodies. In this work, we present a method, which requires O(N) operations and O(N) storage, for the evaluation of periodic Helmholtz, Coulomb, and Yukawa potentials with periodicity in 1-, 2-, and 3-dimensions, using the method of Accelerated Cartesian Expansions (ACE). We present all aspects necessary to effect this acceleration within the framework of ACE including the necessary translation operators, and appropriately modifying the hierarchical computational algorithm. We also present several results that validate the efficacy of this method with respect to both error convergence and cost scaling, and derive error bounds for one exemplary potential.

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