Fast Ewald summation for electrostatic potentials with arbitrary periodicity

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A unified treatment for fast and spectrally accurate evaluation of electrostatic potentials subject to periodic boundary conditions in any or none of the three space dimensions is presented. Ewald decomposition is used to split the problem into a real space and a Fourier space part, and the FFT based Spectral Ewald (SE) method is used to accelerate the computation of the latter. A key component in the unified treatment is an FFT based solution technique for the free-space Poisson problem in three, two or one dimensions, depending on the number of non-periodic directions. The cost of calculations is furthermore reduced by employing an adaptive FFT for the doubly and singly periodic cases, allowing for different local upsampling rates. The SE method will always be most efficient for the triply periodic case as the cost for computing FFTs will be the smallest, whereas the computational cost for the rest of the algorithm is essentially independent of the periodicity. We show that the cost of removing periodic boundary conditions from one or two directions out of three will add up the total runtime marginally. Our comparisons also show that the computational cost of the SE method for the free-space case is typically about four times more expensive as compared to the triply periodic case.

The Gaussian window function, previously used in the SE method, is here compared to an approximation of the Kaiser-Bessel window function that was recently introduced. With a carefully tuned shape parameter that is selected based on an error estimate of this new window function, runtimes for the SE method can be further reduced.