

The Fast Fourier-Poisson method.

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Abstract

The Fast Fourier-Poisson algorithm calculates Coulombic forces and energies between point charges in periodic boundary conditions. It is based on the solution of Poisson's equation on a grid in real space. This equation can be solved either via FFT or via finite-difference approximation combined with multigrid. The later option is preferable when simulating millions of particles on thousands of processors. The FFP method can be also be used to calculate the Coulombic energy of dipoles and higher multipoles. In the latter case it has the advantage that for a set of multipoles of different rank one needs just one solution of Poisson equation or one Fast Fourier transform to calculate the Coulombic energy. This is to be contrasted to several FFTs required by the P3M algorithm in the multipolar case.