

# ENUF of Ewald

Fredrik Hedman and Aatto Laaksonen

Division of Physical Chemistry  
Arrhenius Laboratory  
Stockholm University  
S-106 91 Stockholm, Sweden  
`hedman@phyc.su.se`, `aatto@phyc.su.se`

**Abstract.** We sketch an  $O(N \log N)$  approach, recently proposed by us, that is based on the traditional Ewald summation technique. It can be used to calculate the electrostatic energies and forces in molecular computer simulations and appears to conserve both energy and momentum. The method is straightforward to implement in existing simulation programs. We report here some results from optimizing our implementation, where we utilize widely available libraries, and demonstrate the speed of our approach as well as the expected computational complexity.

## 1 Introduction

In computer simulations of molecular systems, mechanistic ball and spring models are commonly used to give a simple picture of atoms with specific sizes and masses bonded together with covalent bonds. Molecular equilibrium geometries and interactions are defined in so-called force fields where a somewhat arbitrary division between intra- and inter-molecular interactions is made.

The molecular force field models are normally equipped with fractional point charges to give a desired polar character to neutral molecules and charge-group parts of large molecules. Atomic ions (metals and non-metals) in most simulations are modeled as point charges and their sizes are varied by adjusting suitable collision parameters in the short-range part of the interaction potential. By collecting and dividing the diffuse and fluctuating electron densities inside and around molecules on single atomic sites a crude but conceptually simple approximation is made. Interactions between point charges are then calculated using Coulombs law. This is convenient, but comes at a price, since the interactions between point charges exist over *very* long distances.

With more and more experience gained it has gradually become clear that properly and accurately representing these long-range interactions is very important for the quality of a simulation. Ewald summation [1, 2] is still considered as the most reliable choice for calculating the electrostatic interactions and is often used as a reference. With optimal choice of parameters, Ewald summation scales as  $O(N^{3/2})$ , where  $N$  is the number of electrostatic interaction sites in the system. With growing system size, the electrostatic interactions becomes the major computational bottleneck, even for systems of moderate size. Achieving a better

computational complexity is necessary. Several different classes of fast algorithms have been developed that can be used to solve this problem in the context of simulating molecular systems; some examples are multipole methods[3–8], multigrid methods [9–11], particle-particle particle mesh [12, 13], particle mesh Ewald (PME) [14, 15] and large variety of lattice summation schemes [16–19].

In this communication we sketch a method recently suggested by us [20]. It is a novel approach to the Ewald summation method and appears to conserve both energy and momentum. The scaling is  $O(N \log N)$ . It can be viewed as a generalization of the PME method. Our method is simple to implement and should considerably simplify the treatment of Coulombic interactions in computer simulations. After briefly describing the method, we present some details on how the method has been optimized.

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