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Multilevel Evaluation of Coulomb Lattice Sums of Charge Systems

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Abstract: Problem statement: Due to the long range nature of interactions of the N-body systems, direct computation of the Coulomb potential energy involves $O(N^2)$ operations. To decrease such complexity, a simple Multilevel Summation method has been developed. **Approach:** In the frame of the Multilevel Summation method, the two-body interaction is decomposed into two parts: a local part and a smooth part. The local part vanishes beyond some cut-off distance; hence, its contribution to the potential energy is calculated in O(N) operations. In contrast to some common fast summation methods, the smooth part is calculated in real space on a sequence of grids with increasing meshsize in O(N) operations. **Results:** The method is tested on the calculation of the Madelung constants of ionic crystals in one, two and three dimensional cases. For a cut-off distance equals three times the meshsize of the ionic crystal, an error less than 0.01% is obtained. **Conclusion:** In computing the coulomb lattice sums of charge systems consisting of *N* bodies, the Multilevel Summation method decreases the complexity to O(N) operations.

Key words: Long range, fast summation, multilevel, local part, madelung constant, smooth part

INTRODUCTION

Accurate and fast calculation of the long-range Coulombic interactions for a large system of charged particles is one of the challenging tasks facing the computer simulations. The purpose of this calculation may be Monte Carlo simulation, energy minimization, or molecular dynamics. The long-range interactions make the computational effort very intensive. However, these interactions are important and there is no way their presence can be neglected. Calculating such interactions is still of great interest and developing an efficient algorithms to reduce the computer demand for the calculations continues to receive considerable attention and has been the focus of numerous approaches during the last and the present centuries (Kolafa *et al*., 2008; Patra *et al*., 2007; Yakub and Ronchi, 2003; Sagui and Darden, 1999; Gronbech-Jensen, 1997; 1999; Darden *et al*., 1997; Procacci *et al*., 1994).

The first effective summation methods for calculating the long-range part of the Coulomb potential energy had been worked out by Madelung (1918) and Ewald (1921) in the case of ionic crystals. Their papers do still remain important references. In the Madelung's method, collections of ions are formed, each collection is a linear element within the crystal. The potential of each collection is calculated and the summation of all potentials gives the potential of the crystal.

The widely used Ewald summation technique was introduced in 1921 to sum the long-range electrostatic interactions of a crystalline lattice. Later, it was incorporated into Monte-Carlo and Molecular Dynamics simulations of N-body systems with periodic boundary conditions (Rappaport, 1997; Hockney and Eastwood, 1981). Actually, the complexity of the Ewald summation method in its traditional form for N-body systems is $O(N^2)$. Many conventional methods have been proposed as improvements of the Ewald's technique (Yakub and Ronchi, 2003; Lage and Bethe, 1947; Nijboer and Wette, 1957; Brush *et al*., 1966; Sangester and Dixon, 1976; Perram *et al*., 1988; Rhee *et al*., 1989; Fincham, 1994; Yakub and Ronchi, 2005; Hunenburger and McCammon, 1999). Unfortunately the complexity of these methods is not less than $O(N^{3/2})$. To reduce this complexity, several alternative approaches have been developed in the last and the present decades. These approaches are mainly based on the Particle-Mesh (PM) methods, the tree based methods and the multigrid methods. In the PM

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methods, the Coulomb interaction is decomposed into two parts: a short-range part which is calculated directly within some cut-off distance and a long-range part which is handled in the reciprocal space through the Fast Fourier Transform (FFT) computed on a mesh. An efficient computation of long-range interaction without Fourier transform can be found in (Tsukerman, 2004). Examples of the PM methods are the Particle-particle-Mesh (P2M) (Hockney and Eastwood, 1981), the Particle-particle-particle-Mesh (P3M) (Hockney and Eastwood, 1981; Pollock and Glosli, 1996; Ghasemi *et al*., 2007; Neelov *et al*., 2007; Beckers *et al*., 1998), the Particle-Mesh Ewald method (PME) (Darden *et al*., 1993; Essmann *et al*., 1995) and the Fast-Fourier Poisson (FFP) method (York and Yang, 1994). The PM methods reduce the complexity to O (NlogN). The theory of Ewald summation is described in details by Tosi (1971) and Kittle (1996). A survey of the Ewald summation techniques is presented by (Toukmaji and Board, 1996).

The tree method was first introduced by (Appel, 1985; Barens and Hut, 1986) to calculate the energies and forces in a system of N particles using a hierarchical approach. The complexity of methods based on this approach are not worse than O (NlogN). The most effective tree based method is the Fast Multipole Method (FMM) (Greengard and Rokhlin, 1987). The (FMM) provides an algorithm for the rapid evaluation of the long-range electrostatic interactions. In the FMM, the pair-wise interactions are divided into two components: the first of which is short-ranged and is directly calculated. The second is due to the distant particles and approximated by their multipole expansions. Theoretically, the complexity of the FMM for the N-body systems is O (N). Ewald's summation method and the FMM are combined to create the multipole based Ewald method (Schmidt and Lee, 1991). This method is compared with the Ewald summation method; the number of particles N at which the two methods are equally fast is not clear.

Alternative approaches to the (FMM) are the multigrid methods. These methods were originally proposed to give numerical solutions to partial differential equations. They are considered as the fastest numerical methods for solving elliptic equations (e.g., Poisson's equation) (Brandt, 1977) and one of the fastest methods for other types of partial differential equations. The conventional iterative relaxation methods (e.g., Gauss Seidel and Jacobi) are very slow because they do not take into account effects at very large length scale. The multigrid methods improve performance by using relaxation at many length scales. In 1973, a linear complexity was achieved by those methods (Brandt, 1972). Many applications in practice are demonstrated in many papers (Sagui and Darden, 2000; Poplau *et al*., 2004; Zaslavsky and Schlick, 1998; Bernholc *et al*., 1997; Fattebert and Bernholc, 2000; Hirano and Hayash, 2000; Skeel *et al*., 2002; Hackbusch, 2010; Trotenberg *et al*., 2001).

For the N-body systems, direct calculation of the total potential energy involves O (N^2) operations. To avoid the slow direct summations, a multilevel algorithm has been developed and presented in this study. The general Multilevel approach in the context of general transformation, many-body problem and matrix multiplication has been initially proposed by Brandt (1991). Performing the statics computational tasks in computing cost that rises only linearly with the number N in the N-body systems is one objective of the multilevel method. This goal is performed and is clearly presented in this study. Another main goal that may be verified using the multilevel algorithm is performing dynamics calculations in O (N) operations. This can be done by invoking this algorithm into the Monte-Carlo simulation method. The method may also facilitates establishing computational tools for development, scale by scale, of material description at increasingly larger scales (Hardy *et al*., 2009; Brandt *et al*., 2006; Sandak, 2001). In the frame of this method, for the N-body systems, the potential exerted on a particle due to all pair-wise interactions can be decomposed into two components: a local and a smooth part. The local part vanishes beyond some cut-off radius r_{cut} and due to the nearby particles, it is computed directly. In contrast to some common fast summation methods, the smooth part is calculated in real space on a sequence of grids with increasing meshsize. The method has potential advantages over other O (N) and O (NlogN) techniques in the case of moving particles; it is also beneficial to large-scale problems such as molecular statics and Monte Carlo simulations. Our topic is motivated in part by the celebrated problem of Madelung-Sum. More details about the multilevel approach in the case of N-body systems are found in (Suwan, 2006).

MATERIALS AND METHODS

The total Coulomb potential energy arising from a system of N particles in a cubic box of size L and their infinite replicas in periodic boundary conditions is given by Eq. 1:

$$u = \frac{1}{2}\sum_{i,j=1}^{N}\sum_{n}{}' \frac{q_i q_j}{\left|\vec{r}_i - (r_j - nL)\right|} \quad (1)$$

where, q_i is the point charge of the particle i, $\vec{r}_i$ is its position and n is integer vector. The prime symbol in the summation $(\sum_n')$ indicates that for n = 0, the interaction I = j is omitted. However, atoms do interact with their replica images. The summation in (1) is conditionally convergent (i.e., the result depends on the order of summation (Allen and Tildesley, 1989). For simplicity, we will use $\vec{r}_{jn} = \vec{r}_j - nL$ throughout this study.

The kernel $G(|\vec{r}_i - \vec{r}_{jn}|) = \frac{1}{|\vec{r}_i - \vec{r}_{jm}|}$ is singular at the origin (i.e., when $r = |\vec{r}_i - \vec{r}_{jn}|$ equals zero); and its smoothness increases with the distance between particles. A 'softening' of such kernel can be obtained by splitting it into two parts Eq. 2:

$$G(r) = G_{loc}(r) + G_{smooth}(r), \tag{2}$$

where, the first (local) part of the kernel is short range, contains a singularity and it vanishes beyond some cut-off radius $r = r_{cut}$. This part is defined by Eq. 3:

$$G_{loc}(r) = \begin{cases} G(r) - G_{smooth}(r), & r \le r_{cut} \\ 0, & r > r_{cut} \end{cases}. \tag{3}$$

The second part is smooth and a suitable choice for it could be Eq. 4:

$$G_{smooth}(r) = \begin{cases} P_m(r), & r \le r_{cut} \\ G(r), & r > r_{cut} \end{cases}, \tag{4}$$

where, the function $P_m(r) = \sum_{i=0}^{m} a_i \cdot (r)^{2i}$ is a polynomial of order 2 m. The function $G_{smooth}(r)$ and its first m derivatives are assumed to be continuous at $r = r_{cut}$. So, the set of unknown coefficients $\{a_i\}$ is obtained by solving a system of linear equations. Values of the coefficients $\{a_i\}$ can be universalized by changing the variable r into $x=r/r_{cut}$; So, the values of the coefficients can be determined by the above continuity assumption, but this time, at x=1. This leads to solving the set of Eq. 5:

$$\sum_{i=0}^{m} \binom{2i}{k} a_i = (-1)^k, \tag{5}$$

where, $0 \le k \le m$ and $\binom{2i}{k}$ is the binomial coefficient. The values of these coefficients for different values of m are shown in Table 1. For m=1 and $r_{cut} = 2$, $G_{loc}(r)$ and $G_{smooth}(r)$ are shown in Fig. 1.

Using (2), the energy in (1) can be also split into two parts Eq. 6:

$$U = U_{loc} + U_{smooth}, \tag{6}$$

Where the contribution to the potential energy of the local, short range interactions is defined by Eq. 7:

$$U_{loc} = \frac{1}{2} \sum_{i \ne j}^{N} \sum_n' q_i, G_{loc}(|\vec{r}_i - \vec{r}_{jn}|).q_j \tag{7}$$

If r_{cut} is chosen comparable to the average inter-particle distance, a direct summation in (7) costs O(N) operations. The purpose of our algorithm is calculating the second part of (6) with linear complexity.

The basic idea of the multilevel algorithm is performing recursively a sequence of sets of uniform grid points called coarse levels. By "uniform" we mean a rectangular grid, with constant meshsize in each grid direction. At each coarse level, a set of charges, called coarse-level charges, are created by aggregating the located charges in the finer level into collections positioned at the grid points at the coarse level. The number of grid points at each coarse level is less than these of the finer one. The smooth part of the potential function is also recursively split at each coarse level into local and smooth parts. Consequently, the potential energy is split into two parts. The recursion proceeds until the number of coarse charges is so small that the calculation of their potential at that coarse level is not expensive comparable with the whole algorithm.

The smooth part (4) is nonsingular at r = 0. Therefore, the self-interaction energy U_{self} can be added to and subtracted from the last term in (6). Hence Eq. 8-10:

$$U_{smooth} = U^s_{smooth} + U_{self}, \tag{8}$$

Where:

$$U^s_{smooth} = \frac{1}{2} \sum_{i,j}^{N} \sum_n' q_i . G_{smooth}\left(|\vec{r}_i - \vec{r}_{jn}|\right).q_j \tag{9}$$

And:

$$U_{self} = -\frac{1}{2} a_0 \sum_{i=1}^{N} q_i^2 \tag{10}$$

The self-interaction energy U_{self} is independent of particle locations and calculated once in the procedure. Thus, it is not computationally expensive.

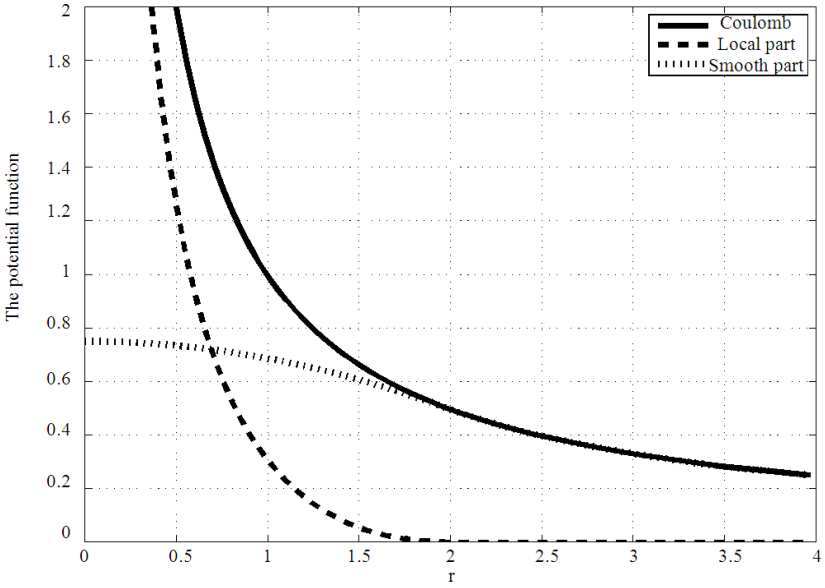

Fig. 1: The Coulomb potential function, the local part and the smooth part

Table 1: Coefficients $\{a_i\}$ in (5)

m	1	2	3	4	5	6
a_0	3/2	15/8	35/16	315/128	693/256	3003/1024
a_1	-1/2	-5/4	-35/16	-105/32	-1155/256	-3003/512
a_2		3/8	21/16	189/64	693/128	9009/1024
a_3			-5/16	-45/32	-495/128	-2145/256
a_4				35/128	385/256	5005/1024
a_5					-63/256	-819/512
a_6						231/1024

In order to approximate the first term in (8), the smoothness property of the kernel is used in the framework of the Multilevel Summation. To perform the multilevel calculations, a coarse-level grid is introduced and defined by a set of gridpoints $\{R_l\}$; the meshsize is H. The value of the smooth part of the kernel (2) for given locations of particles i and j can be interpolated from that grid Eq. 11:

$$\begin{aligned} &G_{smooth}\left(\left|\vec{r}_j - \vec{r}_{JN}\right|\right) = \sum_{l\in\sigma i}\sum_{j\in\sigma_{Jn}} \omega_l(\vec{r}_l) \\ &G_{smooth}\left(\left|R_l - R_{Jn}\right|\right).\omega_J(\vec{r}_{Jn}) + 0(\in) \end{aligned} \tag{11}$$

where, $\omega_l(\vec{r}_j)$ are the Lagrange interpolation coefficients, ε is the error of the interpolation and σ_k is the set of indices of the neighborhoods of the point $\vec{r}_k$. More details about the Lagrange interpolation method can be found in (Faires and Douglas, 1989).

Substitution of (11) in (9) and changing the order of the summation yield to Eq. 12:

$$U^s_{smooth} = \frac{1}{2}\sum_{l,J}\sum_n{}' Q_l.G_{smooth}\left(\left|R_l - R_{Jn}\right|\right).Q_J \tag{12}$$

where, the set of the coarse-level charges $\{Q_l\}$ is defined at the coarse level gridpoints by Eq. 13:

$$Q_l = \sum_{i,l\in\sigma i}\omega_l(\vec{r}_l).q_i \tag{13}$$

The fine-to-coarse transformation (13) is called the adjoint of interpolation, or the anterpolation.

The summation (12) can be carried out recursively using higher levels of coarse grids. Denoting G^1=G for any coarse level l > 1, the potential function $G^l(r)$ is split into a smooth part $G^l_{smooth}(r)$ and a local part $G^l_{loc}(r)$, now on scale $H_l = 2^{l-1}H$ and cut-off radius $R^l_{cut} = 2^{l-1}r_{cut}$ Eq. 14 and 15:

$$G^l_{smooth}(r) = \begin{cases} P^l_m(r), & r \le R^l_{cut} \\ G(r), & r > R^l_{cut} \end{cases} (l = 2,3) \tag{14}$$

And:

$$G^l_{loc}(r) = \begin{cases} G^{l-1}_{smooth}(r) - G^l_{smooth}(r), & r \le R^l_{cut} \\ 0, & r > R^l_{cut} \end{cases}. \tag{15}$$

The coefficients of the 2m-order polynomial $P^l_m(r)$ is calculated using the continuity of the function $G^l_{smooth}(r)$ and its first m derivatives at the point $r = R^l_{cut}$.

Since the function G^{l}_{loc} (r) is defined on a uniform grid, its values can be stored in a precalculated table. The charges at the gridpoints of level l are anterpolated from the finer-level grid. Continuing recursively splitting the smooth part at each level, we conclude Eq. 16:

$$G = \sum_{l=1}^{M_l} G^{l}_{loc}(r) + G^{M_l}_{smooth}(r) \quad (16)$$

where, M_l is the maximum coarse level.

RESULTS

For a periodic identical charge system where charges are placed at sites of some lattice, the Coulomb potential energy at any point i where a charge q is located can be defined by (Rappaport, 1997) Eq. 17:

$$U_i = -\frac{q^2}{h} C_M, \quad (17)$$

where, C_M, which is called Madelung constant, is a summation over the lattice points and depends only on the geometry of the crystal. h is the minimum distance between neighboring charges and q is the charge of the ion. Evaluating U in (1) for the ionic crystal leads to evaluating C_M in (17). The task is to evaluate C_M in the case of lattices with charges of opposite signs, such their sum vanishes. To illustrate the multilevel method, the lattices shown in Fig. 2 are considered.

The exact analytical expression for C_M can be obtained for the one-dimensional system in Fig. 2. In this case, an approximation of C_M denoted by C_{MA} can be defined by the following direct lattice sum Eq. 18:

$$C_{MA}(r_{cut}) = -2\sum_{i=1}^{[r_{cut}]} \frac{(-1)^i}{i} \quad (18)$$

where, […] denotes the integer part of a real number. The exact value of C_M is $\lim_{r_{cut}\to\infty} C_{MA}(r_{cut})$, which is 2ln(2) ≈ 1.3862944.

The convergence of the naive summation (18) to C_M is shown in Fig. 3 and the error versus r_{cut} is presented in Fig. 4. The convergence of the multilevel approach is shown in Fig. 5 and the error versus r_{cut} is demonstrated in Fig. 6.

As seen from Fig. 6, only a few neighbor charges should be taken into account in the local part of the potential. The same is true for more complicated lattices. The obtained Madelung constants for one, two and three-dimensional cases are shown in Table. 2. The convergence of the Multilevel approach for the Madelung constant in two and three-dimensional case are shown in Fig. 7 and 8, respectively.

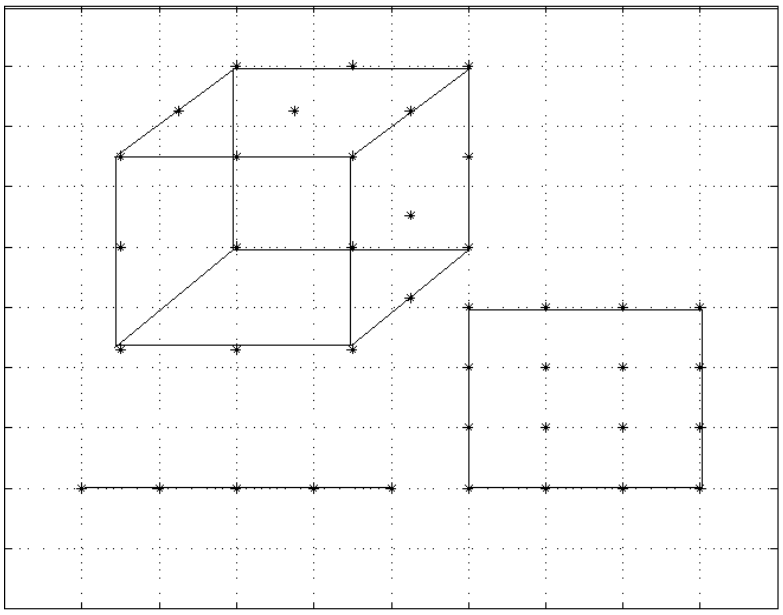

Fig. 2: The lattices for which the Madelung constant is calculated

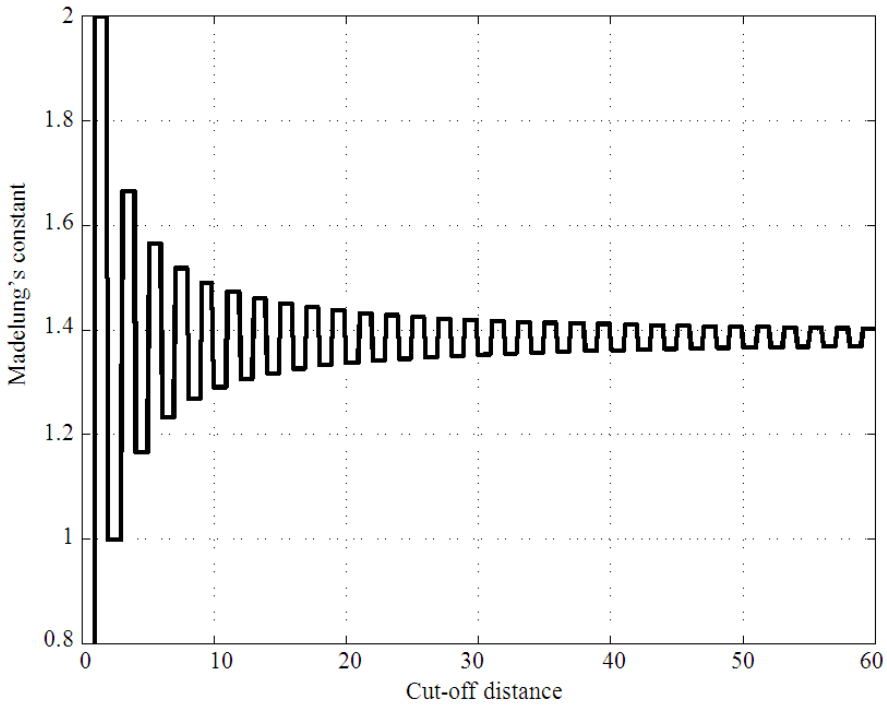

Fig. 3: The naive summation of the Madelung constant

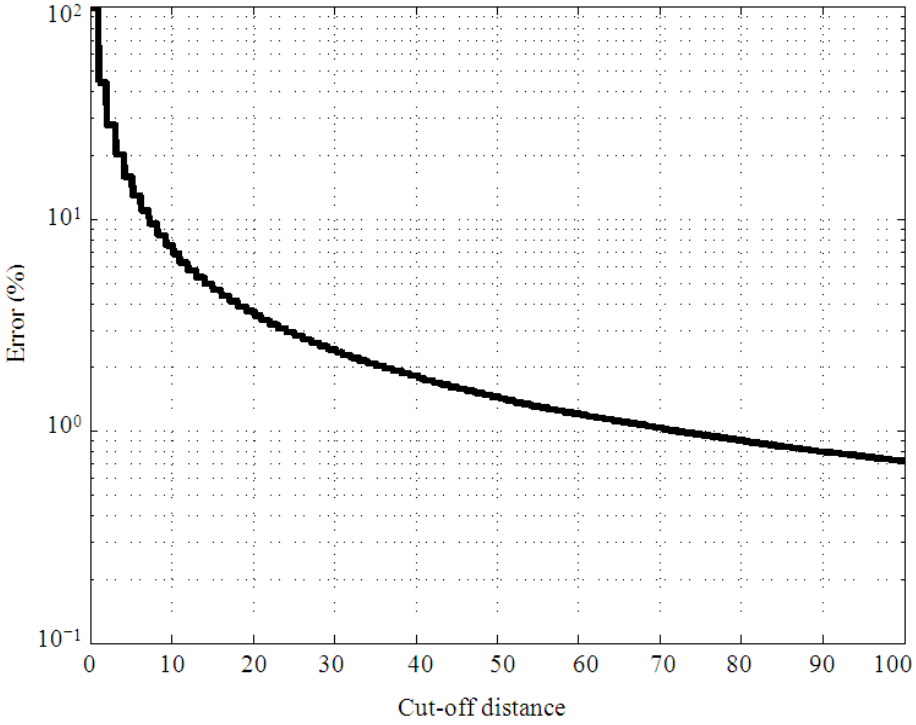

Fig. 4: The percentage error of the naive calculations

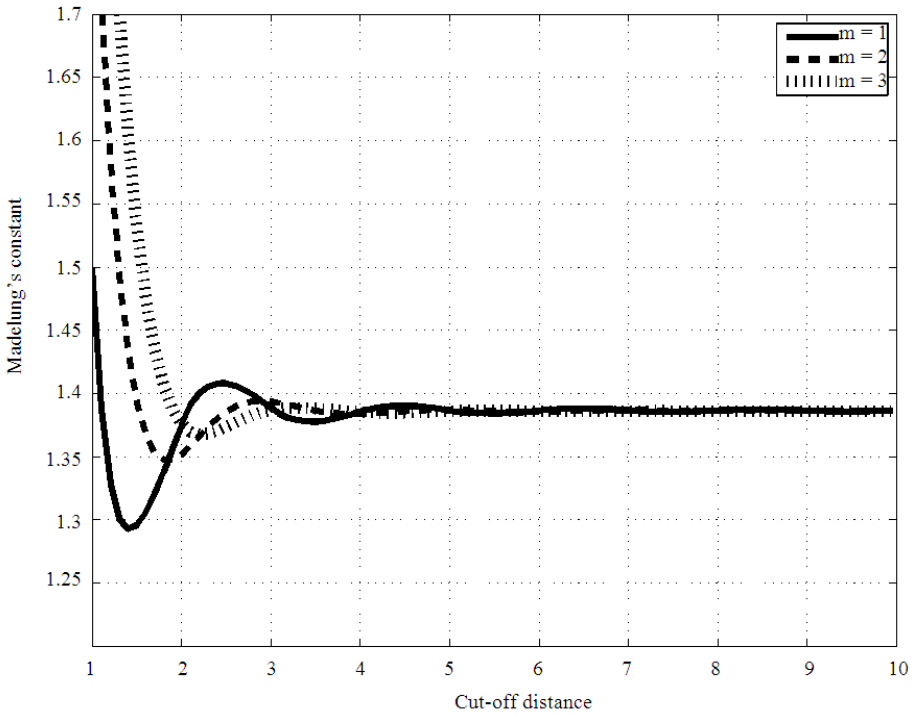

Fig. 5: The Multilevel convergence for the one dimensional case

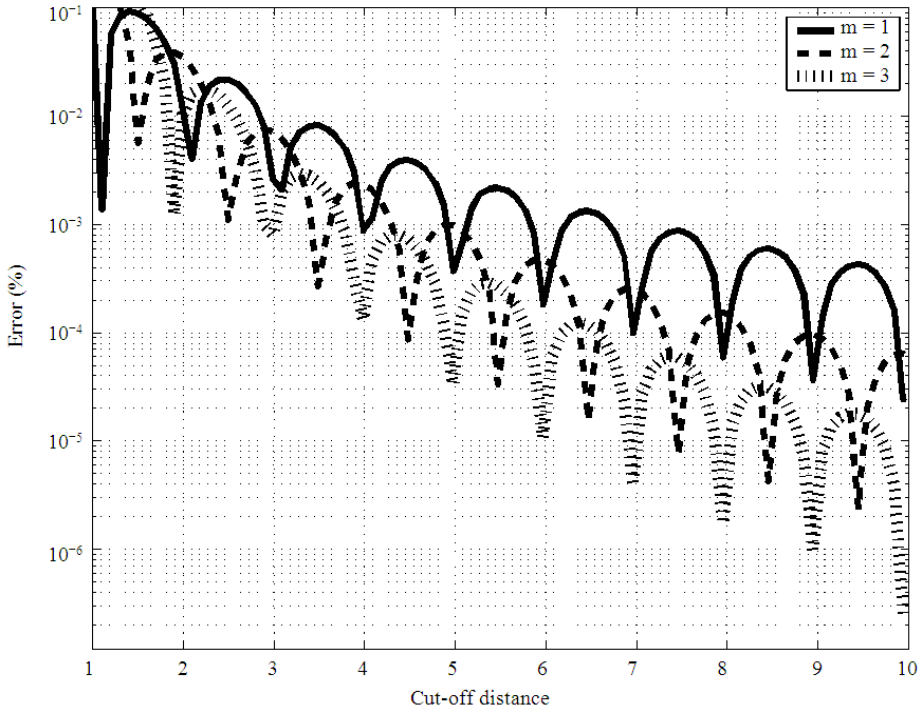

Fig. 6: The error in the multilevel calculations in the one-dimensional case

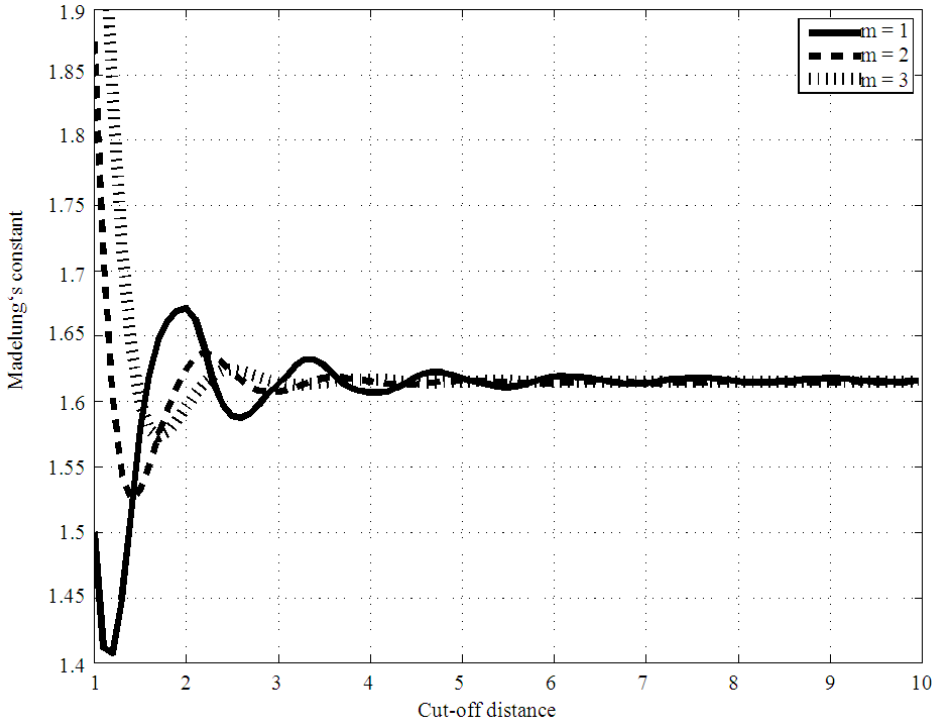

Fig. 7: The Multilevel convergence for the two-dimensional case

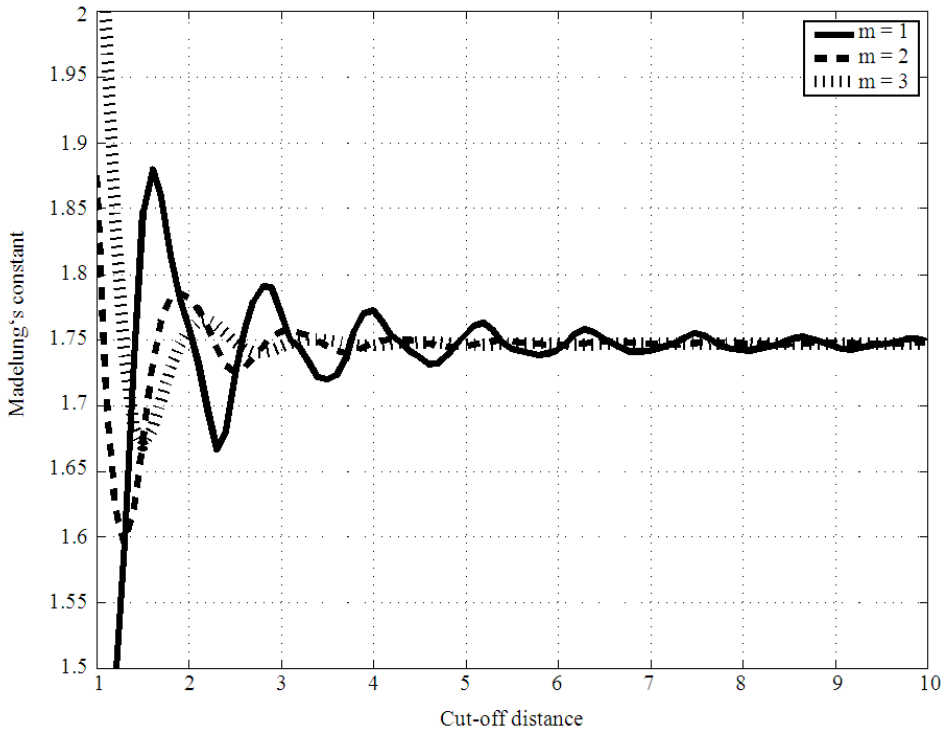

Fig. 8: The Multilevel convergence for the three-dimensional case

Table 2: Madelung constants obtained by the multilevel approach

Charge location	C_M
1D lattice (straight line shape)	1.3862944
2D (square shape)	1.61554263
3D (NaCl type shape)	1.74756460

DISCUSSION

Knowing the value of C_M is important in studying both the mechanical stability of the ionic crystals and the microscopic properties of the atoms consisting it. The more accurate the approximation of the Madelung constant, the more understanding of the ionic structure is expected.

It is necessary to define the coarse-level grid. For charge displacements, a suitable choice is a rectangular grid with meshsize H = 2h along the direction. It is convenient at first to anterpolate charges by (13). Then as we calculate the potential at a given point i, we will have to subtract, in accordance with (8), the contribution of the charge q_i from the coarse-level background. It follows from the symmetry of the lattice that the anterpolation in the case under consideration leads to constants and hence zero charges at all coarse-level gridpoints. This result is independent of the position of the coarse-level grid (as long as its meshsize in each direction is an integer multiple of the corresponding fine-level meshsize h). Therefore it is possible to shift the coarse-level grid so that calculations will be simplified. A convenient disposition of the coarse-level grid is so that a coarse gridpoint is placed at the charge for which the energy has to be calculated. The interpolation of the smooth part of the potential (12) is also done from this gridpoint with unity weight.

For the evaluation of the total potential energy (8), the coarse-level grid is defined as a first step. Then, the following entire algorithm is performed: calculating of the coarse-level charges $\{Q_l\}$ by the anterpolation using (13); then, computing the lattice sums at the coarse-level gridpoints using (12). Calculation of (12) can be carried out recursively for increasingly coarser grids. Each coarse grid is obtained by omitting every other gridpoints from the finer grid. The recursion proceeds until the number of coarse-level charges is so small that the direct calculation of their potential does not cost very much. The self potential (10) of any particle does not need any multilevel calculations; this potential is interpolated to the location of that particle and then subtracted from the potential of the system at that point.

Evaluating the Madelung constant C_M for one, two and three-dimensional cases are carried out in order to illustrate the Multilevel method and to show its efficiency. In the one-dimensional case, a comparison between the multilevel results and the exact value of C_M shows how the convergence is fast and how the obtained value of C_M is close to the exact value of the Madelung constant.

CONCLUSION

Concluding notes: A Multilevel algorithm of fast summation of long range potential for N-body systems has been demonstrated in the present work. The method is tested on the calculation of lattice sums for charge systems with charges of opposite signs, such their sum is zero. The convergence of the method is tested; independently of the dimension, the convergence is obtained. This convergence becomes faster and the accuracy becomes better by increasing m. In this method, the two-body interaction is decomposed into two parts: the local part which vanishes beyond a distance r_{cut} and the smooth part which is calculated on a sequence of grids (a coarse-level). For the estimation of the smooth part, it is necessary to calculate only anterpolated charges on these grids and interaction between them. If the dimension of the fine-level is more than one, higher-dimensional coarsening can be obtained by one-dimensional coarsening at a time, alternating the coarsening directions. The simple fast summation algorithm presented in this study allows calculating the energy in real space and a high accuracy is reached by using small values of the cut-off radius r_{cut}. Hence, for the lattice sums, the complexity of the algorithm is O (N). To test the method, Madelung constant in one, two and three dimensional cases are calculated. At $r_{cut} \geq 3h$, an error less than 0.01% is obtained.

Future prospects: The present approach is a first step towards a general and efficient scheme. The fast summation algorithm can be incorporated into the multiple 'time step' Monte Carlo algorithms (Hetenyi *et al*., 2002; Gelb, 2003). One sweep of this method consists of two steps: Monte Carlo sweeps with local part of the potential and the following acceptance, or rejection of the generated configuration in accordance with the long-range smooth part of the potential energy. The acceptance rate in this method decreases with increasing size of the periodicity cell. This obstacle is expected to be avoided by calculating the smooth part of the potential energy and checking the trial configurations several times during a sweep of the first step. This calculation can be done by applying the present algorithm.

A basic problem which is the incapability of the local simulations to move the system from a local minimum across large-scale energy barriers is expected to be solved

using the present fast summation algorithm. Moves of a more collective nature comparable with the scale of the energy landscape features can be used. For this purpose, a multilevel Monte Carlo algorithm can be developed and the anterpolated charges can be considered as the coarse-level variables.

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