JOURNAL OF COMPUTATIONAL PHYSICS 107, 403–405 (1993)

NOTE

On the Fast Multipole Method for Computing the Energy of Periodic Assemblies of Charged and Dipolar Particles

In two dimensions, it is convenient to represent the coordinates (x, y) of particles as complex numbers $z = x + iy$. The energy of interaction of two point charges q_1 and q_2 at points represented by the complex numbers z_1 and z_2 is then

$$-\mathrm{Re}\{q_1 q_2 \ln(z_1 - z_2)\} \tag{1}$$

since the natural logarithm is the singular part of the Greens function for the two-dimensional Laplace equation.

In performing molecular dynamics and Monte Carlo simulations of neutral systems of charged particles or of point dipoles, it is necessary to compute the energies and forces of an infinite periodic system in which the N charges or dipoles at the points $z_1 \cdots z_N$ resident in the primary (usually square) simulation cell are replicated everywhere in the plane. The energy to be calculated is thus

$$U = \tfrac{1}{2} \sum_j \sum_k \sum_\omega{}^{*} \mathrm{Re}\{q_j q_k \ln(z_j - z_k + \omega L)\}, \tag{2}$$

where L is the length of the square box and ω is a complex number whose real and imaginary parts are integers. The asterisk on the sum over the lattice vectors ω indicates that the term $\omega = 0$ is omitted if $j = k$. Coulomb lattice sums of the type in Eq. (2) are traditionally calculated using the Ewald transformation [1], which results in an algorithm of complexity $N^{3/2}$ [2]. The methodology for doing this correctly in three dimensions is known [3] and has also been given for the two-dimensional case [4].

The reason for restricting ourselves to the two-dimensional case is that Greengard and Rokhlin [5] have recently proposed the FMM for evaluating sums of the form (2) based on nested multipole expansions which leads to an algorithm of complexity N. As part of our investigation [6] of the values of N for which one method becomes more efficient than the other, we have implemented both. We were unable to obtain the same numerical values from both methods, within the accuracy of the computations, which led us to look deeper into the reason for the discrepancy.

When we look at the lattice sum given in Eq. (2) we observe that it is conditionally convergent; i.e., its value depends on the order of summation [3]. To obtain isotropic properties of the system, the summation should be carried out over a large circular region D_0 immersed in a vacuum of dielectric constant unity. We obtain the potential energy [4]

$$U(N, D_0) = -\tfrac{1}{2} \sum_{\omega_0}{}^{*} \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} q_\alpha q_\beta \times \mathrm{Re}\{\log(z_\alpha - z_\beta + \Omega_{m,n})\}, \tag{3}$$

where $\Omega_{m,n} = mL + inL$, and ω_0 indicates a sum over all $\Omega_{m,n}$ inside D_0, and the asterisk indicates that $\Omega_{0,0}$ is omitted when $\alpha = \beta$.

Using the two-dimensional theta-function transformation [4], the limit of Eq. (3) as the radius of the D_0 goes to infinity can be evaluated as

$$\begin{aligned} U(N, D_0^\infty) = &-\frac{1}{4}(\gamma + \log \alpha^2) \sum_{j=1}^{N} q_j^2 + \frac{\pi}{2}\left(\sum_{j=1}^{N} q_j \mathbf{R}_j\right)^2 \\ &+ \frac{1}{4} \sum_{\mathbf{n}}{}^{*} \sum_{i=1}^{N} \sum_{j=1}^{N} q_i q_j E_1(\alpha^2 |\mathbf{R}_i - \mathbf{R}_j + \mathbf{n}|^2) \\ &+ \frac{1}{4\pi} \sum_{\mathbf{n}} \mathbf{n}^{-2} \exp(-\pi^2 \mathbf{n}^2 \alpha^{-2}) \\ &\times \left| \sum_{j=1}^{N} q_j \exp(2\pi i \mathbf{n} \cdot \mathbf{R}_j) \right|^2, \end{aligned} \tag{4}$$

where γ is Euler's constant and where the result is stated in real coordinates. The $\mathbf{R}_j$'s are vectors in $\mathbb{R}^2$ whose components are (x_j, y_j) scaled with respect to L, and $\mathbf{n}$ runs over all two-dimensional vectors with integer components. E_1 is the exponential integral function. The result is independent of the parameter α, whose value is chosen to minimize the total computing overhead for evaluating Eq. (4). For this value of α, the complexity may be shown to be $N^{3/2}$.

Another shape of summation could be a large rectangle D_1 of sides a and b, where the summation is over complex numbers $z = m + in$, where $|m| < a$ and $|n| < b$. The energy is

$$U(N, D_1) = -\tfrac{1}{2} \sum_{\omega_1}{}^{*} \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} q_\alpha q_\beta \times \mathrm{Re}\{\log(z_\alpha - z_\beta + \Omega_{m,n})\}, \tag{5}$$

0021-9991/93 $5.00

581/107/2-14

where ω_1 indicates a sum over all $\Omega_{m,n}$ inside D_1. The limit as the size of the rectangle goes to infinity keeping b/a fixed is not identical to Eq. (4) but is related to it by [4]

$$U(N, D_1^{\infty}) = U(N, D_0^{\infty}) - \mathrm{Re}\left\{\left[(\tfrac{1}{2}L)\sum_{j=1}^{N} q_j z_j\right]^2 \times [2\pi - 8\tan^{-1}(b/a)]\right\}. \quad (6)$$

When the rectangle is a square ($a=b$) we obtain

$$U(N, D_1^{\infty}) = U(N, D_0^{\infty}). \quad (7a)$$

When $b/a=0$ (a sum over infinitely long strips) we obtain

$$U(N, D_1^{\infty}) = U(N, D_0^{\infty}) - 2\pi\,\mathrm{Re}\left\{\left[(\tfrac{1}{2}L)\sum_{j=1}^{N} q_j z_j\right]^2\right\} \quad (b/a \to 0). \quad (7b)$$

For symmetry reasons one might expect the same result when b/a goes to infinity, but this is not the case since we obtain

$$U(N, D_1^{\infty}) = U(N, D_0^{\infty}) + 2\pi\,\mathrm{Re}\left\{\left[(\tfrac{1}{2}L)\sum_{j=1}^{N} q_j z_j\right]^2\right\} \quad (b/a \to \infty). \quad (7c)$$

Thus it seems unreasonable to use any other shape than summation of the circle (or square).

In the fast multipole method [5] a corresponding lattice summation problem is obtained when the coefficients for the local expansions arising from all the other cells in the periodic array are evaluated. The formula for the jth coefficient arising from p-term multipole expansions is [5]

$$b_j = \sum_{k=1}^{p} a_k \binom{j+k+1}{k+1}(-1)^k \left(\sum_s (z_0)^{-(j+k)}\right), \qquad j=1, \ldots, p, \quad (8)$$

where a_k are the kth coefficient of the multipole expansion of the computational cell, and S is the set of all complex numbers $m+in$, where m and n are integers and where $|m|>1$ or $|n|>1$. When $j+k>2$ the sum over S is absolutely convergent and can be evaluated directly. When $j+k=1$ the result is zero for any shape of summation mentioned above. The problem arises when $j+k=2$. In [5] the result

$$\sum_s (z_0)^{-2} = \pi \quad (9)$$

is stated on the basis of a symmetry argument for the energy of a one-dimensional array of dipoles.

We evaluated the result for the potential energy using the result of Eq. (9) in the FMM and compared it with the result of Eq. (4) for the Ewald summation method. We found that they were NOT identical. The reason is that to obtain the result (4), the sum over S has to be done over circular shapes as well, for which the sum in Eq. (9) is zero. We are left with the question of what summation order the result in Eq. (9) corresponds. Since this result—as stated in [5]—corresponds to the requirement that the points $-\frac{1}{2}+0i$ and $\frac{1}{2}+0i$ are equivalent, we expected this result to correspond to a summation over a rectangle in the complex plane with horizontal side a and vertical side b in the case that $b/a \to 0$. We used Eq. (7b) to find the potential energy for the Ewald method and found that it was identical to the result for the FMM method. This case corresponds to slab geometry in three dimensions [7, 8], so the FMM boundary conditions may be used when an external field is imposed in the x-direction.

In the Appendix it is proved directly that

$$\sum_n \left(\sum_m^{*} (m+in)^{-2}\right) = \pi, \quad (10)$$

where the m-summations must be evaluated before the n-summation, and the asterisk indicates that $m=0$ is omitted when $n=0$.

As mentioned above, the only physically useful form of the left-hand side of Eq. (9) is found when a circular shape of summation is used. For this order of summation, we can use obvious symmetry properties to obtain the result

$$\sum_s (z_0)^{-2} = 0. \quad (11)$$

When we used this result in the FMM we found that the potential energy was equal to $U(N, D_0)$ as given by the Ewald method.

APPENDIX

In this section we give a proof that the value of the conditionally convergent double sum

$$S = \sum_n \left(\sum_m^{*} (m+in)^{-2}\right) \quad (A1)$$

over all pairs of integers (n, m), apart from $(0, 0)$, is π if the sum over m is performed first.

We observe first that

$$\sum_m \left(\sum_n^{*} (m+in)^{-2}\right) = \sum_m \left(\sum_n^{*} -(im+n)^{-2}\right) = -S. \quad (A2)$$

We now construct a complex function f in order to change summation into integration. Let $z = x + iy$, we then define f as

$$f(z) = \begin{cases} (m+in)^{-2}, & m-\frac{1}{2} \leqslant x < m+\frac{1}{2}; \\ & n-\frac{1}{2} \leqslant y < n+\frac{1}{2}; (m,n) \neq (0,0) \\ 0, & -\frac{1}{2} \leqslant x < \frac{1}{2}; -\frac{1}{2} \leqslant y < \frac{1}{2}. \end{cases}$$

By the definition of f we have

$$\int_{-\infty}^{\infty} dy \left\{ \int_{-\infty}^{\infty} dx\, f(x+iy) \right\} = S \tag{A3}$$

and analogous to (A2) we have

$$\int_{-\infty}^{\infty} dx \left\{ \int_{-\infty}^{\infty} dy\, f(x+iy) \right\} = -S. \tag{A4}$$

We now construct yet another function $g(z)$ as

$$g(z) = \begin{cases} 0, & -\frac{1}{2} \leqslant x < \frac{1}{2}; -\frac{1}{2} \leqslant y < \frac{1}{2} \\ (x+iy)^{-2}, & \text{otherwise.} \end{cases}$$

Let now T be given as

$$T = \int_{-\infty}^{\infty} dy \left\{ \int_{-\infty}^{\infty} dx\, g(x+iy) \right\}. \tag{A5}$$

Again we observe

$$-T = \int_{-\infty}^{\infty} dx \left\{ \int_{-\infty}^{\infty} dy\, g(x+iy) \right\}. \tag{A6}$$

In the square $m-\frac{1}{2} \leqslant x < m+\frac{1}{2}$; $n-\frac{1}{2} \leqslant y < n+\frac{1}{2}$; $(m,n) \neq (0,0)$ we can regard $f(z)$ as a zero-order Taylor expansion of $g(z)$ around (m,n). When $|z| \to \infty$ we find

$$\begin{aligned} |f(z) - g(z)| &\leqslant \max_{\tau} \{ g'(\tau)/\sqrt{2} \} = \max_{\tau} \{ \sqrt{2}/\tau^3 \} \\ &\leqslant \text{const}(|z| - \sqrt{2})^3, \end{aligned} \tag{A7}$$

where we have used that τ has to lie in the square. Thus

$$\int_{-\infty}^{\infty} dy \left\{ \int_{-\infty}^{\infty} dx\, |f(x+iy) - g(x+iy)| \right\} < \infty. \tag{A8}$$

Thus the integral

$$\int_{-\infty}^{\infty} dy \left\{ \int_{-\infty}^{\infty} dx\, (f(x+iy) - g(x+iy)) \right\}$$

is absolutely convergent, so we can interchange the order of integration:

$$\begin{aligned} S - T &= \int_{-\infty}^{\infty} dy \left\{ \int_{-\infty}^{\infty} dx\, (f(x+iy) - g(x+iy)) \right\} \\ &= \int_{-\infty}^{\infty} dx \left\{ \int_{-\infty}^{\infty} dy\, (f(x+iy) - g(x+iy)) \right\} = T - S. \end{aligned} \tag{A9}$$

Thus $S = T$, so we shall just prove that

$$S = \int_{-\infty}^{\infty} dy \left\{ \int_{-\infty}^{\infty} dx\, (x+iy)^{-2} \right\}$$

is π. The x-integration yields

$$\int_{-\infty}^{\infty} dx\, (x+iy)^{-2} = \begin{cases} 0, & y \leqslant -\frac{1}{2} \text{ or } y \geqslant \frac{1}{2} \\ (y^2 + \frac{1}{4})^{-1}, & -\frac{1}{2} \leqslant y < \frac{1}{2}. \end{cases} \tag{A10}$$

Thus we find that

$$S = \int_{-1/2}^{1/2} dy\, (y^2 + \tfrac{1}{4})^{-1} = \pi. \tag{A11}$$

ACKNOWLEDGMENT

The authors are grateful to Uffe Haggerup for pointing out the method of proof given in the Appendix.

REFERENCES

1. M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Oxford Univ. Press, London, 1987).
2. S. W. de Leeuw, J. W. Perram, and H. G. Petersen, *Mol. Phys.* **65**, 875 (1988).
3. S. W. de Leeuw, J. W. Perram, and E. R. Smith, *Proc. R. Soc. A* **373**, 27 (1980).
4. J. W. Perram and S. W. de Leeuw, *Physica A* **109**, 237 (1981).
5. L. Greengard and V. Rokhlin, *J. Comput. Phys.* **73**, 325 (1987).
6. D. Christiansen, Ph.D. thesis, Odense University, in preparation.
7. E. R. Smith, *Proc. R. Soc. A* **375**, 475 (1981).
8. S. W. de Leeuw, J. W. Perram, and E. R. Smith, *Proc. R. Soc. A* **388**, 177 (1983).

Received January 30, 1992; revised July 8, 1992

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