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# Four Cheap Improvements to the Particle-Mesh Code

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The two dimensional electrostatic particle-mesh code is improved in four ways at no significant cost in computation. The exact spectrum of the potential periodic in both $k$- and real space is derived. The particle shape is adjusted to reduce the dependence of the particle potential on the mesh position. Field errors are halved by using a mesh offset from that used during the charge assignment. Non-central forces are reduced by a factor typically about 10 by modifying the spectrum.

## 1. INTRODUCTION

Great advances in the accuracy of two dimensional electrostatic particle-mesh computations have been made since the earliest nearest-grid-point codes, but each advance has been made only at the expense of increasing the computation required. The purpose of this paper is to propose several simple improvements to existing codes which either need no extra computation at all, or else only affect the initialisation and so do not increase the cycle time. The four proposals presented are quite independent and they can be used either in conjunction or one at a time.

The first proposal is to use the exact potential of a system which is periodic in real space and in $k$-space, instead of relying on the approximations used previously. The spectrum of the Green's function is derived in Section 2. The fields and potentials acting upon the particles should, as far as possible, depend only on the positions of the other particles, and not on the location of the mesh points. The unwanted mesh dependence is minimised in Section 3 by a simple adjustment of the parameters of the triangular shaped particle. The remaining proposals are concerned with improvements to the inter-particle force law in codes which obtain the field by differencing the potential array. This is done by a new difference scheme (Section 4) and by modification of the spectrum (Section 5).

## 2. THE EXACT SPECTRUM OF THE POTENTIAL

In particle-mesh codes, the charge at each mesh point is obtained from the known positions of the particles by a suitable charge-sharing scheme. The potential at these same mesh points is then computed from the charge, usually by Fourier transfor-



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mation in both dimensions. In order to do this, it is necessary to know the Fourier transform, $S(k, l)$, of the Green's function representing the potential at every mesh point, $V(x, y)$, caused by a single particle at the origin. In an infinite system, $V(x, y) = \ln(x^2 + y^2)$, but, once the system is made finite by imposing periodic boundary conditions in both directions, $V$ can only be expressed as a complicated combination of Jacobi elliptic functions [1]. Fourier transformation of this result has not proved possible and, hitherto, no expression has been available for the spectrum $S(k, l)$. Indeed Buneman [2] has pointed out that no expression could yield the logarithmic divergence of $V$ at the origin. In consequence, approximations for $S$ have had to be used: these have either been based on a truncation of the ideal $(k^2 + l^2)^{-1}$ spectrum, or else on one of the many finite difference representations of the Laplacian operator.

In Section 2.1 we will consider the effect of the discrete mesh and obtain the resulting spectrum $S_1(k, l)$, and in 2.3 the periodicity in real space will be allowed for giving the final spectrum $S_2(k, l)$.

### 2.1. *The Spectrum of a Discrete Potential*

We require that $S_1(k, l)$ reproduce the potential correctly at the mesh points, but is unimportant what happens to $V$ between mesh points because such values are never used in the calculation. This leaves $S_1$ undetermined apart from certain conditions on its aliases, but this ambiguity can be resolved as follows. We start with the ideal spectrum

$$S_0(k, l) = (k^2 + l^2)^{-1}, \tag{1}$$

which is the transform of $\ln(x^2 + y^2)$, and take the mesh interval as our unit of length. Then we set $V$ to zero everywhere except at the mesh points by multiplying it by the "bed of nails" function

$$\sum_{M,N} \delta(x - M)\,\delta(y - N), \qquad M, N \text{ integers},$$

which confounds $S_0$ with all of its aliases and gives [3]

$$S_1(k, l) = \sum_{m,n} S_0(k + 2\pi m, l + 2\pi n), \qquad m, n \text{ integers}. \tag{2}$$

The summation over one index, say $m$, can be performed giving a result in terms of a cotangent of complex argument [4]

$$S_1(k, l) = \sum_{n}{}' -\frac{1}{2} b^{-1} \operatorname{Im} \cot\left(\frac{1}{2}k + i\frac{1}{2}b\right),$$

where $b = |l + 2\pi n|$. This expression can be rewritten in a more convenient form as

$$S_1(k, l) = \sum_{n}{}' \frac{\sinh(b)}{b(4\sinh^2(\frac{1}{2}b) + 4\sin^2(\frac{1}{2}k))}. \tag{3}$$

The spectrum $S_1$ can be evaluated directly from (3), but it is more convenient to sum it now, rather than to retain an infinite sum throughout the calculation [5], and thus obtain a spectrum $S_1$ whose periodicity in $k$ and $l$ represents the discrete nature of the mesh potential.

2.2. *A Series Expansion for* $S_1(k, l)$

The dominant contribution in (3) comes from the term with $n = 0$, $S_1^{(0)}$. First the variables $u = 4\sin^2(\frac{1}{2}k)$ and $v = 4\sin^2(\frac{1}{2}l)$ are introduced, and the denominator is expanded, to give

$$S_1^{(0)}(k, l) = \frac{\sinh(l)}{(u+v)l} \sum_{v \geqslant 0}' \left( \frac{v - 4\sinh^2(\frac{1}{2}l)}{u+v} \right)^v. \tag{4}$$

Then the hyperbolic functions are written as series in $l^2$,

$$l^{-1}\sinh(l) = 1 + l^2/3! + l^4/5! + \cdots, \tag{5a}$$

$$2\sinh^2(\tfrac{1}{2}l) = l^2/2! + l^4/4! + \cdots. \tag{5b}$$

Finally each power of $l^2$ is written in terms of $v$ using

$$\begin{aligned} l^2 &= (2\arcsin(\tfrac{1}{2}v^{1/2}))^2 \\ &= v + v^2/12 + v^3/90 + \cdots. \end{aligned} \tag{6}$$

(Only an outline of the expansion procedure is given here, as a copy of the tabulated coefficients and the FORTRAN program used to obtain them is available on request from the author.)

To evaluate the sum over the $n \neq 0$ terms, $S_1^{(n)}$, Eq. (3) is rewritten by using yet another form of the complex cotangent [4], and by expanding $b^{-1}$ in powers of $l$,

$$S_1^{(n)}(k, l) = \sum_{n \neq 0} \left( \sum_{\mu > 0} \cos(\mu k)\, e^{-\mu b} - \frac{1}{2} \right) \sum_{\lambda \geqslant 0} \frac{(-\mathrm{sign}(n) l)^\lambda}{(2\pi n)^{\lambda+1}}. \tag{7}$$

The terms in (7) independent of $\mu$ are just sums over $n$ of reciprocal powers which are proportional to the Riemann zeta function [6]. To evaluate the terms in $\mu$, the series

$$\sum_{n > 0} e^{-\mu 2\pi n} (2\pi n)^{-\lambda-1}, \tag{8}$$

which converge very rapidly, are summed numerically. The resulting series in $l^\lambda$ is then multiplied by the expansion of $e^{-\mu l}$. Adding in the contribution from the negative $n$ values cancels terms of odd order in $l$. Thus we obtain a result of the form

$$S_1^{(n)}(k, l) = \sum_{\mu\lambda} F_{\mu\lambda} \cos(\mu k)\, l^{2\lambda}. \tag{9}$$

The only coefficient that appears to cause any problem here is $F_{00}$, which is logarithmically divergent. However, this is the very term in $S_1(k, l)$ which is independent of $k$ and $l$, and so it represents the transform of the value of the potential $V$ at the origin. No wonder then that $F_{00}$ is infinite. In any practical computer code, $V(0, 0)$ has to be reduced to a more manageable value, so $F_{00}$ is left as a free parameter $\gamma$ to be determined at the user's discretion.

Expansion (9) is next converted into a series in $u$ (using the recurrence relation for cosines of multiple angles and $\cos k = 1 - \frac{1}{2}u$) and $v$ (using Eq. (6)). At this stage the combination of $S_1^{(0)}$ and $S_1^{(n)}$ is a rather lobsided function of $u$ and $v$, although numerically it is symmetric in these variables. We therefore average by interchanging $k$ and $l$.

$$S_1(k, l) = \tfrac{1}{2}(S_1^{(0)}(k, l) + S_1^{(0)}(l, k) + S_1^{(n)}(k, l) + S_1^{(n)}(l, k)),$$

which permits a further transformation to symmetrised variables $p = u + v$ and $q = uv/(u + v)$. This allows cancellation of the inverse powers of $p$ in Eq. (4) and the final result is then

$$S_1(k, l) = p^{-1} \sum_{\mu,\lambda} G_{\mu\lambda} p^{\mu} q^{\lambda}, \tag{10}$$

where $G_{10}$ is the free parameter $\gamma$ mentioned above. The lowest order coefficients $G_{\mu\lambda}$ are given in Table I, but an explicit Padé approximant is

$$\begin{aligned} S_1(k, l) = p^{-1} &\left(\frac{1 + 0.5054P + 0.0754P^2 + 0.0008P^3}{1 - 0.1587P}\right) \\ &\times \left(1 - \left(\frac{q}{6} - \frac{P}{3}\right) \frac{1 + 0.4278P}{1 + 0.1587P - 0.0634P^2}\right)^{-1}, \end{aligned} \tag{11}$$

where $P = p/8$. This expression provides a more economic way of computing $S_1$ than the power series (10), and it is accurate to better than $10^{-4}$ over any part of its range.

The question might be asked, Was the transformation from the variables $u$ and $l$, which appeared naturally, worth the effort? We require a spectrum which is periodic in $l$, but no *finite* Taylor series of the form (9) can give periodic behaviour. By converting from $l$ to $v$ (which is a sinusoidal function of $l$), we automatically get a periodic $S_1$ even with a truncated Taylor series. The final choice of variables, $p$ and $q$, is justified by the more economic form of the series, and by their physical meaning: when $p$ is small, $p$ is the square of the wave vector, $k^2 + l^2$, and $q/p$ gives a purely angular dependence $(1 - \cos 4\theta)/8$.

### 2.3. *The Spectrum of a Periodic Potential*

The final stage of the analysis is to allow for the periodicity in $V(x, y)$. The spectrum then becomes

$$S_2(k, l) = \textstyle\sum_{m,n} S_1(k, l)\, \delta\left(k - \dfrac{2\pi m}{L}\right) \delta\left(l - \dfrac{2\pi n}{L}\right), \tag{12}$$

where $m$ and $n$ are integers and $L$ is the periodic length. Overall charge neutrality in the periodic system is ensured by setting $S_2(0, 0) = 0$. This completes the Fourier transformation of the mesh potential: although the combination of elliptic functions could not be transformed directly, we have achieved the same result by starting with the ideal logarithmic potential and summing the aliases in $k$-space.

### 2.4. *Comparison with Alternative Spectra*

We shall now consider the various approximations to $S_1$ that have been proposed. The list is meant to be exhaustive of all the schemes that have been described in this *Journal* (and one extra scheme is thrown in for good measure), but no attempt has been made to be exhaustive regarding their authorship, as several approximations have been proposed more than once. The schemes are presented in order of increasing complexity. They are all accurate when $k$ and $l$ tend to zero, but a comparison of the coefficients $G_{\mu\lambda}$ in Table I shows that some large discrepancies will occur at larger wavenumber. To estimate the overall accuracy the maximum difference from the exact $S_1$ is given in Table II (this usually but not invariably occurred at $(\pi, \pi)$).

Eastwood and Hockney [1] discuss three proposals, the simplest one being to base the spectrum on the usual five point difference formula for the Laplacian operator. The spectrum which results from this is

$$S_1 = p^{-1}. \tag{13}$$

Here all the $G_{\mu\lambda}$ coefficients, apart from $G_{00}$ and $G_{10}$, are zero. The diagonal version of the five point formula [1] yields

$$S_1 = p^{-1}(1 - p/8)(1 - q/2)^{-1}. \tag{14}$$

We see from Table I that this is a poorer choice because the coefficients are too large, and in particular the dependence on $q$ is much too strong.

By combining the five point schemes, nine point schemes may be generated. The version of Lewis and Nielson [7],

$$S_1 = p^{-1}(1 - q/3)^{-1}, \tag{15}$$

is based on a template which emphasises the diagonal form of the $\nabla^2$ operator, and the table shows that once again the coefficients are too large. A consideration of the $G_{01}$ term would suggest that a better nine point scheme would be made by combining the axial and diagonal operators in the ratio 2 to 1, and this is what the next two authors use.

Buneman's scheme [2] gives

$$S_1 = p^{-1}(1 - q/6)^{-1}, \tag{16}$$

TABLE I

Series Expansion Coefficients $G_{\mu\lambda}\, p^{\mu} q^{\lambda}$ for the Exact Spectrum $S_1$ and the Approximations Made to It

| Name | Eq. | $G_{01}$ | $G_{20}$ | $G_{11}$ | $G_{02}$ | $G_{30}$ | $G_{21}$ | $G_{12}$ | $G_{03}$ |
|---|---|---|---|---|---|---|---|---|---|
| 5 point | (13) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Diagonal | (14) | $\frac{1}{2}$ | 0 | $-\frac{1}{16}$ | $\frac{1}{4}$ | 0 | 0 | $-\frac{1}{32}$ | $\frac{1}{8}$ |
| 9 point [2] | (15) | $\frac{1}{3}$ | 0 | 0 | $\frac{1}{9}$ | 0 | 0 | 0 | $\frac{1}{27}$ |
| 9 point [7] | (16) | $\frac{1}{6}$ | 0 | 0 | $\frac{1}{36}$ | 0 | 0 | 0 | $\frac{1}{216}$ |
| 9 point [1] | (17) | $\frac{1}{6}$ | 0 | $-\frac{1}{72}$ | $\frac{1}{36}$ | 0 | 0 | $-\frac{1}{432}$ | $\frac{1}{216}$ |
| 9 point axial | (18) | $\frac{1}{6}$ | $\frac{1}{144}$ | $-\frac{1}{36}$ | $\frac{1}{36}$ | $-\frac{1}{1728}$ | $\frac{1}{288}$ | $-\frac{1}{144}$ | $\frac{1}{216}$ |
| 25 point | (19) | $\frac{1}{6}$ | $\frac{1}{576}$ | $-\frac{7}{1440}$ | $\frac{1}{36}$ | $\frac{1}{3456}$ | $\frac{-1}{3840}$ | $\frac{-1}{576}$ | $\frac{1}{216}$ |
| Poor Man | (20) | $\frac{1}{6}$ | $-\frac{1}{240}$ | $\frac{1}{180}$ | $\frac{1}{36}$ | $-\frac{61}{136{,}080}$ | $\frac{41}{30{,}240}$ | $\frac{1}{1680}$ | $\frac{1}{216}$ |
| Exact | (10) | $\frac{1}{6}$ | $-3.00 \times 10^{-4}$ | $\frac{1}{180}$ | $\frac{1}{36}$ | $5.61 \times 10^{-7}$ | $-2.10 \times 10^{-4}$ | $\frac{1}{1680}$ | $\frac{1}{216}$ |

*Note.* $G_{00}$ is unity and $G_{10}$ is arbitrary in every case.

and now all the $G_{0\lambda}$ terms are correct, although the other coefficients are all zero. Buneman in fact specified $\gamma = -1/12$, but as discussed in Section 2.2 above, the choice of $\gamma$ is arbitrary. The classic nine point formula gives Eq. (16) with $\gamma = 0$ and so it is represented by the same line in Table I. Eastwood and Hockney [1] obtain a slightly different operator, which gives

$$S_1 = p^{-1}(1 - p/12)(1 - q/6)^{-1}. \tag{17}$$

The nine point extended axis form of the Laplacian [8] could also be used to generate a spectrum:

$$S_1 = p^{-1}(1 + p/12 - q/6)^{-1}. \tag{18}$$

It is interesting to note that each of the schemes (16), (17), (18) contains an effective constant term $\gamma$ of $-1/12$. When it appears explicitly (16) it is harmless, but otherwise it introduces extra terms into the power series which all have the wrong sign. It is clear that the considerations in numerical analysis about the properties of the finite difference approximations to the Laplacian, which called for this term $-1/12$, are not appropriate to the problem of modelling $S_1$.

Finally, in this category we consider the 25 point scheme devised by Lewis [9, 10], which has spectrum

$$S_1 = p^{-1}(1 - p/8 + pq/64)^2(1 - p/6 - q/6 + pq/20 - pq^2/360)^{-1}. \tag{19}$$

Now the coefficient $G_{21}$ is very close to its required value (and $G_{0\lambda}$ are all correct), but there are still several discrepancies in the table.

TABLE II

Comparative Performances

| Name | Eq. | $\Delta S$% | $\Delta V$% | Fluct.% |
|---|---|---|---|---|
| 5 point | (13) | 6.86 | 4.1 | 0.55 |
| Diagonal | (14) | 8.33 | 4.1 | 0.46 |
| 9 point [2] | (15) | 18.14 | 9.8 | 0.72 |
| 9 point [7] | (16) | 0.61 | 0.47 | 0.47 |
| 9 point [1] | (17) | 4.78 | 3.0 | 0.41 |
| 9 point axial | (18) | 1.65 | 2.1 | 0.47 |
| 25 point | (19) | 6.55 | 2.6 | 0.47 |
| Poor Man | (20) | 3.34 | 3.1 | 0.38 |
| Truncated | (20) | 19.35 | 7.8 | 0.39 |
| Padé | (11) | 0.006 | 0.012 | 0.22 |
| & offset mesh | | | | 0.117 |
| & particle shape | | | | 0.107 |
| & improved force | | | | 0.098 |

*Note.* The column $\Delta S$ shows the maximum deviation from the exact spectrum. The error in the resulting potentials are shown in column $\Delta V$. The final column gives the energy fluctuation level for each spectrum and for the other recommendations of this paper.

An alternative to this approach is Boris' "Poor Man's Poisson Solver" [11]:

$$\begin{aligned} S_1 &= (k^2 + l^2)^{-1} \\ &= p^{-1}(1 + p/12 - q/6 + p^2/90 - pq/30 + \cdots)^{-1}. \end{aligned} \tag{20}$$

As far as the power series is concerned, this wins hands down by getting five coefficients correct. However, its performance at large wave number is poor as it does not give the required zero gradient at $k$ or $l = \pi$ which all the other schemes provide. An attempt is often made to circumvent this problem by truncating the spectrum (20), for instance, by setting $S_1 = 0$ if $k^2 + l^2 > \pi$, but the resulting step in $S_1$ is not realistic.

The problem is that we are trying to model the Fourier transform of a continuous function, and so the domain of $S$ never terminates. Once we restrict our attention to the potential at the mesh points, then three options are open to us: we can use the ideal spectrum $S_0$ and include the region beyond $\pm\pi$ by explicitly summing the aliases (Eq. (2)); or we can use the Poor Man's philosophy and arbitrarily cut off $S_0$ at $\pm\pi$ (or indeed at any smaller wavenumber) recognising that we will not then be able to reproduce $V$ correctly; or we can let someone else perform the aliasing for us once and for all and use a spectrum $S_1$ that does terminate at $\pm\pi$. All the approximations, (11), (13)–(19), do this, so it is a matter of selecting the one with the most desirable properties. An overall comparison will be made in Section 6, but on the basis of the $G$ coefficients and the maximum error $\Delta S$, the Padé approximant (11) is the first choice, with Buneman's nine point formula (16) as runner up.

### 2.5. *Accuracy of the Potential*

As a further test of the various spectra, each one has been Fourier transformed on a $64 \times 64$ mesh and the resulting Green's function has been compared with the exact periodic potential [1] at each mesh point. The peak errors, expressed as percentages of the value of $V(1, 0)$ when the mean value of $V$ over the mesh is zero, are given in Table II. Once again Eqs. (11) and (16) come first and second in accuracy.

## 3. The Optimum Triangular Shaped Particle

Eastwood and Hockney [1] discuss charge assignment schemes of different order, and show how improved performance is achieved by sharing the charge over a greater number of mesh points. Of course the improvement is only obtained at the expense of more computation, so it is a moot point which order to take. We show here that a significant improvement can be made to their recommended TSC scheme without involving any more computation.

The TSC scheme assigns the charge of each particle to the nine adjacent mesh points $m'$, $n'$ by a biquadratic weighting function $w(m'; m, x)\, w(n'; n, y)$, where $m$

and $n$ are the nearest integers to the particle coordinates $m+x$ and $n+y$. The function $w$ distributes the charge onto the three nearest integers in the proportions

$$\begin{aligned} w(m-1;m,x) &= \tfrac{1}{2}(c-x+x^2), \\ w(m;m,x) &= 1-c-x^2, \\ w(m+1;m,x) &= \tfrac{1}{2}(c+x+x^2). \end{aligned} \tag{21}$$

The constant $c$ was taken to be $\frac{1}{4}$ as this gives the quadratic spline profile. It is also the natural choice if the TSC is considered as the convolution of two top hat cloud-in-cell functions. There is, however, no real necessity to take $c=\frac{1}{4}$ and we now investigate alternative choices. We consider three different criteria in the following subsections.

3.1. *Minimal Distortion in k-Space*

As the weighting function in two dimensions is the product of one dimensional functions (21), the effect on the Fourier harmonics is similarly the product of factors for each direction. In place $f(k,x)=\exp(ik(m+x))$ for a particle at $m+x$, the distributor $w$ gives

$$g(k,x) = (1+ix\sin k + (c+x^2)(\cos k - 1))\exp(ikm). \tag{22}$$

The effect of the finite particle size is to degrade the $k$ harmonic in the ratio $g/f$. If we average over all particle positions we obtain

$$\langle g/f\rangle = \sin^3(\tfrac{1}{2}k)(8k^{-3}+k^{-1}-4ck^{-1}). \tag{23}$$

This is a generalisation of the result $\operatorname{sinc}^3(\frac{1}{2}k)$ obtained by several authors for the case $c=\frac{1}{4}$.

We note that $\langle g/f\rangle$ falls off as $k$ increases, and we could try to compensate for this by reducing $c$. The choice which keeps $\langle g/f\rangle$ as close as possible to 1 in a least squares sense over the whole range of $k$ is $c=-0.15$. However, we do not recommend this choice (which magnifies the high frequency noise) for the following reason. The harmonics are not built up to average contributions $\langle g/f\rangle$ but actual contributions $g(x)/f(x)$. What we ought to be doing is to try to keep $g/f$ constant as $x$ varies, because the whole purpose of spreading the charge out over several mesh points is to try to make the force independent of the location of the mesh (see Section 3.3 below).

3.2. *Minimal Distortion in Real Space*

To assess how well the TSC distributor $w$ follows different functions (potential, field or whatever), we can do a Taylor expansion about the point $x=m$ and look at each power in turn. In place of $x^t$, we get

$$\begin{aligned} \sum_{m'} w(m';m,x)\,m'^t &= 1, && \text{for } t=0, \\ &= x, && \text{for } t \text{ odd}, \\ &= c+x^2, && \text{for } t \text{ non-zero even}. \end{aligned} \tag{24}$$

Thus the constant and linear terms are followed exactly, the quadratic is followed but with a constant discrepancy $c$, and the higher terms are not reproduced properly. If our criterion were to choose the TSC scheme which distorts the function as little as possible, we would have to choose $c = 0$. The particle shape would then be the standard (TSC) triangle of height 1 and base 2, with the addition of $\delta$-functions (nearest-grid-point contributions) with strength $-\frac{1}{8}$ at the edges and $+\frac{1}{4}$ at the apex. This choice is analogous to the subtracted dipole scheme [12], which is motivated by similar considerations. In that scheme, a rectangular particle shape of height $\frac{1}{2}$ and base 2, having weighting function $w$ shown in Fig. 10 of [12], is modified by $\delta$-functions, $-\frac{1}{4}$ at the edges and $+\frac{1}{2}$ at the centre, to give $w$ as in Fig. 9.

### 3.3. *Independence of the Mesh Position*

However, we are not really worried about constant discrepancies: we could compensate for them by an alteration of the function we are trying to follow, i.e., by weighting the spectral components as discussed in Section 5 below. What is much more important is to choose $c$ to minimise the dependence of the inter-particle potential (and hence force) on the location of the particles with respect to the mesh. A rather tedious piece of algebra shows that the constant and linear components of the inter-particle potential are reproduced correctly by the distributor, and so is the quadratic term apart from a constant discrepancy $2c$, which does not affect the forces between particles. In place of the cubic term $(m + x - X)^3$ in the interaction of particles at $m + x$ and $0 + X$, we have

$$A_3 = m^3 + 6mc + (3m^2 + 1 + 3c)(x - X) + 3m(x - X)^2 + 3(xX^2 - x^2X).$$

This is made up of the desired cubic term, a linear term $6c(m + x - X)$ which is removable by the modification of the spectrum, and an error term

$$A_3' = (1 - 3c)(x - X) - (x^3 - X^3). \tag{25}$$

This final term represents an unwanted dependence on the absolute positions of the particles within the cells of the mesh. It is minimised by choosing $c = 17/60$ giving a mean square noise level

$$\int_{-1/2}^{1/2} \int_{-12}^{1/2} A_3'^2 \, dx \, dX = 3.19 \times 10^{-4}$$

compared with $2.94 \times 10^{-3}$ for $c = \frac{1}{4}$ and a very noisy 0.122 at $c = 0$.

We conclude that the simple change of $c$ from 1/4 to 17/60 cuts the rms noise level to less than a third. The particle shape is then the triangle plus $1/60$ $\delta$-functions at the edges minus a $1/30$ $\delta$-function at the apex. With $c = 17/60$ there is a very small discontinuity in the force when a particle crosses a cell boundary, but its amplitude depends only on the fourth derivative of the potential and its harmful effect is more than offset by the overall reduction in the noise level.

## 4. A Difference Scheme on an Offset Mesh

The proposals in Sections 4 and 5 are applicable when, as is usual, the electric fields at each mesh point are generated from the potentials $V(m, n)$ by a difference scheme of the form

$$E_x(m, n) = \tfrac{1}{2}[V(m+1, n) - V(m-1, n)], \tag{26}$$

the mesh interval being unity. Acting on the logarithmic potential $V = \ln r^2$, this gives (to order $r^{-3}$) a radial field $E_r = 2r^{-1} + \frac{2}{3}r^{-3}\cos 4\theta$, and an azimuthal field $E_\theta = -\frac{2}{3}r^{-3}\sin 4\theta$. An improvement can be made by relaxing the usual restriction that a single mesh be used throughout the computation: we show how that this halves the error in the field.

Let the charge of each particle be assigned to the mesh points and the potentials be deduced in the usual way. Then, when calculating the fields that each particle sees, distribute the charge to the nine nearest centres of the cells instead of the nearest cell corners; i.e., let $m, n, m', n'$ be half integers in Eq. (21). We may then use the formulae

$$\begin{aligned} E_x(m, n) &= E_+ + E_-, \\ E_y(m, n) &= E_+ - E_-, \end{aligned} \tag{27}$$

where

$$E_\pm(m, n) = \tfrac{1}{2}[V(m + \tfrac{1}{2}, n \pm \tfrac{1}{2}) - V(m - \tfrac{1}{2}, n \mp \tfrac{1}{2})].$$

This gives $E_r = 2r^{-1} - \frac{1}{3}r^{-3}\cos 4\theta$ and $E_\theta = +\frac{1}{3}r^{-3}\sin 4\theta$, so that the errors have been halved.

Further improvements are possible, but these would need increased computational effort, so they do not fall within the scope of this paper. A particularly attractive idea be to add the results of (26) and (27) in the proportions $\frac{1}{3}$ and $\frac{2}{3}$ as then the leading error term in $E_\theta$ falls to $+(1/15)\,r^{-5}\sin 4\theta$.

Lest there should be any misconception, the use of the offset mesh is not the same as the interlacing [3] used to reduce aliases during the Fourier transformation. In that method, several meshes are used consecutively to give the effect of a finer mesh without any extra storage space being needed, but here we just have one mesh, albeit displaced from its original position.

Only one problem arises with the use of (27): we do not have exact momentum conservation and so the self-induced field seen by the particles is not automatically zero [13, 14]. The discrepancy is small and its mean value is zero, but its exact value depends on the potential at the mesh points near the origin hand hence on the arbitrary constant $\gamma$. By selecting $\gamma$ to make $V(0, 0)$ equal to $V(1, 0)$, the error field is reduced to $\leqslant \frac{1}{2}\%$ of the field at one mesh interval. This is considerably less than the unavoidable noise arising in the interaction between pairs of particles.

## 5. Improvement of the Inter-particle Force

The spectrum can be adjusted to improve the force between particles except when the particles get very close together. Buneman [2] used a factor which made his charge sharing scheme equivalent to a quadratic spline fitting. However, the purpose of our correction will be to reduce the effect of errors introduced by the finite difference scheme.

The goal used in this paper is to reduce $E_\theta(\mathbf{r})$ to zero and to ensure that $(2\pi)^{-1}\int E_r(\mathbf{r})\,d\theta = 2/r$. Thus we are aiming for a purely central force with the correct mean strength. Unfortunately any improvement to $E_\theta$ makes $E_r$ worse and vice versa, and this is the reason why we recommend using the offset mesh (Section 4) so as to start from as good a position as possible. A similar technique could be used if we preferred to make $E_r$ independent of $\theta$ at the expense of a larger non-central component.

We can avoid a complicated calculation over the mesh structure by first finding the effect of the difference operator on a continuous logarithmic potential, and then introducing the effect of the aliases. The spurious azimuthal field arising from the logarithmic potential is

$$E_\theta = \frac{1}{2h}\sum_{\lambda=1}^{4} \sin(\theta + \tfrac{1}{2}\lambda\pi)\ln(h^2 - 2hr\cos(\theta + \tfrac{1}{2}\lambda\pi) + r^2), \tag{28}$$

where $\theta$ is taken to be zero along one of the difference vectors $\mathbf{h}$ used in the difference scheme. With the conventional scheme $h$ is the mesh interval unity, but using the offset mesh $h$ is $\times 2^{-1/2}$ smaller. By resolving $E_\theta$ into its harmonic components, we find that $E_\theta$ is the derivative of a potential

$$\begin{aligned} U(\mathbf{r}) &= \sum_{v\geqslant 1} \frac{r^{4v}}{2vh^{4v}}\left[\frac{1}{4v-1} - \frac{r^2}{h^2(4v+1)}\right]\cos 4v\theta, \qquad r \leqslant h, \\ &= \sum_{v\geqslant 1} \frac{h^{4v}}{2vr^{4v}}\left[\frac{r^2}{h^2(4v-1)} - \frac{1}{4v+1}\right]\cos 4v\theta, \qquad r > h. \end{aligned} \tag{29}$$

This result is exact: if the approximation for $E_\theta$ in Section 4 had been used in its derivation, a much less tractable result would have been obtained.

The Hankel transform of $U(\mathbf{r})$ is

$$B_0(\mathbf{k}) = \sum_{v\geqslant 1} \frac{8}{k^4h^2} J_{4v}(kh)\cos 4v\theta, \tag{30}$$

and this sum over harmonic components can be performed to give

$$B_0(\mathbf{k}) = \frac{8}{k^4h^2}\left[\cos(\mathbf{k}\cdot\mathbf{h}) + \cos(\mathbf{k}\times\mathbf{h}) - 2J_0(kh)\right]. \tag{31}$$

The radial field is calculated in a similar way and we find that there is no need to correct for the error in $\int E_r \, d\theta$ as this is identically zero for all $r \geqslant h$. We thus correct for the spurious $E_\theta$ by subtracting $B_0$ from $S_0(\mathbf{k})$.

Nothing can be done to improve the mesh-calculated force for separations less than $h$, so for small $h$ we obtain a very simple result,

$$B_0(\mathbf{k}) = \frac{h^2}{48} \cos 4\theta. \tag{32}$$

Thus the correcting potential depends only on the direction of $\mathbf{k}$, not on its magnitude, except for the point $\mathbf{k} = 0$, where it is not analytic. Allowing for aliases and transforming to the periodic variables $p$ and $q$ gave a Padé approximant for $B_1$. A one term approximant is nearly as good as more complicated expressions (because of the smearing out caused by the finite particle size), so we recommend a correction

$$B_1(\mathbf{k}) = \frac{1.1h^2 q}{6p} \tag{33}$$

to be added to $S_1(\mathbf{k})$ when the offset mesh is used, and subtracted with the conventional mesh. The factor 1.1 was chosen empirically to compensate for the particle size. The effect of this $B_1$ is to reduce the non-central force by a factor of between 3, at short distances ($r \leqslant 4$), and 10 or more, at larger separations. If it is desired to eliminate $\partial E_r / \partial \theta$ rather than $E_\theta$, then the sign of $B_1$ should be reversed.

## 6. Conclusion

The purpose of this paper has been to show that significant improvements can be made to the performance of the particle-mesh code, without incurring extra computation. The four proposals are easy to implement and can be adopted as a group or singly (for instance, the modified particle shape is also the ideal choice for three dimensional codes). Similarly in codes which form gradients in $k$-space and prepare separate arrays for $E_x$ and $E_y$, the results of Section 3 are still applicable and techniques analogous to those in Sections 2 and 5 could be devised.

The degrees of improvement obtainable with each proposal were discussed in the appropriate sections above, and their overall usefulness has been assessed by measuring the energy fluctuation level in the simulation of a guiding-centre plasma. The Padé approximant (11) gives a 0.22% fluctuation level, which is less than that given by any of the alternative spectra (see Table II), the Poor Man formula being runner up in this test. Clearly the proper spectrum (11) is the one to use, but the approximation which is the safest alternative (the one that does least badly over the whole set of tests) is Hockney's nine point scheme (17).

The other recommendations in this paper reduce the fluctuation level further.

Changing to the offset mesh brings down the fluctuation level to 0.117%, and altering the particle shape to $c = 17/60$ further reduces it to 0.107%. Finally the modification to the spectrum (33) gives a level of 0.098%.

Once the restriction to cheap improvements is lifted, then more radical changes to the existing codes become possible: for instance, Eastwood has considered the optimal design of a one dimensional code [5] and in three dimensions has recommended a four point difference scheme [15]. The present paper should be considered as complementary rather than alternative to that approach. After all, proposals of the kind discussed here can be applied to codes of any degree of sophistication, and it is the author's opinion that most practitioners would prefer to sharpen their familiar tools rather than feel obliged to buy new ones.

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