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# Quiet High-Resolution Computer Models of a Plasma

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We introduce two new computer models in which the influence of the finite potential mesh is, for most practical purposes, eliminated. The Quiet Particle–Mesh model (QPM) uses a Gaussian-shaped charge cloud and careful shaping of the potential solution in either real or transform space. The QPM model is measured to be 150 times less noisy than the conventional CIC model and is suitable for large collisionless plasma simulations with $10^5$ or more particles. This is achieved at little or no cost in computing time. The hybrid Particle–Particle/Particle–Mesh model (PPPM), on the other hand, adds to the above mesh calculation contributions from nearby particles by direct summation. This model has a spatial resolution which is independent of the mesh spacing and may be a small fraction of a mesh cell. It is more time-consuming and is suitable for high-resolution sub-Debye length investigations with a smaller number of particles ($\sim 10^4$). Applied to molecular dynamics, the PPPM model can simulate systems with approximately 100 times the number of particles than conventional methods.

## 1. INTRODUCTION

The spatial resolution of conventional computer models of plasmas, such as the NGP [1] and CIC [2] models, is limited by the density of mesh points on which the fields are defined. Theoretical [3, 15, 16] and experimental [8, 17] work has shown that, in the case of collisionless plasmas, the finite sampling density of the fields causes increased collision times, nonconservation of energy, and mesh-induced growth of plasma waves. The desirable lengthening of collision times may be physically interpreted by ascribing a finite size to the representative particles, whereas the other two effects, which arise from mesh-induced force fluctuations (aliases in transform space), are totally unrealistic and unacceptable. We describe here a quiet particle–mesh model (QPM) in which the unwanted force fluctuations are almost completely suppressed, and a related hybrid particle–particle/particle–mesh (PPPM) model [5] in which the charge shape may be specified independently of the mesh spacing. On the one hand, the QPM version provides an improvement on the CIC method for use in collisionless simulations with large ($\sim 10^5$) numbers of particles, while, on the other hand, the PPPM version is capable of studying the

microscopic (sub-Debye length) plasma properties with a smaller ($\sim 10^4$) number of particles. Both methods are applicable in one, two, or three dimensions.

In the PPPM model, the force between two particles is composed of a slowly varying long-range mesh force, **E**, which is present for all separations, $r$, of the particles, together with a rapidly varying short-range particle–particle (PP) component, **F**, which is present only if $r < a$ (the cutoff radius). We shall see that the total force, $\mathbf{E} + \mathbf{F}$, can be of arbitrary shape; however, we will restrict the subsequent description to the special case of the coulomb interaction in two dimensions which is appropriate in the plasma application. The QPM version is simply the PPPM model in the absence of the short-range-part **F**.

## 2. The QPM Model

### 1. *Gaussian-Shaped Cloud*

The mesh force is obtained in the usual way [1, 2] by the assignment of charge to a fixed potential mesh, the solution of Poisson's equation, and the differencing of the potential to obtain the field at each mesh point. The coordinates of each particle are taken to be the center of a truncated Gaussian-Shaped Cloud (GSC) with charge density

$$\begin{aligned} N(x_i) &\propto \exp\left(-\sum_{i=1}^{d} x_i^2/2\sigma^2\right) && |x_i| \leqslant H, \\ &= 0 && |x_i| > H, \\ & 1 \leqslant i \leqslant d, \qquad \sigma = 0.455, \end{aligned} \tag{1}$$

where $H$ is the distance between mesh points, $x_i$ is the coordinate in the $i$th dimension relative to the center of the particle, and $d$ is the dimensionality.

The GSC spreads the charge of a particle over the surrounding nine cells (in two dimensions) in proportion to the charge of the cloud lying in each cell. Similarly, the total force on a particle is taken as the weighted sum of the forces in the surrounding nine cells using the same proportional weights, just as in the CIC method.

The force obtained with GSC interpolation is continuous in the first and all higher derivatives to within $\sim 10\%$ of either the first or second derivative of the field. It is therefore smoother and quieter than the CIC model which has large discontinuities in the first derivative, approximately equal in magnitude to the second derivative of the field. By comparison, quadratic spline interpolation, as discussed by Buneman [4], has exact continuity in the first derivative, large discontinuities of the second derivative, and exact continuity of all higher deriv-

atives [10]. Here, we have adopted the GSC which spreads the total amount of discontinuity over all higher derivatives rather than concentrating the effect in one derivative (a comparative analysis of the effect of different charge-sharing algorithms on the mesh force **E** is given by Eastwood [12]).

## 2. *Potential Correction*

The potential, $\phi$, is obtained from the charge distribution, $\rho$, by using the Fast Fourier Transform (FFT) [6] and the relation

$$\hat{\phi}_{k,\ell} = \hat{G}_{k,\ell}\hat{q}_{k,\ell}\,, \tag{2}$$

where

$$q = -4\pi\rho H^2 \qquad \text{in esu.}$$

The hat denotes the finite double Fourier transform of the mesh values, and $G$ is a Green's or influence function for a unit point source, which may be of arbitrary shape [7].

We split $\hat{G}(= \hat{G}' + \hat{G}'')$ into two parts:

$$\begin{aligned} &\hat{G}'_{k,\ell} = (A + 4)/(4B + 8A - 20) \qquad k, \ell = 1, 2, \ldots, m/2, \\ &\hat{G}'_{0,0} = 0, \end{aligned} \tag{3}$$

where

$$A = \cos(2\pi k/m) + \cos(2\pi\ell/m)$$

and

$$B = \cos(2\pi k/m)\cos(2\pi\ell/m),$$

which is derived from the 9-point difference approximation to Poisson's equation, $\nabla^2\phi = -4\pi\rho$, on an $(m \times m)$ mesh and solves that equation well except at short range, and a correction term.

$$\hat{G}''_{k,\ell} = \sum_{s,t} c_{s,t}\cos(2\pi ks/m)\cos(2\pi\ell t/m) \tag{4}$$

which for small values of $s$ and $t$ alters the Greens function $G_{s,t}$ only at short range (i.e., for $r < a$).

The mesh assigned part of the force between two particles depends both on their separation and on the angle, $\theta$, between the separation vector and the axis of the mesh. For the NGP and CIC methods, we have found the maximum difference between the mesh force measured along $\theta = 0°$ and $\theta = 45°$ to be $\sim 50\,\%$ of the force at one mesh distance. This angular anisotropy is immediately reduced to $5\,\%$ by the use of the GSC and to $0.5\,\%$ by a careful choice of eight independent

constants $c_{s,t}$. A least-squares procedure is used with the requirement that **E** be any function of $r$ for $r < a$ and the coulomb field for $r > a$. The required total force is then obtained by suitably choosing the short-range force, **F**. The result is valid for any position of the particles within a mesh cell. A set of optimum constants has been found for the GSC on a 256 × 256 potential mesh with doubly periodic boundary conditions using the 9-point difference equations (3). These are:

$$\begin{gathered} c_{00} = 0.2804, \quad c_{01} = c_{10} = 0.2698, \quad c_{11} = 0.1775, \\ c_{02} = c_{20} = 0.0213, \quad c_{12} = c_{21} = 0.0878, \quad c_{22} = -0.0443, \\ c_{03} = c_{30} = 0.0067, \quad c_{13} = c_{31} = -0.0351. \end{gathered} \tag{5}$$

The constants are independent of the number of mesh points, $m$, and the mesh spacing $H$. The use of the constant $c_{00}$ by itself tampers with the Fourier transform in the way discussed by Buneman [4, p. 253].

The interpretation of the influence function $G_{s,t}$ is simply related to the physical realization of Green's function in continuum electrostatics. The convolution integral arising from the application of Green's method to Poisson's equation

$$\phi(\mathbf{x}) = \int_{\mathbf{x}} G(\mathbf{x} - \mathbf{x}')\, \rho(\mathbf{x}')\, d\mathbf{x}' \tag{6}$$

becomes the convolution sum on the mesh

$$\phi_{s,t} = \sum_{s',t'} G_{s-s',t-t'} \rho_{s',t'}, \tag{7}$$

the finite transform of which is the harmonic equation (2). Comparison of Eqs. (6) and (7) immediately reveals that $G_{s,t}$ gives the potential on mesh point $(s, t)$ due to a unit charge at the origin. Thus, since the global shaping of $\hat{G}_{k,\ell}$ by $\hat{G}''_{k,\ell}$ corresponds to independently changing values of $G_{s,t}$ in each octant by amounts $c_{s,t}$, $\hat{G}''_{k,\ell}$ may be seen as the correction to offset the "squareness" produced by charge sharing and differencing errors on the rectangular mesh [9, 10].

The use of the FFT to solve for the potential, and smoothing by shaping the transform, are not themselves new. The efficacy of these ideas have been recognized and exploited previously by, for instance, Hockney [7, 8] and Orens *et al.* [14] in the simulation of plasmas, and by Hohl and Hockney [11] in galaxy simulations. However, to our knowledge, methodically shaping the transform by varying individual values of $G_{s,t}$ (subject to the eightfold symmetry requirements of the mesh) is without precedent. The great advantage of our novel method is that with a finite difference approximation for the electric field, changes in the values $c_{s,t}$

result in spatially localized changes in the force. Accordingly, by limiting values of $s$ and $t$ to approximately the circle such that $s^2 + t^2 < 10$, we are able to find the best values of coefficients $c_{s,t}$ to smooth the short-range force variations without affecting the mesh force at long range. Assuming that we adopt the physically meaningful interparticle force profile as a measure of the width of the charged clouds [8–10], then, for the QPM version, the optimal values cited in Eq. (5) yield almost mesh independent cylindrically symmetric rods of width $3.2H$ (cf. $\sim H$ for NGP and CIC). We have used here the distance to the peak in the force law $F(r)$ as the value of width. This provides an easy measure, agreeing well with collision measurements. The increased width and smoothness have the desirable effect of lengthening both the collision time and heating time [8, 10]. Indeed, it is evident that the stochastic heating rate [8] and coherent particle–mesh interactions [3] should be considerably reduced, for our method provides an interparticle force whose dependence on the mesh is two orders of magnitude weaker than that of the standard CIC algorithm. This is what we mean by a Quiet Model.

The quality of a plasma simulation may be measured in terms of the collision time (the time on average for a plasma particle in a thermal plasma to deflect through 90°) and the heating time (the time for kinetic energy of the electrons to increase by $kT$ due to stochastic effects). We have extended the measurements of these quantities previously made by Hockney [8] on the CIC and NGP models to the new QPM model and some other variants.

## 3. *Noise Measurements*

The collision time, $\tau_{\text{coll}}$, is related empirically to the Debye length, $\lambda_D$, plasma density, $n$, and particle width, $W$, by the relation

$$\tau_{\text{coll}}/\tau_{pe} = 0.98n(\lambda_D{}^2 + W^2). \tag{8}$$

Further, the heating time, $\tau_H$, is related to the collision time by the equation

$$\tau_H/\tau_{\text{coll}} = K_H/(H/\lambda_D)^2 \tag{9}$$

provided that a sensible choice is made of the time step, $DT$ optimum, from

$$\omega_{pe}DT_{\text{opt}} = \min[1, \tfrac{1}{2}(H/\lambda_D)]. \tag{10}$$

$K_H$ (previously called $K_4$) will be referred to as the heating constant.

These relations show that for a quiet, collisionless simulation we want a large value of $W$ (but not so large as to lose too much spatial resolution) and a large value of $K_H$. The measured values for various models in descending order of merit are as follows:

| | | | | | | |
|---|---|---|---|---|---|---|
| (1) | GSC, | 9, | YES = QPM | $W = 3.0$, | $K_H = 3000$, | $f = 150$ |
| (2) | CIC, | 9, | YES = QCIC | $W = 2.8$, | $K_H = 600$, | $f = 26$ |
| (3) | CIC, | 5, | YES | $W = 2.8$, | $K_H = 200$, | $f = 9$ |
| (4) | GSC, | 9, | NO = GSC | $W = 1.8$, | $K_H = 150$, | $f = 3$ |
| (5) | CIC, | 9, | NO = CIC | $W = 1.0$, | $K_H = 100$, | $f = 1$ |
| (6) | CIC, | 5, | NO = CIC | $W = 1.0$, | $K_H = 100$, | $f = 1$ |
| (7) | CIC, | 5, | NO = CIC [8] | $W = 1.0$, | $K_H = 40$, | $f = 1/2.5$ |
| (8) | NGP, | 5, | NO = NGP [8] | $W = 1.0$, | $K_H = 5$, | $f = 1/20$ |

In the above table, the first three letters designate the type of charge sharing used; the number 9 or 5, the number of finite difference points used in the approximation to Poisson's equation; and YES or NO refers to whether or not the potential correction term $\hat{G}''$ and coefficients $c_{s,t}$ are included. The merit figure, $f$, is proportional to the heating time in units of plasma period for a typical problem with $(H/\lambda_D) = 1$. It includes the contribution of both $W$ and $K_H$ to the quietness in a particular application.

Model (1) is the QPM model as described in this paper which is shown, as expected, to be 150 times quieter than the tranditional CIC models (5) or (6). The next-best model number (2) is obtained by adding the correction coefficients $c_{s,t}$ to the traditional CIC model (5) with the 9-point Poisson approximation. These coefficients given in Eq. (5), although chosen to compensate for a GSC charge-sharing scheme, improve the CIC model by a factor 26. We call this the quiet CIC model (QCIC). The same coefficients are somewhat less successful in quietening a (CIC) model using the 5-point finite difference approximation, presumably because the coefficients were chosen for a 9-point approximation, but a factor of almost 10 improvement even in this case is remarkable. Model (4) is the model using GSC charge sharing and no potential correction. The unexpectedly small improvement over CIC of a factor 3, which is mostly due to increased particle width, may not justify the use of this model because of the extra computing time required by GSC charge sharing. The difference between the measurements of the same CIC model listed under models (6) and (7) probably indicates a systematic difference between the earlier measurements [8] and the current ones. The reason may be the greater care now taken to establish thermal equilibrium before the heating rate measurement is taken.

## 4. *Real-Space Smoothing*

We emphasize that the QPM model presented is only one of a class of QPM models. The introduction of the short-range correction $\hat{G}''$ is a general method that can be used to reduce the mesh dependence of the force obtained from any charge sharing and double FFT Poisson-solving algorithm. The ensuing improvements are

achieved at no extra cost in computer time, since $\hat{G}''$ is absorbed into the precalculated multiplying factor $\hat{G}$. In particular, it can be used, with appropriately chosen values of $c_{s,t}$ to improve the commonly used CIC scheme, as the above measurements confirm.

In the event that a Fourier-transform potential solver is not being used, the potential correction can be applied in real-space entirely externally to the potential solver, again at little or no cost in computing time. In fact, an improvement of computer speed may result if a faster method than FFT is used to solve Poisson's equation. The process may be regarded as a smoothing operation applied either to the charge distribution prior to the potential solution or to the potential after the solution of Poisson's equation. The Poisson-solving routine, whatever its nature, is used as a "black box".

The required potential is given by

$$\boldsymbol{\phi} = [(\nabla_h^2)^{-1}) + G]\,\mathbf{q}, \tag{11}$$

where $\nabla_h^2$ is the matrix operator describing the finite-difference equations and $G$ is the matrix containing the coefficients $c_{s,t}$ which describe the potential correction. Both $\nabla_h^2$ and $G$ represent localized operations and are therefore sparse matrices; $\boldsymbol{\phi}$ and $\mathbf{q}$ are vectors containing the ordered mesh values of the potential and charge distribution.

Equation (11) may be computed in two stages:

$$\mathbf{q}^* = [1 + \nabla_h^2 G]\,\mathbf{q}, \tag{12}$$

followed by

$$\boldsymbol{\phi} = (\nabla_h^2)^{-1}\,\mathbf{q}^*, \tag{13}$$

where (12) represents the smoothing of the given charge distribution to obtain $\mathbf{q}^*$ and (13) is the application of any existing Poisson-solving routine to the smoothed function. Equally well, the smoothing may be performed after solving for the potential by computing

$$\boldsymbol{\phi}^* = (\nabla_h^2)^{-1}\,\mathbf{q} \tag{14}$$

followed by

$$\boldsymbol{\phi} = [1 + G\nabla_h^2]\,\boldsymbol{\phi}^*. \tag{15}$$

It is easy to see that sines and cosines are the eigenfunctions of both $G$ and $\nabla_h^2$; consequently, these matrices commute and the two smoothing operators in (12) and (15) are in fact the same. The number of computer operations required to compute $\boldsymbol{\phi}$ from $\mathbf{q}^*$ or $\boldsymbol{\phi}^*$ from $\mathbf{q}$ is $63m^2$ for an $(m \times m)$ potential mesh, where we have made use of any symmetries in the coefficients $c_{s,t}$ to reduce the number of multiplications. This extra computing may be compensated for by using, for example, the FACR algorithm [7] for the solution of Poisson's equation with an

operation count of $2.5m^2 (\log_2 m + 2.4)$ in place of the Fourier transform DFA [7] method with an operation count of $10m^2 (\log_2 m - 2.8)$. A comparison of the total operations required shows that real-space and $k$-space potential correction take closely the same time for $m = 256$ and that real-space smoothing wins for larger values of $m$. However, there may be other reasons for favoring the calculation of $k$-space.

## 3. The PPPM Model

The PPPM version of the model is formed by adding the particle–particle force **F**, which is found by directly summing contributions from the neighbors of each particle (i.e., those for which the separation $r < a$). The contribution added is the force necessary to bring the mesh force **E** up to the required value. It is found by table look-up and can clearly be of arbitrary shape. The effective particle size, as determined by the total force of interaction $\mathbf{E} + \mathbf{F}$, can therefore be adjusted to any required value and becomes *independent of the mesh spacing*, $H$. Thus the particle size is no longer determined by the region of the mesh over which the charge of the particle is distributed, as is the case with the CIC or QPM models. In particular, the effective width of the QPM particle can be reduced from a value of $\sim 3.2H$ to an arbitrary small fraction of a cell.

Buneman [4] has given an interpolation scheme, using splines, which reduces the uncertainty in position of the center of a particle cloud to a fraction of a cell; however, the distance at which two particles may be recognized as distinct (the resolution in the astronomical sense) is still approximately the mesh size. In the PPPM model, this "astronomical" resolution may be reduced to a fraction of a cell. This is what we mean by High Resolution.

### 1. *Linked-List Technique*

We find the neighbors by a linked-list technique. A mesh of chain cells is introduced over the region of the calculation and all particles in each cell are linked together in a chain. If the side of a chain cell is of length $a$, then all neighbors of a particle are to be found either in its own chain cell or in one of the eight cells touching it. To form the chains, one needs an array containing the particle number of the first particle in the chain for each cell—the "head of chain" array— and an additional coordinate for each particle. This link coordinate is the particle number of the next particle of the chain, with the convention that a zero value for the link means the end of the chain.

After clearing the "head of chain" array, the chain can be built-up by scanning the particle coordinates in sequence and performing the steps (a)–(c), given below. Let the particle being examined be number $n$ and the total number of particles $N$; then,

(a) find the chain cell from the particle coordinates, say cell $(i, j)$;

(b) transfer the present contents of the "head of chain" array $(i, j)$ to the link coordinate of particle $n$;

(c) place $n$ in the "head of chain" array $(i, j)$.

The formation of the chains may conveniently be done while the charge distribution is being built-up and takes only $2N$ divisions and a storage typically of $1\frac{1}{5}N$. The technique is described in detail because some frequently used methods for tracing neighbors, e.g., in molecular dynamics, take $\sim N^2$ operations and a great deal more storage. Such $N^2$ methods cannot be used with large assemblies.

The linked-list technique may be extended to simulations where only parts of the field array and a subset of the particle coordinates may be held simultaneously in random access memory. The extension involves splitting configuration space into slabs, each slab having its own (variable length) linked-list and head-of-chain table; particles passing from slab $a$ to slab $b$ are transferred from slab $a$ to a transfer table, and thence to slab $b$ when that region is being processed. Naturally, the increased bookwork leads to greater overheads, but the operation count remains proportional to $N$.

## 4. Computer Timings

A PPPM model has been used successfully to simulate a two-dimensional assembly of 10,000 ions and had a time-step cycle of 8.7 sec on the IBM 360/195. The potential mesh was ($256 \times 256$), the chain mesh ($64 \times 64$), $a = 4H$, and the average number of neighbors was 12. Charge assignement and the formation of links took 0.7 sec, the potential solution 2 sec and the particle pushing (i.e., differencing of the potential and movement of particles) 6 sec. The program ran in a region size of $800K$ Bytes.

The above model was also run as a QPM code by eliminating the particle–particle contribution. The cycle time was then 4.3 sec of which the particle pushing took 1.1 sec. This time corresponds to 110 $\mu$sec per particle which will seem slow compared to some existing highly optimized CIC codes (for example, Orens, Boris, and Haber report $\sim 12$ $\mu$sec[1] per particle for an NRL CIC code using word packing and integer arithmetic [14]). However, the times quoted in this paper refer to an unoptimized development program written in Fortran and compiled under the Fortran $H$ opt $= 2$. There is no reason, based on the number of computer operations, why the particle pushing of the QPM code using the 9-point GSC cloud should be more than twice as slow as the 4-point CIC algorithm. This is confirmed

[1] Scaled from a figure of $\sim 20$ $\mu$sec on the IBM360/91 using the comparative machine speeds reported by Hockney [13].

by the following comparative measurements for the particle-pushing phase of different models which were all made with Fortran programs written with the same level of care and run on the IBM 360/195 under Fortran $H$ opt $= 2$ compiler, on the same day:

NGP 1-point scheme; 23 $\mu$sec per particle
CIC 4-point scheme; 44 $\mu$sec per particle
QPM 9-point scheme; 104 $\mu$sec per particle
PPPM (9-point + PP); 550 $\mu$sec per particle.

## 5. Conclusions

The quiet high-resolution model conspicuously exhibits qualities hitherto unattained in particle–mesh models. In the absence of the direct particle–particle force contribution (QPM version), the short-range correction $\hat{G}''$ enables the mesh-induced force fluctuations to be supressed, while at the same time retaining the maximum physically meaningful information; we stress again that this correction can be used to improve any existing codes (e.g., CIC) which use a FFT method for determining the potential, without any increase in cycle time. The addition of the short-range force to form the PPPM model provides new flexibility to the established particle–mesh methods, bringing the study of microscopic properties of large ensembles of ionized particles within the compass of practicable simulations.

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