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Density-Conserving Shape Factors for Particle Simulations in Cylindrical and Spherical Coordinates

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It is shown that, in cylindrical and spherical coordinates, particle-to-grid weighting based on conventional particle-in-cell (PIC) and cloud-in-cell (CIC) shape factors results in non-uniform grid densities even for uniform particle distributions. Instead, alternative, density-conserving weighting schemes are discussed, including modified PIC and CIC weighting.

I. INTRODUCTION

The use of particle methods in numerical plasma simulation is now well established [1, 2]. In such calculations, electric potentials and fields are solved on a computational grid, while individual particles move within this grid, each representing a "cloud" of ions or electrons. An important step in such calculations is the assignment of particle charges to the grid, a process which is governed by a particle shape factor. Generally, this shape factor is not defined a priori, and there is considerable flexibility in choosing an appropriate expression. Examples of common shape factors are those based on particle-in-cell (PIC) or cloud-in-cell (CIC) weighting [1, 2], nearest-grid-point (NGP) weighting [1, 2], spline-weighting [1–4], gaussian-averaged-particle weighting [1], inverse distance weighting [5], and kernel methods that do not require a spatial grid but still carry the notion of finite particle clouds [6].

While an arbitrary number of requirements can be imposed in deriving expressions for a shape factor, any reasonable model must conserve charge. That is, for each particle, the sum of the fractional charges assigned to the grid must be equal to the total charge carried by the particle. In Section II, we argue that another reasonable requirement for a shape factor is that it must conserve charge *density* as well. That is, a uniform distribution of particles should render a uniform charge density on the grid upon particle-to-grid weighting. Although, in cartesian coordinates, this requirement appears to be satisfied for all of the weighting schemes mentioned above, we show in Section III that it is not satisfied for the common PIC and CIC weighting schemes in cylindrical and spherical coordinates.

To reconcile this situation, two approaches are possible. The first one is to modify the expression for the shape factor for a given problem. This is done in Sections IV and V, where alternative PIC and CIC weighting factors are derived, and density-conserving formulations of NGP weighting and spline weighting are discussed. The other approach relies on redefining the normalization volume that is used to obtain the charge density at a grid point from the charge on the grid point. This approach is described in Section VI. Conclusions are stated in Section VII.

II. PROBLEM STATEMENT

Let us define the particle shape factor for a given problem by $S_g(\mathbf{x}_p)$, where $\mathbf{x}_p$ is the coordinate of the particle, and the index g indicates the dependence on the grid. Charge localization is generally taken to imply that $S_g(\mathbf{x}_p)$ has a maximum (usually unity) when the particle is located exactly at a grid point ($\mathbf{x}_p = \mathbf{x}_g$) and falls to zero, roughly monotonically, within some distance, called the support or smoothing length of the shape factor. The requirement of charge conservation can now be expressed as

$$\sum_g S_g(\mathbf{x}_p) = 1, \qquad \text{all } \mathbf{x}_p. \tag{2.1}$$

In practice, the summation in Eq. (2.1) is only over a few grid points, namely those for which the shape factor is non-zero.

Next, in order to specify charge density, we note that in most particle calculations each grid point is embedded in a computational cell, whose boundaries are in between grid points. These cells are used, for example, to discretize Poisson's equation and to calculate the electric field on the grid from the potentials on the grid. Throughout our discussion, we assume that these cells are the natural choice for

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calculating charge densities from the charges on the grid points (the same is done, for example, in Ref. [1, p. 334], in deriving charge densities on a cylindrical grid using PIC weighting). Denoting the volume of these cells by V_g, we can thus define, for each cell, a charge density

$$\rho_g \equiv \frac{1}{V_g} \int S_g(\mathbf{x}_p)\, d\mathbf{x}_p, \tag{2.2}$$

where the integral is, in principle, over the entire computational domain, or, in practice, over only those cells for which the shape factor is non-zero. The normalized density from Eq. (2.2) may be interpreted as the expectation value of the charge density at individual grid points, given an infinite ensemble of homogeneously distributed particles with unit charge density on the grid. The requirement of conservation of charge density, then, we argue, is that for each gridpoint

$$\rho_g = 1, \qquad \text{all } g. \tag{2.3}$$

In other words, if a very large number of, say, equally charged particles is distributed homogeneously over the computational domain, the number of particles in each cell should be proportional to the volume of that cell.

For a further development of this concept we confine our discussion to a single coordinate and assume a bounded, not necessarily uniform, grid with grid points x_n, where n ranges from 0 through N, and where x_0 may or may not be at the origin of the coordinate system. This grid may represent either a one-dimensional, cartesian system ($D=1$), a two-dimensional cylindrical system ($D=2$), or a three-dimensional spherical system ($D=3$). The intervals on the grid thus represent line segments, circular rings, or spherical shells, respectively. The cell boundaries, located between grid points, are denoted by $x_{n\pm 1/2}$. Quite generally, these boundaries can be expressed in terms of the grid coordinates as

$$x_{n+1/2} = \alpha_n x_{n+1} + (1-\alpha_n)\, x_n = x_n + \alpha_n\, \Delta x_n, \tag{2.4}$$

where $\Delta x_n = x_{n+1} - x_n$, and $0 < \alpha_n < 1$. Usually, but not necessarily, $\alpha_n = \frac{1}{2}$, so that the cell boundaries are located midway between grid points.

Furthermore, we confine our discussion to shape factors with two-point support. Such two-point shape factors can be written in terms of a left-hand and a right-hand part as follows

$$S_n(x_p) = \begin{cases} S_n^-(x_p), & x_{n-1} \leqslant x_p \leqslant x_n, \\ S_n^+(x_p), & x_n \leqslant x_p \leqslant x_{n+1}, \\ 0, & \text{otherwise}, \end{cases} \tag{2.5}$$

where $S_n^-(x_n) = S_n^+(x_n)$ and it is understood that the factors $S_0^-(x_p)$ and $S_N^+(x_p)$ are not defined, since they fall outside of the computational domain. Charge localization is now expressed by the requirements

$$\begin{aligned} S_n^-(x_n) &= S_n^+(x_n) = 1, \\ S_n^-(x_{n-1}) &= S_n^+(x_{n+1}) = 0, \end{aligned} \tag{2.6}$$

and the charge conservation requirement from Eq. (2.1) implies that the right-hand and left-hand shape factors of neighboring grid points are simply related by

$$S_n^+(x_p) + S_{n+1}^-(x_p) = 1, \qquad x_n \leqslant x_p \leqslant x_{n+1}. \tag{2.7}$$

Because of this simple relationship, it suffices to specify only the, say, right-hand shape factors $S_n^+(x_p)$, as we do in the following.

With Eqs. (2.2) and (2.3), the requirement that charge density be conserved upon particle-to-grid weighting can be written as

$$\int_{x_{n-1}}^{x_{n+1}} S_n(x_p)\, x_p^{D-1}\, dx_p = \frac{1}{D}\,(x_{n+1/2}^D - x_{n-1/2}^D), \qquad x_n \leqslant x \leqslant x_{n+1}, \tag{2.8}$$

where the expression on the right-hand side is essentially the D-dimensional cell volume V_g from Eq. (2.2). For the zeroth grid point, both $x_{n-1/2}$ and x_{n-1} in Eq. (2.8) are replaced by x_0, whereas, for the last grid point, both $x_{n+1/2}$ and x_{n+1} are replaced by x_N. It is easy to show that, on a bounded or semi-infinite grid, the requirement from Eq. (2.8) must be satisfied for each half cell individually. That is, the right-hand shape factors $S_n^+(x_p)$ from Eq. (2.5) must satisfy the condition

$$\int_{x_n}^{x_{n+1}} S_n^+(x_p)\, x_p^{D-1}\, dx_p = \frac{1}{D}\,(x_{n+1/2}^D - x_n^D), \tag{2.9}$$

namely for all $0 \leqslant n < N$.

Below, we show how the common PIC and CIC weighting schemes violate this density conservation requirement in cylindrical and spherical coordinates, and we derive some alternative expressions without this difficulty. However, we offer no further justification for the density conservation requirement itself, beyond that mentioned above: namely, the notion that a homogeneous distribution of unit charges should populate each of the cells of the computational domain uniformly.

III. CONVENTIONAL PIC AND CIC WEIGHTING

Two charge assignment schemes that are commonly used in particle simulations are those based on particle-in-cell

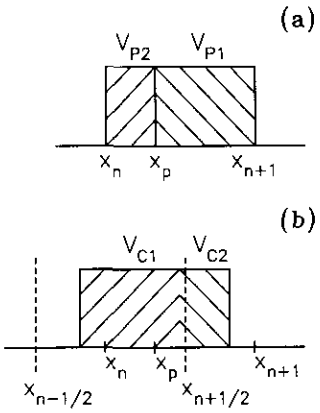

FIG. 1. Illustration of particle-in-cell (a) and cloud-in-cell weighting (b) for a particle at x_p, located between grid points x_n and x_{n+1}. In both cases, the width of the "cloud" is $\Delta x_n = x_{n+1} - x_n$, and the charge assigned to x_n is proportional to the shaded area with subscript "1." In (b), the values $x_{n\pm 1/2}$ indicate the cell boundaries.

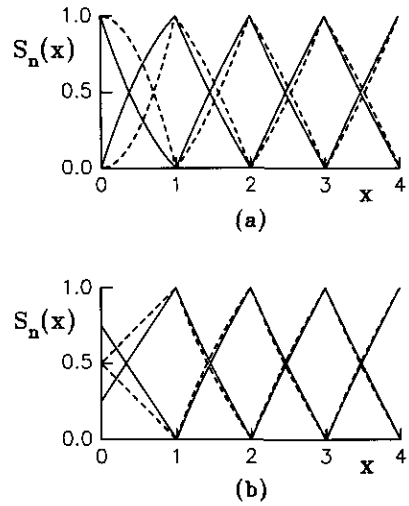

FIG. 2. Examples of cylindrical shape factors for a uniform grid with cell boundaries midway between grid points: (a) PIC weighting; (b) CIC weighting. The dashed curves correspond to the conventional, non-density-conserving shape factors from Section III. The solid curves represent the alternative, density-conserving shape factors from Section IV.

and cloud-in-cell weighting. Following the discussion in Ref. [1], shape factors for these methods are found, essentially, by inspection of a diagram like that shown in Fig. 1 (see also the figures on pages 21 and 309 in Ref. [1]).

In the PIC scheme, the shape factor is found by linear interpolation, area-weighting, or volume-weighting. Thus, a particle at position x_p, located between the grid points x_n and x_{n+1}, gives a right-hand shape factor

$$S_n^+(x_p) = \frac{V_{P1}}{V_{P1}+V_{P2}} = \frac{x_{n+1}^D - x_p^D}{x_{n+1}^D - x_n^D}, \tag{3.1}$$

where the volumes V_{P1} and V_{P2} are indicated in Fig. 1a. (We will use the term volume for each of the cases considered here, namely for dimensions $D=1$, $D=2$, as well as $D=3$.) Note that this PIC shape factor is independent of the cell boundaries between grid points, both in form and principle. Note also that this general shape factor satisfies the localization condition from Eq. (2.6), namely that it is equal to unity when the particle is located exactly at a grid point and that it falls to zero exactly at the neighboring grid points.

In the CIC scheme, the particle is conceived as a "rectangular" cloud of unit density, distributed symmetrically around the particle position x_p, with a width Δx_n equal to the distance between the two grid points that surround x_p. In this scheme, the shape factor is given by the fraction of the cloud which falls within the boundaries of the cell in which the nearest grid point is embedded. With the volumes V_{C1} and V_{C2} from Fig. 1b, the right-hand CIC shape factor is thus given by

$$S_n^+(x_p) = \frac{V_{C1}}{V_{C1}+V_{C2}} = \frac{(x_n + \frac{1}{2}\Delta x_n)^D - (x_p - \frac{1}{2}\Delta x_n)^D}{(x_p + \frac{1}{2}\Delta x_n)^D - (x_p - \frac{1}{2}\Delta x_n)^D}, \tag{3.2}$$

where $\Delta x_n = x_{n+1} - x_n$ and it has been assumed that the cell boundaries are midway between gridpoints, that is, $x_{n+1/2} = x_n + \frac{1}{2}\Delta x_n$. Note that Eq. (3.2) can be applied, without difficulty, at the boundaries of the grid. However, at the origin of a cylindrical coordinate system (that is, $D=2$ and $x_0 = 0$), the shape factor does not satisfy the usual localization condition from Eq. (2.6). Instead, $S_0^+(0) = S_1^-(0) = \frac{1}{2}$ for this case. Examples of PIC and CIC shape factors in both cylindrical and spherical coordinates are shown by the dashed curves in Figs. 2 and 3.

In order to address the conservation of charge density, then, let us first consider the case of cartesian coordinates. For this case, with $D=1$, it is easily seen that the PIC and CIC shape factors are identical for arbitrary choices of grid and particle coordinates [1, pp. 21, 309]. Also, it is easily verified that this linear PIC/CIC weighting satisfies Eq. (2.9) for arbitrary x_n and x_{n+1}, implying that the requirement for the conservation of charge density is satisfied.

Still, despite this seemingly obvious behavior in cartesian coordinates, some confusion exists over the application of the linear PIC/CIC shape factors at the boundaries of a computational domain. For example, in [7, p. 257], which

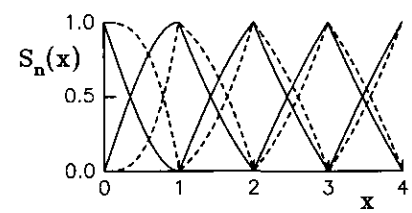

FIG. 3. Same as Fig. 2a for spherical PIC shape factors.

deals with a one-dimensional, bounded, cartesian grid, we read: "Thus, for diagnostic purposes, if nothing else, it is necessary to double the charge collected at the boundary to obtain the physical charge density." Actually, as stated in the same paragraph, the volume of the boundary cells is less than that of the other cells—namely one half. Thus, in this particular example, the correct approach to obtain the charge densities at the boundaries is not to double the charge density, but rather to divide the boundary charge by only half a "normal" cell volume.

While it may be argued that, in this example from Ref. [7], the results with either approach are the same and that, therefore, any confusion, if any, is over nomenclature only, a more serious problem exists in cylindrical and spherical coordinates, as is shown below. But before addressing the non-conservation of charge density in these systems, we point out that, unlike for the cartesian coordinates, PIC and CIC weighting give rise to different expressions for the shape factor. It appears that this fact has not been widely recognized; no comparitive discussions of PIC versus CIC weighting in non-cartesian coordinates are known to the author. An example of PIC weighting in cylindrical coordinates—simply referred to as area-weighting—can be found in Section 14–11 of Ref. [1]; an example of CIC weighting in cylindrical coordinates—although referred to as PIC weighting—can be found in Ref. [8]; another example of weighting in cylindrical coordinates can be found in Ref. [9], where it appears that a variation of CIC weighting is used.

So let us consider the issue of non-conservation of charge density with PIC and CIC weighting schemes in cylindrical and spherical coordinates. In cylindrical coordinates ($D=2$), the PIC shape factor from Eq. (3.1), using Eqs. (2.2), (2.4)—with $\alpha_n=\frac{1}{2}$, (2.5), (2.7), and (2.8), gives, for $0<n<N$, a normalized charge density

$$\rho_n=\frac{2(x_{n+1}+x_{n-1})}{x_{n+1}+2x_n+x_{n-1}}. \tag{3.3}$$

For $n=0$ and $n=N$, the correct normalized charge densities can be calculated either separately, or they can be obtained from Eq. (3.3) by setting $x_{n-1}=0$ and $x_{n+1}=0$, respectively. From Eq. (3.3), it follows that $\rho_n\neq 1$, in general, implying non-conservation of charge density. For a uniform grid with $x_{n\pm1}=x_n\pm\Delta x$, where Δx is constant for the whole grid, the situation may seem a little better. Namely, for such a uniform grid, $\rho_n=1$ for all interior points on the grid. However, non-unit densities result at the boundaries. In particular, $\rho_N\simeq\frac{2}{3}$ at the outer boundary, and, for $x_0=0$, $\rho_0=2$ at the inner boundary. We emphasize that, unlike in the example from Ref. [7] discussed above, these non-unit densities at the boundaries are *not* merely the result of confusion over the correct choice of the normalization volume. Rather, they are intrinsic to the PIC area-weighting scheme. Also, we emphasize that one cannot resolve this difficulty by modifying the PIC shape factor only at the grid boundaries, because, in the process of particle-to-grid weighting, cells generally collect charge from particles both to the left as well as to the right of the embedded grid point. That one cannot suffice by altering the shape factors only at the boundaries follows also by inspection of Eq. (2.7), which shows that, if S_0^+ is modified, S_1^- must be modified also. In turn, then, S_1^+ must be modified to retain unit density in the first cell, and so on.

A similar discussion applies to the cylindrical CIC shape factors from Eq. (3.2). For these, the normalized charge densities become, again assuming cell boundaries midway between grid points ($\alpha_n=\frac{1}{2}$ in Eq. (2.4)),

$$\rho_n=\frac{2}{3}\left(\frac{x_{n+1}+4x_n+x_{n-1}}{x_{n+1}+2x_n+x_{n-1}}\right), \tag{3.4}$$

valid for $0<n<N$. Again, the normalized densities at the boundaries may be obtained by setting $x_{n-1}=0$ for $n=0$, and by setting $x_{n+1}=0$ for $n=N$. As in the case of PIC weighting in cylindrical coordinates, CIC weighting produces unit charge densities at the interior points of a uniform grid. But this time, the density at the inner boundary is too small, namely $\rho_0=\frac{2}{3}$ for $x_0=0$, and the density at the outer boundary is too large, namely $\rho_N\simeq\frac{10}{9}$. As is the case for the PIC scheme, one cannot simply correct these results by modifying the shape factors at the boundaries.

Finally, we consider briefly the case of spherical coordinates ($D=3$). After the above discussion, it should not come as a surprise that, for this case, neither PIC nor CIC weighting conserve charge density in general. In fact, not even at the interior points of a uniform grid is the correct density produced. For example, for uniform grids with $x_0=0$ and $\alpha_n=\frac{1}{2}$, spherical PIC weighting yields the normalized densities

$$\rho_n=\begin{cases}(12n^2+4)/(12n^2+1), & 0\leqslant n<N,\\ (4N^2-8N+4)/(7N^2-5N+1), & n=N.\end{cases} \tag{3.5}$$

That is, $\rho_0=4$ at the origin, a particularly poor value, and $\rho_N\simeq\frac{4}{7}$ at the outer boundary. For spherical CIC weighting, some rather complicated expressions result. Here we suffice by stating that the normalized density at the origin of a spherical grid is given by

$$\rho_0=\tfrac{1}{3}+\tfrac{2}{9}\ln 13-(\operatorname{atan}\sqrt{12})/\sqrt{12}\simeq 0.531, \tag{3.6}$$

a value worse than that obtained at the origin of a cylindrical coordinate system with CIC weighting.

In summary, although PIC and CIC weighting conserve charge density for a cartesian coordinate system, charge density is not conserved in cylindrical and spherical coordinates. Non-conservation of the charge density is

particularly noticeable at the boundaries of the grid, and it is worse for spherical coordinates than it is for cylindrical coordinates. Also, it is worse for PIC weighting than it is for CIC weighting. In the next section, we show how this situation can be remedied easily by alternative choices for the shape factors.

IV. ALTERNATIVE PIC AND CIC SHAPE FACTORS

In this section we derive several cylindrical and spherical shape factors that conserve charge density on an arbitrary radial grid. We refer to these as alternative PIC and CIC shape factors primarily because their mathematical form is very similar to the conventional PIC and CIC shape factors discussed in Section III. In Sections V and VI, we consider several more particle-to-grid weighting schemes that conserve charge density also.

Let us start with the following general polynomial expression for the (right-hand) shape factor of the nth cell:

$$S_n^+(x)=\frac{x_{n+1}-x}{x_{n+1}-x_n}\left[1+(x-x_n)\times\left(\frac{a_{-1}}{x}+a_0+a_1x+\cdots\right)\right]. \tag{4.1}$$

For convenience, we have used x for the particle position x_p, and the a_j's are arbitrary parameters. This shape factor satisfies the localization conditions from Eq. (2.6) for arbitrary coefficients a_j, namely $S_n^+(x_{n+1})=0$, and $S_n^+(x_n)=1$, unless $x=x_n=0$ and $a_{-1}\neq 0$, as is the case for the cylindrical CIC shape factor from Eq. (3.2). Substitution of the general expression from Eq. (4.1) into the charge density conservation requirement from Eqs. (2.8) or (2.9) now yields a requirement for the parameters a_j, solution of which renders the coefficients a_j in terms of the dimension D, the grid points x_n and x_{n+1}, and the cell boundary parameters α_n.

So let us consider application of this procedure to a cylindrical grid with cell boundaries midway between grid points ($\alpha_n=\frac{1}{2}$). For this case, the conventional PIC shape factor from Eq. (3.1) can be written in the form of Eq. (4.1) using only one of the coefficients a_j, namely $a_0=(x_n+x_{n+1})^{-1}$. Retaining, again, only the coefficient a_0 in the general polynomial from Eq. (4.1), but requiring conservation of charge density as expressed by Eq.(2.9), we find, in terms of the above value of a_0, the requirement that $a_0'=-\frac{1}{2}a_0$. Substituting this new value a_0' back into Eq. (4.1), the alternative, charge-density-conserving cylindrical PIC shape factor becomes

$$S_n^+(x)=\frac{3}{2}\left(\frac{x_{n+1}-x}{x_{n+1}-x_n}\right)-\frac{1}{2}\left(\frac{x_{n+1}^2-x^2}{x_{n+1}^2-x_n^2}\right)=\frac{(x_{n+1}-x)(2x_{n+1}+3x_n-x)}{2(x_{n+1}^2-x_n^2)}. \tag{4.2}$$

That is, the alternative form of the cylindrical PIC shape factor is a linear combination of the conventional linear and cylindrical PIC shape factors. Note that the latter expression is more computationally efficient than the former, because, with appropriate precalculated factors, only one multiplication and one division are required per particle position x. This alternative cylindrical PIC shape factor is illustrated by the solid curves in Fig. 2a. The difference with the conventional PIC shape factors, illustrated by the dashed curves in Fig. 2a, is most noticeable near the origin, where, as shown in Section III, conventional PIC weighting gives rise to the largest violation of conservation of charge density.

Similarly, we note that the conventional cylindrical cloud-in-cell shape factor from Eq. (3.2) can be expressed in terms of the general polynomial from Eq. (4.1) with only a single non-vanishing coefficient a_j, namely $a_{-1}=-\frac{1}{2}$. With Eq. (2.9), it follows that charge density is conserved, instead, with the alternative value $a'_{-1}=\frac{1}{2}a_{-1}=-\frac{1}{4}$. Thus, an alternative, charge-density-conserving formulation of cylindrical CIC weighting is given by the shape factor

$$S_n^+(x)=\frac{x_{n+1}-x}{x_{n+1}-x_n}\left(\frac{3+x_n/x}{4}\right). \tag{4.3}$$

This alternative CIC shape factor is illustrated by the solid curves in Fig. 2b, along with the conventional CIC shape factors, represented by the dashed curves. Again, the difference between the two sets of shape factors is most noticeable near the origin. Note also that, just as for the conventional cylindrical CIC shape factors, a non-unit value of the shape factor results for $x=x_0=0$, namely $S_0^+(0)=\frac{3}{4}$. If this feature is undesirable, one could replace, on the interval $x_0\leqslant x<x_1$, the CIC shape factor from Eq. (4.3) by the PIC shape factor from Eq. (4.2). Indeed, because the PIC and CIC shape factors from Eqs. (4.2) and (4.3) conserve charge density for each half cell individually, one can choose different expressions for the shape factor on each grid interval, if desired.

Next, we consider the case of PIC weighting in spherical coordinates. Expressing the PIC shape factors from Eq. (3.1), with $D=3$, in terms of the general polynomial from Eq. (4.1), we find that two of the coefficients a_j are non-vanishing, namely a_0 and a_1, which are given by $a_0=(x_{n+1}+x_n)\,a_1=(x_n^2+x_nx_{n+1}+x_{n+1}^2)^{-1}$. To conserve charge density, alternative values must be chosen, namely so as to satisfy Eq. (2.9). Although an infinite number of combinations of a_0 and a_1 can be found with this property, an aesthetically pleasing result is obtained by retaining the same ratio between the two coefficients a_0 and a_1. This gives, in terms of the above values, $a_0'=-\frac{1}{2}a_0$ and $a_1'=-\frac{1}{2}a_1$. Substitution of these values into Eq. (4.1) then yields a shape factor that can be written as a linear combina-

tion of the linear and spherical PIC shape factors from Section III, namely,

$$S_n^+(x)=\frac{3}{2}\left(\frac{x_{n+1}-x}{x_{n+1}-x_n}\right)-\frac{1}{2}\left(\frac{x_{n+1}^3-x^3}{x_{n+1}^3-x_n^3}\right). \qquad (4.4)$$

Note the strong similarity of this expression for the alternative spherical shape factor with that for the alternative cylindrical shape factor from Eq. (4.2). As is the case for the alternative PIC shape factor from Eq. (4.2), the expression in Eq. (4.4) may be rewritten slightly to reduce the number of operations that are required during actual computation. Conventional and alternative spherical PIC shape factors are shown in Fig. 3. Again, the differences between the two are most noticeable near the origin.

Finally, we consider very briefly the case of spherical CIC weighting. In this case, it is actually too cumbersome to write the shape factor from Eq. (3.2) in terms of Eq. (4.1), because of the occurrence of a factor $12x^2+(x_{n+1}-x_n)^2$ in the denominator—it is this type of denominator that gives rise to the non-rational result for the charge density in Eq. (3.6). Of course, it is still possible to derive alternative expressions for the shape factor that do conserve charge density. However, we leave this exercise for the interested reader.

V. NEAREST-GRID-POINT AND SPLINE WEIGHTING

In most applications, especially those in which conventional PIC and CIC weighting have been used, the alternative PIC and CIC shape factors from the previous section should be adequate. Here, we discuss several more density-conserving shape factors that are variations on weighting schemes that have been used elsewhere, namely nearest-grid-point weighting and spline weighting, which are, respectively, coarser and smoother than either PIC or CIC weighting.

First, we consider the case of nearest-grid-point (NGP) weighting. In this method, the value of the shape factor is either unity or zero, and all of the charge carried by the particle is assigned to the grid point nearest to the particle. From the density conservation requirement from Eq. (2.9), it is immediately obvious that this weighting scheme conserves charge density in an arbitrary coordinate system as long as the concept of nearness is interpreted as the particle being located inside of the cell to which the charge is to be assigned. For two-point weighting with cell boundaries midway between grid points, the two criteria are equivalent. But, for example, for cylindrical coordinates with azimuthal dependence, they are not. This is illustrated in Fig. 4, in which particles that are located inside the shaded region are closer to the grid point (r_n, ϕ_n), yet need to be assigned to the grid point (r_{n+1}, ϕ_n) to achieve conservation of charge density. Thus, in this particular example, the term "nearest" should apply, independently, to the radial and azimuthal coordinates, rather than to the actual distance from the particle to the grid points. Similar considerations apply in the case of spherical or other coordinates.

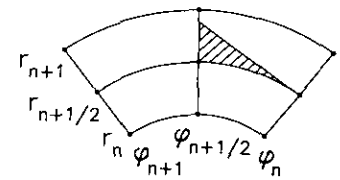

FIG. 4. Illustration of nearest-grid-point weighting for cylindrical coordinates with azimuthal dependence. To conserve charge density, particles located inside the shaded area must be assigned to the upper right grid point, even though they are actually closer to the lower right grid point.

Returning to the case of two-point, single-coordinate shape factors, we now derive some further density-conserving weighting schemes. But, before doing this, let us consider, for simplicity, a dimensionless formulation of the problem. Specifically, we introduce a dimensionless particle coordinate $\xi_n \equiv (x_p-x_n)/(x_{n+1}-x_n)$, which varies from 0 to 1 as the particle moves between the grid points x_n and x_{n+1}, and we write the corresponding right-hand shape factor as $\tilde{S}_n^+(\xi_n)$. The requirement for conservation of charge density from Eq. (2.9) can now be expressed in terms of the moments $M_{n,k}$ of the shape factor, defined by

$$M_{n,k}=\int_0^1 \tilde{S}_n^+(\xi_n)\,\xi_n^k\,d\xi_n. \qquad (5.1)$$

Namely, for arbitrary grid coordinates x_n and x_{n+1}, arbitrary dimensions D, and arbitrary cell boundary parameters α_n, conservation of charge density as imposed by Eq. (2.9) is assured if these moments satisfy the condition

$$\sum_{k=0}^{D-1}\binom{D-1}{k}x_n^{D-1-k}(x_{n+1}-x_n)^k \times\left(M_{n,k}-\frac{\alpha_n^{k+1}}{k+1}\right)=0. \qquad (5.2)$$

In addition, localization of the shape factor can be imposed by the usual boundary conditions

$$\tilde{S}_n^+(0)=1, \qquad \tilde{S}_n^+(1)=0. \qquad (5.3)$$

With Eqs. (5.1)–(5.3), it is straightforward to solve for any adjustable parameters in a given general expression for the shape factor, such as that of Eq. (4.1) in the previous section.

With reference to the requirement of conservation of charge density as expressed by Eq. (5.2), we note that not each of the terms in the summation from Eq. (5.2) have to vanish separately. However, if they do, namely if the moments satisfy the condition

$$M_{n,k} = \alpha_n^{k+1}/(k+1), \qquad 0 \leqslant k \leqslant D-1, \qquad (5.4)$$

the special situation is obtained in which the dimensionless shape factor is independent of the grid coordinates x_n and x_{n+1}. Such is the case, for example, for linear PIC/CIC weighting with grid boundaries midway between grid points. Namely, in this case, $\tilde{S}_n^+(\xi_n) = 1 - \xi_n$, so that the zeroth moment is equal to $\frac{1}{2}$, and Eq. (5.4) is satisfied indeed. Generally, however, more complicated expressions for the shape factor result if it is required to satisfy the stricter requirement from Eq. (5.4) as opposed to the sufficient requirement from Eq. (5.2). For example, to satisfy Eqs. (5.3) and (5.4) for cell boundaries midway between grid points in cylindrical coordinates, a cubic polynomial is required, namely $\tilde{S}_n^+(\xi_n) = 1 + \frac{3}{2}\xi_n - \frac{15}{2}\xi_n^2 + 5\xi_n^3$. Of course, in terms of the required number of operations per particle position, this expression is less economical than the quadratic form of the alternative cylindrical PIC shape factor from Eq. (4.2) in the previous section.

Requiring only the general requirement from Eq. (5.4) to be satisfied—as opposed to the stricter requirement from Eq. (5.2)—we mention here two more two-point weighting schemes that do not only satisfy the localization requirements from Eq. (5.3) and conserve charge density, but that possess another property as well: namely, that they vary smoothly as the particle moves through a computational cell. In particular, we impose, in addition to the boundary condition from Eq. (5.3), the requirement that $d\tilde{S}_n^+/d\xi_n = 0$ for both $\xi_n = 0$ and for $\xi_n = 1$. The simplest shape factor with this property, in terms of the required number of operations per particle-to-grid weighting, is given by the quadratic spline

$$\tilde{S}_n^+(\xi_n) = \begin{cases} 1 - \xi_n^2/s_n, & 0 \leqslant \xi_n \leqslant s_n, \\ (1-\xi_n)^2/(1-s_n), & s_n \leqslant \xi_n \leqslant 1, \end{cases} \qquad (5.5)$$

where the knots s_n are found by substituting Eq. (5.5) into Eqs. (5.1) and (5.2). In the case of spherical coordinates, this leads to a cubic equation for the knots s_n. For cylindrical coordinates, a quadratic expression results, for example, $2ps_n^2 + 2s_n = 1$ for grid boundaries midway between grid points, where p is given in terms of the grid coordinates x_n and x_{n+1}, namely, $p = (x_{n+1} - x_n)/(x_{n+1} + 3x_n)$. For values of the cell boundary parameter α_n other than $\frac{1}{2}$, the resulting values of s_n are in the proper range, namely $0 < s_n < 1$, as long as $1/\sqrt{6} < \alpha_n < \frac{2}{3}$, or $0.408 \lesssim \alpha_n \lesssim 0.667$.

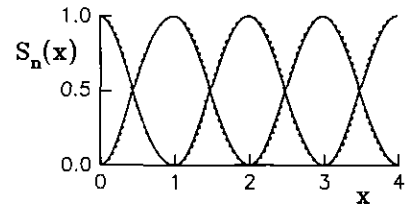

FIG. 5. Illustration of the smoothly varying, density-conserving shape factors from Section V; solid and dashed curves represent the spline from Eq. (5.5), and the equivalent expression from Eq. (5.6), respectively.

Another expression for the shape factor that has zero derivatives at the grid points is given by the polynomial

$$\tilde{S}_n^+(\xi_n) = [1 - \xi_n^2(1 - t_n + t_n\xi_n)]^2. \qquad (5.6)$$

This expression requires at least four multiplications per particle-to-grid weighting, but does not require a logical operation as does the above spline—and may therefore be programmed on a machine with vector-processing capabilities. For cylindrical coordinates, conservation of charge density as imposed by Eqs. (5.1) and (5.2) leads again to a quadratic expression, namely in terms of the parameter t_n. This expression has well-behaved solutions if $(\frac{18}{175})^{1/2} < \alpha_n < \frac{9}{14}$, or $0.321 \lesssim \alpha_n \lesssim 0.643$—for smaller values, the value of t_n becomes complex; for larger values, $\tilde{S}_n^+(\xi_n)$ becomes larger than unity on part of the interval $0 < \xi_n < 1$. Figure 5 displays the smoothly varying shape factors from Eqs. (5.5) and (5.6) for the case of cell boundaries midway between grid points. Note that, on the entire interval, the difference between the two cases is quite small. For the case of spherical coordinates, the general expressions from Eqs. (5.5) and (5.6) can be used as well. In this case, cubic expressions for the parameters s_n and t_n have to be solved before the shape factors can be calculated.

VI. REVERSE APPROACH: CHOOSING CELL BOUNDARIES

Finally, we discuss one more approach to achieving correct charge densities in the process of particle-to-grid weighting. This approach is, in essence, the reverse of the techniques discussed above. Namely, instead of selecting a density-conserving shape factor for a given choice of cell boundaries, this approach seeks to adjust the cell boundaries so that, for a given shape factor, the correct densities are obtained. Thus, instead of choosing an expression for the shape factor whose moments satisfy Eq. (5.2) for a given value of α_n, the cell boundary parameter α_n is chosen to satisfy Eq. (5.2) for a given shape factor. Or, equivalently, in terms of the non-dimensionless expressions for the conservation of charge density in Section II, the cell boundaries $x_{n+1/2}$—which depend on α_n as expressed in Eq. (2.4)—are chosen so as to satisfy Eq. (2.9).

As an example of this approach, let us consider the conventional PIC weighting scheme for cylindrical coordinates as given by Eq. (3.1) with $D=2$. As shown in Section III, this shape factor does *not* produce the correct charge densities for the conventional choice of cell boundaries midway between grid points. However, as is easily verified with Eqs. (2.4) and (2.9), or with Eqs. (5.1) and (5.2) in the previous section, correct charge densities result if the cell boundaries $x_{n+1/2}$ are chosen according to

$$x_{n+1/2}^2 = \tfrac{1}{2}(x_n^2 + x_{n+1}^2). \tag{6.1}$$

For example, the cell boundary enclosing the origin would be located at $x_{n+1/2} = x_1/\sqrt{2}$ instead of at $x_{n+1/2} = x_1/2$, as is normally the case. However, if one takes the approach that cell boundaries can be freely adjusted to render correct charge densities for arbitrary shape factors, one could just as well use the linear PIC weighting scheme in cylindrical coordinates, namely that given by Eq. (3.1) with $D=1$. Namely, using the approach of adjusting cell boundaries, correct densities are again obtained in cylindrical coordinates, even for linear PIC/CIC weighting, if the values of $x_{n+1/2}$ are chosen according to

$$x_{n+1/2}^2 = \tfrac{1}{3}(x_{n+1}^2 + x_{n+1}x_n + x_n^2), \tag{6.2}$$

yielding, for example, a cell boundary at $x_{n+1/2} = x_1/\sqrt{3}$ around the origin. Similarly, either linear, quadratic, or cubic (conventional) PIC weighting can be rendered density-conserving in spherical coordinates if cell boundaries are adjusted in an appropriate manner. Quite generally, it follows from Eq. (5.2) that, for any given shape factor, the dimensionless cell boundary parameters α_n are in the range

$$0 < M_{n,0} < \alpha_n \leqslant (DM_{n,D-1})^{1/D} \leqslant 1, \tag{6.3}$$

where the upper limit applies at the origin of the coordinate system, namely at $x_0 = 0$, and the lower limit applies at the outer boundary, where $1 - x_n/x_{n+1} \ll 0$.

From a practical standpoint, the "reverse approach" of selecting cell boundaries so as to yield correct charge densities is as straightforward to implement as the approach of selecting an expression for the shape factor that conserves charge density for a given choice of cell boundaries. However, the question arises if this approach is consistent with the finite difference techniques that are used simultaneously with particle-to-grid weighting in typical particle simulations. For example, if the discretization scheme for Poisson's equation assumes grid boundaries midway between grid points, it seems inconsistent to choose cell boundaries in different locations merely for the purpose of calculating charge densities. This matter of consistency will not be addressed further here, as it requires a more complete analysis of the particle simulation method, which is beyond the scope of this work. However, from consistency considerations alone, it seems, at least to the author, that the techniques from Sections III–V constitute the more desirable approach, namely, to select an expression for the shape factor that, for a given choice of cell boundaries, yields correct charge densities on the computational grid.

VII. CONCLUSIONS

We have shown that, although, in plasma particle simulations, it is taken for granted that the total charge in the system must be conserved in the process of particle-to-grid weighting, conservation of charge density is not guaranteed for arbitrary weighting schemes, particularly for cylindrical and spherical coordinates. Namely, for these latter two systems, we have shown that the much-used PIC and CIC weighting schemes do not result in uniform charge densities on the grid, even for a uniform distribution of particles. This effect is most pronounced at the boundaries of the grid, but is, actually, intrinsic to the definition of the shape factor for the whole grid. Thus, one cannot apply a correction factor only at the boundaries to remedy the situation.

Instead, we have shown, quite generally, how the nonconservation of charge density can be overcome, and we have derived, specifically, a number of alternative shape factors that conserve charge as well as charge density. These are given in Eqs. (4.2) and (4.3) for alternative PIC and CIC weighting in cylindrical coordinates, and in Eq. (4.4) for alternative PIC weighting in spherical coordinates. Mathematically, these alternative shape factors are no more complicated than the conventional, non-density-conserving expressions, so that they can be implemented without any penalty of increased computational time.

A second approach has been presented also, namely one in which no modification to a given shape factor is required, but, instead, the location of cell boundaries is modified. Thus, different normalization volumes are obtained by which charges on the grid can be converted to charge densities on the grid. Since, however, cell boundaries are normally chosen as the basis for a finite difference formulation of the electrostatic or electromagnetic interactions between the plasma particles, the conceptual difficulty arises with this alternative approach of having two different sets of cell boundaries in the same calculation. A comparative study of the merits of the two methods, namely adjusting the shape factor on the one hand and adjusting the normalization volumes on the other hand, is beyond the scope of this discussion, but warrants further investigation.

It was also beyond the scope of this work to carry out a series of numerical simulations to compare the performance and accuracy of conventional and alternative PIC and CIC weighting factors. Differences between the two should be most pronounced in calculations in which relatively few grid points are used and in situations where large gradients in particle densities exist near the origin in cylindrical or spherical grids. Finally, it would seem logical that, when

using the alternative weighting schemes discussed here, identical schemes be used for particle-to-grid weighting and for the reverse process of grid-to-particle weighting for the purpose of calculating electric and magnetic fields at the particle positions. However, this subject, also, may warrant some further analysis.

In summary, then, this work has shown that care must be taken when calculating charge densities in plasma particle simulations on non-cartesian grids, and we have described several approaches that circumvent the problem of yielding non-uniform charge densities for uniform plasma distributions, as is the case with conventional weighting schemes.

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