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# Symmetric Spline Weighting for Charge and Current Density in Particle Simulation

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A general method for computing charge and current density source terms for Maxwell's equations from particles weighted to a mesh is described. The method presented here eliminates the need for correction factors often applied in curvilinear coordinates to compensate for errors at the edge of the system, and applied in the interior as well for nonuniform meshes. Generality is achieved by weighting volume elements using a spline symmetric to that by which particle charge and current are weighted to the mesh. The method presented has a number of desirable properties, including conservation of charge, preservation of a uniform distribution, and generality on nonuniform meshes with arbitrary particle–mesh interpolation schemes. The method recovers the exact answer in the limit of mesh sizes approaching zero. 

*Key Words:* PIC; particle; weighting; radial; cylindrical; spherical; correction.

## 1. INTRODUCTION

In charge and current accumulation schemes commonly used in particle-in-cell codes, a systematic error occurs on the boundary cells in curvilinear coordinates. The error is particularly severe on the axis in cylindrical and spherical models, with systematic errors 33 and 100% larger than the theoretical value for either charge or current density in cylindrical and spherical coordinates, respectively. Additional error occurs at the outer edge of the system, and throughout the interior for nonuniform meshes. This error leads to similar errors in the forces calculated at those points, as well as to the exacerbation of radial noise due to particle statistics, which is largest near $r = 0$. The errors in density do *not* decrease with decreasing mesh size. This problem is not present in Cartesian coordinates, even for nonuniform meshes.

The issue of radial correction factors for the charge density term has been addressed in recent works by Ruyten [1] and by Larsen *et al.* [2]. These works derive the error for linear weighting to uniform meshes in cylindrical coordinates and propose correction terms.



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In [1], the author states that the axial behavior is beyond the scope of the work. In [2], the analysis carried out includes the origin, and the proposed correction is shown to approach the theoretical value for large numbers of particles. We demonstrate that the result of [2] is exact for the uniform charge density case despite errors shown in that paper for charge density at the axis.

In this work, the error is analyzed for the uniform particle density distribution for the charge density, $\rho$. A general scheme is developed which applies the same interpolation scheme to both the particle and the volume or surface element in order to obtain a density which eliminates the systematic error in curvilinear coordinates. The new scheme is compared with analytic theory in cylindrical and spherical coordinates. The algorithm is extended to the current density, $J$.

## 2. DENSITY ERRORS

In this section, the errors in the most common interpolation scheme used in particle simulation [3], linear weighting, are demonstrated for uniform density in one dimension on a nonuniform mesh in cylindrical and spherical coordinates. For an arbitrary continuum particle distribution specified by $f(r)$, the exact density in cylindrical coordinates is given by

$$n(r) = \frac{\int_r^{r+dr} f(r')\,dr'}{\int_r^{r+dr} 2\pi r'\,dr'}. \tag{1}$$

For the uniform particle distribution, $f(r) = 2\pi r$, and we obtain $n(r) = 1$. Similarly, in spherical coordinates for the uniform particle distribution $f(r) = 4\pi r^2$ we obtain

$$n(r) = \frac{\int_r^{r+dr} f(r')\,dr'}{\int_r^{r+dr} 4\pi (r')^2\,dr'} = 1. \tag{2}$$

In the classical particle scheme [3], the cell volumes are computed from geometric considerations independently of the weighting scheme used to accumulate charge to the grid. Because the volume elements are nonlinear in the spatial variable for curvilinear coordinates, this leads to systematic errors. This conceptual error is precisely why the previous works [1, 2] describe corrections to the weighting scheme. For linear weighting on a nonuniform mesh in cylindrical coordinates, we can write the density at an arbitrary intermediate node for an arbitrary particle distribution $f(r)$ in the standard way [3] in order to make the conceptual error more apparent. That is,

$$n_j = \frac{\int_{r_{j-1}}^{r_j} f(r)\frac{r - r_{j-1}}{r_j - r_{j-1}}\,dr + \int_{r_j}^{r_{j+1}} f(r)\frac{r_{j+1} - r}{r_{j+1} - r_j}\,dr}{\int_{r_{j-1/2}}^{r_{j+1/2}} 2\pi r\,dr}, \tag{3}$$

where $r_j$ refers to the position of the $j$th mesh, and $r_{j+1/2} \equiv (r_j + r_{j+1})/2$. The edge

densities are written (valid also on axis, $r_0 = 0$) as

$$n_0 = \frac{\int_{r_0}^{r_1} f(r)\frac{r_1 - r}{r_1 - r_0}\,dr}{\int_{r_0}^{r_{1/2}} 2\pi r\,dr} \tag{4}$$

and

$$n_N = \frac{\int_{r_{N-1}}^{r_N} f(r)\frac{r - r_{N-1}}{r_N - r_{N-1}}\,dr}{\int_{r_{N-1/2}}^{r_N} 2\pi r\,dr}. \tag{5}$$

For a uniform particle distribution, $f(r) = 2\pi r$, the standard discrete densities in Eqs. (3)–(5) become

$$n_j = \frac{4}{3}\frac{r_{j-1} + r_j + r_{j+1}}{r_{j-1} + 2r_j + r_{j+1}}, \tag{6}$$

$$n_0 = \frac{4}{3}\frac{2r_0 + r_1}{3r_0 + r_1}, \tag{7}$$

and

$$n_N = \frac{4}{3}\frac{r_{N-1} + 2r_N}{r_{N-1} + 3r_N}. \tag{8}$$

On a nonuniform mesh, the linear weighting with uncorrected volumes always produces the incorrect result for all cells. For a uniform mesh, we see from inspection of Eq. (6) that the correct solution is produced for the interior cells, but the systematic error persists at the edges. For nonuniform meshes, the error occurs at interior points as well. The systematic error is $1/3$ on axis for meshes which include the axis and is independent of grid spacing $\Delta_r$. Note that the error in the outer edge is small for $N \gg 1$. The uncorrected results for a uniform and nonuniform mesh are plotted in Fig. 1.

A similar development for linear weighting in spherical coordinates for the uniform particle distribution, $f(r) = 4\pi r^2$, gives

$$n_j = 2\frac{r_{j-1}^2 + r_{j-1}r_j + r_{j-1}r_{j+1} + r_j^2 + r_j r_{j+1} + r_{j+1}^2}{r_{j-1}^2 + 3r_{j-1}r_j + r_{j-1}r_{j+1} + 3r_j^2 + 3r_j r_{j+1} + r_{j+1}^2}, \tag{9}$$

$$n_0 = 2\frac{3r_0^2 + 2r_0 r_1 + r_1^2}{7r_0^2 + 4r_0 r_1 + r_1^2}, \tag{10}$$

and

$$n_N = 2\frac{r_{N-1}^2 + 2r_{N-1}r_N + 3r_N^2}{r_{N-1}^2 + 4r_{N-1}r_N + 7r_N^2}. \tag{11}$$

For uniform mesh spacing, $\Delta_r$, Eqs. (9)–(11) become

$$n_j = 2\frac{6r_j^2 + \Delta_r^2}{12r_j^2 + \Delta_r^2}, \tag{12}$$

$$n_0 = 2\frac{6r_0^2 + 4r_0\Delta_r + \Delta_r^2}{12r_0^2 + 6r_0\Delta_r + \Delta_r^2}, \tag{13}$$

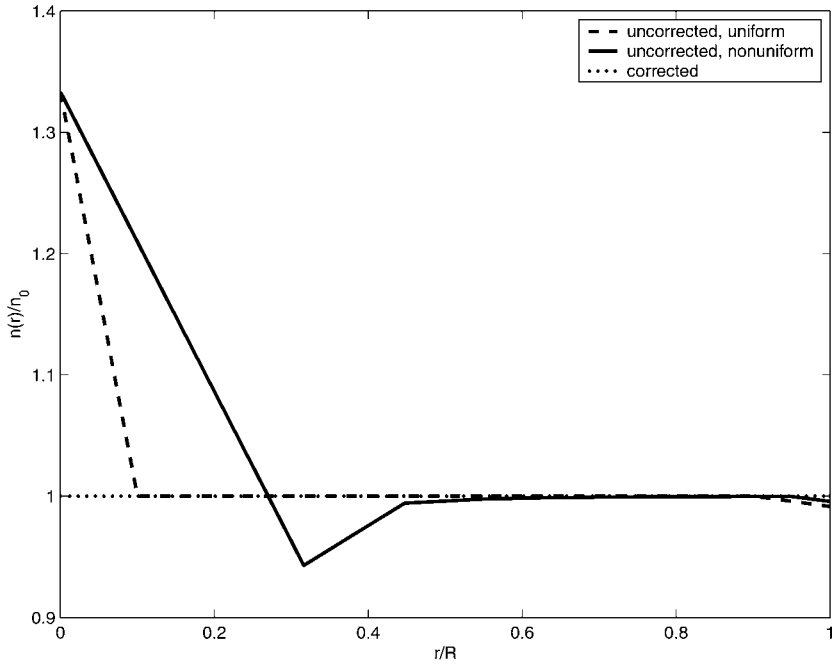


**FIG. 1.** Mesh densities computed using standard linear weighting (uncorrected) on a uniform and nonuniform mesh in cylindrical coordinates, as well as the corrected density on both meshes. The uniform mesh has $N = 10$ steps; the nonuniform mesh is computed from $r_j = \sqrt{r_{j-1}^2 + (r_N^2 - r_0^2)/N}$, such that the interval contains $N = 10$ equal volumes.

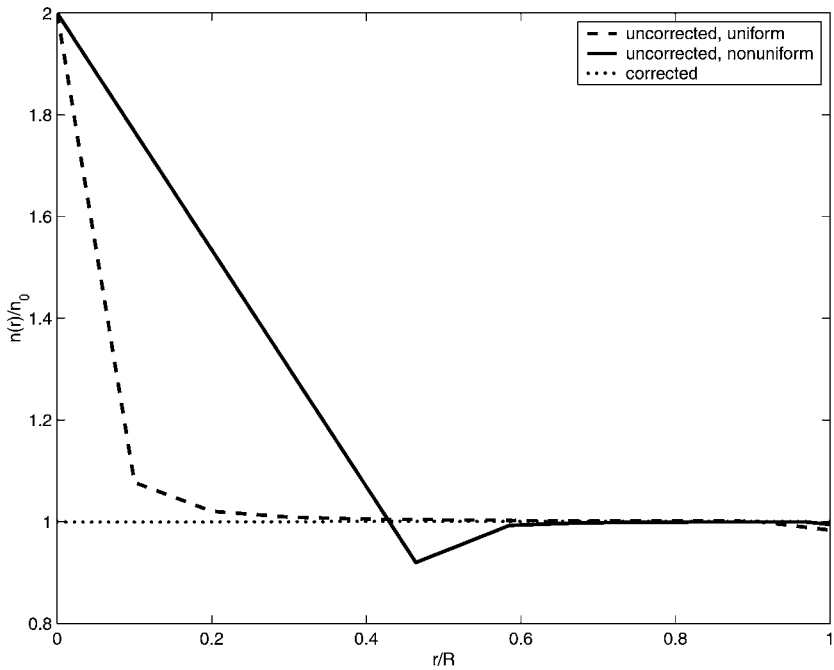


**FIG. 2.** Mesh densities computed using standard linear weighting (uncorrected) on a uniform and nonuniform mesh in spherical coordinates, as well as the corrected density on both meshes. The uniform mesh has $N = 10$ steps; the nonuniform mesh is computed from $r_j = [r_{j-1}^3 + (r_N^3 - r_0^3)/N]^{1/3}$, such that the interval contains $N = 10$ equal volumes.

and

$$n_N = 2\frac{6r_N^2 - 4r_N\Delta_r + \Delta_r^2}{12r_N^2 - 6r_N\Delta_r + \Delta_r^2}. \tag{14}$$

Note that the uncorrected density for the spherical case is always in error, approaching the correct solution only for $r_j \gg \Delta_r$. The uncorrected results for a uniform and nonuniform mesh are plotted in Fig. 2. The systematic error is 100% on axis for meshes which include the axis, independent of grid spacing $\Delta_r$.

## 3. IMPROVED DENSITY-WEIGHTING ALGORITHM

In this section, a general algorithm is developed for computing the charge density in nonuniform meshes for curvilinear coordinates using arbitrary particle–mesh interpolation. Consider a modified calculation for the volume in which differential volume elements are weighted to the mesh using the same algorithm as the charge weighting. A general method is suggested by the definition of density in cylindrical (Eq. (1)) and spherical (Eq. (2)) coordinates, weighting both the charge and the volume. That is,

$$n_{\mathbf{j}} = \frac{\int_{\mathbf{r}} f(r) W_{\mathbf{j}}(\mathbf{r})\, dr}{\int_{\mathbf{r}} W_{\mathbf{j}}(\mathbf{r})\, dV}, \tag{15}$$

where $W_{\mathbf{j}}(\mathbf{r})$ is an interpolation function which weights particles at position $\mathbf{r}$ to mesh $\mathbf{j}$, and $dV$ is a volume element, given in one dimension by $dV = 2\pi r\, dr$ in cylindrical coordinates and $dV = 4\pi r^2 dr$ in spherical coordinates.

For linear weighting in cylindrical coordinates, the density can then be written

$$n_j = \frac{\int_{r_{j-1}}^{r_j} f(r)\frac{r-r_{j-1}}{r_j-r_{j-1}}\, dr + \int_{r_j}^{r_{j+1}} f(r)\frac{r_{j+1}-r}{r_{j+1}-r_j}\, dr}{\int_{r_{j-1}}^{r_j} 2\pi r\frac{r-r_{j-1}}{r_j-r_{j-1}}\, dr + \int_{r_j}^{r_{j+1}} 2\pi r\frac{r_{j+1}-r}{r_{j+1}-r_j}\, dr}. \tag{16}$$

The edge densities are found simply by dropping the out-of-bounds integrals,

$$n_0 = \frac{\int_{r_0}^{r_1} f(r)\frac{r_1-r}{r_1-r_0}\, dr}{\int_{r_0}^{r_1} 2\pi r\frac{r_1-r}{r_1-r_0}\, dr} \tag{17}$$

and

$$n_N = \frac{\int_{r_{N-1}}^{r_N} f(r)\frac{r-r_{N-1}}{r_N-r_{N-1}}\, dr}{\int_{r_{N-1}}^{r_N} 2\pi r\frac{r-r_{N-1}}{r_N-r_{N-1}}\, dr}. \tag{18}$$

For $f(r) = 2\pi r$, we obtain the exact solution for all $0 \le j \le N$, $n_j = 1$. For more general particle distributions (specifically when $f$ is not a linear function of $r$), Eqs. (16)–(18) result in an error term which depends on the weighting scheme; for example, the linear weighting function results in an error proportional to $\Delta_r^2$.

This can be implemented in a standard linear weighting scheme simply by modifying the volumes used to compute $n_j$. Taking the cell size in the $z$-direction to be $\Delta_z$, the volumes

become

$$V_j = \Delta_z \frac{\pi}{3}[r_{j+1}(r_j + r_{j+1}) - r_{j-1}(r_{j-1} + r_j)], \tag{19}$$

$$V_0 = \Delta_z \frac{\pi}{3}(r_1 - r_0)(2r_0 + r_1), \tag{20}$$

and

$$V_N = \Delta_z \frac{\pi}{3}(r_N - r_{N-1})(r_{N-1} + 2r_N). \tag{21}$$

The corrected and uncorrected densities have been implemented in the XOOPIC [4] and XPDC1 [5] codes, and comparisons of the results are shown in Fig. 1. The comparisons shown are valid when there is at least one particle per cell. Total charge and volume are also identically conserved with the corrected method. This method can be easily extended to arbitrary weighting functions by using the desired weighting in Eqs. (16)–(18).

For linear weighting in spherical coordinates the density can be written

$$n_j = \frac{\int_{r_{j-1}}^{r_j} f(r)\frac{r-r_{j-1}}{r_j-r_{j-1}}\,dr + \int_{r_j}^{r_{j+1}} f(r)\frac{r_{j+1}-r}{r_{j+1}-r_j}\,dr}{\int_{r_{j-1}}^{r_j} 4\pi r^2\frac{r-r_{j-1}}{r_j-r_{j-1}}\,dr + \int_{r_j}^{r_{j+1}} 4\pi r^2\frac{r_{j+1}-r}{r_{j+1}-r_j}\,dr}, \tag{22}$$

with edge densities again obtained by dropping out-of-bounds integrals.

For the uniform particle distribution, $f(r) = 4\pi r^2$, we again obtain the exact solution for all $0 \le j \le N$, $n_j = 1$. For more general particle distributions we obtain the same result as that of the cylindrical case above.

Similar to the cylindrical case, the method can be implemented for the spherical scheme by precomputing the volumes using the denominator of Eq. (22). That is,

$$V_j = \frac{\pi}{3}(r_{j+1} - r_{j-1})\left(r_{j-1}^2 + r_{j-1}r_j + r_{j-1}r_{j+1} + r_j^2 + r_j r_{j+1} + r_{j+1}^2\right), \tag{23}$$

$$V_0 = \frac{\pi}{3}(r_1 - r_0)\left(3r_0^2 + 2r_1 r_0 + r_1^2\right), \tag{24}$$

and

$$V_N = \frac{\pi}{3}(r_N - r_{N-1})\left(r_{N-1}^2 + 2r_{N-1}r_N + 3r_N^2\right). \tag{25}$$

The densities computed with the method presented here are compared to the uncorrected densities for linear weighting on a uniform and nonuniform mesh in Fig. 2.

## 4. CURRENT DENSITY

This algorithm can be applied to current density for the electromagnetic source term in a straightforward manner by using $J = nqv$. The quantity $qv$ is weighted to the mesh for each particle, and the result is divided by the surface area, **S**. To obtain the surface area, consider the differential elements of the components in cylindrical coordinates,

$$dS_r = r\,d\theta\,dz, \tag{26}$$

$$dS_\theta = dr\,dz, \tag{27}$$

and

$$dS_z = r\,dr\,d\theta. \tag{28}$$

It is evident from Eqs. (26)–(28) that only the axial component of **S** will result in a nonlinear dependence on $r$ when computing the surface area from $S = \int WdS$, where $W$ is the particle–mesh weighting used. The results for the axial component of the current density are trivially different from the charge density results derived above, and the comparison plots are identical.

## 5. CONCLUSIONS

An algorithm for obtaining the correct charge and current densities in curvilinear coordinate systems for arbitrary particle interpolation schemes is described. Volumes and surface areas are weighted to the mesh using the same interpolation scheme used to weight particles. The method recovers the charge density correction factors for linear weighting in cylindrical coordinates [2] but extends to the more general case. The method has the notable beneficial properties of conserving charge and current as well as total volume and surface area on a general orthogonal mesh. The algorithm yields the exact answer for the uniform particle distribution, as demonstrated here. Arbitrary distributions are similarly correct to the mesh resolution, becoming exact as the mesh size approaches zero for continuum distributions; the corresponding electric field can also be shown to approach the exact solution in the same limit. This is a significant conceptual departure from the previous scheme of computing using incorrect volumes and then using correction factors designed for special cases [2]. The results are easily extended to two and three dimensions.

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