JOURNAL OF COMPUTATIONAL PHYSICS 89, 31–40 (1990)

An Analysis and Optimization of the Pseudo-current Method

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Received October 19, 1988; revised May 10, 1989

The pseudo-current method proposed by B. Marder for eliminating charge conservation errors in electromagnetic particle-in-cell codes has been analyzed and extended. The new method has been shown to be effective and efficient in removing high frequency, short wavelength errors caused by the choice of charge deposition algorithms. To maintain the physical properties of the electromagnetic field the choice of the free parameter in the originally proposed method has been restricted. It is found that the parameter should be homogeneous spatially and that an error minimization technique can be used to determine its value. A comparison is made between this adaptive pseudo-current method and the effects of spatial smoothing on the transverse and longitudinal components of the electromagnetic field.

INTRODUCTION

In electromagnetic particle-in-cell (PIC) codes the most widely used algorithms for particle charge and current attribution on a discretized mesh do not conserve charge exactly. The discrepancy between the particle charge and the charge conservation law implied by field solve algorithms can result in errors which lead to numerical instabilities characterized by the addition of noise in the high k part of the spectrum and non-conservation of energy. It is the purpose of this paper to examine in detail one of the newest techniques for overcoming this problem, namely the pseudo-current method proposed by Barry Marder [1].

Historically there have been two solutions proposed for the problem of charge conservation errors: (1) the use of a Poisson correction [2–4] and (2) the use of more complicated charge and current deposition algorithms which are exactly charge conserving [5–7]. In electromagnetic PIC codes charge nonconservation

581/89/1-3

0021-9991/90 $3.00

is a local phenomenon and is sometimes intertwined with the use of smoothing or filtering for the elimination of high frequency, short wavelength noise [8, 9]. These two strategies have advantages and disadvantages. A Poisson correction is exact. It works well in simple geometries where the Poisson solution can be implemented using fast direct solvers, such as FFTs. However, it can be difficult or expensive to implement in complicated geometries when irregular structures are present on the mesh. Such complications call for iterative Poisson solvers or capacitance matrix methods coupled to a fast FFT solver [10]. Exact deposition algorithms eliminate the charge conservation problem completely. They are, however, more complicated and are therefore more difficult to code and expensive to run. The deposition of currents on a mesh involves a scalar indirect index operation which is generally acknowledged to be the principal performance bottleneck in electromagnetic PIC codes. Exact charge consevation is obtained at the cost of expanding the deposition stencil to more of the surrounding meshpoints (up to 12 points in two dimensions). Conservative methods are also characterized by noise at short wavelengths due to the "nearest gridpoint" nature of the current deposition [4, 6].

Smoothing charge and current terms is effective in postponing or hiding the effects of charge non-conservation because the conservation errors are local. This means that conservation errors are of a wavelength for which smoothing is most effective. The use of smoothing, however, is not limited to charge conservation errors, and has important effects of its own.

The recent paper by Barry Marder introduced a method for managing charge conservation errors in electromagnetic PIC codes which elegantly avoids the problems associated with the usual methods described above. We have analyzed this new method which is based on a correction term to the electric field advance and which depends on the choice of an algebraic coefficient. The analysis suggests an optimal choice for the correction coefficient and a generalization of the method.

Generalization of the Pseudo-current Method

The basic equation of the pseudo-current method is an augmented Ampere's equation:

$$\frac{\partial \vec{\mathbf{D}}}{\partial t} = \nabla \times \vec{\mathbf{H}} - \vec{\mathbf{J}} + \frac{\alpha \nabla \delta\rho}{\Delta t}, \tag{1}$$

where

$$\delta\rho = \nabla \cdot \vec{\mathbf{D}} - \rho_p. \tag{2}$$

The quantity $\delta\rho$ was shown to satisfy an inhomogeneous diffusion equation driven by a source term representing charge conservation errors due to imperfect charge and current deposition. As first described, the constant α was left as a free

parameter, which for numerical stability in one dimension has to satisfy the condition:

$$\frac{2\alpha}{\Delta x^2} < 1. \tag{3}$$

This augmented Ampere's equation is differenced in a straightforward manner to time advance the electric fields. When the equation is differenced a question arises as to which electric fields should be used in the divergence calculation. Since the particle contribution to the charge density, ρ, is known at the "new" positions x^{N+1}, then the electric field should also be used at the advanced time t^{N+1}. This is most easily accomplished by recasting the equation for advancing E into two steps: a normal Ampere's equation,

$$\vec{\mathbf{D}}_0^{N+1} = \vec{\mathbf{D}}^N + \Delta t[\nabla \times \vec{\mathbf{H}}^{N+1/2} - \vec{\mathbf{J}}^{N+1/2}], \tag{4}$$

followed by the addition of the pseudo-current term using fields at t^{N+1}:

$$\vec{\mathbf{D}}_1^{N+1} = \mathbf{D}_0^{N+1} + \alpha\nabla(\nabla \cdot \vec{\mathbf{D}}_0^{N+1} - \rho_p^{N+1}). \tag{5}$$

When cast in this manner it is natural to allow repeated applications of the correction term using progressively more accurate values of the time advanced electric fields in the difergence term. The iteration formula is

$$\vec{\mathbf{D}}_{m+1}^{N+1} = \vec{\mathbf{D}}_{m+1}^{N+1} + \alpha_{m+1}\nabla(\nabla \cdot \vec{\mathbf{D}}_m^{N+1} - \rho_P^{N+1}). \tag{6}$$

By taking the curl of the above equation it can be seen that as long as the curl of the gradient vanishes for the differencing scheme chosen and the coefficient α does *not* vary spatially, this iteration term will not affect the transverse or radiating part of the electric field. While the convergence of this iteration formula is not especially fast (being a time distributed Picard iteration) other faster iteration schemes may not preserve the longitudinal character of the correction fields.

As suggested by Langdon, an alternate form of the iteration scheme which we have not explored is

$$\vec{\mathbf{D}}_{m+1}^{N+1} = \vec{\mathbf{D}}_{m+1}^{N+1} + \nabla(\alpha_{m+1}(\nabla \cdot \vec{\mathbf{D}}_m^{N+1} - \rho_P^{N+1})). \tag{6b}$$

The virtue of this formulation is that only the longitudinal component is affected and that α can be varied spatially. This is probably important for rapid convergence when using non-uniform meshes.

The proposed correction eliminates the error in the longitudinal component of $\vec{\mathbf{D}}$. Noise in the longitudinal component caused by particle statistics and noise in the transverse component of $\vec{\mathbf{D}}$ due to either statistics or deposition errors in the transverse currents is unaffected.

This scheme is conceptually a time distributed iterative solution to Poisson's equation for the correction charge, and while different from Marder's method it is based on his initial introduction of the pseudo-current. Although a large number of iterations would asymptotically approach a complete solution of Poisson's equation, in practice a few iterations are sufficient. The approach is consequently much more efficient than performing a complete solution by direct methods such as FFT or ICCG.

Strategies for the Choice of the Pseudo-Current Coefficient α

The effect on the error of this iterative correction depends on the choice of the coefficient α. If we define the error to be

$$\delta\rho_m = (\nabla \cdot \vec{\mathbf{D}}_m^{N+1} - \rho_p^{N+1}), \tag{7}$$

then taking the divergence of the iteration equation and subtracting ρ_p^{N+1} from both sides we obtain

$$\delta\rho_{m+1} = \delta\rho_m + \alpha_{m+1}\nabla^2\,\delta\rho_m. \tag{8}$$

Decomposing $\delta\rho_{m+1}$ in eigenvalues of ∇^2, we obtain

$$\delta\rho_{m+1}^k = \delta\rho_m^k(1 - \alpha_{m+1}k^2). \tag{9}$$

When $|1 - \alpha_{m+1}k^2| < 1$ for all k then the charge conservation error will decay for repeated iterations. This expression sets the convergence criteria for the algorithm. Since errors in the current and charge deposition to the mesh are local in nature it is reasonable to assume that most of the error is at short wavelengths or high k number. The natural choice for α then becomes

$$\alpha_{m+1} = \frac{1}{k_{\max}^2} = \left[4\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)\right]^{-1}. \tag{10}$$

For short wavelength errors the iteration term is very effective.

Instead of chosing a constant factor α_{m+1} for each iteration, the technique can be improved by one of several approaches. A popular method for minimizing the error over an interval is to fix the number of iterations and select the coefficients α_{m+1} in such a way that the resulting filter function polynomial is minimized over the desired part of the spectrum. In this case,

$$\delta\rho_N^k = \delta\rho_0^k \prod_{i=1}^{N} (1 - \alpha_i k^2) = \delta\rho_0^k P_N(k^2). \tag{11}$$

and the coefficients α_i are identical for each timestep.

It is also possible to adaptively calculate an α_{m+1} in such a way as to minimize the mean squared error in the fields at each iteration. If we choose the norm and define the error to be

$$\varepsilon = \sum_{\text{mesh}} (\delta\rho_{m+1})^2 \, \text{Vol}_{\text{zone}}, \tag{12}$$

then substituting the iteration formula from Eq. (8) yields

$$\varepsilon = \sum_{\text{Mesh}} (\delta\rho_m^2 + 2\alpha_{m+1} \, \delta\rho_m \nabla^2 \, \delta\rho_m + \alpha_{m+1}^2 \, (\nabla^2 \, \delta\rho_m)^2) \, \text{Vol}_{\text{zone}}. \tag{13}$$

If the above error is minimized with respect to α_{m+1} by differentiation and set equal to zero we can solve for the α_{m+1}. Doing this we obtain

$$\alpha_{m+1} = \frac{-\sum_{\text{Mesh}} \delta\rho_m \nabla^2 \, \delta\rho_m \, \text{Vol}_{\text{zone}}}{\sum_{\text{Mesh}} (\nabla^2 \, \delta\rho_m)^2 \, \text{Vol}_{\text{zone}}}. \tag{14}$$

RESULTS

To test the algorithm, an example based on the behavior of a doubly periodic, hot, low density, charge neutral plasma was selected. This simple geometry was chosen for two reasons. First, Marder's original paper has already demonstrated that the pseudo-current term being applied in each iteration can be performed for general boundary conditions, as in his magnetron example. Second, a doubly periodic problem will allow a direct and simple diagnosis of errors in k-space. For each simulation several diagonostics were taken. First, the α obtained from the adaptive calculation above was plotted versus time. Second, the RMS charge error (or correction charge) was measured and normalized to the maximum charge magnitude on the mesh; and

$$E_{\text{relative}} = \frac{\langle \delta\rho \rangle}{\max(|\rho_e|, \rho_i)}, \tag{15}$$

which represents the relative error, is then plotted versus time. Finally, the spectrum of the correction charge was measured and plotted versus wavenumber k for various combinations of pseudocurrent corrections and a simple centered spatial smoothing iteration.

For these simulations the zone size chosen was 0.01 m. Therefore the optimal static α should be 1.25×10^{-5}. Figure 1 shows how the adaptively calculated α compares with our a priori estimate. As can be seen the least squares calculation yields an α which is 1.7 times the static value. When the larger value of α is used, the region of strongest error reduction is moved away from the highest wavenumbers towards the midrange of the spectrum where there are many more modes.

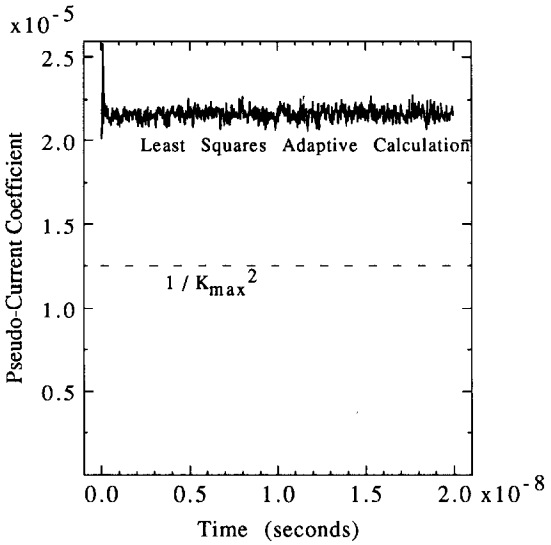

FIG. 1. A comparison between the adaptively calculated α and the a priori static estimate.

Although not shown here the calculated α was also measured in the case where a single spatial smoothing iteration was performed on the deposited currents and charge before the pseudo-current correction was applied. The prescription for the spatial smoothing was to perform alternating sweeps in each direction using

$$\rho_k^{M+1} = \frac{1}{4}\rho_{k+1}^{M} + \frac{1}{2}\rho_k^{M} + \frac{1}{4}\rho_{k-1}^{M}, \tag{16}$$

where M is the number of smoothing steps. The calculated α was centered around 2.5×10^{-5}, exactly double the static α. This is to be expected since the spatial smoothing already reduced the error strongly at high wavenumber. If α were to exceed 2.5×10^{-5} then the errors at the highest wavenumber are changed in sign and magnified. When two pseudo-current iterations are performed for a single time step the calculated α reported from the last iteration is about 1.5 times the static value. This indicates that the first iteration is focused on midrange k wavenumbers and then subsequent iterations move towards higher wavenumbers.

Charge errors are further reduced as additional iterations are performed. Figure 2 shows the normalized correction charge versus time for six runs. From top to bottom they are the history of the correction charge for 0 to 5 pseudo-current iterations. No correction gives charge errors on the order of 15%. A single pseudo-current iteration leaves errors of 0.7%! Further iterations reduce the error although in lessening degree.

The effect of applying a simple spatial smoothing operation on the deposited charges and currents before applying the pseudo-current correction will have the effect shown in Fig. 3. Smoothing alone without any pseudo-current correction

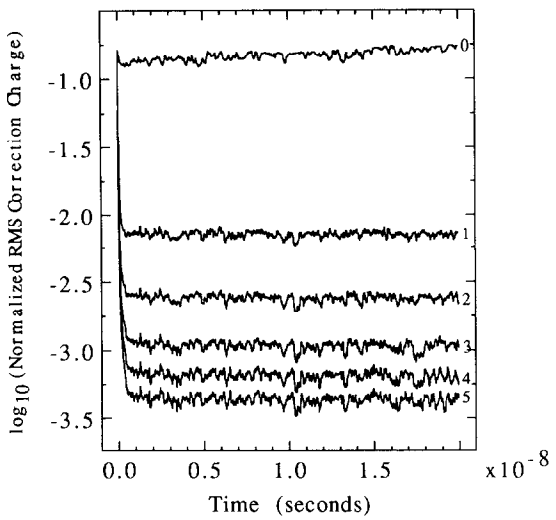

FIG. 2. A comparison of normalized correction charge for differing numbers of correction iterations. Shown are zero through five iterations.

only lowers the normalized error to about 4% compared with 0.7%. When the correction term is iterated, the relative improvement of each iteration is the same as the case without smoothing.

The effect of both the pseudo-current iteration and spatial smoothing is further shown by examining the correction charge spectrum as a function of wavenumber for various numbers of smoothings and correction terms. Figure 4 shows the correction charge spectrum for 0 to 5 pseudo-current iterations without any prior spatial

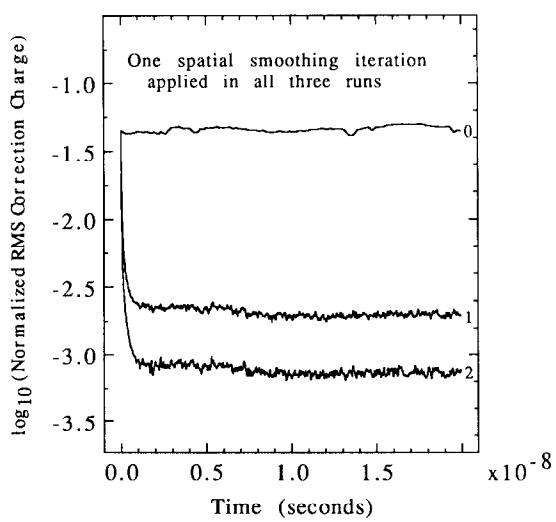

FIG. 3. A comparison of normalized correction charge for differing numbers of correction iterations. One spatial smoothing pass was done before applying the pseudo-current corrections.

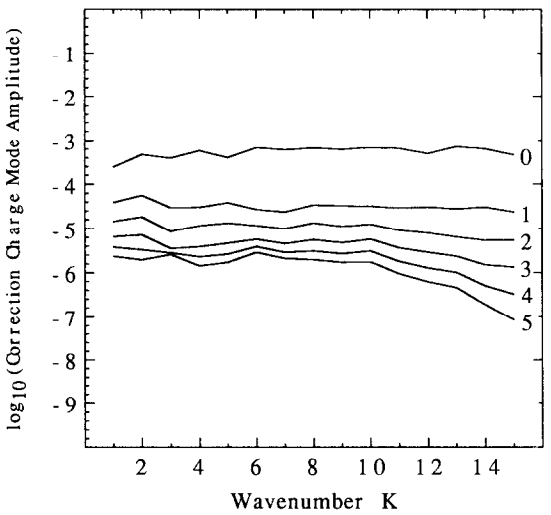

FIG. 4. Correction charge spectrum for different numbers of pseudocurrent correction with no spatial smoothing.

smoothing of currents or charge. Errors continue to be reduced with increasing iteration number even for low to moderate wavenumber. Figure 5 is a display of the same data but for many more iterations, namely 0 to 50 in increments of 5. After the first five iterations, the rate at which errors are reduced has clearly become more strongly dependent on the value of k and seems focused at the highest wavenumbers. After 25 iterations, the error at the highest wavenumbers is not further reduced because it has reached machine roundoff.

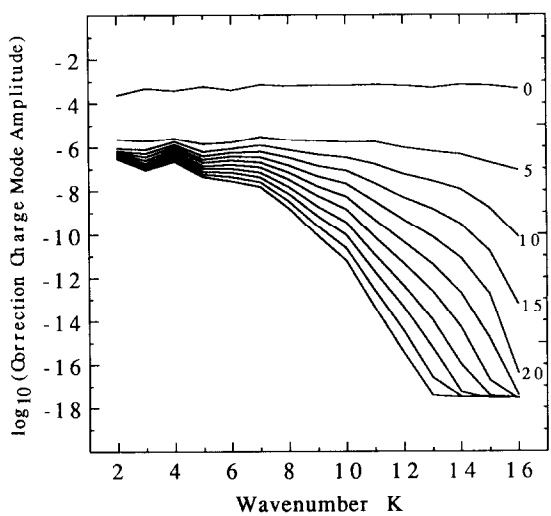

FIG. 5. Same as Fig. 4 except that the effect of many more (up to 50) iterations is shown.

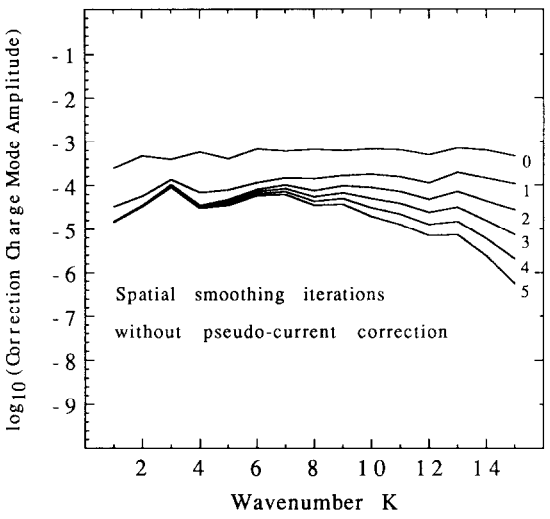

FIG. 6. The effect of iterating the spatial smoothing formula on the correction charge spectrum is shown.

The effects of iterating the spatial smoothing formula is shown in Fig. 6. These runs included no pseudo-current corrections, and display the correction charge spectrum for 0 to 5 iterations of the spatial smoothing formula. The large drop in the spectrum for all wavenumbers between 0 and 1 iteration is due to the fact that errors accumulate with no smoothing. The step to step effect is really only evident as you go from iteration 1 to 2 and above. It is clear that spatial smoothing has very little effect at low wavenumber. It also appears that even where spatial smoothing is most effective (at high wavenumber), the pseudo-current correction will reduce divergence errors more rapidly than spatial smoothing. Over all wavenumbers, the first iteration of the pseudo-current correction is about four times as effective as one iteration of spatial smoothing.

CONCLUSIONS

The pseudo-current method has proven to be effective at eliminating charge conservation errors, especially when applied with a coefficient calculated to minimize the RMS charge errors. It is effective not only for high k-number errors but also at middle and lower k numbers. That the method is more effective at this than the spatial smoothing of currents and charge is not surprising. It was specifically designed to remove divergence errors while smoothing simply damps short wavelength source terms without discriminating between conservation errors and correct sources.

While the pseudo-current method is limited to affecting only longitudinal fields, smoothing affects both longitudinal and transverse sources. Application of smooth-

ing to the charge and current density permits residual non-conservation errors to persist during future timesteps. Once source errors have been allowed to drive errors in the fields, those errors will remain indefinitely. Pseudo-current correction, on the other hand, will be continually working to reduce the charge conservation errors in the fields from step to step.

Even though the ability to maintain fields with the correct divergence is very important, it is also true that a correct, charge conserving and energy conserving simulation may still be noisy. In this case a judicious application of current and charge smoothing will be one way to reduce noise. This will be a simpler choice now that the issue of charge conservation error has been separately addressed by a more discriminating and effective tool.

ACKNOWLEDGMENTS

This research was performed in part under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract No. W.7405-Eng-48.

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