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Interesting modelling of intense electron flow has been done with implicit "particle-in-cell" simulation codes [1–4]. In this report, the "direct" implicit PIC simulation approach [5–8] is applied to simulations that include full electromagnetic fields. The resulting algorithm offers advantages relative to "moment" implicit electromagnetic algorithms [4], and may help in our quest for robust and simpler implicit codes.

Implicit fields reproduce electromagnetic waves at long wavelengths ($\gg c\Delta t$). At short wavelengths, the electrostatic, magnetostatic, and inductive electric fields are retained, as in a "Darwin" code [9]. At all wavelengths, Langmuir waves are stabilized, as in a direct implicit electrostatic code. The electrostatic fields are accurate for wavelengths longer than the electron transit distance ($v_{te}\Delta t$). These properties make an implicit electromagnetic code attractive e.g. to modeling of intense electron flow which is subject to pinching, Weibel instability [4], and other processes generating magnetic fields which alter the electron flow [1].

Time Differencing of the Particle and Field Equations

To begin our outline of an implicit algorithm we select the "D_1" time-differencing scheme [10] for the particles:

$$\frac{x_{n+1} - x_n}{\Delta t} = v_{n+\frac{1}{2}}; \qquad \frac{v_{n+\frac{1}{2}} - v_{n-\frac{1}{2}}}{\Delta t} = \bar{a}_n + \frac{v_{n+\frac{1}{2}} + v_{n-\frac{1}{2}}}{2} \times \frac{qB_n}{mc} \tag{1ab}$$

$$\text{where } \bar{a}_n = \tfrac{1}{2}[\bar{a}_{n-1} + \frac{q}{m}E_{n+1}(x_{n+1})]. \tag{1c}$$

Desired features of the implicit differencing of the Maxwell equations include:

- At long wavelengths, accuracy in dispersion Re $\omega(k)$, and weak damping (e.g. $\mathrm{Im}\,\omega(k)/ck = \mathcal{O}(ck\Delta t)^3$; k is the wavevector).

- Stability (preferably damping) at short wavelengths $\gtrsim 2\Delta x$ –stability despite $c\Delta t \geq \Delta x$ (violation of the Courant condition for *explicit* differencing), and dissipation of inaccurately calculated short wavelengths.

- Compatible with implicit particles.

- Adaptable to general boundary conditions.

- Simplicity, and economy in storage.

- Optionally recover the centered 2nd order scheme now commonly used for the fields.

- Optionally recover the centered Darwin scheme [9].

For the fields, we adapt implicit schemes developed for the particle equations of motion. For example, in the particle equations (1), we drop the $v\times B$ term, replace x by E, v by $c\nabla\times B$, and $\bar{a}$ by $-c^2\nabla\times\nabla\times\bar{E}$ to obtain the Maxwell equations (in rationalized cgs units):

$$c\nabla\times B_{n+\frac{1}{2}} = J_{n+\frac{1}{2}} + \frac{E_{n+1} - E_n}{\Delta t} \tag{2a}$$

$$-c\nabla\times\bar{E}_n = \frac{B_{n+\frac{1}{2}} - B_{n-\frac{1}{2}}}{\Delta t} \tag{2b}$$

where $\bar{E}_n = \frac{1}{2}[\bar{E}_{n-1} + E_{n+1}]$ (2c)

is the result of a recursive low-pass filter with phase error $\mathcal{O}(\Delta t^3)$. This phase error is an advance, not a lag as one gets if E_{n+1} is not used, so it provides stability when $ck\Delta t \gg 1$.

The code must solve the coupled set of equations (1ab) and (2). A price of implicit differencing is that time-cycle splitting, of the particle and the field time advances, is more complicated.

To advance the field values implicitly, eliminate E_{n+1} or $B_{n+\frac{1}{2}}$ from the coupled equations (2) to obtain a single elliptic equation. Eliminating $B_{n+\frac{1}{2}}$ to form an equation for E_{n+1}:

$$E_{n+1} + \tfrac{1}{2}c^2\Delta t^2\nabla\times\nabla\times E_{n+1} = E_n - J_{n+\frac{1}{2}}\Delta t + c\Delta t\nabla\times[B_{n-\frac{1}{2}} - \tfrac{1}{2}c\Delta t\nabla\times\bar{E}_{n-1}] \tag{3}$$

–or, eliminate E_{n+1} to form an equation for $B_{n+\frac{1}{2}}$:

$$B_{n+\frac{1}{2}} - \tfrac{1}{4}c^2\Delta t^2\nabla^2 B_{n+\frac{1}{2}} = B_{n-\frac{1}{2}} + \tfrac{1}{2}c\Delta t\nabla\times[J_{n+\frac{1}{2}} - E_{n-1} - E_n]$$

In either case, the right-hand-side is composed of known fields. The left-hand-sides have well-behaved elliptic operators.

To form a B_n for use in the particle mover, we use e.g.

$$B_n = B_{n-\frac{1}{2}} - \frac{\Delta t}{2} c\nabla\times E_n \tag{4}$$

Eqs. (2a-2b) differ from the popular centered "leap-frog" scheme only in that the electric field in Faraday's law here is $\bar{E}_n$ instead of E_n. *If we replace* $\bar{E}_n$ *in* (2b) with the linear combination $\alpha\bar{E}_n + (1-\alpha)E_n$, then with $\alpha=1$ we obtain the D_1 scheme above, and the leap-frog scheme with $\alpha=0$. For intermediate values the upper bound on Δt increases as $\alpha \to 1$. In problems where most cells are large and the undamped leap-frog scheme is preferred, but some cells are much smaller (e.g. near a boundary, or for $r\to 0$ in cylindrical or spherical coordinates), one might use $\alpha=0$ for the large cells and increase α to maintain stability where cells are smaller.

The Direct Method for Implicit Particles and Fields

The essence of the "direct" method is that we work *directly* with the particle equations of motion and the particle/field coupling equations. These are linearized about an estimate (extrapolation) for their values at the new time level n+1. The future values of $\{x,v\}$ are divided into two parts:

- increments $\{\delta x,\delta v\}$ which depend on the (unknown) fields at the future time level n+1, and

- extrapolations $\{x^{(0)}_{n+1},v^{(0)}_{n+\frac{1}{2}}\}$ which incorporate *all* other contributions to the equation of motion

The increments $\{\delta x,\delta v\}$ are evaluated by linearization of each equation o motion [5,6,7]; here, we have

$$\delta x_{n+1}/\Delta t = \delta v_{n+\frac{1}{2}} = \tfrac{1}{2}(I+R)\cdot(q\Delta t/2m)E_{n+1}(x_{n+1}), \tag{5}$$

where the operator R effects a rotation through angle $-qB_n\Delta t/mc$.

The corresponding densities $\{\rho^{(0)}_{n+1},J^{(0)}_{n+\frac{1}{2}}\}$ and $\{\delta\rho,\delta J\}$ are inserted into Maxwell's equations.

Evaluation of $\{\rho_{n+1}^{(0)}, J_{n+\frac{1}{2}}^{(0)}\}$, the extrapolated densities.

The extrapolated current and charge densities are evaluated the same as in explicit codes, such as ZOHAR [11] and WAVE, from $x_{n+1}^{(0)}$, $v_{n+\frac{1}{2}}^{(0)}$ and x_n. At the grid point located at X_j,

$$\rho_{n+1}^{(0)} = \sum qS(X_j - x_{n+1}^{(0)}) \tag{6}$$

$$J_{n+\frac{1}{2}}^{(0)} = \sum qv_{n+\frac{1}{2}}^{(0)} S(X_j - \tfrac{1}{2}[x_n + x_{n+1}^{(0)}]) \tag{7a}$$

or
$$= \sum qv_{n+\frac{1}{2}}^{(0)} \tfrac{1}{2}[S(X_j - x_n) + S(X_j - x_{n+1}^{(0)})] \tag{7b}$$

To correct the small error in $\nabla\cdot J_{n+\frac{1}{2}}^{(0)}$ (due to the slightly nonconservative but otherwise beneficial method of collection of J [12,11]), we replace $J_{n+\frac{1}{2}}^{(0)}$ by

$$J'_{n+\frac{1}{2}} = J_{n+\frac{1}{2}}^{(0)} - (\nabla\psi)/\Delta t, \tag{8a}$$

where $-\nabla^2\psi = \rho_{n+1}^{(0)} + \nabla\cdot[\Delta t J_{n+\frac{1}{2}}^{(0)} - E_n]$. (8b)

Evaluation of $\{\delta\rho, \delta J\}$, the increments due to future fields.

The care with which $\{\delta\rho, \delta J\}$ are formed is a compromise between complexity and strong convergence [5,7]. They may be evaluated rigorously if necessary as derivatives of equations (6) and (7) ("strict differencing"; [5], section 4), or as simplified difference representations [5,7] of

$$\delta\rho = -\nabla\cdot[\rho\delta x], \tag{9}$$

$$\delta J = \rho\delta v - \tfrac{1}{2}\nabla \times (J \times \delta x) \tag{10}$$

for each species. This form for δJ trivially conserves charge: $\delta\rho + \Delta t\nabla\cdot\delta J = 0$. This property can easily be preserved in the spatial differencing of δJ.

The terms in Eq. (10) have both analytic and pictorial justifications; see Figure. A heuristic derivation of δJ uses an analogy to magnetization current. The magnetic moment of the current loop in the last diagram is

$$(1/2c)\int x \times dx = (q/2c\Delta t)\delta x \times (v_{n+\frac{1}{2}}^{(0)}\Delta t).$$

The current due to a density n of these is

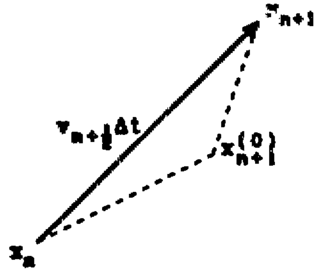
$$\delta J = c\nabla\times M = c\nabla\times[n(q/2c\Delta t)\ \delta x \times v_{n+\frac{1}{2}}^{(0)}\Delta t] = \tfrac{1}{2}\nabla\times[\delta x \times \rho v_{n+\frac{1}{2}}^{(0)}]$$

which leads to the last term in (10).

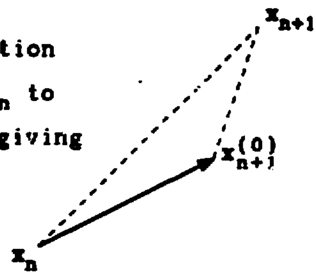
We now have everything needed to write an equation for E_{n+1}. On

Geometric Interpretation of the Terms in $J = J^{(0)} + \delta J$

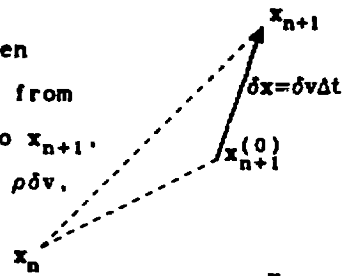
While $J_{n+\frac{1}{2}}$ corresponds to moving the particle directly from x_n to x_{n+1}, it can be regarded as the sum of 3 motions:



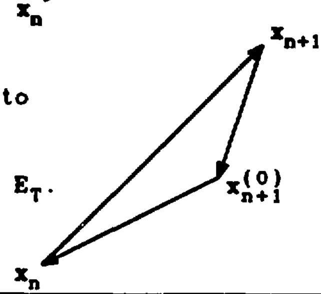
(1) motion from x_n to $x^{(0)}_{n+1}$, giving $J^{(0)}_{n+\frac{1}{2}}$,



(2) then motion from $x^{(0)}_{n+1}$ to x_{n+1}, giving $\rho\delta v$,



plus (3) a circulation term $-\frac{1}{2}\nabla\times(J\times\delta x)$ to cancel the "detour" to $x^{(0)}_{n+1}$. This is not needed to get ρ_{n+1} but does affect B and E_T.



substituting our expressions for $\rho^{(0)}_{n+1}$, $\delta\rho$, $J^{(0)}_{n+\frac{1}{2}}$ and δJ into the field equations (2–3), we have

$$c\nabla \times \left[B_{n+\frac{1}{2}} + (J'_{n+\frac{1}{2}} \times \delta x)/2c \right] = J'_{n+\frac{1}{2}} + \rho^{(0)}_{n+1}\delta v + \frac{E_{n+1} - E_n}{\Delta t} \qquad (11a)$$

$$-\frac{1}{2}\, c\nabla \times \left[\bar{E}_{n-1} + E_{n+1}\right] = \frac{B_{n+\frac{1}{2}} - B_{n-\frac{1}{2}}}{\Delta t} \qquad (11b)$$

These equations, together with (5), are the simplest yet proposed for implicit field prediction, both in themselves and in what one must accumulate from the particles.

The divergence of the Ampere–Maxwell equation recovers *exactly* our electrostatic implicit field equation [5,6]

$$\rho^{(2)}_{n+1} = \nabla\cdot[I+\chi]\cdot E_{n+1}$$

where the implicit susceptibility $\chi = (\rho^{(0)}_{n+1} q\delta t^2/2m)(I+R)/2$ is a tensor due to the rotation R induced by B.

Generalizations

To include relativity, one would linearize the relativistic particle equation-of-motion [11,12]. Electron-ion collisions ($\nu \lesssim \Delta t^{-1}$) may be described as an addition to the rotation R in the equation-of-motion.

If a component of the plasma is modeled by fluid equations then those equations are linearized to find $\{\delta\rho, \delta J\}$ [8]. Combining fluid and particle descriptions is difficult, but not more so in the direct method than in the moment method.

Loose Ends

Some questions remain for analysis and/or experimentation. For example, in a straightforward implementation of Eq. (11), a careful examination of the locations at which E and B are evaluated shows a $\mathcal{O}(kv\Delta t)^2$ error. This error is the same type as in [7], where it seemed not to cause problems in their applications. This report does not discuss spatial differencing, which I anticipate would follow in spirit the "simplified differencing" of Refs. [5, 7]. As in Refs. [5, 7, 13], the "strict direct method" provides tools for analysis of the convergence and stability of differencing schemes that are simpler than those derived by strict application of the direct method, and are simpler (and less restrictive in some respects) than the moment method.

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