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DIRECT IMPLICIT ELECTROMAGNETIC PLASMA SIMULATION*

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The essence of any implicit PIC algorithm is to use part of the future fields in the evolution of the particle/field equations so that stability with a large time step can be maintained.[1] The big impediment in developing implicit methods for PIC techniques has been the difficulty of solving the field rapidly and robustly in the parameter regimes of general interest. We describe here a new implementation[2] of the Direct Implicit algorithm[1] with a field solution that greatly reduces these concerns.

Overview of the Direct Implicit PIC Method

The particle integration scheme in the direct implicit algorithm is implemented in two conceptual steps. First we advance the particles to the ~ level using everything **except** the advanced $\underline{E}$ field. For each particle we use

$$\tilde{\underline{v}}_{n+1/2} = \underline{v}_{n-1/2} + 1/2\Delta t[\bar{\underline{a}}_{n-1} + (\tilde{\underline{v}}_{n+1/2} - \underline{v}_{n-1/2})/2 \times qB_n(\underline{x}_n)/mc] \tag{1a}$$

$$\tilde{\underline{x}}_{n+1} = \underline{x}_n + \Delta t\tilde{\underline{v}}_{n+1/2} \tag{1b}$$

followed by the accumulation of some particle-derived source terms at this ~ level. The ~ level source terms are constructed such that the advanced source terms can be obtained from the ~ source terms when the new $\underline{E}$ field is known. The expressions we use are

$$\rho_{n+1}(\underline{X}_j) = \tilde{\rho}_{n+1}(\underline{X}_j) - \underline{\nabla}\cdot\underline{\chi}\cdot\underline{E}_{n+1} \tag{2a}$$

$$\Delta t\underline{J}_{n+1/2}(\underline{X}_j) = \Delta t\tilde{\underline{J}}_{n+1/2}(\underline{X}_j) + \underline{\chi}\cdot\underline{E}_{n+1} - c\Delta t\ \underline{\nabla}\times\underline{\zeta}\cdot\underline{E}_{n+1} \tag{2b}$$

where $\tilde{\rho}$ and $\tilde{J}$ result from summations over ~ level particle quantities as are the tensors $\underline{\chi}$ and $\underline{\zeta}$ whose precise form is discussed elsewhere.[2-4] These expressions are substituted into the D_1-scheme Maxwell's equations

$$\underline{E}_{n+1} - \underline{E}_n = c\Delta t\ \underline{\nabla}\times\underline{B}_{n+1/2} + 4\pi\Delta t\ \underline{J}_{n+1/2} \tag{3a}$$

$$\underline{B}_{n+1/2} - \underline{B}_{n-1/2} = -c\Delta t\ \underline{\nabla}\times\bar{\underline{E}}_n \tag{3b}$$

$$\underline{B}_{n+1} - \underline{B}_{n+1/2} = -1/2c\Delta t\underline{\nabla}\times\underline{E}_{n+1} \tag{3c}$$

$$\bar{\underline{E}}_n = 1/2(\underline{E}_{n+1} + \bar{\underline{E}}_{n-1}) \tag{3d}$$

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so that we may solve for the advanced fields. The solution of these field equations becomes a numerical task independent of the particle equations --given these particle-derived source terms. Our new field solution technique is described below. Assuming the advanced fields have been calculated, the particle advance can now be completed with these new fields. The final advance is given, for each particle, by

$$\underline{\delta v} = 1/2\Delta t[q/m\ \underline{E}_{n+1}(\overset{N}{\underline{x}}_{n+1}) + \underline{\delta v}/2 \times q\underline{B}_n(\underline{x}_n)/mc] \tag{4a}$$

$$\underline{x}_{n+1} = \tilde{\underline{x}}_{n+1} + \Delta t\ \underline{\delta v} \tag{4b}$$

$$\underline{v}_{n+1/2} = \tilde{\underline{v}}_{n+1/2} + \underline{\delta v} \tag{4c}$$

$$\bar{\underline{a}}_n = 1/2\ [\ \bar{\underline{a}}_{n-1} + q/m\ \underline{E}_{n+1}(\tilde{\underline{x}}_{n+1})\ ] \tag{4d}$$

Further discussion of this method can be found in Refs. 1-4.

Solution of the Implicit Field Equations

Substituting the expression for $\underline{J}_{n+1/2}$ into eqs. (3a-3d) and eliminating $\underline{B}$, the equation for $\underline{E}$ is

$$\underline{E} - 1/2c^2\Delta t^2[\nabla^2\underline{E} - \underline{\nabla}(\underline{\nabla}\cdot\underline{E})] + 4\pi(\underline{\chi}\cdot\underline{E} - c\Delta t\ \underline{\nabla}\times\underline{\zeta}\cdot\underline{E}) = \underline{Q} \tag{5}$$

$$= \underline{E}_n - 4\pi\Delta t\ \tilde{\underline{J}} + c\Delta t\ \underline{\nabla}\times\underline{B}_{n-1/2} - 1/2c^2\Delta t^2\ \underline{\nabla}\times\underline{\nabla}\times\bar{\underline{E}}_n$$

where the $\underline{E}$ without subscript is $\underline{E}_{n+1}$. The solution of eq. (5) must satisfy

$$\underline{\nabla}\cdot(\underline{I} + 4\pi\underline{\chi})\cdot\underline{E}_{n+1} = 4\pi\tilde{\rho}_{n+1} \tag{6}$$

our best statement of the Gauss law $\nabla\cdot\underline{E}_{n+1} = 4\pi\rho_{n+1}$. Taking the divergence of (5) shows that $\underline{E}_{n+1}$ satisfies instead $\nabla\cdot(\underline{I} + 4\pi\underline{\chi})\cdot\underline{E} = \nabla\cdot\underline{Q}$. In general $\nabla\cdot\underline{Q} \neq 4\pi\tilde{\rho}_{n+1}$, due both to the method of forming $\tilde{\underline{J}}$ and inconsistencies on previous time steps. Ignoring this issue permits $\nabla\cdot\underline{E}$ to drift far away from ρ, because ρ appears nowhere in (5).

An adjustment for $\underline{Q}$ analogous to that used explicit EM codes--correcting the irrotational part of $\tilde{\underline{J}}$ that goes into $\underline{Q}$--is not adequate for at least two reasons. First, in simulations with large values of $\Omega\nabla t$, it is known[1] that the resulting field $\underline{E}_{n+1}$ is wrong due to spuriously large currents across $\underline{B}$. The correction $\underline{\nabla}\psi$ was computed without information about the anisotropy caused by $\underline{B}$. Secondly, we found that abrupt changes in density (plasma-vacuum interfaces) causes spuriously large fields $\underline{E}_{n+1}$ in the low density region. Information about the plasma conditions corresponding to both these situations is carried by $\underline{\chi}$.

Motivated by these observations to include $\underline{\chi}$ in the correction process, our present solution to both these problems is to take a new form[1,2] for the correction; we subtract $(\underline{I} + 4\pi\underline{\chi})\cdot\underline{\nabla}\psi$ from $\underline{Q}$. Substitution into the divergence of eqn. (5) yields an elliptic equation for ψ,

$$\underline{\nabla}\cdot[\underline{I} + 4\pi\underline{\chi}]\cdot\underline{\nabla}\psi = \underline{\nabla}\cdot\underline{Q} - 4\pi\tilde{\rho} \tag{7}$$

Numerical Implementation of the Field Solution

Eq. (5) involves a coupling of $\underline{E}$ components and plasma source terms that has proven difficult to solve if not properly arranged. Early 1-D tests[3] revealed the advantage of solving all components simultaneously with a linear system solver. Once $\underline{E}_{n+1}$ is known, the other field equations, eqs. (3b-3d), can simply be evaluated point by point. Since a direct solve in 2D requires too much storage, an iterative solution based on ADI has been implemented.[2,3]

When the coefficient $1/2c^2\Delta t^2/\Delta_\xi^2 >> \underline{\chi}$, the term arising from $\underline{\nabla}\times\underline{\nabla}\times$ dominates the equation. The convergence rate slows down in this case--presumably because this operator does not fit symmetrically into the splitting scheme. This limit occurs in low density regions in which the collisionless skin depth is well resolved. To make these terms more tractable in such regions, we split $\underline{E}$ into irrotational and solenoidal parts, denoted by $\underline{E}_\ell$ and $\underline{E}_t$, respectively. Since $\underline{E}_\ell = \underline{\nabla}\Phi$ where Φ is the electrostatic potential, we self-consistently compute the n+1 time level of four 2-D quantities. Equation (5) still determines the total advanced electric field although it only provides three component equations. An additional equation is needed to serve as a constraint condition on Φ.

The divergence of eq. (5) provides a satisfactory constraint equation and when coupled with eq. (5)

$$\underline{E}_t - \underline{\nabla}\Phi - 1/2c^2\Delta t^2\nabla^2\underline{E}_t + 4\pi[\underline{\chi}\cdot(\underline{E}_t - \underline{\nabla}\Phi) - c\Delta t\ \underline{\nabla}\times\underline{\zeta}\cdot(\underline{E}_t - \underline{\nabla}\Phi)] = \underline{Q} \tag{8a}$$

$$\underline{\nabla}\cdot(\underline{I} + 4\pi\underline{\chi})\cdot(\underline{E}_t - \underline{\nabla}\Phi) = \nabla\cdot\underline{Q} \tag{8b}$$

provides a set of four coupled elliptic equations which offer symmetry in the terms associated with each coordinate direction. The essential feature of this decomposition is that we can obtain the correct cancellation of the terms $[\underline{\nabla}^2\underline{E}_\ell - \underline{\nabla}(\underline{\nabla}\cdot\underline{E}_\ell)]$ **analytically** if we use an interleaved mesh.[2]

The strong coupling of these equations makes simultaneous solution necessary; an AD procedure[2] has been devised that works well in parameter regimes of interest. The necessary precision (we generally require 1 part in 10^3 for all components) is usually obtained with only 7-12 iterations.

Test Cases

We have used electron beam filamentation as a test problem with which we can easily vary the resolution of the collisionless skin depth--a situation in which the importantance of the simultaneous solution is apparent. Our algorithm works well in both regimes; we have recovered filamentation growth rates in good agreement with simple theory and will present these results. Preliminary studies of magnetic reconnection will also be presented.

If we assume 30 particles per cell on a 40 x 32 mesh, our present code will use about 50% of the effort in the field solve. Since the particle advance consists of two pieces, we find AVANTI takes about four times the CPU effort of the corresponding explicit algorithm--but with time steps up to fifty times larger. We find no stability limit on time step. Implementation details, now used in the code AVANTI, can be found in reference 2.

References

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