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2.5D EM Direct Implicit PIC Simulation using AVANTI

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An appealing feature of the well-known PIC algorithm for plasma simulations is the intuitive connection of the plasma representation with real plasmas. Working directly with macro "particles" provides intuition about plasma behavior but at greater computational expense for the extra detail that the method provides. Further, traditional explicit fully electromagnetic PIC algorithms still have stability and accuracy constraints that demand microscopic details be resolved in time and space. Recent progress in making the PIC algorithm implicit have been successful in allowing selective resolution in space and time of only those plasma phenomena of interest. We present here an overview of one of these procedures known as the direct implicit method as implemented in the LLNL code AVANTI[1].

Basic Equations of the Direct Implicit D_1 Scheme

The desired implicit particle advance with the direct implicit D_1 scheme is given by

$$\mathbf{v}_{n+\frac{1}{2}} = \mathbf{v}_{n-\frac{1}{2}} + \Delta t\left[\bar{\mathbf{a}}_n + \frac{q}{m}\frac{\mathbf{v}_{n+\frac{1}{2}} + \mathbf{v}_{n-\frac{1}{2}}}{2c} \times \mathbf{B}_n(\mathbf{x}_n)\right] \qquad (1a)$$

where $\mathbf{x}_n$ and $\mathbf{v}_n$ represent each particles's position and velocity at time level n such that $t_n = n\Delta t$. $\mathbf{E}$ and $\mathbf{B}$ are the electromagnetic fields. $\bar{\mathbf{a}}_n$ is given by the recurrence relation $\bar{\mathbf{a}}_n = \frac{1}{2}[\bar{\mathbf{a}}_{n-1} + \frac{q}{m}\mathbf{E}_{n+1}(\mathbf{x}_{n+1})]$. The position advance is given by

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \Delta t\ \mathbf{u}_{n+\frac{1}{2}}. \qquad (1b)$$

Note that the explicit scheme is recovered by taking $\bar{\mathbf{a}}_n = \frac{q}{m}\mathbf{E}_n$.

Maxwell's equations, finite differenced using the D_1 scheme, become

$$\mathbf{E}_{n+1} - \mathbf{E}_n = c\Delta t\nabla \times \mathbf{B}_{n+\frac{1}{2}} + 4\pi\Delta t\mathbf{J}_{n+\frac{1}{2}} \qquad (2a)$$

$$\mathbf{B}_{n+\frac{1}{2}} - \mathbf{B}_{n-\frac{1}{2}} = -c\Delta t\nabla \times \bar{\mathbf{E}}_n \qquad (2b)$$

with $\bar{\mathbf{E}}_n$ given by the recurrence $\bar{\mathbf{E}}_n = \frac{1}{2}(\mathbf{E}_{n+1} + \bar{\mathbf{E}}_{n-1})$. As with the particle equations, the explicit scheme could be recovered by taking $\bar{\mathbf{E}}_n = \mathbf{E}_n$.

These equations provide time stability for large Δt. Using only the advanced quantity instead of the time averaged recurrence, in both the particle and field time integration, provides stability but excessive damping of low frequency phenomena; including some time history through the time recursion represents those phenomena just resolved by the time step with less dispersion[2,3,4].

What remains is to discuss the solution technique. Obviously it is not feasible to solve the whole system by matrix inversion–each particle quantity is an unknown making the matrix hopelessly big in most interesting situations.

Overview of the Direct Implicit PIC Method

The particle integration scheme in this direct implicit algorithm is implemented in two conceptual steps. First we advance the particles to the *tilde* level using everything *except* the advanced **E** field. For each particle we use

$$\tilde{\mathbf{v}}_{n+\frac{1}{2}} = \mathbf{v}_{n-\frac{1}{2}} + \frac{\Delta t}{2}\bar{\mathbf{a}}_{n-1} + (\tilde{\mathbf{v}}_{n+\frac{1}{2}} + \mathbf{v}_{n-\frac{1}{2}}) \times \boldsymbol{\theta} \qquad (3a)$$

where $\boldsymbol{\theta} = \frac{q\,\Delta t\,\mathbf{B}_n(\mathbf{x}_n)}{2\,m\,c}$ and

$$\tilde{\mathbf{x}} = \mathbf{x}_n + \Delta t\,\tilde{\mathbf{v}}_{n+\frac{1}{2}}. \qquad (3b)$$

The particle time advance to the *tilde* level is followed by the accumulation of some particle-derived source terms at this *tilde* level. The *tilde* level source terms are constructed such that the advanced source terms can be obtained when the new **E** field is known. The expressions we use are

$$\rho_{n+1}(\mathbf{x}_g) = \tilde{\rho}_{n+1}(\mathbf{x}_g) - \nabla \cdot \chi(\mathbf{x}_g) \cdot \mathbf{E}_{n+1}(\mathbf{x}_g) \qquad (4a)$$

and

$$\mathbf{J}_{n+\frac{1}{2}}(\mathbf{x}_g) = \tilde{\mathbf{J}}_{n+\frac{1}{2}}(\mathbf{x}_g) + \frac{\chi(\mathbf{x}_g)}{\Delta t} \cdot \mathbf{E}_{n+1}(\mathbf{x}_g) - c\nabla \times \zeta(\mathbf{x}_g) \cdot \mathbf{E}_{n+1}(\mathbf{x}_g) \qquad (4b)$$

where $\tilde{\rho}$ and $\tilde{\mathbf{J}}$ result from summations over *tilde* level particle quantities and the argument $\mathbf{x}_g$ indicates a mesh quantity.

The tensors χ and ζ provide the connection between the charge and current densities obtained from summations over particle *tilde* positions and velocities and the fully advanced quantities that can be obtained only after the advanced E is calculated. Not surprisingly, these tensors are expressed in terms of the contributions $\delta\mathbf{v}$ and $\delta\mathbf{x}$ that result when the new $\mathbf{E}_{n+1}$ is finally applied to the particles. The derivation, given in [1,2,3], begins with the usual expression for $\rho_{n+1}(\mathbf{x}_g) = \sum_i q_i S(\mathbf{x}_g - \mathbf{x}_{n+1})$ which, for each particle, is expanded about the *tilde* position. After some rearrangement and "simplified" differencing, we obtain

$$\chi(\mathbf{x}_g) = \sum_s \frac{\Delta t^2}{4}\frac{q_s}{m_s}\tilde{\rho}_s(\mathbf{x}_g)[\mathbf{I} + \mathbf{R}_s(\mathbf{x}_g)] \qquad (5)$$

in which the sum of particle source terms is over particle species. **I** and **R** are identity and rotation operators associated with the particle advance but expressed on the mesh. A similar expression, also evaluated on the computational mesh, is obtained for ζ. With these expression for the tensors χ and ζ, eqs. (4a) and (4b) are used in Maxwell's equations so that we may solve for the advanced fields. The solution of these field equations becomes an independent numerical task given these particle-derived source terms.

Assuming the advanced fields have been calculated, the particle advance can be completed. The final advance is given, for each particle, by

$$\delta\mathbf{v} = \tfrac{1}{2}\Delta t\frac{q}{m}\mathbf{E}_{n+1}(\tilde{\mathbf{x}}_{n+1}) + \delta\mathbf{v} \times \boldsymbol{\theta} \qquad (6a)$$

$$\mathbf{x}_{n+1} = \tilde{\mathbf{x}}_{n+1} + \Delta t\,\delta\mathbf{v} = \tilde{\mathbf{x}}_{n+1} + \delta\mathbf{x} \qquad (6b)$$

$$\mathbf{v}_{n+\frac{1}{2}} = \tilde{\mathbf{v}}_{n+\frac{1}{2}} + \delta \mathbf{v}. \tag{6c}$$

These expressions are just the pieces of eqs. (1) left out of eqs. (3).

The details of the procedures are important to the overall robustness of the direct implicit algorithm. Several variants were considered during development of the algorithm; only the most successful survived[1,2,5].

Solution of the Implicit Field Equations

a) Consistency

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

$$\mathbf{E} - \tfrac{1}{2}c^2\Delta t^2[\nabla^2\mathbf{E} - \nabla(\nabla\cdot\mathbf{E})] + 4\pi(\chi\cdot\mathbf{E} - c\Delta t\nabla\times\zeta\cdot\mathbf{E}) = \mathbf{Q}'$$

$$= \mathbf{E}_n - 4\pi\Delta t\tilde{\mathbf{J}} + c\Delta t\nabla\times\mathbf{B}_{n-\frac{1}{2}} - \tfrac{1}{2}c^2\Delta t^2\nabla\times\nabla\times\bar{\mathbf{E}}_n \tag{7}$$

where the $\mathbf{E}$ without subscript is $\mathbf{E}_{n+1}$. The solution of eq. (7) must satisfy

$$\nabla\cdot(\mathsf{I} + 4\pi\chi)\cdot\mathbf{E} = 4\pi\tilde{\rho}_{n+1}, \tag{8}$$

our best statement of Gauss' law, $\nabla\cdot\mathbf{E} = 4\pi\rho_{n+1}$. Taking the divergence of (6) shows that $\mathbf{E}$ satisfies instead $\nabla\cdot(\mathsf{I}+4\pi\chi)\cdot\mathbf{E} = \nabla\cdot\mathbf{Q}'$. In general $\nabla\cdot\mathbf{Q}' \neq 4\pi\tilde{\rho}_{n+1}$, due both to the method of forming $\tilde{\mathbf{J}}$ and to inconsistencies on previous time steps. Ignoring this issue permits $\nabla\cdot\mathbf{E}$ to drift far away from ρ, because ρ appears nowhere in (6).

An adjustment for $\mathbf{Q}'$ analogous to that used explicit EM codes–correcting the irrotational part of $\tilde{\mathbf{J}}$ that goes into $\mathbf{Q}'$–is not adequate for at least two reasons. First, in simulations with large values of $\omega_{ce}\Delta t$, it was found by Barnes[1] that the resulting field $\mathbf{E}$ is wrong due to spuriously large currents across $\mathbf{B}$. Secondly, we found that abrupt changes in density (plasma-vacuum interfaces) causes spuriously large fields $\mathbf{E}$ in the low density region. Information about the plasma conditions corresponding to both these situations is carried by χ.

Motivated by these observations to include χ in the correction process, we take a new form[1,2] for the correction; we subtract $(\mathsf{I} + 4\pi\chi)\cdot\nabla\psi$ from $\mathbf{Q}'$ to form a "corrected" $\mathbf{Q}$. Substitution into the divergence of eq. (6) yields an elliptic equation for ψ,

$$\nabla\cdot[\mathsf{I} + 4\pi\chi]\cdot\nabla\psi = \nabla\cdot\mathbf{Q}' - 4\pi\tilde{\rho}. \tag{9}$$

b) Numerical Implementation of the Field Solution

Early 1-D tests[6] revealed the advantage of solving all components of $\mathbf{E}$ simultaneously with a linear system solver. Since a direct solve in 2D requires too much storage, an iterative solution based on ADI has been implemented[1]. First attempts at this solution encountered several difficulties. In low density regions in which the collisionless skin depth is well resolved, the coefficient of $\nabla\times\nabla\times$ can exceed χ and dominates the equation. The convergence rate slows down in this case because this operator does not fit symmetrically into the splitting scheme. The solution is to split $\mathbf{E}$ into irrotational and solenoidal parts so that we obtain the correct cancellation of the terms irrotational part of $\nabla\times\nabla\times$ *analytically* using an interleaved mesh[1].

Since $\mathbf{E}_l = -\nabla\Phi$, where Φ is the electrostatic potential, we self-consistently compute the $n+1$ time level of four 2-D scalars.

The divergence of eq. (7) provides the extra equation for Φ and, when coupled with the vector decomposition of $\mathbf{E}$, gives

$$\mathbf{E}_t - \nabla\Phi - \tfrac{1}{2}c^2\Delta t^2\nabla^2\mathbf{E}_t + 4\pi[\boldsymbol{\chi}\cdot(\mathbf{E}_t - \nabla\Phi) - c\Delta t\nabla\times\boldsymbol{\zeta}\cdot(\mathbf{E}_t - \nabla\Phi)] = \mathbf{Q}. \qquad (10a)$$

$$\nabla\cdot(\mathbf{I} + 4\pi\boldsymbol{\chi})\cdot(\mathbf{E}_t - \nabla\Phi) = \nabla\cdot\mathbf{Q}. \qquad (10b)$$

In general the strong tensorial coupling of these equations reinforces the need for simultaneous solution; the ADI procedure 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. Further details of this splitting procedure can be found in reference 1.

Examples demonstrating the capabilities of AVANTI will be shown.

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