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RELATIVISTIC EXTENSION OF THE ELECTROMAGNETIC DIRECT IMPLICIT PIC ALGORITHM

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Relativistic Extension of the Electromagnetic Direct Implicit PIC Algorithm

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The PIC model provides a very complete representation of plasma behavior that is essential when investigating phenomena requiring velocity space information such as laser-plasma interactions. New implicit PIC algorithms have expanded considerably in both space and time the scope of problems that may be addressed with this model. Applications of the new code AVANTI [1], based on our version of the Direct Implicit PIC algorithm [2,3,4], frequently require a relativistic representation of the plasma. We present here a relativistic extension of the plasma representation of this method.

As with explicit PIC codes [5], the relativistic generalization consists of a modification of the particle equations of motion so that the relativistic particle momentum is integrated in time rather than the particle velocity. Maxwell's equations, already built into the model [1], are relativistically correct. The implicit D_1 adaptation of the relativistic particle advance is given by

$$\mathbf{u}_{n+\frac{1}{2}} = \mathbf{u}_{n-\frac{1}{2}} + \Delta t\big[\bar{\mathbf{a}}_n + \frac{q}{m}\frac{\mathbf{u}_{n+\frac{1}{2}} + \mathbf{u}_{n-\frac{1}{2}}}{2\gamma_n c} \times \mathbf{B}_n(\mathbf{x}_n)\big] \tag{1a}$$

where

$$\bar{\mathbf{a}}_n = \tfrac{1}{2}\big[\bar{\mathbf{a}}_{n-1} + \frac{q}{m}\mathbf{E}_{n+1}(\mathbf{x}_{n+1})\big] \tag{1b}$$

and Boris' definition of γ_n [5],

$$\gamma_n^2 = 1 + (\mathbf{u}_{n-\frac{1}{2}} + \tfrac{1}{2}\bar{\mathbf{a}}_n\Delta t)^2/c^2, \tag{1c}$$

is time-centered because it is also equal to $1 + (\mathbf{u}_{n+\frac{1}{2}} - \frac{1}{2}\bar{\mathbf{a}}_n\Delta t)^2/c^2$; the position advance is given by

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \Delta t\frac{\mathbf{u}_{n+\frac{1}{2}}}{\gamma_{n+\frac{1}{2}}} \tag{1d}$$

where

$$\gamma_{n+\frac{1}{2}}^2 = 1 + \frac{u_{n+\frac{1}{2}}^2}{c^2} \tag{1e}$$

and we defined $\mathbf{u} \equiv \gamma\mathbf{v}$, the relativistic momentum divided by the rest mass; $\mathbf{x}$ is the position vector and $\mathbf{E}$ and $\mathbf{B}$ are the electromagnetic fields. Note that the explicit relativistic scheme is given by taking $\bar{\mathbf{E}}_n = \mathbf{E}_n$ just as it is in the nonrelativistic case [3,4].

Our implicit algorithm splits the time advance into two parts: the first part, the PREPUSH, advances the particles to a *tilde* level using all the field contributions *except* those due to the advanced electric field $\mathbf{E}_{n+1}$; the second part, the FINALPUSH adds on the contribution due to $\mathbf{E}_{n+1}$ after it has been computed. The PREPUSH takes the form

$$\tilde{\mathbf{u}}_{n+\frac{1}{2}} = \mathbf{u}_{n-\frac{1}{2}} + \tfrac{1}{2}\bar{\mathbf{a}}_{n-1}\Delta t + \frac{\tilde{\mathbf{u}}_{n+\frac{1}{2}} + \mathbf{u}_{n-\frac{1}{2}}}{\tilde{\gamma}_n} \times \boldsymbol{\theta} \tag{2a}$$

where

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

and

$$\tilde{\gamma}_n^2 = 1 + (\mathbf{u}_{n-\frac{1}{2}} + \tfrac{1}{4}\bar{\mathbf{a}}_{n-1}\Delta t)^2/c^2 \tag{2b}$$

and the *tilde* position coordinates are advanced by

$$\tilde{\mathbf{x}} = \mathbf{x}_n + \Delta t \frac{\tilde{\mathbf{u}}_{n+\frac{1}{2}}}{\tilde{\gamma}_{n+\frac{1}{2}}} \tag{2c}$$

where $\tilde{\mathbf{u}}_{n+\frac{1}{2}}$ can be found using the Boris solution [5], with

$$\tilde{\gamma}_{n+\frac{1}{2}}^2 = 1 + \frac{\tilde{u}_{n+\frac{1}{2}}^2}{c^2}. \tag{2d}$$

The direct implicit algorithm computes the advanced electric and magnetic fields using information from the *tilde* level. The plasma source terms at the advanced time level must be eliminated in Maxwell's equations before we can solve for the advanced fields. Expanding the particle-mesh shape weighting factor about the *tilde* positions and velocities, we can express the advanced charge and current densities on the mesh as [1,2]

$$\rho_{n+1} = \tilde{\rho}_{n+1} - \nabla \cdot \tilde{\rho}_{n+1}\delta\mathbf{x}$$

$$\mathbf{J}_{n+\frac{1}{2}} = \tilde{\mathbf{J}}_{n+\frac{1}{2}} + \tilde{\rho}_{n+1}\delta\mathbf{v} - \tfrac{1}{2}\nabla \times (\tilde{\mathbf{J}}_{n+\frac{1}{2}} \times \delta\mathbf{x})$$

Not surprisingly, ρ_{n+1} and $\mathbf{J}_{n+\frac{1}{2}}$ are expressed as sums over the contributions $\delta\mathbf{u}$ and $\delta\mathbf{x}$ that result when the new $\mathbf{E}_{n+1}$ is applied to the particles. Keeping all contributions linear in $\mathbf{E}_{n+1}$, we write

$$\rho_{n+1} = \tilde{\rho}_{n+1} - \nabla \cdot \boldsymbol{\chi} \cdot \mathbf{E}_{n+1} \tag{3a}$$

$$\mathbf{J}_{n+\frac{1}{2}} = \tilde{\mathbf{J}}_{n+\frac{1}{2}} + \boldsymbol{\chi} \cdot \mathbf{E}_{n+1}/\Delta t - c\nabla \times \boldsymbol{\zeta} \cdot \mathbf{E}_{n+1} \tag{3b}$$

The dimensionless tensors $\boldsymbol{\chi}$ and $\boldsymbol{\zeta}$ provide the connection in the source terms 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.

In order to get expressions for $\boldsymbol{\chi}$ and $\boldsymbol{\zeta}$, we first must obtain expressions for the pieces $\delta\mathbf{u}$ and $\delta\mathbf{x}$ that express the difference between the *tilde* level and the advanced time. Beginning with the simpler adjustment to $\tilde{\mathbf{x}}$ to get $\mathbf{x}_{n+1}$, linearization of Eqs. (1d-1e) about the *tilde* values (2c-2d) provides

$$\delta\mathbf{x} = \frac{\Delta t}{\tilde{\gamma}_{n+\frac{1}{2}}}\left[\mathbf{I} - \frac{\tilde{\mathbf{u}}_{n+\frac{1}{2}}\tilde{\mathbf{u}}_{n+\frac{1}{2}}}{\tilde{\gamma}_{n+\frac{1}{2}}^2 c^2}\right] \cdot \delta\mathbf{u}. \tag{4a}$$

Linearization of Eqs. (1a-1c) provides

$$\delta\mathbf{u} = \frac{q\Delta t}{2m}\mathbf{E}_{n+1}(\tilde{\mathbf{x}}) + \frac{1}{\tilde{\gamma}_n}\left[\delta\mathbf{u} - (\tilde{\mathbf{u}}_{n+\frac{1}{2}} + \mathbf{u}_{n-\frac{1}{2}})\frac{\delta\gamma}{\tilde{\gamma}_n}\right] \times \boldsymbol{\theta} \tag{4b}$$

From (1c) and (2d),

$$\tilde{\gamma}_n\delta\gamma = (\mathbf{u}_{n-\frac{1}{2}} + \tfrac{1}{4}\bar{\mathbf{a}}_{n-1}\Delta t)/c^2 \cdot \frac{q\Delta t}{4m}\mathbf{E}_{n+1} \tag{4c}$$

From which

$$\delta\mathbf{u} = \left\{ \mathsf{I} - \frac{1}{2\tilde{\gamma}_n^3 c^2}(\tilde{\mathbf{u}}_{n+\frac{1}{2}} + \mathbf{u}_{n-\frac{1}{2}}) \times \boldsymbol{\theta}\,(\mathbf{u}_{n-\frac{1}{2}} + \tfrac{1}{4}\bar{\mathbf{a}}_{n-1}\Delta t) \right\} \cdot \frac{q\Delta t}{2m}\mathbf{E}_{n+1} + \delta\mathbf{u} \times \boldsymbol{\theta}/\tilde{\gamma}_n \quad (4d)$$

The δ terms are just the pieces that are left over when Eqs. (2) are subtracted from Eqs. (1). Eq. (4d) can be solved in the form

$$\delta\mathbf{u} = \tfrac{1}{2}\left[\mathsf{I} + \mathsf{R}(\boldsymbol{\theta}/\tilde{\gamma}_n)\right] \cdot \left\{\ldots\right\} \cdot \frac{q\Delta t}{2m}\mathbf{E}_{n+1} \quad (4e)$$

where R is the gyro rotation; explicitly

$$\tfrac{1}{2}\left[\mathsf{I} + \mathsf{R}(\boldsymbol{\theta})\right] = \left[\mathsf{I} + \boldsymbol{\theta}\boldsymbol{\theta} - \boldsymbol{\theta} \times \mathsf{I}\right]/(1 + \theta^2)$$

A significant difference between the nonrelativistic and relativistic algorithm is now apparent. In the nonrelativistic case the corresponding expression Eq. (4a) does not have the $\tilde{\mathbf{u}}\tilde{\mathbf{u}}$ tensor contribution, and the factor $\{\ldots\}$ in (4d-4e) slows the evaluation of $\delta\mathbf{u}$ relative to the explicit Boris push. Further, this coupling must also be considered when summations are made over the δ quantities to find expressions for the tensors $\boldsymbol{\chi}$ and $\boldsymbol{\zeta}$. In the nonrelativistic case using simplified differencing [2,3], we find these two tensors can be made from combinations of $\tilde{\rho}_{n+1}$ and $\tilde{\mathbf{J}}_{n+\frac{1}{2}}$ summed over species. In the relativistic case, we find *tensor* quantities for each particle i which must be summed over to find the contribution of the δ quantities to the advanced source terms:*

$$\boldsymbol{\chi}_i = \frac{\Delta t^2}{2}\frac{q_i^2}{m_i}\frac{1}{\tilde{\gamma}_{n+\frac{1}{2}}}\left[\mathsf{I} - \frac{\tilde{\mathbf{u}}_{n+\frac{1}{2}}\tilde{\mathbf{u}}_{n+\frac{1}{2}}}{\tilde{\gamma}^2_{n+\frac{1}{2}}c^2}\right] \cdot [\mathsf{I} + \mathsf{R}] \cdot \{\ldots\}, \quad (5c)$$

$$\boldsymbol{\zeta}_i = \frac{\Delta t^2}{4}\frac{q_i^2}{m_i c}\frac{\tilde{\mathbf{u}}_{n+\frac{1}{2}}}{\tilde{\gamma}_{n+\frac{1}{2}}} \times [\mathsf{I} + \mathsf{R}] \cdot \{\ldots\}. \quad (5d)$$

In the summations over particles the tensors $\boldsymbol{\chi}_i$ and $\boldsymbol{\zeta}_i$ are weighted to the mesh at positions $\tilde{\mathbf{x}}_{i,n+1}$. The representation on the interleaved mesh is given in [1], Appendix A. A simplicity that is lost with the relativistic extension is that it is necessary to sum over particles to accumulate these tensors; they depend on particle velocity as well as position and cannot be evaluated simply on the spatial mesh.

These equations constitute a relativistic direct implicit PIC algorithm using simplified differencing. It is similar in most respects to the nonrelativistic model now implemented in AVANTI [1]. The field solution algorithm and most data structures need no modification to work with this extension. The code TESS [6] has already provided a useful test bed for some of these ideas in the 1D electrostatic limit.

There are difficulties in the extension of implicit codes to include relativistic effects. The extra computer time required for the "scattering" steps required to accumulate the tensors from the particles is an obvious concern. In many problems, however, it may be acceptable to treat

* In (5d), the factor $[\mathsf{I} - \tilde{\mathbf{u}}\tilde{\mathbf{u}}/\tilde{\gamma}^2 c^2]$ does not appear because of the $\tilde{\mathbf{u}}_{n+\frac{1}{2}} \times \ldots$ operation.

only some species relativistically so that the extra expense is paid only for those species. Because $u^2/c^2\gamma^2 \rightarrow 1$ for $\gamma \gg 1$, we are cautious about making approximations to the form of (4a). Similarly, simplification of (4d) is evident only for $\theta/\gamma \ll 1$.

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