A PIC algorithm for collisionless plasma

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1 Equations

1.1 Kinetic equations

A kinetic plasma model regards the plasma as charged particles interacting with an electromagnetic field. In the case of a collisionless kinetic plasma model, the particles do not interact directly with one another, but are directly coupled only to the electromagnetic field, so the equations are:

$$[d_t(\gamma \mathbf{v}) = (q/m)(\mathbf{E} + \mathbf{v} \times \mathbf{B})]_{\mathrm{p}},$$
$$[d_t \mathbf{x} = \mathbf{v}]_{\mathrm{p}},$$
$$\partial_t \mathbf{E} = c^2 \nabla \times \mathbf{B} - \mathbf{J}/\epsilon_0,$$
$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E},$$

where t is time, $\gamma := \big(1 - (v/c)^2\big)^{-1/2}$, p denotes particle index, m_{p} denotes particle mass, $\mathbf{x}_{\mathrm{p}}(t)$ denotes particle position, $\mathbf{v}_{\mathrm{p}}(t)$ denotes particle velocity. $\mathbf{E}$ is the electric field, $\mathbf{B}$ is the magnetic field, ϵ_0 is vacuum electric permittivity, $\mathbf{J} = \sum_{\mathrm{p}} (qSv)_{\mathrm{p}}$ is the current, and $S_{\mathrm{p}}(x,t) = S_{\mathrm{p}}(\mathbf{x} - \mathbf{x}_{\mathrm{p}}(t))$ is the distribution in space ("shape") of particle p. We assume that $\int_{\mathbb{R}^d} S_{\mathrm{p}} = 1$. (For physical plasmas, S can be taken to be a unit impulse (Dirac delta) function; our numerical model will take S to be a more spread-out distribution to avoid numerical noise.)

Physical solutions satisfy

$$\nabla \cdot \mathbf{E} = \sigma/\epsilon_0,$$
$$\nabla \cdot \mathbf{B} = 0,$$

where $\sigma = \sum_{\mathrm{p}} (qS)_{\mathrm{p}}$ is the (net) charge density.

2 Algorithm

2.1 PIC algorithm

We describe a particle-in-cell (PIC) algorithm. It assumes a rectilinear mesh.

$$\Big[\mathbf{v}^{n+\frac{1}{2}} = \mathbf{v}^{n-\frac{1}{2}} + \Delta t (q/m)\big(\mathbf{E}^n(x^n) + \frac{1}{2}(\mathbf{v}^{n+\frac{1}{2}} + \mathbf{v}^{n-\frac{1}{2}}) \times \mathbf{B}^n(\mathbf{x}^n)\big)\Big]_{\mathrm{p}},$$
$$[\mathbf{x}^{n+1} = x^n + \mathbf{v}^{n+\frac{1}{2}} \Delta t]_{\mathrm{p}},$$
$$\mathbf{E}^{n+1} = \mathbf{E}^n - \Delta t \Big(c^2 (\nabla \times \mathbf{B})^{n+\frac{1}{2}} - \mathbf{J}^{n+\frac{1}{2}}/\epsilon\Big)$$

The differential operators here are discretized versions that are cell-centered. For the explicit Yee scheme, the magnetic field is time-staggered. Note that all values

2.2 Explanation of PIC algorithm

Since we aim for second order accuracy, we are free to use space-centered and time-centered differencing. Using centered differences in space means that the discrete curl of the discrete gradient and the discrete divergence of the discrete curl both vanish exactly, just as for the corresponding continuous differential operators. Therefore, just as in the continuous case, taking the discrete divergence of Maxwell's evolution equations shows that if the discrete versions of the divergence constraints are initially exactly satisfied, they remain satisfied for all time. (We assume here that the discrete version of charge conservation, $\sigma + \nabla \cdot \mathbf{J} = 0$, holds exactly; we can ensure this by using a finite volume method and requiring $\mathbf{J}$ to be the flux of σ).

Applying centered differences to Maxwell's equations for d dimensions of space (where for the moment we take $\mathbf{J} = 0$) results in a scheme that partitions the quantity values at mesh points in space and time into 2^{d+1} completely decoupled sets of self-coupled mesh point values: for each quantity, mesh points that are adjacent either in space or time belong to different sets. Note that for a given coupled set of mesh points, values for different physical quantities are staggered in space and time with respect to another. The resulting scheme, restricted to one of the self-coupled sets, and expressed using half-integer indices to indicate the staggering, is called the *Yee scheme*. Since we intend to couple our algorithm to a finite-volume algorithm, we prefer to regard the domain as partitioned into cubes whose centers are the integral mesh points, and prefer to think of flux components (such as current components) as located at (and oriented perpendicular to) cell faces.

For $\mathbb{R}^3$, this leads us to locate the components of vectors, such as $\mathbf{J}$ and $\mathbf{E}$, so that each components is at the center of a face and points perpendicular to it, whereas we locate the components of pseudovectors, such as $\mathbf{B}$ or $\nabla \times \mathbf{E}$, at the center of cell edges so that each component points along the edge on which is lies.

Thus, in the generality of the three-dimensional Yee scheme, $\sigma_{i,j,k}$ denotes charge density located at the cell center, $\mathbf{E}^1_{i+\frac{1}{2},j,k}$ denotes the first component of the electric field located at (and pointing perpendicular to) a cell face, and $\mathbf{B}^1_{i,j+\frac{1}{2},k+\frac{1}{2}}$ denotes a component of the magnetic field located at (and pointing along) an edge. For two dimensions, we simply project these components onto the first two dimensions by omitting the third spatial index. For one dimension, only the first spatial index remains.

We elect to regard σ_j as at integer values in space and time. Then $\mathbf{J}$ must be staggered in space in time. So $\partial_t \mathbf{E}$ and $\nabla \times \mathbf{B}$ are staggered in time. So $\mathbf{E}$ is not staggered in time, and for the explicit Yee scheme, $\mathbf{B}$ must be staggered in time. (For the implicit Yee scheme, $(\nabla \times \mathbf{B})^{n+\frac{1}{2}} := \frac{1}{2}[(\nabla \times \mathbf{B})^n + (\nabla \times \mathbf{B})^{n+1}]$, and no time staggering is needed.)