Symplectic Particle-in-Cell

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Outline

Symplectic tracking:

- What is a symplectic code?
- Advantages/drawbacks
- How do you check symplecticity?

Symplectic PIC: from plasma physics to particle accelerators

- Low's Hamiltonian (relativistic)
- Transformation to Frenet-Serret coordinates

What is a symplectic code?

1. Find a Hamiltonian,
2. derive equations of motion from it,
3. plugged them into a symplectic integrator,
4. do nothing else.

What do you gain?

- You cannot get nonphysical results;
- You may still get inaccurate results.

What is the price to pay?

- Need knowledge of potentials: $\mathbf{A}$, ϕ.
- When $H(p, q)$: need to use an implicit integrator (slower).

How do you check symplecticity?

Symplectic PIC

My starting point: H. Qin *et al.* (arXiv:1503.08334).

We start from the canonical Poisson bracket and Hamiltonian for the Vlasov-Maxwell equations [26],

$$\{F, G\} \equiv \int f \left\{ \frac{\delta F}{\delta f}, \frac{\delta G}{\delta f} \right\}_{\mathbf{xp}} d\mathbf{x} d\mathbf{p} + \int \left(\frac{\delta F}{\delta \mathbf{A}} \frac{\delta G}{\delta \mathbf{Y}} - \frac{\delta G}{\delta \mathbf{A}} \frac{\delta F}{\delta \mathbf{Y}} \right) d\mathbf{x}. \tag{1}$$

$$H(f, \mathbf{A}, \mathbf{Y}) = \frac{1}{2} \int (\mathbf{p} - \mathbf{A})^2 f d\mathbf{x} d\mathbf{p} + \frac{1}{2} \int \left[\mathbf{Y}^2 + (\nabla \times \mathbf{A})^2 \right] d\mathbf{x}. \tag{2}$$

Here, F, G, and the Hamiltonian H are functionals of the distribution function f, vector potential $\mathbf{A}$, and $\mathbf{Y} \equiv \partial \mathbf{A}/\partial t$. The bracket $\{h, g\}_{\mathbf{xp}}$ inside the first term on the right hand side of Eq. (1) is the canonical Poisson bracket for functions h and g of canonical phase space $(\mathbf{x}, \mathbf{p})$. The temporal gauge, i.e., $\phi = 0$, has been explicitly chosen for this Poisson bracket

$\Longrightarrow$ 12 equations of motion integrated numerically with the same symplectic integrator.

Relativistic Hamiltonian

$$H(\mathbf{X}, \boldsymbol{\mathcal{P}}, \mathbf{A}, -\boldsymbol{\mathcal{E}}; t) =$$

$$\iint \sqrt{\tilde{m}^2 + (\boldsymbol{\mathcal{P}} - \tilde{q}\mathbf{A}(\mathbf{X}))^2} \mathrm{d}\mathbf{v}_1 \mathrm{d}\mathbf{x}_1 + \int \frac{\boldsymbol{\mathcal{E}}^2}{2} + \frac{(\nabla \times \mathbf{A})^2}{2} \, \mathrm{d}\mathbf{x}_1 \,, \qquad (1)$$

with $\tilde{m} = fm$, $\tilde{q} = fq$, and $\boldsymbol{\mathcal{P}} = f\,(\mathbf{p} + q\mathbf{A})$.

See arXiv:1603.02976.

Equations of Motion:

Like for single particles, equations of motion are obtained from:

$$\dot{q} = \{q, H\} \tag{2}$$
$$\dot{p} = \{p, H\}\ . \tag{3}$$

The canonical Poisson bracket is:

$$\{F, G\} := \iint \frac{\delta F}{\delta \mathbf{X}} \frac{\delta G}{\delta \boldsymbol{\mathcal{P}}} - \frac{\delta F}{\delta \boldsymbol{\mathcal{P}}} \frac{\delta G}{\delta \mathbf{X}}\, \mathrm{d}^3 v_1 \mathrm{d}^3 x_1 - \int \frac{\delta F}{\delta \mathbf{A}} \frac{\delta G}{\delta \boldsymbol{\mathcal{E}}} - \frac{\delta F}{\delta \boldsymbol{\mathcal{E}}} \frac{\delta G}{\delta \mathbf{A}} \mathrm{d}^3 x_1 \tag{4}$$

where δ stand for functional derivatives.

Twelve Equations of Motion:

$$\dot{\mathbf{X}} = \frac{(\boldsymbol{\mathcal{P}} - \tilde{q}\mathbf{A})}{\sqrt{\tilde{m}^2 + (\boldsymbol{\mathcal{P}} - \tilde{q}\mathbf{A})^2}} \tag{5}$$

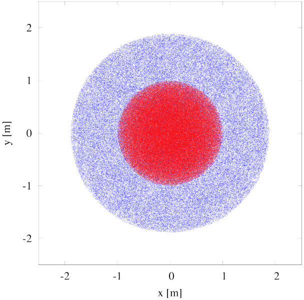
$$\dot{\boldsymbol{\mathcal{P}}} = \tilde{q}\nabla(\dot{\mathbf{X}} \cdot \mathbf{A}) \tag{6}$$

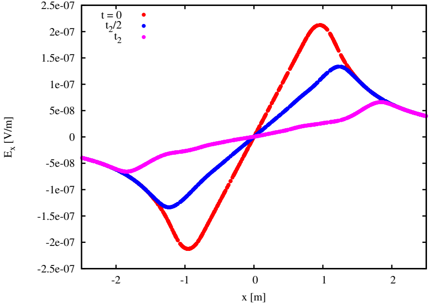
$$\dot{\mathbf{A}} = -\boldsymbol{\mathcal{E}} \tag{7}$$

$$-\dot{\boldsymbol{\mathcal{E}}} = -\nabla \times \nabla \times \mathbf{A} + \int \tilde{q}\dot{\mathbf{X}}\,\mathrm{d}^3 v_1\,. \tag{8}$$

Code Testing: Debunching Sphere

My student Paul Jung plugged those 12 equations into a **second order symplectic Störmer-Verlet** integrator:



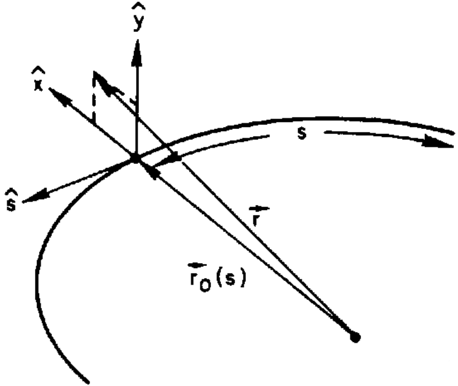


In the non-relativistic limit the time needed for the sphere to double its size is given by:

$$t_2 = (\text{arcsinh}(1) + \sqrt{2})\sqrt{\frac{2\pi m R_0^3}{qQ}} \tag{9}$$

But that is about how far we got...

Frenet-Serret Coordinates



Canonical Transformation to Frenet-Serret

To make use of J. Struckmeier's work I need a Hamiltonian written under a single integral: $H = \int \mathcal{H}$. I propose:

$$H = \int \sqrt{\tilde{m}^2 + (\boldsymbol{\mathcal{P}} - \tilde{q}\mathbf{A}(\mathbf{X}))^2} + \frac{3}{8\pi}\left(\boldsymbol{\mathcal{E}}^2 + (\nabla \times \mathbf{A})^2\right) \mathrm{d}^3 v_1 \mathrm{d}^3 x_1 \mathrm{d}t_1 \,. \quad (10)$$

given that $\int \mathrm{d}^3 v_1 = \frac{4\pi}{3}$. Canonical pairs are: $(\mathbf{X}, \boldsymbol{\mathcal{P}})$, $(\mathbf{A}, -\boldsymbol{\mathcal{E}})$, $(t, -\mathcal{H})$.

Canonical Transformation to Frenet-Serret

The Poisson bracket writes:

$$\{F, G\} := \int \left(\sum_i \frac{\delta F}{\delta q_i} \frac{\delta G}{\delta p_i} - \frac{\delta F}{\delta p_i} \frac{\delta G}{\delta q_i} \right) \mathrm{d}^3 v_1 \mathrm{d}^3 x_1 \mathrm{d} t_1 \tag{11}$$

Canonical Transformation to Frenet-Serret

$(X, Y, Z, t) \to (x, y, s, \Delta t)$:

$$F_3 = \boldsymbol{\mathcal{P}} \cdot \mathbf{X} - \mathcal{H} \cdot t - \boldsymbol{\mathcal{E}} \cdot \mathbf{A} \tag{12}$$

It is a generating function of the type "new positions old momenta" which requires derivatives w.r.t. old momenta to be the old positions. For a proof and more explanations follow this link.

Canonical Transformation to Frenet-Serret

New momenta are given by derivatives w.r.t. new positions:

$$
\begin{aligned}
\boldsymbol{\mathcal{P}}_x &= \frac{\partial F_3}{\partial x} = \boldsymbol{\mathcal{P}} \cdot \hat{\mathbf{x}} \\
\boldsymbol{\mathcal{P}}_y &= \frac{\partial F_3}{\partial y} = \boldsymbol{\mathcal{P}} \cdot \hat{\mathbf{y}} \\
\boldsymbol{\mathcal{P}}_s &= \frac{\partial F_3}{\partial s} = (1 + \frac{x}{\rho})\boldsymbol{\mathcal{P}} \cdot \hat{\mathbf{s}} - \frac{\mathcal{H}}{\beta_0} \\
-\mathcal{H} &= \frac{\partial F_3}{\partial \Delta t} = -\mathcal{H} \\
-\boldsymbol{\mathcal{E}}_x &= \frac{\partial F_3}{\partial \mathbf{A}_x} = -\boldsymbol{\mathcal{E}} \cdot \hat{\mathbf{x}} \\
-\boldsymbol{\mathcal{E}}_y &= \frac{\partial F_3}{\partial \mathbf{A}_y} = -\boldsymbol{\mathcal{E}} \cdot \hat{\mathbf{y}} \\
-\boldsymbol{\mathcal{E}}_s &= \frac{\partial F_3}{\partial \mathbf{A}_s} = -\boldsymbol{\mathcal{E}} \cdot \hat{\mathbf{s}}
\end{aligned}
\tag{13}
$$

Canonical Transformation to Frenet-Serret

$$\mathcal{H} = \frac{3}{8\pi}\left(\boldsymbol{\mathcal{E}}^2 + (\nabla \times \mathbf{A})^2\right) + \sqrt{\tilde{m}^2 + (\boldsymbol{\mathcal{P}}_x - \tilde{q}\mathbf{A}_x(\mathbf{x}))^2 + (\boldsymbol{\mathcal{P}}_y - \tilde{q}\mathbf{A}_y(\mathbf{x}))^2 + \left(\frac{\boldsymbol{\mathcal{P}}_s + \frac{\mathcal{H}}{\beta_0}}{1 + \frac{x}{\rho}} - \tilde{q}\mathbf{A}_s(\mathbf{x})\right)^2} \tag{14}$$

Canonical Transformation to Frenet-Serret

$$\mathcal{H}_s = -\boldsymbol{\mathcal{P}}_s =$$

$$\frac{\mathcal{H}}{\beta_0} - (1 + \frac{x}{\rho}) \left(\tilde{q}\mathbf{A}_s(\mathbf{X}) + \sqrt{\left(\mathcal{H} - \frac{3}{8\pi} \left(\boldsymbol{\mathcal{E}}^2 + (\nabla \times \mathbf{A})^2\right)\right)^2 - \tilde{m}^2 - (\boldsymbol{\mathcal{P}}_x - \tilde{q}\mathbf{A}_x(\mathbf{X}))^2 - (\boldsymbol{\mathcal{P}}_y - \tilde{q}\mathbf{A}_y(\mathbf{X}))^2} \right) \tag{15}$$

Equations of motion with s as independent variable:

$$
\begin{aligned}
x' &= (1+\frac{x}{\rho})\frac{\mathcal{P}_x - \tilde{q}\mathcal{A}_x(\mathbf{x})}{\sqrt{\cdots}} \\
y' &= (1+\frac{x}{\rho})\frac{\mathcal{P}_y - \tilde{q}\mathcal{A}_y(\mathbf{x})}{\sqrt{\cdots}} \\
\Delta t' &= (1+\frac{x}{\rho})\frac{\mathcal{H}_b}{\sqrt{\cdots}} - \frac{1}{\beta_0} \\
\boldsymbol{\mathcal{P}}' &= \tilde{q}\nabla(\mathbf{v}\cdot\mathbf{A}) + \sqrt{\cdots}\,\nabla(1+\frac{x}{\rho}) \\
\mathbf{A}' &= -\frac{3}{4\pi}(1+\frac{x}{\rho})\boldsymbol{\mathcal{E}}\int \frac{\mathcal{H}_b}{\sqrt{\cdots}}\,\mathrm{d}^3 v_1 \\
\boldsymbol{\mathcal{E}}' &= \frac{3}{4\pi}\nabla\times\nabla\times\mathbf{A}\int\frac{\mathcal{H}_b}{\sqrt{\cdots}}\,\mathrm{d}^3 v_1 - \int \tilde{q}\mathbf{v}\,\mathrm{d}^3 v_1 \\
\mathcal{H}' &= 0
\end{aligned}
\tag{16}
$$

Equations of motion with s as independent variable:

where

$$\mathbf{v} = \begin{bmatrix} x' \\ y' \\ 1 + \frac{x}{\rho} \end{bmatrix}, \tag{17}$$

with

$$\mathcal{H}_b = \mathcal{H} - \frac{3}{8\pi} \left(\boldsymbol{\mathcal{E}}^2 + (\nabla \times \mathbf{A})^2 \right) \ , \tag{18}$$

and

$$\sqrt{\ldots} = \sqrt{\left(\mathcal{H} - \frac{3}{8\pi} \left(\boldsymbol{\mathcal{E}}^2 + (\nabla \times \mathbf{A})^2 \right) \right)^2 - \tilde{m}^2 - (\mathcal{P}_x - \tilde{q}\mathcal{A}_x(\mathbf{x}))^2 - (\mathcal{P}_y - \tilde{q}\mathcal{A}_y(\mathbf{x}))^2} \, . \tag{19}$$