STRUCTURE-PRESERVING SECOND-ORDER INTEGRATION OF RELATIVISTIC CHARGED PARTICLE TRAJECTORIES IN ELECTROMAGNETIC FIELDS

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What is structure preservation, and why is it important?

- Structure = invariants
  - Integrals of motion (energy, momentum, …), motion lies on topological circules
  - Differential (Poincaré invariants, including Liousville = volume) regions neither expand nor contract
- Structure preserving integration:
  - Preserve an invariant exactly, even though integrator is accurate to only a certain order
- Structure preserving integration can
  - Require less computational work
  - Better preserve other integral invariants

Outline

- Symplectic integration
- Motion in EM fields (absence of a general symplectic integrator)
- Boris push
- Spatial Boris push (muon collider sims) & numerical results
- Volume preservation
- Vay push preserves ExB motion
- Higuera-Cary push preserves ExB and volume
- Numerical results

Long been a belief in need for symplectic integration

- Hadron beams propagating in accelerator lattice: collection of single particle Hamiltonian systems, neglecting radiation, collisions, self-fields
- Courant-Snyder invariants: transverse and longitudinal actions conserved: *invariant actions*
- Perturbations are always present
  - Lattice errors
  - Sextupoles (chromaticity)
- KAM theorem: Tori of invariant actions are preserved by small perturbations

Simple example: Euler versus leap frog

$$\frac{dx}{dt} = p_0 \qquad \frac{dp}{dt} = -\omega^2 x$$

- Not Symplectic (Euler – diverges, long-time exponentially unstable)

$$x(\Delta t) = x_0 + p_0 \Delta t$$
$$p(\Delta t) = p_0 - \omega^2 x_0 \Delta t$$
$$J = 1 + (\omega \Delta t)^2$$

- Symplectic (Leap frog, product of symplectics)

$$x(\Delta t) = x_0 + p_0 \Delta t \qquad p(\Delta t) = p_0 - \omega^2 x(\Delta t)$$

An integrator is a solution of the equations of motion valid to some order

- Canonical momentum, p
- Kinetic momentum, u
- Propagation
- Lorentz force

$$\mathbf{E}(\mathbf{x}, t) \quad \mathbf{B}(\mathbf{x}, t)$$

$$q = m = c = 1$$

$$\dot{\mathbf{x}} = (\mathbf{p} - \mathbf{A})/\gamma \equiv \mathbf{v}(\mathbf{u})$$

$$\mathbf{u} \equiv \mathbf{p} - \mathbf{A}$$

$$\dot{\mathbf{u}} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$

$$\mathbf{x}(\Delta \mathrm{t}) \equiv \mathbf{x}_0 + \Delta\mathbf{x}(\mathbf{x}_0, \mathbf{p}_0, \Delta t) + O(\Delta t^2)$$

$$\mathbf{p}(\Delta t) \equiv \mathbf{p}_0 + \Delta\mathbf{p}(\mathbf{x}_0, \mathbf{p}_0, \Delta t) + O(\Delta t^2)$$

A symplectic integrator: the solution is exactly a canonical transformation

$$\mathbf{x}(\Delta t) \equiv \mathbf{x}_0 + \Delta\mathbf{x}(\mathbf{x}_0, \mathbf{p}_0, \Delta t)$$

$$\mathbf{p}(\Delta t) \equiv \mathbf{p}_0 + \Delta\mathbf{p}(\mathbf{x}_0, \mathbf{p}_0, \Delta t)$$

$$\frac{\partial x_i}{\partial \mathbf{x}_0} \cdot \frac{\partial x_j}{\partial \mathbf{p}_0} - \frac{\partial x_i}{\partial \mathbf{p}_0} \cdot \frac{\partial x_j}{\partial \mathbf{x}_0} = 0 \qquad \frac{\partial x_i}{\partial \mathbf{x}_0} \cdot \frac{\partial p_j}{\partial \mathbf{p}_0} - \frac{\partial x_i}{\partial \mathbf{p}_0} \cdot \frac{\partial p_j}{\partial \mathbf{x}_0} = \delta_{i,j}$$

- And two more relations
- To be a symplectic integrator, the above relations must hold *exactly*

Ruth, Nuclear Science, IEEE Trans. on. (1983)
Forest and Ruth; Yoshida (1990)
Candy and Rozmus (1991)

- The expression in terms of kinetic momenta is more complicated: non-canonical Poisson brackets

Littlejohn (198?)
Cary, Littlejohn (1983)

The KAM theorem indicates stability of numerical integration

- One symplectic transformation (the actual motion)
- Another symplectic transformation (the numerically found trajectory)
- With a small perturbation, invariant tori with sufficiently irrational tunes of the first survive in the second
- Find a numerical integration method that, while only approximate, is symplectic exactly, then for sufficiently small time step, it will behave for *long times* like the actual system

Operator splitting: path to second order

$$\dot{\mathbf{x}} = \mathbf{v}(\mathbf{u}) = \mathbf{u}/\gamma \qquad \mathbf{x} = \mathbf{x}_0 + \mathbf{v}\Delta t$$

$$\dot{\mathbf{u}} = \mathbf{E} + \mathbf{v}\times\mathbf{B} \qquad \Delta\mathbf{x} = \mathbf{v}\Delta t$$

- Integrate the first equation holding u constant
- Integrate the second equation holding x constant – cannot be done if E and B are time varying
- Cannot be done in a simulation when variation of E, B depend on particle motion
- Know E, B at a given time, find change in u by time-centered difference (implicit)

$$\Delta\mathbf{u} = (\mathbf{E} + \bar{\mathbf{v}}\times\mathbf{B})\Delta t$$

- Average so far unspecified

Plasma simulation long relied on the "Boris push"

- Operator splitting again
  - Half acceleration
  - Rotation (γ=constant)
  - Half acceleration
- Time centered as starts and ends with half acceleration

$$\Delta \mathbf{u} = (\mathbf{E} + \bar{\mathbf{v}} \times \mathbf{B})\Delta t$$

$$\mathbf{u}_- = \mathbf{u}_0 + \frac{1}{2}\mathbf{E}\Delta t$$

$$\mathbf{u}_+ - \mathbf{u}_- = \frac{\mathbf{u}_+ + \mathbf{u}_-}{2\gamma} \times \mathbf{B}\Delta t$$

$$\mathbf{u}_f = \mathbf{u}_+ + \frac{1}{2}\mathbf{E}\Delta t$$

- Unconditionally stable
- Good results since 1971!
- Universal among PIC codes (Vorpal, Osiris, Warp, …)

Spatial analog found in PR ST/AB 5, 094001 (2002)

- Muon collider (Fernow) relied on Runge-Kutta-4 for integration.
- Goal: is there emittance transfer through ionization cooling?
- Problem: is there cooling simply due to the integration
- Boris push modified (Stoltz et al) for spatial integration (tracking) by interchange

$$t \leftrightarrow z \qquad \gamma \leftrightarrow p_z$$

Spatial Boris eliminated numerical, unphysical cooling

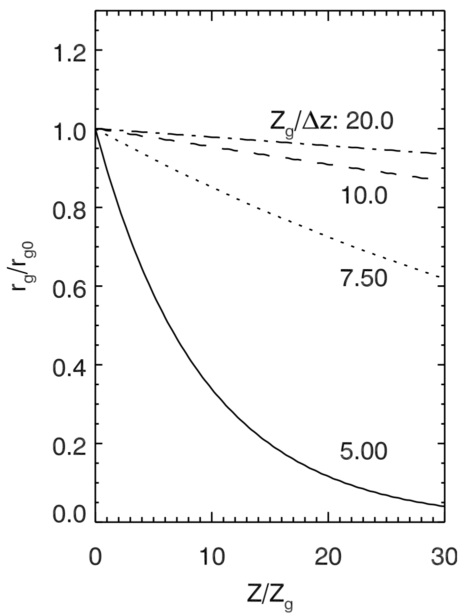
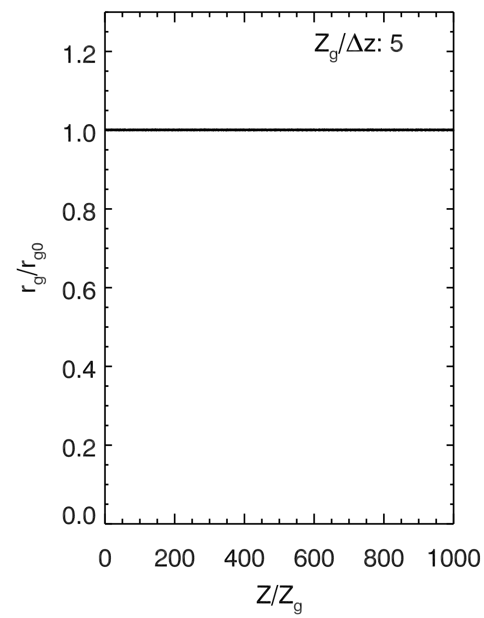


FIG. 1. The gyroradius (normalized to its initial value) as a function of distance (normalized to the gyroperiod) calculated using the fourth-order Runge-Kutta integration scheme. Plots are shown for step sizes of 5, 7.5, 10, and 20 steps per gyroperiod. The curves for perpendicular momentum as a function of distance are similar to these.



RK4 (4th order) vs Spatial Boris (2nd order)

Special property of Boris push: volume preservation

- NOT symplectic, yet still very good
- Boris push is volume preserving (Qin, 2015) as it is the successive application of
  - Translation in space
  - Half translation in momentum
  - Sheared rotation in momentum
  - Half translation in momentum
- All of which are volume preserving
- But spectral methods have long existed: Cary Doxas, "An Explicit Symplectic Integration Scheme for Plasma Simulations," J. Comp. Phys. 107 (1) 98-104 (1993) shows how to also get low noise, PIC algorithmic scaling

For self-consistent beams, want to preserve ExB balance

- Beam nonequilibrium between E and jxB forces
- Constant focusing model, add in extra “electric field”

The general push can be thought of as a time-centered acceleration

$$\Delta \mathbf{u} = (\mathbf{E} + \bar{\mathbf{v}} \times \mathbf{B}) \Delta \boldsymbol{t}$$

$$\bar{\mathbf{v}}_{Boris} = \frac{\mathbf{v}\left(\mathbf{u}_i + \frac{1}{2}\mathbf{E}\Delta t\right) + \mathbf{v}\left(\mathbf{u}_f - \frac{1}{2}\mathbf{E}\Delta t\right)}{2}$$

- Boris is the above average which corresponds to the translation, rotation, translation, for which the equations were solved long ago.
- But there is no steady solution

$$\Delta \mathbf{u} \Rightarrow (\mathbf{E} + \bar{\mathbf{v}}_B \times \mathbf{B}) = 0$$

- Either $v_{B,||}$ = 0 (not true for intense beams)
- Or u+EΔt/2 = u-EΔt/2 or E = 0 (also not true for relativistic, intense beams)
- Generally, no steady solution

The Vay push uses the average of the velocities

$$\Delta \mathbf{u} = (\mathbf{E} + \bar{\mathbf{v}} \times \mathbf{B})\Delta t$$

$$\bar{\mathbf{v}}_{Vay} = \frac{\mathbf{v}(\mathbf{u}_i) + \mathbf{v}(\mathbf{u}_f)}{2}$$

- Average the velocities
- Allows equilibrium solution
- Zero change gives

$$\mathbf{E} + \bar{\mathbf{v}}_V \times \mathbf{B} = 0$$

$$\mathbf{E} + \bar{\mathbf{v}}_i \times \mathbf{B} = \mathbf{E} + \bar{\mathbf{v}}_f \times \mathbf{B} = 0$$

From Higuera-Cary paper: Center the momentum

$$\Delta \mathbf{u} = (\mathbf{E} + \bar{\mathbf{v}} \times \mathbf{B}) \Delta t$$

$$\bar{\mathbf{v}}_{HC} = \mathbf{v}\left(\frac{\mathbf{u}_i + \mathbf{u}_f}{2}\right)$$

- Compute velcity at average of kinetic momenta
- Allows equilibrium solution
- Zero change gives

$$\mathbf{E} + \bar{\mathbf{v}}_{HC} \times \mathbf{B} = 0$$

$$\mathbf{E} + \bar{\mathbf{v}}_i \times \mathbf{B} = \mathbf{E} + \bar{\mathbf{v}}_f \times \mathbf{B} = 0$$

To study volume preservation, break step into two parts

$$\Delta\mathbf{u} = (\mathbf{E} + \bar{\mathbf{v}}\times\mathbf{B})\Delta\mathrm{t}$$

$$\bar{\mathbf{v}}_{HC} = \mathbf{v}\left(\frac{\mathbf{u}_i + \mathbf{u}_f}{2}\right)$$

$$\mathbf{u}_\mathrm{f} = \bar{\mathbf{u}} + (\mathbf{E} + \mathbf{v}(\bar{\mathbf{u}})\times\mathbf{B})\Delta t/2 \qquad \bar{\mathbf{u}} = \mathbf{u}_i + (\mathbf{E} + \mathbf{v}(\bar{\mathbf{u}})\times\mathbf{B})\Delta t/2$$

- HC: implicit step followed by explicit step
- Volume preservation follows:
  - Jacobian from initial to average is inverse of Jacobian from average to initial, which is the inverse of the same function from average to final. QED.
- Vay turns out to be opposite: explicit followed by implicit. But volume preservation does not follow because evaluated at different kinetic momenta

Only integrator of Higuera-Cary paper meets both desired criteria

All of these integrators have the same accuracy order, but they have different properties regarding exact preservation of differential and integral invariants

Integrator	Exactly Volume preserving	Exactly preserves equilibrium
Boris	✓	No
Vay	No	✓
Higuera and Cary	✓	✓

Maximum effect is moderately relativistic with some E parallel to B

- Vay non-volume-conservation:

$$J_{v,B} = \frac{J(x_0,u_0)}{J(x_0,u_1)} \frac{J(x_1,u_1)}{J(x_1,u_2)} \cdots \frac{J(x_{N-1},u_{N-1})}{J(x_{N-1},u_N)},$$

- Where

$$J_{f,new} = 1 + \frac{\beta^2 + (\vec{\beta}\cdot\bar{u}_{new})^2}{\gamma_{new}^4}.$$

$$\vec{\beta} \equiv \frac{q\vec{B}}{2m}\Delta t,$$

- Important where both B and u change
  - B changes from position change
  - u changes to prevent telescoping
  - Moderately relativistic (compare with changes)

Surfaces of section find that Vay has much larger islands, but basically still integrable

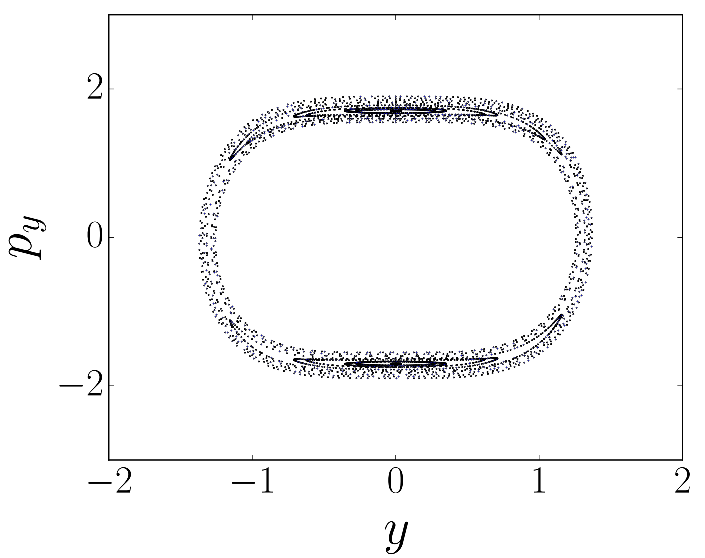
- One model problem

$$\vec{E} = E_x(x)\hat{x} \qquad \vec{A} = A_z(y)\hat{z}.$$

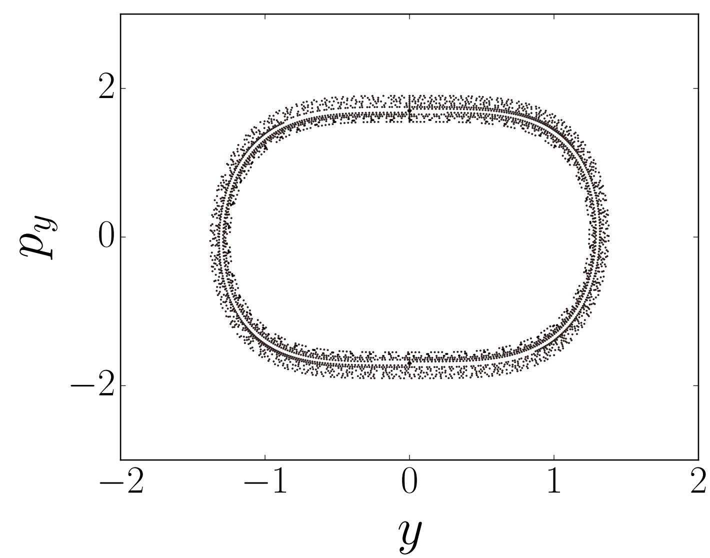
$$\vec{B} = B_x(y)\hat{x},$$

$$H = \sqrt{1 + p_x^2 + p_y^2 + (p_z - A_z(y))^2} + \phi(x)$$

- Invariants in involution: pz, $I_y \equiv p_y^2 + (p_z - A_z(y))^2$
- Surface of section (islands! Chaotic motion?)



$\omega\Delta t = 0.1$



Many more issues to explore

- What happens in the self-consistent (evolving fields) context?
- Could this be a problem in tracking/self-consistent codes?
- Others are right now looking at this in time-domain codes.

Hi John,
Sorry for my late response. Have been swamped this week.
Only glanced at it but looks like a great new particle pusher.
Likely that we will implement and test it soon.
Best, Jean-Luc

Summary and conclusions

- While the KAM theorem can be *proven* for only symplectic integrators, particular cases provide evidence that volume preservation is sufficient
  - 1.5D they are the same
  - Stability seen in spatial tracking studies relevant to muon collider
- Exact beam equilibrium calculations pose additional requirement
- A new integrator has been found to satisfy both
- These dual requirements are not being satisfied by “space-charge-tracking” codes?
- How do we verify that existing computations are giving the right answer for truly intense beams?