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Explicit time-reversible orbit integration in Particle In Cell codes with static homogeneous magnetic field

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ABSTRACT

A new explicit time-reversible orbit integrator for the equations of motion in a static homogeneous magnetic field – called Cyclotronic integrator – is presented. Like Spreiter and Walter's Taylor expansion algorithm, for sufficiently weak electric field gradients this second order method does not require a fine resolution of the Larmor motion; it has however the essential advantage of being symplectic, hence time-reversible. The Cyclotronic integrator is only subject to a linear stability constraint ($\Omega\Delta t < \pi$, Ω being the Larmor angular frequency), and is therefore particularly suitable to electrostatic Particle In Cell codes with uniform magnetic field where Ω is larger than any other characteristic frequency, yet a resolution of the particles' gyromotion is required. Application examples and a detailed comparison with the well-known (time-reversible) Boris algorithm are presented; it is in particular shown that implementation of the Cyclotronic integrator in the kinetic codes SCEPTIC and Democritus can reduce the cost of orbit integration by up to a factor of ten.

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1. Introduction

The Boris integration scheme [1], designed to solve the single particle equations of motion in electric and magnetic fields

$$\begin{cases} \dot{\mathbf{x}} = \mathbf{v} \\ m\dot{\mathbf{v}} = Q(\mathbf{E} + \mathbf{v} \wedge \mathbf{B}) \end{cases} \tag{1}$$

is perhaps the most widely used orbit integrator in explicit Particle In Cell (PIC) simulations of plasmas; here $\mathbf{x}$ and $\mathbf{v}$ are the particle position and velocity, m its mass and Q its charge. The idea of the Boris integrator is to offset $\mathbf{x}$ and $\mathbf{v}$ by half a time-step $\Delta t/2$, and update them alternately using the following *Drift* (D) and *Kick* (K) operators:

$$D_B(\Delta t) := \mathbf{x}' - \mathbf{x} = \Delta t \mathbf{v}, \tag{2}$$

$$K_B(\Delta t) := \mathbf{v}' - \mathbf{v} = \Delta t \frac{Q}{m}\left[\mathbf{E}(\mathbf{x}') + \frac{\mathbf{v}' + \mathbf{v}}{2} \wedge \mathbf{B}(\mathbf{x}')\right]. \tag{3}$$

Although seemingly implicit (the right hand side of Eq. (3) contains both $\mathbf{v}$ and $\mathbf{v}'$, the velocities at the beginning and end of the step), K_B can easily be inverted and the scheme is in practice explicit. The reasons for Boris scheme's popularity are twofold.

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It must first be recognized that the algorithm is extremely simple to implement, and offers second order accuracy while requiring only one force (or field) evaluation per time-step. Other integrators such as the usual or midpoint second order Runge–Kutta [2] require two such evaluations per step, thus considerably increasing the computational cost. The second reason is that for stationary electric and magnetic fields, the errors on conserved quantities such as the energy, or the canonical angular momentum when the system is axisymmetric, are bounded for an infinite time (the error on those quantities is second order in Δt as is the scheme). Those conservation properties, usually observed on long-time simulations of periodic or quasi-periodic orbits, are characteristic of time-reversible integrators [3].

Unfortunately the Boris scheme requires a fine resolution of the Larmor angular frequency $\Omega = Q|\mathbf{B}|/m$, typically $\Omega\Delta t \lesssim 0.3$ for a 1% accuracy [1], which is penalizing if Ω is much larger than any other characteristic frequency of the problem. In the regime of static uniform magnetic field considered in this paper, Spreiter and Walter [4] previously attempted to relax the Larmor constraint, and developed a "Taylor expansion algorithm". Their method however suffers from non time-reversibility, as well as a "weak" unconditional unstability particularly apparent when $\Omega\Delta t \lesssim O(1)$.

We developed an alternative integrator by taking advantage of the fact that in a uniform magnetic field and zero electric field the particle trajectory has a simple analytic form. Using this method, called Cyclotronic integrator, the time-step is in theory only limited by linear stability considerations (leading to $\Omega\Delta t < \pi$). By construction, in static uniform magnetic fields the Cyclotronic integrator is second order and symplectic [5]; in other words it preserves the geometric structure of the Hamiltonian flow, which guarantees excellent conservation properties. The authors' main motivation for the present work was to increase the speed of electrostatic PIC codes such as SCEPTIC [6,7] or Democritus [8], designed to study the electrostatic flow of a uniform magnetoplasma past an electrode. For this system, it is indeed necessary to resolve the Larmor rotation in order to accurately compute the orbit intersections with the collector. The appropriate time-step regime is $\Omega\Delta t \lesssim O(1)$; Spreiter and Walter's algorithm can therefore not be used because of its unstability, while the Boris scheme is too expensive for strongly magnetized plasmas. The Cyclotronic integrator can also be useful to the simulation of other systems, such as intermediately magnetized Penning traps where the magnetic field is not strong enough for a guiding-center approach to be applicable [9].

The paper is organized as follows: After a review of Boris and Spreiter and Walter's algorithms (Section 2), we present a construction of the Cyclotronic integrator where its symplectic character straightforwardly appears (Section 3). A linear stability analysis of the these algorithms is performed in Section 4. We then proceed with the application of the Cyclotronic integrator to the ideal Penning trap system (Section 5) and to the PIC codes SCEPTIC and Democritus (Section 6).

2. Review of previous integrators

2.1. Boris integrator

The Boris integrator [1] is a time-splitting method; the equations of motion (1) are separated in two parts that are successively integrated in a Verlet form:

$$\begin{pmatrix}\mathbf{x}\\ \mathbf{v}\end{pmatrix}(t+\Delta t) = D_B(\Delta t/2)\cdot K_B(\Delta t)\cdot D_B(\Delta t/2)\begin{pmatrix}\mathbf{x}\\ \mathbf{v}\end{pmatrix}(t), \tag{4}$$

where the Boris Drift and Kick operators (D_B and K_B) are defined in Eqs. (2) and (3). If $\overline{\overline{R}}_{\Delta\boldsymbol{\varphi}}$ denotes a rotation of characteristic vector

$$\Delta\boldsymbol{\varphi} = 2\mathrm{atan}\left(\frac{\Delta t}{2}\Omega\right)\frac{\mathbf{B}}{B}, \tag{5}$$

$K_B(\Delta t) := \mathbf{v} \to \mathbf{v}'$ can be split in the following way [1]:

$$K_B(\Delta t) := \begin{cases} \mathbf{v}^* = \mathbf{v} + \frac{Q\mathbf{E}\Delta t}{2m}, \\ \mathbf{v}^{**} = \overline{\overline{R}}_{\Delta\boldsymbol{\varphi}}\mathbf{v}^*, \\ \mathbf{v}' = \mathbf{v}^{**} + \frac{Q\mathbf{E}\Delta t}{2m}. \end{cases} \tag{6}$$

Eqs. (2) and (6) readily show that the Boris integrator is time-reversible, even for non uniform magnetic fields. Indeed the Drift operator does not act on the particle velocity, and the Kick operator does not act on the position. In PIC codes it is customary to define the position and velocity with half a time-step of offset, which amounts to concatenating the two adjacent $D_B(\Delta t/2)$ from successive steps in Eq. (4).

A popular variant of this integrator (known as the "tan" transformation [1]), second order in Δt, consists in letting $\Delta\boldsymbol{\varphi} = \Omega\Delta t\frac{\mathbf{B}}{B}$ in Eq. (6). Regardless of the form used for $\Delta\boldsymbol{\varphi}$ however, the Drift operator (2) requires $\Omega\Delta t \ll \pi$, which is a severe limitation if the other characteristic frequencies (such as the quadrupole harmonic frequency ω_0 introduced in Section 4, or the plasma frequency in dynamic systems) are much smaller than Ω.

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