Large-stepsize integrators for charged particles in a strong magnetic field

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Abstract. This talk considers the numerical treatment of the differential equation that describes the motion of electric particles in a strong magnetic field. A standard integrator is the Boris algorithm which, for small stepsizes, can be analysed by classical techniques. For a strong magnetic field the solution is highly oscillatory and the numerical integration is more challenging. New modifications of the Boris algorithm are discussed, and their accuracy and long-time behaviour are studied with means of modulated Fourier expansions. Emphasis is put on the situation where the stepsize is proportional to (or larger than) the wavelength of the oscillations.

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INTRODUCTION

We consider a charged particle with position $x(t)$ in a magnetic field. Newton's second law together with Lorentz's force equation yield the second order differential equation

$$\ddot{x} = \dot{x} \times B(x) + E(x), \tag{1}$$

where $B(x)$ is a magnetic field and $E(x) = -\nabla U(x)$ is an electric field with scalar potential $U(x)$. The flow in the phase space $(x, \dot{x})$ is volume preserving, and the energy $H(x, \dot{x}) = \frac{1}{2}\dot{x}^\top \dot{x} + U(x)$ is exactly preserved.

The most popular discretisation of (1) is the Boris algorithm [1]

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{h^2} = \frac{x_{n+1} - x_{n-1}}{2h} \times B(x_n) + E(x_n). \tag{2}$$

Here, h is the stepsize, and x_n is an approximation to the solution $x(t)$ of (1) at $t = nh$. The velocity approximation $v_n \approx \dot{x}(nh)$ at the grid points is given by

$$v_n = \frac{x_{n+1} - x_{n-1}}{2h}. \tag{3}$$

Using the velocity approximation at the off-step point $t_{n-1/2} = (n - \frac{1}{2})h$,

$$v_{n-1/2} = \frac{1}{h}\big(x_n - x_{n-1}\big) = v_n - \frac{h}{2} v_n \times B(x_n) - \frac{h}{2} E(x_n), \tag{4}$$

the Boris algorithm (2) is usually written and implemented as a one-step method $(x_n, v_{n-1/2}) \mapsto (x_{n+1}, v_{n+1/2})$,

$$\begin{aligned} v_{n-1/2}^{+} &= v_{n-1/2} + \tfrac{h}{2} E(x_n) \\ v_{n+1/2}^{-} - v_{n-1/2}^{+} &= \tfrac{h}{2}\big(v_{n+1/2}^{-} + v_{n-1/2}^{+}\big) \times B(x_n) \\ v_{n+1/2} &= v_{n+1/2}^{-} + \tfrac{h}{2} E(x_n) \\ x_{n+1} &= x_n + h\, v_{n+1/2}. \end{aligned} \tag{5}$$

The starting value $v_{-1/2}$ is obtained from (4) with $n = 0$. This is a symmetric method of classical order 2. The mapping $(x_n, v_{n-1/2} \mapsto (x_{n+1}, v_{n+1/2})$ is volume preserving, so that $(x_n, v_n \mapsto (x_{n+1}, v_{n+1})$ is conjugate to a volume preserving mapping. What can be said about near energy preservation ?

SMALL STEPSIZES

Assume that the product of the stepsize h with the Lipschitz constant of the vector field in (1) is small. Using backward error analysis [6] the following result can be obtained.

Theorem 1 ([2]) *Assume that at least one of the following conditions is satisfied*

- *the magnetic field* $B(x) = B$ *is constant,*
- *the scalar potential* $U(x) = \frac{1}{2}x^\top Qx + q^\top x$ *is quadratic,*

and that the numerical solution (x_n, v_n) *of the Boris method stays in a compact set. For every truncation index* N*, the error in the energy* $H(x,v) = \frac{1}{2}v^\top v + U(x)$ *is bounded as*

$$|H(x_n, v_n) - H(x_0, v_0)| \le C_{2N} h^2 \quad \text{for} \quad nh \le h^{-2N}$$

with C_{2N} *independent of* n *and* h *as long as* $nh \le h^{-2N}$*, but depending on the truncation index* N*.*

Theorem 1 gives sufficient conditions for near energy preservation. In general, energy is not preserved. Counterexamples with (i) a linear energy drift and (ii) a random walk behaviour of the energy error are given in [2].

LARGE STEPSIZES

We are now interested in stepsizes that are not small compared to the Lipschitz constant of (1). We assume that the stiffness comes from a constant term in $B(x)$, i.e.,

$$B(x) = \frac{1}{\varepsilon}B_0 + B_1(x), \qquad \varepsilon \ll 1, \tag{6}$$

where $\|B_0\| = 1$ (such a scaling is called *maximal ordering* in the plasma physics literature [3]), and we consider large stepsizes $h \approx \varepsilon$, so that the product of the stepsize with the Lipschitz constant of (1) is of size $\mathcal{O}(1)$.

Example 2 Applying the standard Boris algorithm with stepsize $h = 1.5 \cdot \varepsilon$ to the charged particle equation (1) with

$$B(x) = \frac{1}{\varepsilon}\begin{pmatrix}0\\0\\1\end{pmatrix} + \begin{pmatrix}-x_1\\0\\x_3\end{pmatrix}, \qquad U(x) = \frac{1}{\sqrt{x_1^2 + x_2^2}}$$

and initial values $x(0) = (\frac{1}{3}, \frac{1}{4}, \frac{1}{2})^\top$, $v(0) = (\frac{2}{5}, \frac{2}{3}, 1)^\top$, yields an error in position and velocity shown in Figure 1 (red curves). The error in the velocity is $\mathcal{O}(1)$ (top red curve), that in the position $\mathcal{O}(h)$ (second red curve). The velocity approximation has no accuracy at all, the position is only approximated with order 1.

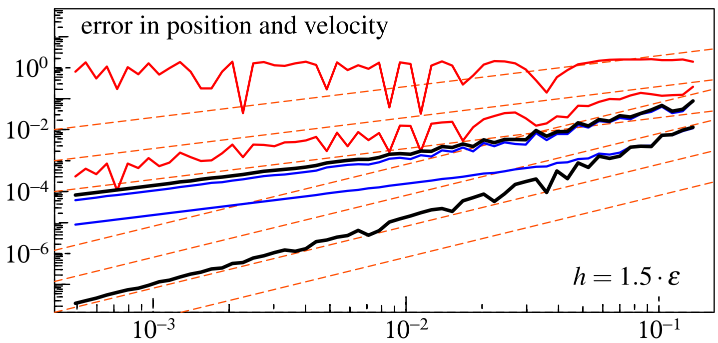

FIGURE 1. Error in position and velocity as a function of the stepsize for the standard Boris method (red), for the filtered Boris method (blue), and for the filtered Boris method with correction (black)

We modify the Boris algorithm with the aim of improving its accuracy. Applying ideas of exponential (trigonometric) integrators [4],[5],[6, Section XIII.2] we introduce filter functions, and we replace the midpoint rule (second line of (5)) by the exponential function. This considerably improves the accuracy in both, velocity and position, see Figure 1 (blue curves). For $h \to 0$, the position and velocity approximations are now of order 1. With a detailed study of the numerical approximations using modulated Fourier expansions (see [8]) a further improvement is achieved, by perturbing the argument in the magnetic field evaluation. The resulting algorithm, as a mapping $(x_n, v_{n-1/2}) \mapsto (x_{n+1}, v_{n+1/2})$, is as follows: let $B_n = B(x_n)$, $\bar{B}_n = B(\bar{x}_n)$ with $\bar{x}_n$ defined by

$$\bar{x}_n = x_n + \big(1 - \theta(h|B_n|)\big)\frac{v_n \times B_n}{|B_n|^2}, \qquad \theta(\xi) = \frac{1}{\operatorname{sinc}^2(\xi/2)},$$

and $E_n = E(x_n)$:

$$\begin{aligned} v^+_{n-1/2} &= v^-_{n-1/2} + \tfrac{h}{2}\,\Psi(h\widehat{B_n})\,E_n \\ v^-_{n+1/2} &= \exp\big(-h\widehat{\bar{B}_n}\big)\,v^+_{n-1/2}. \\ v_{n+1/2} &= v^-_{n+1/2} + \tfrac{h}{2}\,\Psi(h\widehat{B_n})\,E_n \\ x_{n+1} &= x_n + h\,v_{n+1/2}, \end{aligned} \tag{7}$$

where $\Psi(\zeta) = \operatorname{tanch}(\zeta/2)$ with $\operatorname{tanch}(\zeta) = \tanh(\zeta)/\zeta$. The velocity approximation v_n is given by

$$v_n = \Phi_1(h\widehat{\bar{B}_n})\,\frac{x_{n+1} - x_{n-1}}{2h} - h\Upsilon(h\widehat{B_n})E_n, \tag{8}$$

where $\Phi_1(\zeta) = \dfrac{1}{\operatorname{sinch}(\zeta)}$ with $\operatorname{sinch}(\zeta) = \dfrac{\sinh(\zeta)}{\zeta}$, and $\Upsilon(\zeta) = \dfrac{\Phi_1(\zeta) - 1}{\zeta}$. The starting approximation $v_{1/2}$ is computed from

$$v_{n\pm 1/2} = \varphi_1\big(\mp h\widehat{\bar{B}_n}\big)\Big(v_n + h\Upsilon(h\widehat{B_n})E_n\Big) \pm \frac{h}{2}\Psi(h\widehat{B_n})\,E_n, \tag{9}$$

(with $n = 0$) where $\varphi_1(\zeta) = (e^{\zeta} - 1)/\zeta$.

Note that the algorithm is implicit, because $\bar{x}_n$ depends on v_n which itself depends on $\bar{x}_n$ as argument of the magnetic field. It turns out that, starting a fixed-point iteration with $\bar{x}_n = x_n$ convergences very fast, so that typically only one iteration is required. Therefore, the algorithm is essentially explicit.

Theorem 3 ([8]) *Consider the filtered Boris algorithm with at least one correction for $\bar{x}_n$. If the step size satisfies $h \le C\varepsilon$ and the non-resonance condition*

$$\Big|\operatorname{sinc}\big(\tfrac{1}{2}kh|B(x(t))|\big)\Big| \ge c > 0 \qquad \textit{for} \quad k = 1, 2, 3,$$

then we have

$$\begin{aligned} x_n - x(t_n) &= \mathcal{O}(\varepsilon^2) \\ v_n^{\|} - v^{\|}(t_n) &= \mathcal{O}(\varepsilon^2), \qquad v_n^{\perp} - v^{\perp}(t_n) = \mathcal{O}(\varepsilon). \end{aligned}$$

The constants in the $\mathcal{O}$-notation are independent of ε, h, and n with $0 \le t_n = nh \le T$, but depend on T.

Applying this algorithm to the problem of Example 2 shows convergence of order 2 in the position, but only convergence of order 1 in the velocity (see Figure 1, black curves). This confirms the statement of Theorem 3.

For sake of completeness we mention that for a fully implicit variational integrator near-conservation over long times of a modified energy and of a modified magnetic moment are proved in [7].

VERY LARGE STEPSIZES

The previous section considered a strong magnetic field (6) and numerical integrators applied with large stepsizes $h \approx \varepsilon$. Here, we study the same strong magnetic field, but we use even larger stepsizes satisfying

$$0 < \varepsilon \le h^2 \ll 1. \tag{10}$$

The motivation for considering very large stepsizes is the following: for a magnetic field (6) with very small ε, the solution is composed of a fast rotation (with amplitude $\mathscr{O}(\varepsilon)$) around a guiding centre, which moves smoothly. Typically, one is not interested in the high oscillations, but mainly in the guiding centre motion, which can be approximated accurately with large stepsizes.

In addition to the Boris algorithm (2) we consider a related variational integrator. For this we assume that $B(x) = \nabla_x \times A(x)$ with a vector potential $A(x) = -\frac{1}{2}x \times B_0/\varepsilon + A_1(x)$.

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{h^2} = \frac{x_{n+1} - x_{n-1}}{2h} \times B(x_n) + E(x_n) + A'(x_n)\frac{x_{n+1} - x_{n-1}}{2h} - \frac{A(x_{n+1}) - A(x_{n-1})}{2h}. \tag{11}$$

We note that the correction term (compared to the Boris algorithm (2)) vanishes for linear $A(x)$. Consequently, $A(x)$ can be replaced by $A_1(x)$ without changing the method. This shows that the correction term is independent of ε.

The following result is taken from [9]. To reduce the oscillations it is proposed to replace the initial velocity v_0 by

$$v_0 = v_0^{\|} + v_0^{\perp}, \qquad v_0^{\|} = P_0\dot{x}(0), \qquad v_0^{\perp} = \varepsilon\big(v_0^{\|} \times B_1(x_0) + E(x_0)\big) \times B_0, \tag{12}$$

where $P_0 = B_0 B_0^\top$ is the orthogonal projection in direction of B_0.

Theorem 4 ([9]) *Consider the variational integrator* (11) *applied with a stepsize satisfying* (10)*, and assume that the component of the starting velocity orthogonal to B_0 is small, $v_0^{\perp} = \mathscr{O}(\varepsilon)$. If the numerical solution x_n of the variational integrator, applied with starting velocity* (12)*, stays in a compact set K for $0 \le t \le c\,\varepsilon^{-1}$ (with K and c independent of ε and h), the total energy remains $O(h^2)$-close to the initial energy:*

$$|H(x^n, v^n) - H(x^0, v^0)| \le Ch^2, \qquad 0 \le nh \le c\min(\varepsilon^{-1}, h^{-6}). \tag{13}$$

The constant C is independent of ε, h, and n with $0 \le nh \le c/\varepsilon$.

This result shows that the variational integrator works remarkably well for very large stepsizes on a time scale ε^{-1}. We do not know if such a result holds for the standard Boris algorithm. By introducing suitable filter functions in (11) it is possible to prove near energy preservation over much longer time scales ε^{-N} with arbitrary N (see [9]).

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