Numerical treatment of charged particle dynamics in a magnetic field

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In collaboration with Christian Lubich

Charged particle dynamics

Newton's Second Law together with Lorentz's force equation yields (assuming suitable units)

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

where $E(x)$ is the electric field and $B(x)$ the magnetic field.

Boris algorithm

The most simple discretization is

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

J.P. Boris, *Relativistic plasma simulation-optimization of a hybrid code.*
Proc. of 4th Conf. on Numer. Simul. of Plasmas (Nov. 1970)

Outline of the talk

1. **Magnetic field of moderate size**
   - Properties of the Boris algorithm
   - Main result – numerical energy preservation
   - Numerical experiments
   - Proof – backward error analysis
2. **Strong magnetic field**
   - Numerical experiment with the Boris algorithm
   - Filtered Boris algorithm
   - Main result – accuracy in stiff case
   - Proof – modulated Fourier expansion

Properties of the differential equation

We write

$$\ddot{x} = \dot{x} \times B(x) + E(x) \quad \text{as} \quad \begin{aligned} \dot{x} &= v \\ \dot{v} &= v \times B(x) + E(x) \end{aligned}$$

- the flow $\varphi_t(x, v)$ is volume preserving:

$$\mu\big(\varphi_t(K)\big) = \mu(K) \qquad \text{for all } t;$$

- if $E(x) = -\nabla U(x)$, the energy

$$H(x, v) = \tfrac{1}{2} v^\top v + U(x) \qquad \text{is preserved;}$$

- if $E(x) = -\nabla U(x)$ and $B(x) = \nabla_x \times A(x)$, the differential equations are the Euler–Lagrange equations with

$$L(x, v) = \tfrac{1}{2} v^\top v - U(x) + A(x)^\top v$$

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- if

Proof. Divergence of the vector field $= 0$, because $v \times B(x) = \widehat{B}(x)\, v$ with a skew-symmetric matrix $\widehat{B}(x)$.

- if $E(x) = -\nabla U(x)$ and $B(x) = \nabla_x \times A(x)$, the differential equations are the Euler–Lagrange equations with

$$L(x, v) = \tfrac{1}{2} v^T v - U(x) + A(x)^T v$$

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Proof.

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} H\big(x(t), v(t)\big) &= v^\top \dot{v} + \dot{x}^\top \nabla U(x) \\ &= v^\top \big(v \times B(x) - \nabla U(x)\big) + v^\top \nabla U(x) = 0 \end{aligned}$$

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$$\frac{\mathrm{d}}{\mathrm{d}t}\big(\nabla_v L\big) = \nabla_x L$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(v + A(x)\big) = -\nabla_x U + \nabla_x\big(A(x)^\top v\big)$$

- if

and the statement follows from

$$\nabla_x\big(A(x)^\top v\big) - \frac{\mathrm{d}}{\mathrm{d}t}A(x) = \big(A'(x)^\top - A'(x)\big)v = v \times B(x)$$

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Boris algorithm as one-step method

$$\begin{aligned} x_{n+1} - 2x_n + x_{n-1} &= \tfrac{h}{2}\,(x_{n+1} - x_{n-1}) \times B(x_n) + h^2 E(x_n) \\ v_n &= \tfrac{1}{2h}\,(x_{n+1} - x_{n-1}) \end{aligned}$$

With $v_{n+1/2} = \frac{1}{h}(x_{n+1} - x_n) = v_n + \frac{h}{2}\, v_n \times B(x_n) + \frac{h}{2} E(x_n)$ we have

$$v_{n+1/2} - v_{n-1/2} = \tfrac{h}{2}\,(v_{n+1/2} + v_{n-1/2}) \times B(x_n) + h\,E(x_n)$$

and the map $(x_n, v_{n-1/2}) \mapsto (x_{n+1}, v_{n+1/2})$ is implemented as

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

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Boris algorithm as one-step method

With the splitting

$$\begin{pmatrix} \dot{x} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} 0 \\ E(x) \end{pmatrix} + \begin{pmatrix} 0 \\ v \times B(x) \end{pmatrix} + \begin{pmatrix} v \\ 0 \end{pmatrix}$$

we have

Wit

$$\begin{pmatrix} x_{n+1} \\ v_{n+1/2} \end{pmatrix} = \varphi_h^V \circ \varphi_{h/2}^E \circ \Phi_h^B \circ \varphi_{h/2}^E \begin{pmatrix} x_n \\ v_{n-1/2} \end{pmatrix}$$

where φ_t^E and φ_t^V are the exact flows, and Φ_h^B is the discrete flow (mid-point rule) for the vector field in the middle.

and

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

Properties of the Boris algorithm

$$x_{n+1} - 2x_n + x_{n-1} = \frac{h}{2}\,(x_{n+1} - x_{n-1}) \times B(x_n) + h^2 E(x_n)$$
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- the mapping $(x_n, v_{n-1/2}) \mapsto (x_{n+1}, v_{n+1/2})$ is volume preserving. Hence, the Boris method $(x_n, v_n) \mapsto (x_{n+1}, v_{n+1})$ is conjugate to a volume preserving mapping.
- the Boris method is a variational integrator only if $B(x) = Const.$ *(see Ellison & al.)*
- What can be said about near energy preservation in the general case, where $B(x)$ is not a constant vector field? *This is the topic of part I of the present talk.*

C. L. Ellison, J. W. Burby, and H. Qin, *Comment on "Symplectic integration of magnetic systems": A proof that the Boris algorithm is not variational. J. Comput. Phys. 301* (2015), 489–493

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“Particle-in-cell” article from Wikipedia

Because of its excellent long term accuracy, the Boris algorithm is the de facto standard for advancing a charged particle.

It was realized that the excellent long term accuracy of nonrelativistic Boris algorithm is due to the fact it conserves phase space volume, even though it is not symplectic.

The global bound on energy error typically associated with symplectic algorithms still holds for the Boris algorithm, . . .

Energy preservation - main result

Theorem

Assume that at least one of the following conditions is satisfied

- *the magnetic field* $B(x) = B$ *is constant,*
- *the scalar potential* $U(x) = \frac{1}{2} x^\top Q x + q^\top x$ *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 *independent of* n *and* h *as long as* $nh \le h^{-2N}$*.*

What happens if none of the above two conditions is satisfied?

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with C *independent of* n *and* h *as long as* $nh \leq h^{-2N}$.

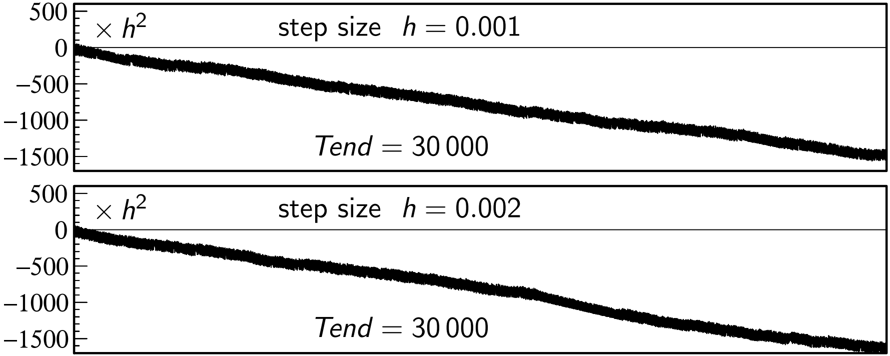
What happens if none of the above two conditions is satisfied?

Example 1: linear growth

We consider the error in the energy for

$$U(x) = x_1^3 - x_2^3 + \frac{1}{5}x_1^4 + x_2^4 + x_3^4, \qquad B(x) = \begin{pmatrix} 0 \\ 0 \\ \sqrt{x_1^2 + x_2^2} \end{pmatrix}$$

$x(0) = (0.0, 1.0, 0.1)^\top$, $v(0) = (0.09, 0.55.0.30)^\top$.



Example 2: random walk

We consider the error in the energy for

$$U(x) = x_1^3 - x_2^3 + \frac{1}{5}x_1^4 + x_2^4 + x_3^4, \qquad B(x) = \frac{1}{2}\begin{pmatrix} x_2 - x_3 \\ x_1 + x_3 \\ x_2 - x_1 \end{pmatrix}$$

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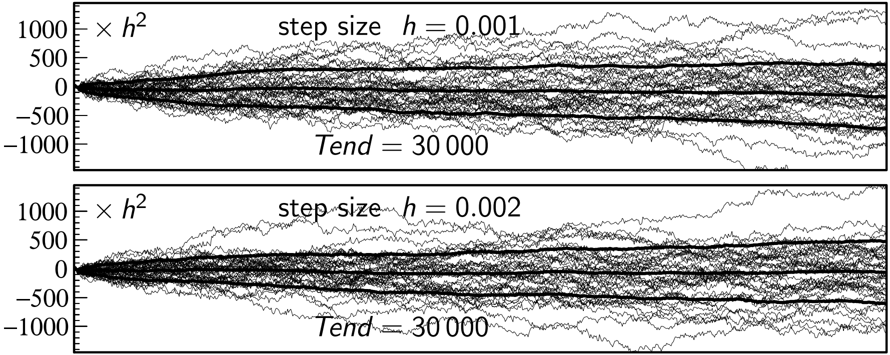

Backward error analysis (Boris algorithm)

For $x_n = y(nh)$ and $t = nh$ the Boris algorithm reads

$$y(t+h)-2y(t)+y(t-h) = \frac{h}{2}\Big(y(t+h)-y(t-h)\Big)\times B\big(y(t)\big)-h^2\nabla U\big(y(t)\big)$$

Expanding into powers of h and dividing by h^2 yields

$$\ddot y + \frac{h^2}{12}\ddddot y + \ldots = \Big(\dot y + \frac{h^2}{6}\dddot y + \ldots\Big)\times B(y) - \nabla U(y)$$

Eliminating third and higher derivatives by differentiation

$$\begin{aligned}\dddot y &= \ddot y \times B(y) + \dot y \times B'(y)\dot y - \nabla^2 U(y)\dot y + \mathcal{O}(h^2)\\ &= -\nabla U(y)\times B(y) + \dot y \times B'(y)\dot y - \nabla^2 U(y)\dot y + \mathcal{O}(h^2)\end{aligned}$$

gives the modified differential equation.

Similarly, we have $v_n = w(nh)$ for $t = nh$, where

$$w(t) = \frac{1}{2h}\Big(y(t+h)-y(t-h)\Big) = \dot y + \frac{h^2}{3!}\dddot y + \frac{h^4}{5!}y^{(5)} + \ldots$$

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Energy conservation - quadratic electric potential

Consider the modified equation with $U(x) = \frac{1}{2} x^\top Q x + q^\top x$

$$\ddot{y} + \frac{h^2}{12} \ddddot{y} + \ldots = \Big(\dot{y} + \frac{h^2}{6} \dddot{y} + \ldots \Big) \times B(y) - \nabla U(y)$$

and take the scalar product with $\big(\dot{y} + \frac{h^2}{6} \dddot{y} + \ldots\big)$. This gives

$$\frac{\mathrm{d}}{\mathrm{d}t} \Big(\frac{1}{2} \dot{y}^\top \dot{y} + U(y) + \frac{h^2}{12} \big(\dot{y}^\top \dddot{y} + \frac{1}{2} \ddot{y}^\top \ddot{y} \big) + \ldots \Big) = -\frac{h^2}{6} \dddot{y}^\top \nabla U(y) + \ldots$$

Theorem

If $U(x) = \frac{1}{2} x^\top Q x + q^\top x$, *there exist* $E_{2j}(x, v)$ *such that*

$$\frac{\mathrm{d}}{\mathrm{d}t} \Big(\frac{1}{2} \dot{y}^\top \dot{y} + U(y) + h^2 E_2(y, \dot{y}) + \ldots + h^{2N} E_{2N}(y, \dot{y}) \Big) = \mathcal{O}(h^{2N+2})$$

along solutions (y, w) *of the modified differential equation.*

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ar

because $\quad \dddot y^\top \nabla U(y) = \dddot y^\top (Qy + q) = \frac{\mathrm{d}}{\mathrm{d}t}\Big(\ddot y^\top Q y - \frac{1}{2} \dot y^\top Q \dot y + \ddot y^\top q \Big)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{1}{2} \dot y^\top \dot y + U(y) + \frac{h^2}{12}\big(\dot y^\top \dddot y + \frac{1}{2} \ddot y^\top \ddot y \big) + \ldots \Big) = -\frac{h^2}{6} \dddot y^\top \nabla U(y) + \ldots$$

Theorem

If $U(x) = \frac{1}{2}\, x^\top Q x + q^\top x$, *there exist* $E_{2j}(x, v)$ *such that*

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{1}{2} \dot y^\top \dot y + U(y) + h^2 E_2(y, \dot y) + \ldots + h^{2N} E_{2N}(y, \dot y) \Big) = \mathcal{O}(h^{2N+2})$$

along solutions (y, w) *of the modified differential equation.*

Outline of the talk

1. Magnetic field of moderate size
   - Properties of the Boris algorithm
   - Main result – numerical energy preservation
   - Numerical experiments
   - Proof – backward error analysis

2. **Strong magnetic field**
   - Numerical experiment with the Boris algorithm
   - Filtered Boris algorithm
   - Main result – accuracy in stiff case
   - Proof – modulated Fourier expansion

Charged particle dynamics in a strong magnetic field

We consider

$$\ddot{x} = \dot{x} \times B(x,t) + E(x), \qquad B(x,t) = \frac{1}{\varepsilon} B_0(\varepsilon x) + B_1(x,t)$$

with $\varepsilon \ll 1$ and an electric field $E(x) = -\nabla U(x)$ given by a potential.

We assume

$$x(0) = \mathcal{O}(1), \qquad \dot{x}(0) = \mathcal{O}(1)$$

so that the energy

$$H(x,\dot{x}) = \frac{1}{2}\,\dot{x}^\top \dot{x} + U(x)$$

is bounded independently of $\varepsilon \le 1$.

Remark. This scaling of $B(x,t)$ is of interest in particle methods in plasma physics and is called *maximal ordering* in
Brizard & Hahm, Found. of nonlinear gyrokinetic theory. Rev. Modern Phys. (2007)

“Particle-in-cell” article from Wikipedia

Even with super-particles, the number of simulated particles is usually very large ($> 10^5$), and often the particle mover is the most time consuming part of PIC, since it has to be done for each particle separately.

Thus, the pusher is required to be of high accuracy and speed and much effort is spent on optimizing the different schemes.

Properties of the differential equation

We write

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

as

$$\begin{aligned} \dot{x} &= v \\ \dot{v} &= v \times B(x,t) + E(x) \end{aligned}$$

- the flow $(x^0, v^0) \mapsto \varphi_t(t^0, x^0, v^0)$ is volume preserving;
- if $E(x) = -\nabla U(x)$, the energy $H(x,v) = \frac{1}{2} v^\top v + U(x)$ is preserved;

Before studying the long-time behaviour we consider the accuracy of the Boris algorithm (which is unconditionally stable)

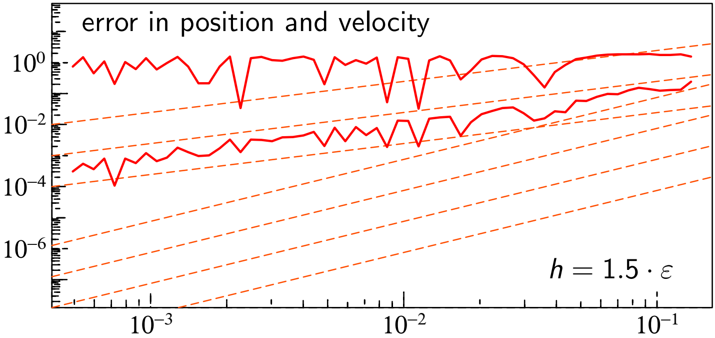
$$\begin{aligned} v_{n-1/2}^{+} &= v_{n-1/2} + \frac{h}{2}\, E(x_n) \\ v_{n+1/2}^{-} - v_{n-1/2}^{+} &= \frac{h}{2}\, (v_{n+1/2}^{-} + v_{n-1/2}^{+}) \times B(x_n, t_n) \\ v_{n+1/2} &= v_{n+1/2}^{-} + \frac{h}{2}\, E(x_n) \\ x_{n+1} &= x_n + h\, v_{n+1/2} \end{aligned}$$

Numerical experiment

Error in position and velocity of the Boris algorithm for

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

with initial values $x(0) = (\frac{1}{3}, \frac{1}{4}, \frac{1}{2})^\top$, $v(0) = (\frac{2}{5}, \frac{2}{3}, 1)^\top$.



Filtered Boris algorithm (explicit)

We consider the Boris algorithm

$$
\begin{aligned}
v^+_{n-1/2} &= v_{n-1/2} + \tfrac{h}{2}\, E(x_n) \\
v^-_{n+1/2} - v^+_{n-1/2} &= \tfrac{h}{2}\,(v^-_{n+1/2} + v^+_{n-1/2}) \times B(x_n, t_n) \\
v_{n+1/2} &= v^-_{n+1/2} + \tfrac{h}{2}\, E(x_n) \\
x_{n+1} &= x_n + h\, v_{n+1/2}
\end{aligned}
$$

the second line is the implicit midpoint rule applied to

$$
\dot v = v \times B(x_n, t_n) = -\widehat{B}(x_n, t_n)\, v, \qquad \widehat{B} = \begin{pmatrix} 0 & -b_3 & b_2 \\ b_3 & 0 & -b_1 \\ -b_2 & b_1 & 0 \end{pmatrix}
$$

we can replace it by the exponential function

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$$\begin{aligned} v_{n-1/2}^{+} &= v_{n-1/2} + \tfrac{h}{2}\, E(x_n) \\ v_{n+1/2}^{-} &= \exp\big(-h\, \widehat{B}(x_n, t_n)\big)\, v_{n-1/2}^{+} \\ v_{n+1/2} &= v_{n+1/2}^{-} + \tfrac{h}{2}\, E(x_n) \\ x_{n+1} &= x_n + h\, v_{n+1/2} \end{aligned}$$

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we can replace it by the exponential function

This method is exact, if $B(x, t) = B$ and $E(x) = 0$.

Filtered Boris algorithm (explicit)

In the spirit of exponential integrators we introduce a filter function Ψ

$$
\begin{aligned}
v_{n-1/2}^{+} &= v_{n-1/2} + \frac{h}{2}\,\Psi\big(h\,\widehat{B}(x_n,t_n)\big)\,E(x_n)\\
v_{n+1/2}^{-} &= \exp\big(-h\,\widehat{B}(x_n,t_n)\big)\,v_{n-1/2}^{+}\\
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x_{n+1} &= x_n + h\,v_{n+1/2}
\end{aligned}
$$

and define

$$
v_n = \Phi\big(h\,\widehat{B}(x_n,t_n)\big)\,\frac{x_{n+1}-x_{n-1}}{2\,h} - \Gamma\big(h\,\widehat{B}(x_n,t_n)\big)\,E(x_n)
$$

where $\Phi(\zeta) = \dfrac{1}{\mathrm{sinch}(\zeta)}, \quad \Gamma(\zeta) = \dfrac{\Phi(\zeta)-1}{\zeta}, \quad \mathrm{sinch}(\zeta) = \dfrac{\sinh(\zeta)}{\zeta}$

Properties of the filtered Boris algorithm

We choose the filter function as

$$\Psi(\zeta) = \mathrm{tanch}\Big(\frac{\zeta}{2}\Big) \qquad \text{where} \qquad \mathrm{tanch}(\zeta) = \frac{\tanh(\zeta)}{\zeta}$$

- If $B(x,t) = B$ and $E(x) = E$ are constant vector fields, then the method produces the exact solution;
- conjugate to a volume preserving method;
- explicit and symmetric.

What can be said about its accuracy ?

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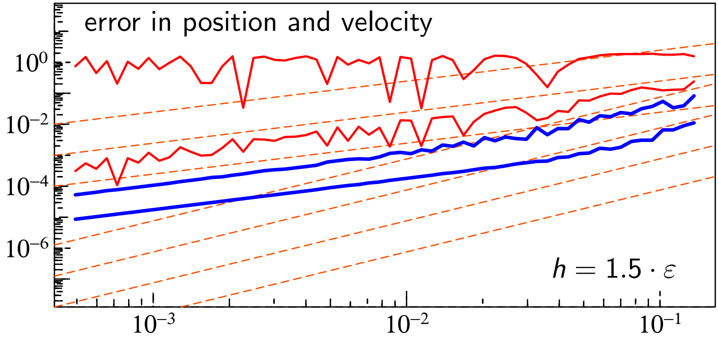
Numerical experiment

- Error of the Boris algorithm – red
- Error of the filtered Boris algorithm – blue



- There is a huge improvement in the velocity approximation!
- Can we do better in the position approximation ?

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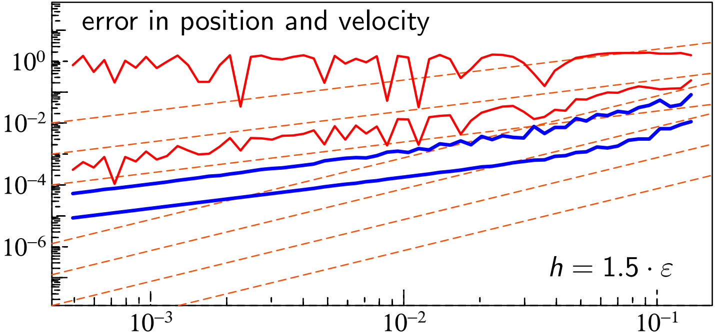

- There is a huge improvement in the velocity approximation!
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Modulated Fourier expansion

We consider

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

and the 2-step formulation of the filtered Boris algorithm ($\widehat{B}_n = \widehat{B}(x_n, t_n)$)

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{h^2} = \frac{2}{h}\tanh\Big(-\frac{h}{2}\widehat{B}_n\Big)\frac{x_{n+1} - x_{n-1}}{2h} + \Psi(h\widehat{B}_n)E(x_n)$$

We separate high oscillations from the smooth motion by the ansatz:

exact solution	numerical solution
$x(t) \approx \sum_{k\in\mathbf{Z}} z^k(t)\,\mathrm{e}^{\mathrm{i}k\phi(t)/\varepsilon}$	$x_n \approx \sum_{k\in\mathbf{Z}} z^k(t_n)\,\mathrm{e}^{\mathrm{i}k\phi(t_n)/\varepsilon}$

Kruskal (1958) for proving the formal existence of an adiabatic invariant;
H. & Lubich (2016) for Hamiltonian systems with solution-dependent high frequency.

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Modulated Fourier expansion

The linear mapping $v \mapsto v \times B(x,t)$ has eigenvalues

$$\lambda_1 = \mathrm{i}|B(x,t)|, \qquad \lambda_0 = 0, \qquad \lambda_{-1} = -\mathrm{i}|B(x,t)|$$

and eigenvectors $v_j(x,t)$ for $j \in \{-1,0,1\}$.
We denote the projectors onto the eigenspaces by $P_j(x,t)$, and split the coefficient functions of the MFE as

$$z^k = z_1^k + z_0^k + z_{-1}^k, \qquad z_j^k(t) = P_j\big(z^0(t),t\big) z^k(t)$$

It turns out that with $\phi(t)$ satisfying $\dot\phi(t) = \varepsilon \big| B(z^0(t),t) \big|$, there exist smooth functions such that

- $z_j^k = \mathcal{O}(\varepsilon^{|k|+1})$ for $|k| \geq 2$
- $z_j^k = \mathcal{O}(\varepsilon^3)$ for $|k| = 1$ and $j \neq k$
- $z_1^1 = \mathcal{O}(\varepsilon)$, $z_{-1}^{-1} = \mathcal{O}(\varepsilon)$
- $z_j^0 = \mathcal{O}(1)$ for $j \in \{-1,0,1\}$.

MFE for the exact solution

Theorem

The phase function satisfies $\dot\phi(t) = \varepsilon\big|B(z^0(t),t)\big|$ *and the coefficient functions are determined by the differential equations*

$$P_0(z^0,t)\ddot z^0 = P_0(z^0,t)\Big(E(z^0) + 2\,\Re\Big(\mathrm{i}\frac{\dot\phi}{\varepsilon} z_1^1 \times B'(z^0,t) z_{-1}^{-1}\Big)\Big) + \mathcal{O}(\varepsilon^2)$$

$$P_{\pm 1}(z^0,t)\dot z^0 = \pm \mathrm{i}\varepsilon\dot\phi^{-1} P_{\pm 1}(z^0,t)E(z^0) + \mathcal{O}(\varepsilon^2),$$

$$\dot z_{\pm 1}^{\pm 1} = \mathcal{O}(\varepsilon^2)$$

with initial values

$$z^0(0) = x(0) + \frac{\dot x(0) \times B\big(x(0),0\big)}{\big|B\big(x(0),0\big)\big|^2} + \mathcal{O}(\varepsilon^2),$$

$$\dot z_0^0(0) = P_0(x(0),0)\dot x(0) + \dot P_0(x(0),0)x(0) + \mathcal{O}(\varepsilon^2),$$

$$z_{\pm 1}^{\pm 1}(0) = \mp\,\mathrm{i}\varepsilon\dot\phi(0)^{-1} P_{\pm 1}(x(0),0)\dot x(0) + \mathcal{O}(\varepsilon^2).$$

MFE for the numerical solution

Theorem

The phase function satisfies $\dot\phi(t) = \varepsilon \big| B(z^0(t), t) \big|$ *and the coefficient functions are determined by the differential equations*

$$
\begin{aligned}
P_0(z^0,t)\ddot z^0 &= P_0(z^0,t)\Big(E(z^0) \\
&\qquad + 2\,\Theta\Big(\frac{h}{\varepsilon}\dot\phi\Big)\,\Re\Big(\mathrm{i}\frac{\dot\phi}{\varepsilon} z_1^1 \times B'(z^0,t) z_{-1}^{-1}\Big)\Big) + \mathcal{O}(\varepsilon^2) \\
P_{\pm 1}(z^0,t)\dot z^0 &= \pm \mathrm{i}\varepsilon \dot\phi^{-1} P_{\pm 1}(z^0,t) E(z^0) + \mathcal{O}(\varepsilon^2), \\
\dot z_{\pm 1}^{\pm 1} &= \mathcal{O}(\varepsilon^2)
\end{aligned}
$$

where $\Theta(\xi) = \mathrm{sinc}^2(\xi/2)$*.*

The initial values satisfy the same relations as for the exact solution.

Consequence of the theorem

a) The filtered method has an error of size $\mathcal{O}(\varepsilon^2)$ if for all $z \in \mathbb{C}^3$

$$P_0(x,t)\,\Im\big(z \times B'(x,t)\,\overline{z}\big) = \mathcal{O}(\varepsilon)$$

This is the case if $B(x,t) = B(t)$ only depends on time.

b) The coefficient functions for the exact solution satisfy the differential equations with $\Theta(\xi) = 1$.

Can we modify the filtered method to get $\Theta(\xi) = 1$?

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Filtered Boris algorithm (implicit)

Idea (Christian): perturb the argument of $B(x,t)$

$$
\begin{aligned}
v_{n-1/2}^{+} &= v_{n-1/2} + \tfrac{h}{2}\,\Psi\big(h\,\widehat{B}(x_n,t_n)\big)\,E(x_n)\\
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x_{n+1} &= x_n + h\,v_{n+1/2}
\end{aligned}
$$

where, with $B_n = B(x_n,t_n)$

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

and

$$
v_n = \Phi\big(h\,\widehat{B}(\bar{x}_n,t_n)\big)\frac{v_{n+1/2}^{-} + v_{n-1/2}^{+}}{2} - \Gamma\big(h\,\widehat{B}(x_n,t_n)\big)E(x_n)
$$

Filtered Boris algorithm (implicit)

- The mapping $(x_n, v_{n-1/2}) \mapsto (x_{n+1}, v_{n+1/2})$ is volume preserving. Hence, the Boris method $(x_n, v_n) \mapsto (x_{n+1}, v_{n+1})$ is conjugate to a volume preserving method.

Theorem

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

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

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.

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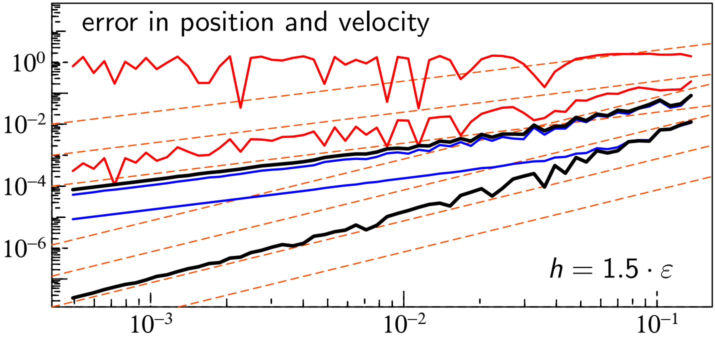
Numerical experiment

- Error of the Boris algorithm – red
- Error of the filtered Boris algorithm (explicit) – blue
- Error of the filtered Boris algorithm (implicit) – black



Conclusion

Nonstiff charged particle dynamics

- Longtime behaviour of the Boris algorithm and near energy preservation are well understood.

Charged particle dynamics in a strong magnetic field

- A new filtered Boris algorithm is presented.
- Stiff order 2 (for $h \approx \varepsilon$) for position and stiff order 1 for velocity is proved with help of modulated Fourier expansions.

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Thank you !

More details can be found in

E. Hairer & Ch. Lubich, *Energy behaviour of the Boris method for charged particle dynamics*. BIT (2018).

E. Hairer & Ch. Lubich, *Long-term analysis of a variational integrator for charged-particle dynamics in a strong magnetic field*. Numerische Mathematik, to appear.

E. Hairer, Ch. Lubich & Bin Wang, *A filtered Boris algorithm for charged-particle dynamics in a strong magnetic field*. Submitted.