ETH zürich

Seminar in Physics for CSE

A filtered Boris algorithm for charged-particle dynamics in a strong magnetic field

Ernst Hairer, Christian Lubich, Bin Wang

Presented by Carla López

13 Dec 2024

Outline

1. Introduction
2. Presentation of algorithms
   Standard Boris algorithm
   Filtered Boris algorithm
   Two-point filtered Boris algorithm
3. Results
4. Conclusion

Outline

1. Introduction
2. Presentation of algorithms
   - Standard Boris algorithm
   - Filtered Boris algorithm
   - Two-point filtered Boris algorithm
3. Results
4. Conclusion

Introduction

Propose and analyse a numerical integrator for the equations of motion of a charged particle

$$\ddot{x}(t) = \dot{x}(t) \times B(x(t), t) + E(x(t), t), \quad x(t), B(x,t), E(x,t) \in \mathbb{R}^3 \tag{1}$$

Introduction

Propose and analyse a numerical integrator for the equations of motion of a charged particle

$$\ddot{x}(t) = \dot{x}(t) \times B(x(t),t) + E(x(t),t), \quad x(t), B(x,t), E(x,t) \in \mathbb{R}^3 \tag{1}$$

in a strong inhomogeneous magnetic field

$$B(x,t) = \frac{1}{\varepsilon} B_0(\varepsilon x) + B_1(x,t) \quad \text{for } 0 < \varepsilon \ll 1 \tag{2}$$

Outline

1. Introduction
2. Presentation of algorithms
   Standard Boris algorithm
   Filtered Boris algorithm
   Two-point filtered Boris algorithm
3. Results
4. Conclusion

Standard Boris algorithm

De facto algorithm for charged particles in a magnetic field.

$$(x^n, v^{n-1/2}) \mapsto (x^{n+1}, v^{n+1/2})$$

$$v_+^{n-1/2} = v^{n-1/2} + \frac{h}{2} E(x^n, t^n) \tag{3}$$

$$v_-^{n+1/2} - v_+^{n-1/2} = \frac{h}{2} \left(v_-^{n+1/2} + v_+^{n-1/2} \right) \times B(x^n, t^n) \tag{4}$$

$$v^{n+1/2} = v_-^{n+1/2} + \frac{h}{2} E(x^n, t^n) \tag{5}$$

$$x^{n+1} = x^n + h v^{n+1/2} \tag{6}$$

Guiding center approximation

$$x^n_\odot = x^n + \frac{v^n \times B(x^n, t^n)}{|B(x^n, t^n)|^2}$$ guiding center approximation

$$\bar{x}^n = \theta^n x^n + (1 - \theta^n) x^n_\odot$$ point on the straight line connecting x and $x_\odot$

$$\theta^n = \theta(h|B(x^n, t^n)|)$$

$$\theta(\xi) = \frac{1}{\mathrm{sinc}(\xi/2)^2} \quad \text{with} \quad \mathrm{sinc}(\xi) = \frac{\sin(\xi)}{\xi}$$

Notation

$$B^n = B(x^n, t^n)$$
$$\bar{B}^n = B(\bar{x}^n, t^n)$$
$$E^n = E(x^n, t^n)$$

We will also express $v \times B = -\hat{B}v$, where $B = (b_1, b_2, b_3)$, and so

$$\hat{B} = \begin{pmatrix} 0 & -b_3 & b_2 \\ b_3 & 0 & -b_1 \\ -b_2 & b_1 & 0 \end{pmatrix} \tag{7}$$

Filtered Boris

$$(x^n, v^{n-1/2}) \mapsto (x^{n+1}, v^{n+1/2})$$

$$\begin{aligned}
v^{n+1/2} &= v^{n-1/2} + \frac{h}{2}\Psi(h\hat{B}^n)E^n && (8)\\
v_-^{n+1/2} &= \exp(-h\hat{\hat{B}}^n)v^{n-1/2} && (9)\\
v^{n+1/2} &= v_-^{n+1/2} + \frac{h}{2}\Psi(h\hat{B}^n)E^n && (10)\\
x^{n+1} &= x^n + hv^{n+1/2} && (11)
\end{aligned}$$

Filtered Boris

$$(x^n, v^{n-1/2}) \mapsto (x^{n+1}, v^{n+1/2})$$

$$v^{n+1/2} = v^{n-1/2} + \frac{h}{2}\Psi(h\hat{B}^n)E^n \tag{8}$$

$$v_-^{n+1/2} = \exp(-h\hat{\hat{B}}^n)v^{n-1/2} \tag{9}$$

$$v^{n+1/2} = v_-^{n+1/2} + \frac{h}{2}\Psi(h\hat{B}^n)E^n \tag{10}$$

$$x^{n+1} = x^n + hv^{n+1/2} \tag{11}$$

where $\Psi(\zeta) = \mathrm{tanch}(\zeta/2)$ with $\mathrm{tanch}(\zeta) = \tanh(\zeta)/\zeta$.

Filtered Boris

Evaluation of matrix functions, for example $\Psi(h\hat{B})$, can be done efficiently using the Rodriguez formula by taking advantage of the fact that $\hat{B}$ is skew-symmetric.

Filtered Boris

Evaluation of matrix functions, for example $\Psi(h\hat{B})$, can be done efficiently using the Rodriguez formula by taking advantage of the fact that $\hat{B}$ is skew-symmetric.

$\Psi(h\hat{B})$ can therefore be expressed as:

$$\Psi(h\hat{B}) = I + \frac{1 - \operatorname{tanc}(h|B|/2)}{|B|^2}\hat{B}^2 \tag{12}$$

Filtered Boris

Since we have

$$v_{-}^{n+1/2} = \exp(-h\hat{\bar{B}}^{n})v^{n-1/2}, \tag{9}$$

and

$$\begin{aligned}\bar{x}^{n} &= \theta^{n}x^{n} + (1-\theta^{n})x_{\odot}^{n},\\ x_{\odot}^{n} &= x^{n} + \frac{v^{n}\times B^{n}}{|B^{n}|^{2}},\end{aligned}$$

Filtered Boris

Since we have

$$v_-^{n+1/2} = \exp(-h\hat{B}^n)v^{n-1/2}, \tag{9}$$

and

$$\begin{aligned}
\bar{x}^n &= \theta^n x^n + (1-\theta^n)x_\odot^n, \\
x_\odot^n &= x^n + \frac{v^n \times B^n}{|B^n|^2},
\end{aligned}$$

we need to compute v^n with the following approximation,

$$v^n = \Phi_1(hB^n)\frac{v_-^{n+1} - v_+^{n-1}}{2} - h\Gamma(hB^n)E^n, \tag{13}$$

where $\Phi_1(\zeta) = \frac{1}{\mathrm{sinch}(\zeta)}$ with $\mathrm{sinch}(\zeta) = \frac{\sinh(\zeta)}{\zeta}$, and $\Gamma(\zeta) = \Phi_1(\zeta) - 1$.

Filtered Boris

Since we have

$$v_-^{n+1/2} = \exp(-h\hat{\hat{B}}^n)v^{n-1/2}, \tag{9}$$

and

$$\bar{x}^n = \theta^n x^n + (1-\theta^n)x_\odot^n,$$
$$x_\odot^n = x^n + \frac{v^n \times B^n}{|B^n|^2},$$

we need to compute v^n with the following approximation,

$$v^n = \Phi_1(hB^n)\frac{v_-^{n+1} - v_+^{n-1}}{2} - h\Gamma(hB^n)E^n, \tag{13}$$

where $\Phi_1(\zeta) = \frac{1}{\mathrm{sinch}(\zeta)}$ with $\mathrm{sinch}(\zeta) = \frac{\sinh(\zeta)}{\zeta}$, and $\Gamma(\zeta) = \Phi_1(\zeta) - 1$.

We therefore need to solve the equation with a fixed-point iteration to get v^n.

Variants

When $\theta(x,t) = 1 \quad \rightarrow \quad \bar{x^n} = x^n$, and so the algorithm is explicit, we will call it **Exp-A**

Variants

When $\theta(x,t) = 1 \quad \rightarrow \quad \bar{x^n} = x^n$, and so the algorithm is explicit, we will call it **Exp-A**

When $\theta(x,t) = \frac{1}{\text{sinc}(h|B(x,t)|/2)^2} \quad \rightarrow$ algorithm is implicit, we will call it **Imp-A**

Two-Point Filtered Boris Algorithm

$$(x^n, v^{n-1/2}) \mapsto (x^{n+1}, v^{n+1/2})$$

$$v_+^{n-1/2} = v^{n-1/2} + \frac{h}{2}\Psi(h\hat{B}^n)E^n \tag{14}$$

$$\Phi_2(h\hat{B}_\odot^n)(v_-^{n+1/2} - v_+^{n-1/2}) = \frac{h}{2}\Phi_1(h\hat{B}^n)(v_-^{n+1/2} + v_+^{n-1/2}) \times B^n \tag{15}$$

$$v^{n+1/2} = v_-^{n+1/2} + \frac{h}{2}\Psi(h\hat{B}^n)E^n \tag{16}$$

$$x^{n+1} = x^n + hv^{n+1/2} \tag{17}$$

Two-Point Filtered Boris Algorithm

$$(x^n, v^{n-1/2}) \mapsto (x^{n+1}, v^{n+1/2})$$

$$v_+^{n-1/2} = v^{n-1/2} + \frac{h}{2}\Psi(h\hat{B}^n)E^n \tag{14}$$

$$\Phi_2(h\hat{B}_\odot^n)(v_-^{n+1/2} - v_+^{n-1/2}) = \frac{h}{2}\Phi_1(h\hat{B}^n)(v_-^{n+1/2} + v_+^{n-1/2}) \times B^n \tag{15}$$

$$v^{n+1/2} = v_-^{n+1/2} + \frac{h}{2}\Psi(h\hat{B}^n)E^n \tag{16}$$

$$x^{n+1} = x^n + hv^{n+1/2} \tag{17}$$

where $\Psi(\zeta) = \mathrm{tanch}(\zeta/2)$ and $\Phi_1(\zeta) = \frac{1}{\mathrm{sinch}(\zeta)}$ and $\Phi_2(\zeta) = \frac{1}{\mathrm{sinch}(\zeta/2)^2}$.

Two-Point Filtered Boris Algorithm

This method is also implicit.

The fixed-point iteration for $x_{\odot}^{n}$ requires:

- the evaluation of matrix functions by the Rodriguez formula
- and the solution of a linear system with the 3x3 matrix $\Phi_2(h\hat{B_{\odot}^{n}}) + \frac{1}{2}h\hat{B^{n}}\Phi_1(h\hat{B^{n}})$.

Outline

1. Introduction
2. Presentation of algorithms
   - Standard Boris algorithm
   - Filtered Boris algorithm
   - Two-point filtered Boris algorithm
3. Results
4. Conclusion

Numerical experiment

$$
\begin{aligned}
B(x,t) &= \nabla \times \frac{1}{\epsilon}\begin{pmatrix}0 & x_1 & 0\end{pmatrix} + \nabla \times \begin{pmatrix}0 & x_1 x_3 & 0\end{pmatrix} \\
&= \frac{1}{\epsilon}\begin{pmatrix}0 & 0 & 1\end{pmatrix} + \begin{pmatrix}-x_1 & 0 & x_3\end{pmatrix} \\
E(x,t) &= -\nabla_x U(x) \\
U(x) &= \frac{1}{\sqrt{x_1^2 + x_2^2}}
\end{aligned}
$$

Initial conditions:

$$
\begin{aligned}
x(0) &= \left(\frac{1}{3}, \frac{1}{4}, \frac{1}{2}\right)^\top \\
v(0) &= \left(\frac{2}{5}, \frac{2}{3}, 1\right)^\top \\
0 \leq\ & t \leq 1
\end{aligned}
$$

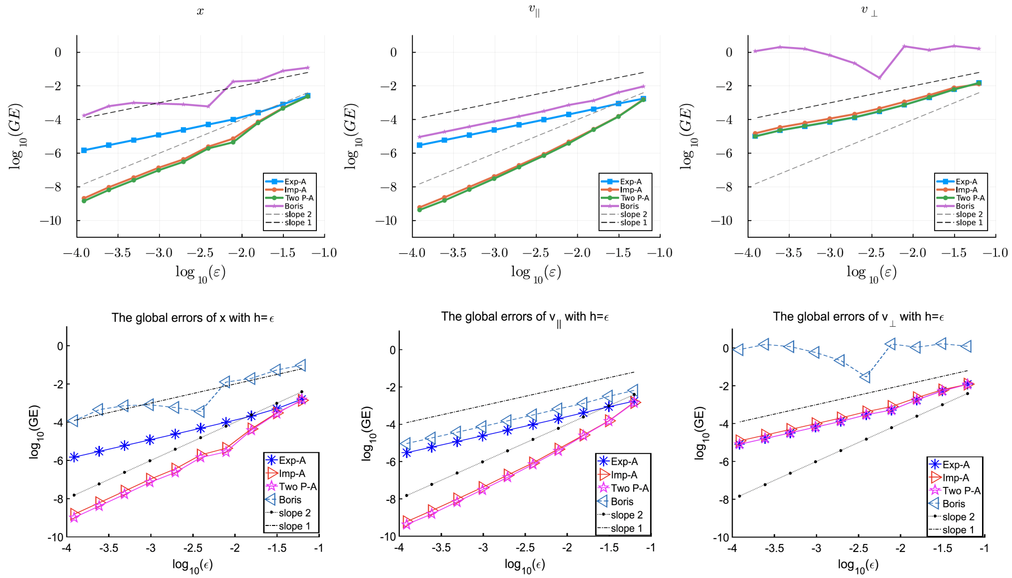


Figure: The logarithm of the global error at t=1 against the logarithm of ϵ for $h = 1\epsilon$

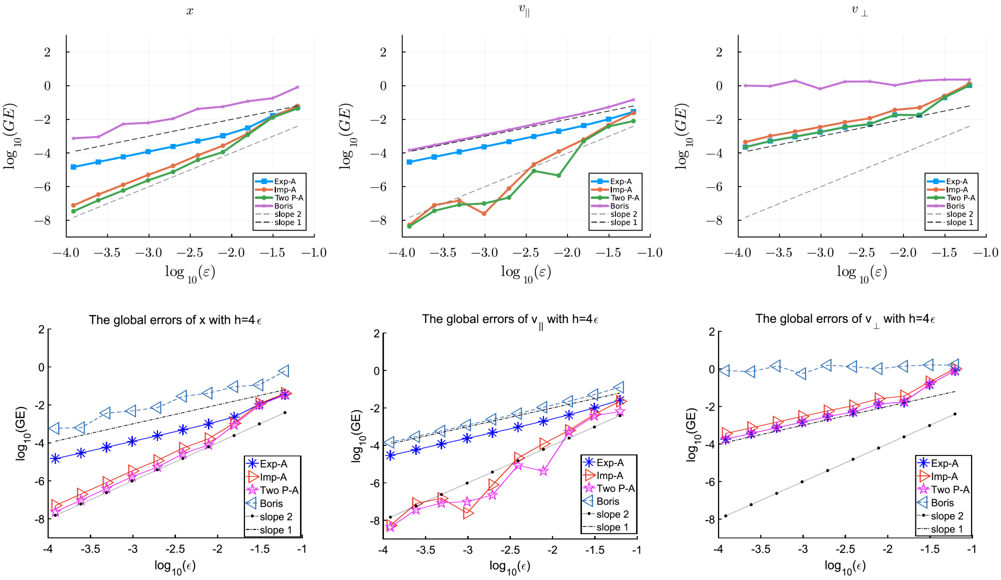


Figure: The logarithm of the global error at t=1 against the logarithm of ϵ for $h = 4\epsilon$

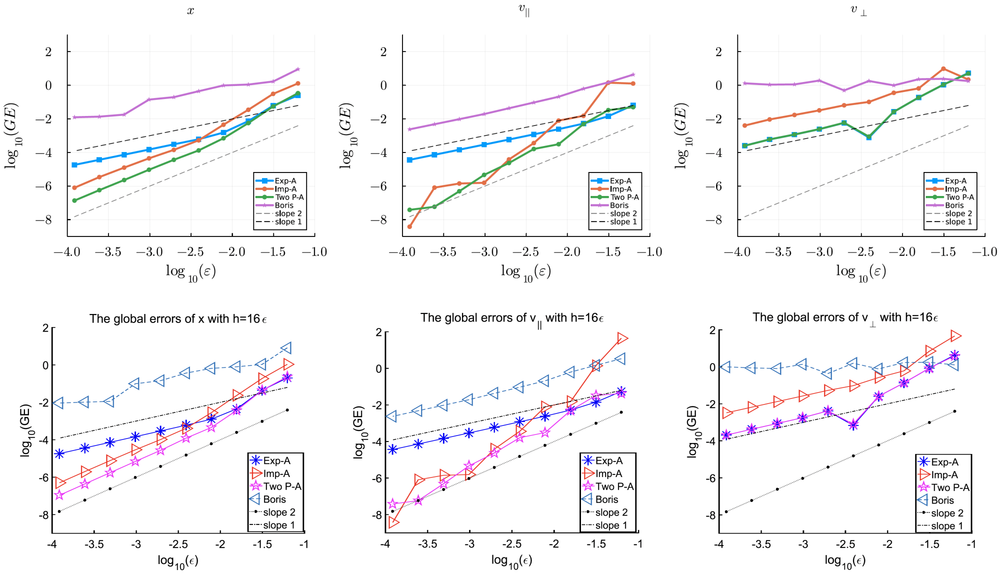


Figure: The logarithm of the global error at t=1 against the logarithm of ϵ for $h = 16\epsilon$

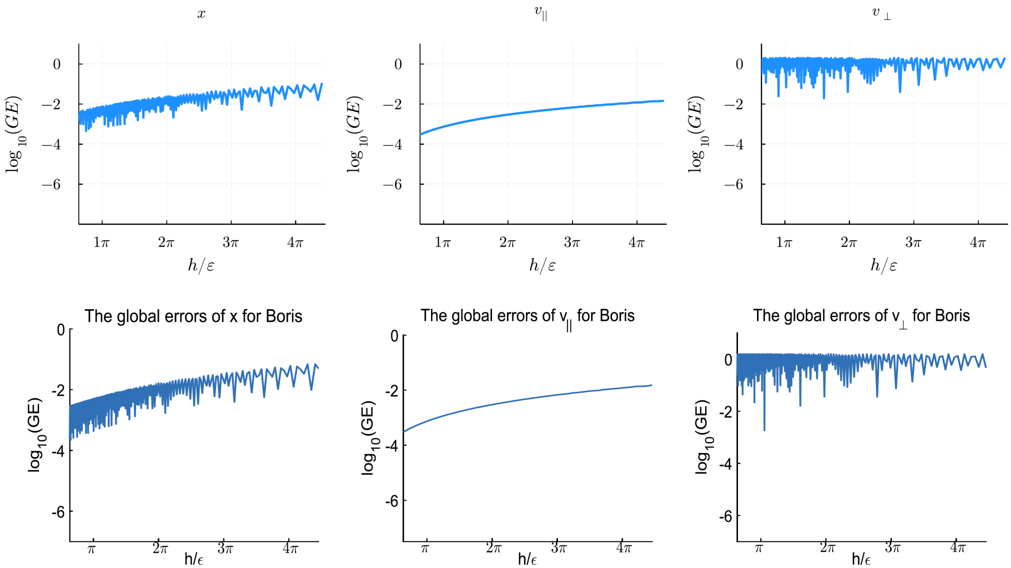
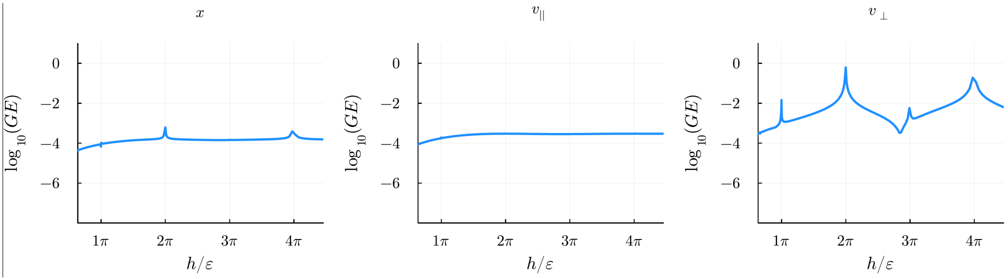


Figure: The logarithm of the global error at $t = 1$ against h/ϵ for $\epsilon = (1/2)^{10}$ and $h = 1/k$, $k = 60, 61, ..., 600$



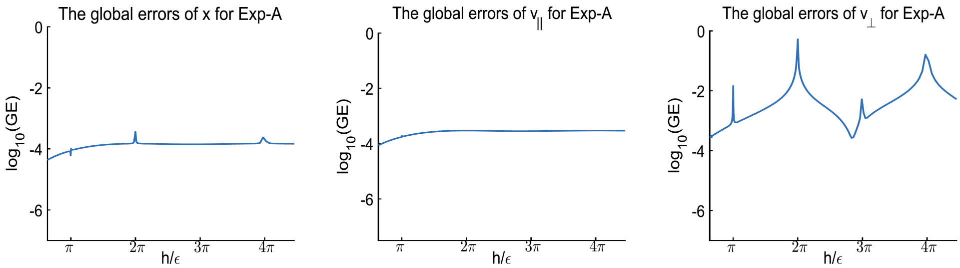


Figure: The logarithm of the global error at $t = 1$ against h/ϵ for $\epsilon = (1/2)^{10}$ and $h = 1/k$, $k = 60, 61, ..., 600$

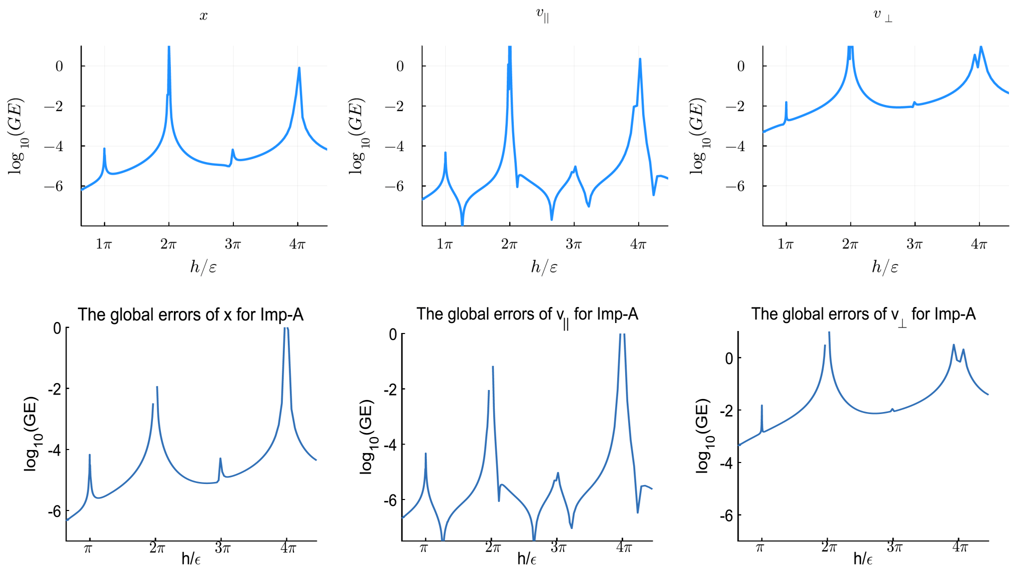


Figure: The logarithm of the global error at $t = 1$ against h/ϵ for $\epsilon = (1/2)^{10}$ and $h = 1/k$, $k = 60, 61, ..., 600$

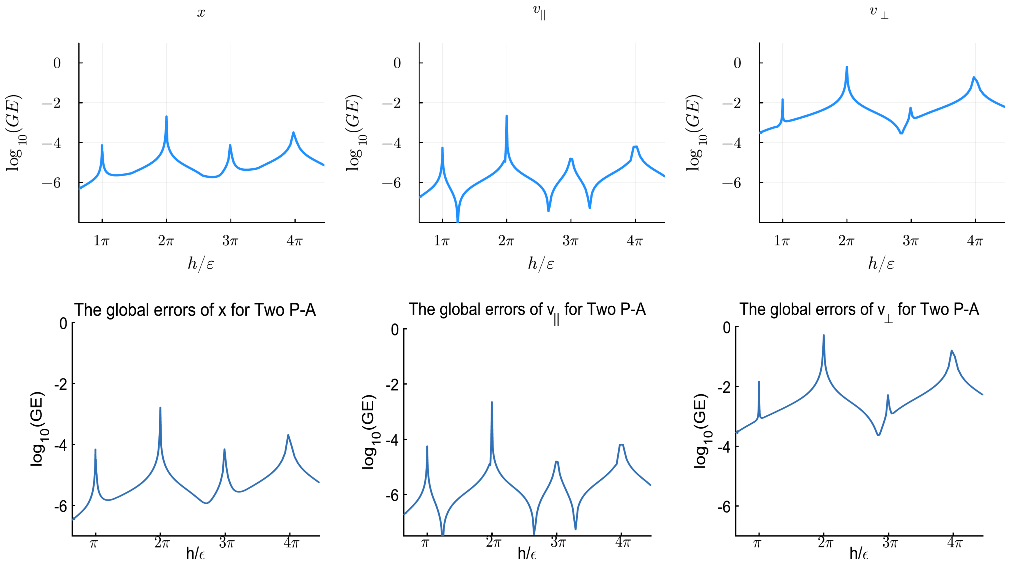


Figure: The logarithm of the global error at $t = 1$ against h/ϵ for $\epsilon = (1/2)^{10}$ and $h = 1/k$, $k = 60, 61, ..., 600$

Challenges

- Reference solution of the ODE was not stated, solved it using RK ode45 equivalent in Julia with appropriate tolerance.
- Most standard libraries/ programming languages (Julia, Python, Matlab but not Mathematica!) implement $\mathrm{sinc}(\zeta)$ as $\sin(\pi\zeta)/(\pi\zeta)$ which gave incorrect results since the authors used $\sin(\zeta)/\zeta$.
- Derivation of the efficient computation of filter functions using a Rodriguez type formula was included in the Appendix of the paper but does not include intermediate steps, and not much literature is found regarding this.
- This and the miscalculation of sinc lead me to believe that the derivation of the matrix filter functions using Rodriguez like formula was incorrect.
- Which in turn lead me to try other computation methods for the matrix functions using matrix identities which yielded correct results.
- However, with one concrete example, the derivation of the rest of the filter functions using the Rodriguez like formula is straightforward and I was able to verify the results and derive the not explicitly stated filter functions.

Outline

1. Introduction
2. Presentation of algorithms
   Standard Boris algorithm
   Filtered Boris algorithm
   Two-point filtered Boris algorithm
3. Results
4. Conclusion

Conclusion

- It is observed that all three filtered Boris methods improve considerably over the standard Boris method, and the optimally filtered methods Imp-A and Two P-A show second order, whereas method Exp-A only shows first order.
- Methods Imp-A and Two P-A behave very similar away from stepsize resonances, but method Two P-A appears more robust near stepsize resonances.

Thank you for your attention!

Carla López
calopez@student.ethz.ch