Boris-type particle integrators in particle-in-cell (PIC) simulation

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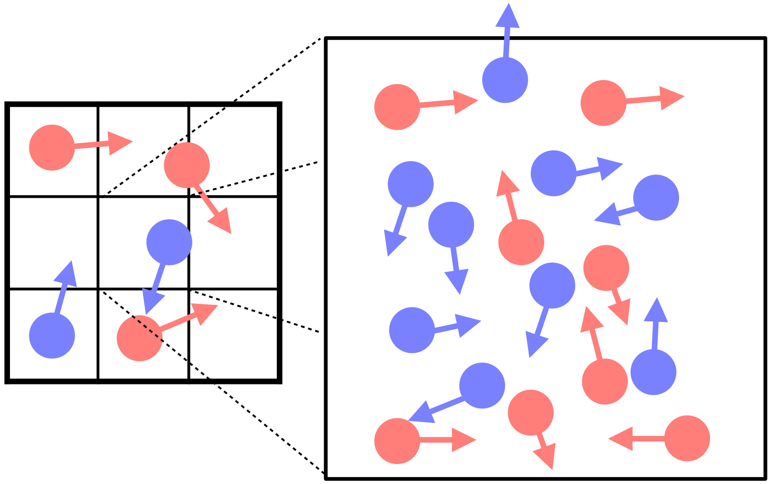
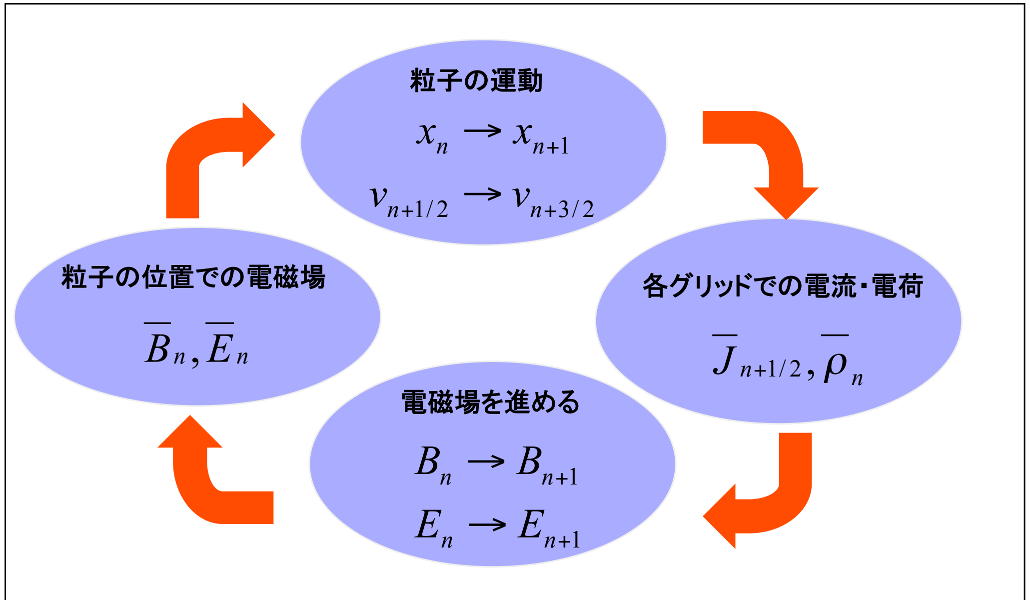
Particle-in-cell (PIC) simulation





Accurate modeling of particle motion is important for studying kinetic plasma processes (reconnection, shocks, kinetic turbulence…)

Particle solver

- Particle solver

$$\frac{\boldsymbol{x}^{t+\Delta t}-\boldsymbol{x}^{t}}{\Delta t}=\frac{\boldsymbol{u}^{t+\frac{1}{2}\Delta t}}{\gamma^{t+\frac{1}{2}\Delta t}}$$

$$\boxed{m\,\frac{\boldsymbol{u}^{t+\frac{1}{2}\Delta t}-\boldsymbol{u}^{t-\frac{1}{2}\Delta t}}{\Delta t}=q\left(\boldsymbol{E}^{t}+\frac{\boldsymbol{u}^{t}}{\gamma^{t}}\times\boldsymbol{B}^{t}\right)}$$

$$\gamma^2=1+(u/c)^2$$

$$\boldsymbol{u}=\gamma\boldsymbol{v}$$

- Time-splitting

$$\boldsymbol{u}^{-}=\boldsymbol{u}^{t-\frac{1}{2}\Delta t}+\frac{q}{m}\boldsymbol{E}^{t}\frac{\Delta t}{2}$$

1/2-acceleration by E

$$\boxed{\frac{\boldsymbol{u}^{+}-\boldsymbol{u}^{-}}{\Delta t}=\frac{q}{m}\left(\boldsymbol{v}^{t}\times\boldsymbol{B}^{t}\right)}$$

gyration about B

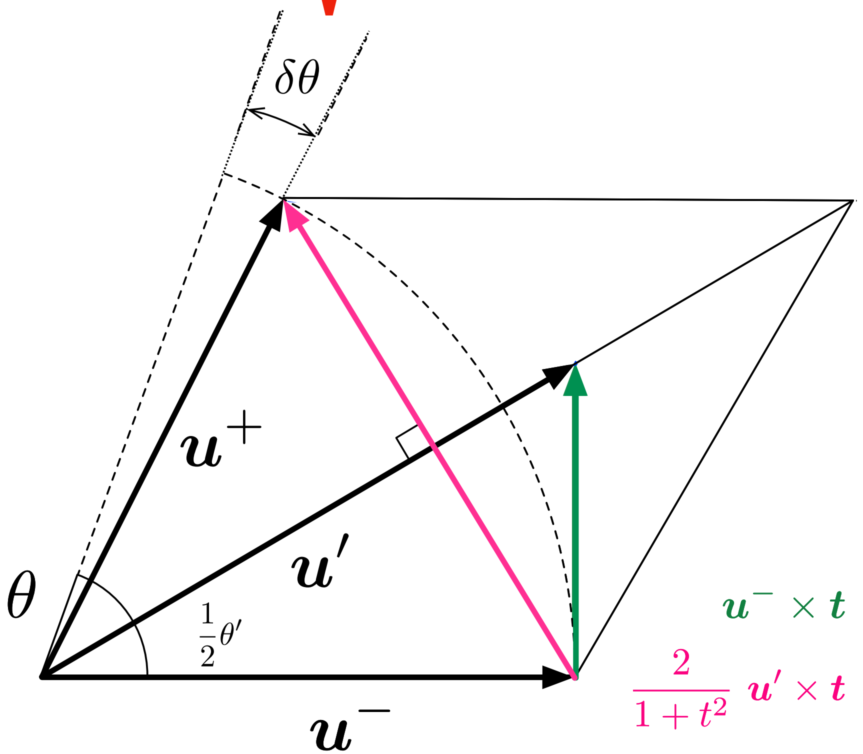
$$\boldsymbol{u}^{t+\frac{1}{2}\Delta t}=\boldsymbol{u}^{+}+\frac{q}{m}\boldsymbol{E}^{t}\frac{\Delta t}{2}$$

1/2-acceleration by E

Boris solver (2-step Boris solver)

$$\delta\theta = \theta\left(\frac{1}{12}\theta^2 - \frac{1}{80}\theta^4 + \cdots\right)$$

- Second-order accuracy in angle



$$\boldsymbol{t} \equiv \frac{q\Delta t}{2m\gamma^-}\boldsymbol{B}$$

$$\boldsymbol{u}' = \boldsymbol{u}^- + \boldsymbol{u}^- \times \boldsymbol{t}$$

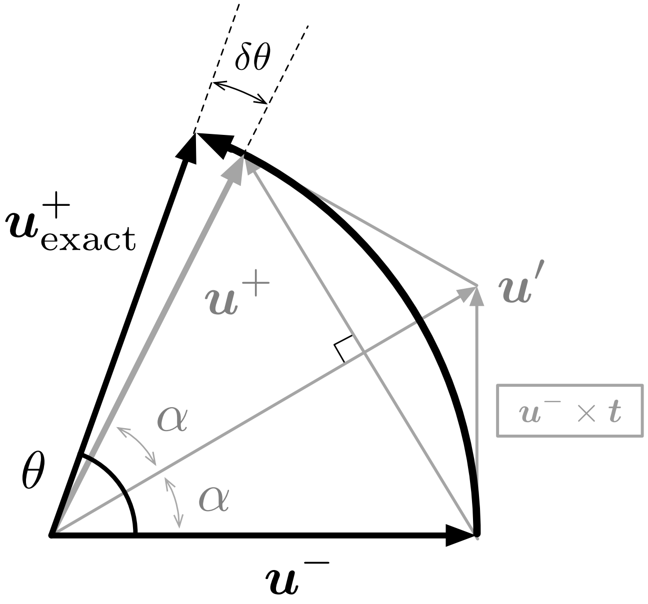
$$\boldsymbol{u}^+ = \boldsymbol{u}^- + \frac{2}{1+t^2}\boldsymbol{u}' \times \boldsymbol{t}$$

Boris 1970
Hockney & Eastwood 1981
Birdsall & Langdon 1985

Can we eliminate this error?

(Solution 0: tan correction by [Boris 1970])

Solution 1: From a different angle…



(a) Boris solver

$$\boldsymbol{t} \equiv \frac{q\Delta t}{2m\gamma^-}\boldsymbol{B}$$

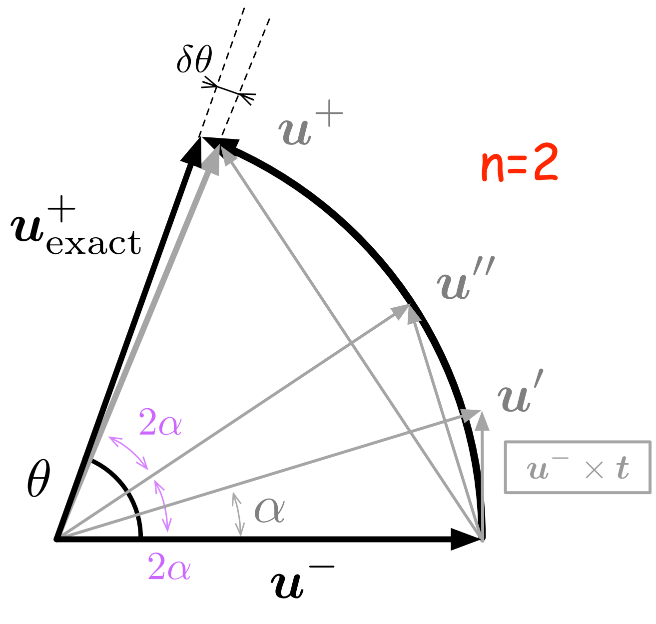
$$\boldsymbol{u}' = \boldsymbol{u}^- + \boldsymbol{u}^- \times \boldsymbol{t}$$

$$\boldsymbol{u}^+ = \boldsymbol{u}^- + \frac{2}{1+t^2}\,\boldsymbol{u}' \times \boldsymbol{t}$$

$$\begin{aligned}
\boldsymbol{u}^+ &= \frac{1}{1+t^2}\Big((1-t^2)\boldsymbol{u}^- + 2(\boldsymbol{u}^- \times \boldsymbol{t}) + 2(\boldsymbol{u}^- \cdot \boldsymbol{t})\boldsymbol{t}\Big) \\
&= \boldsymbol{u}^- \cos 2\alpha + (\boldsymbol{u}^- \times \hat{\boldsymbol{b}}) \sin 2\alpha + (1-\cos 2\alpha)\boldsymbol{u}^-_{\parallel} \\
&= (\boldsymbol{u}^- - \boldsymbol{u}^-_{\parallel}) \cos 2\alpha + (\boldsymbol{u}^- \times \hat{\boldsymbol{b}}) \sin 2\alpha + \boldsymbol{u}^-_{\parallel},
\end{aligned}$$

Rotation by an approximate angle 2α

Solution 1: Multiple Boris solvers



(b) Double Boris solver

n=2

- We repeat Boris procedure multiple times (Inspired by Umeda 2018)

$$\boldsymbol{t} \equiv \frac{\theta}{2n}\hat{\boldsymbol{b}}, \qquad \alpha \equiv \arctan t.$$

$$\theta \equiv \frac{q\Delta t}{m\gamma^-}B$$

$$\boldsymbol{u}_n^+ = (\boldsymbol{u}^- - \boldsymbol{u}_\parallel^-)\cos(2n\alpha) + (\boldsymbol{u}^- \times \hat{\boldsymbol{b}})\sin(2n\alpha) + \boldsymbol{u}_\parallel^-$$

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Solution 1: Multiple Boris solvers

$$\boldsymbol{u}_n^+ = (\boldsymbol{u}^- - \boldsymbol{u}_\parallel^-)\cos(2n\alpha) + (\boldsymbol{u}^- \times \hat{\boldsymbol{b}})\sin(2n\alpha) + \boldsymbol{u}_\parallel^-$$

$$= c_{n1}\boldsymbol{u}^- + c_{n2}\ (\boldsymbol{u}^- \times \boldsymbol{t}) + c_{n3}(\boldsymbol{u}^- \cdot \boldsymbol{t})\boldsymbol{t}$$

General form for an arbitrary n

$$t \equiv \frac{qB\Delta t}{2nm\gamma^-}$$

$$p \equiv \cos 2\alpha = \frac{1 - t^2}{1 + t^2}$$

$$c_{n1} = T_n(p)$$

$$c_{n2} = (1+p)U_{n-1}(p)$$

$$c_{n3} = \begin{cases} 1+p & (\text{for } n=1) \\ (1+p)\ \Big(U_k(p) + U_{k-1}(p)\Big)^2 & (\text{for } n = 2\text{k}+1) \\ 2\ \Big((1+p)U_{k-1}(p)\Big)^2 & (\text{for } n = 2\text{k}) \end{cases}$$

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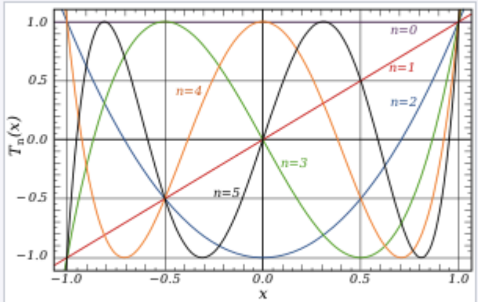
Reminder: Chebyshev polynomials

First kind [edit]

The first few Chebyshev polynomials of the first kind are OEIS: A028297

$$T_0(x) = 1$$
$$T_1(x) = x$$
$$T_2(x) = 2x^2 - 1$$
$$T_3(x) = 4x^3 - 3x$$
$$T_4(x) = 8x^4 - 8x^2 + 1$$
$$T_5(x) = 16x^5 - 20x^3 + 5x$$
$$T_6(x) = 32x^6 - 48x^4 + 18x^2 - 1$$
$$T_7(x) = 64x^7 - 112x^5 + 56x^3 - 7x$$
$$T_8(x) = 128x^8 - 256x^6 + 160x^4 - 32x^2 + 1$$
$$T_9(x) = 256x^9 - 576x^7 + 432x^5 - 120x^3 + 9x$$
$$T_{10}(x) = 512x^{10} - 1280x^8 + 1120x^6 - 400x^4 + 50x^2 - 1$$
$$T_{11}(x) = 1024x^{11} - 2816x^9 + 2816x^7 - 1232x^5 + 220x^3 - 11x$$

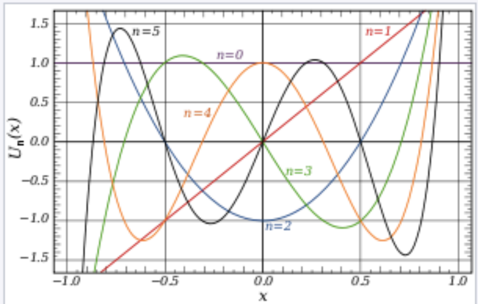


The first few Chebyshev polynomials of the first kind in the domain $-1 < x < 1$: The flat T_0, T_1, T_2, T_3, T_4 and T_5.

Second kind [edit]

The first few Chebyshev polynomials of the second kind are OEIS: A053117

$$U_0(x) = 1$$
$$U_1(x) = 2x$$
$$U_2(x) = 4x^2 - 1$$
$$U_3(x) = 8x^3 - 4x$$
$$U_4(x) = 16x^4 - 12x^2 + 1$$
$$U_5(x) = 32x^5 - 32x^3 + 6x$$
$$U_6(x) = 64x^6 - 80x^4 + 24x^2 - 1$$
$$U_7(x) = 128x^7 - 192x^5 + 80x^3 - 8x$$
$$U_8(x) = 256x^8 - 448x^6 + 240x^4 - 40x^2 + 1$$
$$U_9(x) = 512x^9 - 1024x^7 + 672x^5 - 160x^3 + 10x$$

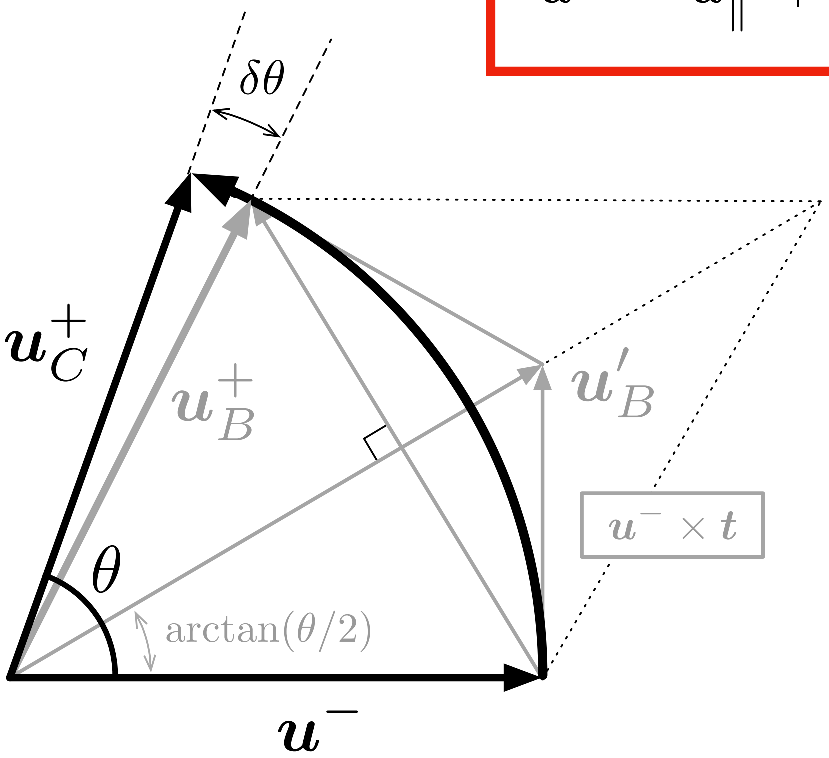


The first few Chebyshev polynomials of the second kind in the domain $-1 < x < 1$: The flat U_0, U_1, U_2, U_3, U_4 and U_5. Although not visible in the image, $U_n(1) = n + 1$ and $U_n(-1) = (n + 1)(-1)^n$.

https://en.wikipedia.org/wiki/Chebyshev_polynomials#Examples

Solution 2: Exact-gyration solver

$$\boxed{\begin{aligned} \boldsymbol{u}^-_{\parallel} &= \frac{(\boldsymbol{u}^- \cdot \boldsymbol{B})\ \boldsymbol{B}}{|B|^2} \\ \boldsymbol{u}^+ &= \boldsymbol{u}^-_{\parallel} + (\boldsymbol{u}^- - \boldsymbol{u}^-_{\parallel}) \cos\theta + \frac{\boldsymbol{u}^- \times \boldsymbol{B}}{|B|} \sin\theta \end{aligned}}$$



- Rotation angle

$$\theta = \frac{q\Delta t}{m\gamma^-} B$$

- Equivalent to the Boris solver with a gyro-phase correction

Zenitani & Umeda 2018

Stability: Volume preservation

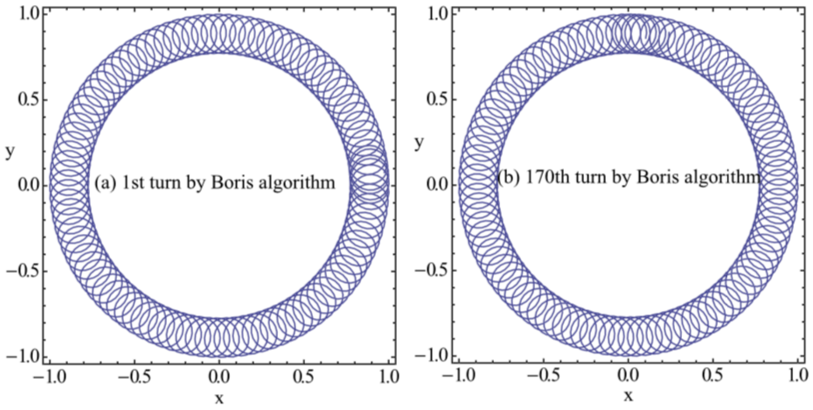
- Stable scheme preserves a volume in the phase space during the temporal evolution (Qin et al. 2013).
- We have formally proved this property in our paper.

$$(\boldsymbol{x}^{t-\frac{1}{2}\Delta t}, \boldsymbol{u}^{t-\frac{1}{2}\Delta t}) \rightarrow (\boldsymbol{x}^{t+\frac{1}{2}\Delta t}, \boldsymbol{u}^{t+\frac{1}{2}\Delta t})$$

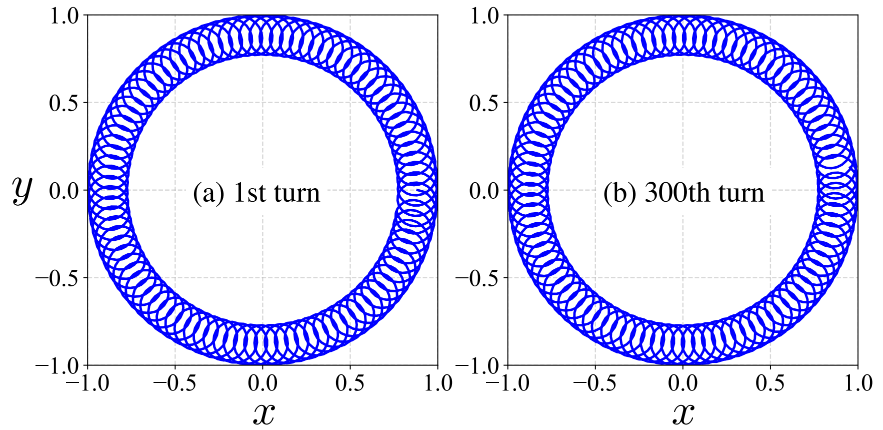
$$\left|\frac{\partial(\boldsymbol{x}^{t+\frac{1}{2}\Delta t}, \boldsymbol{u}^{t+\frac{1}{2}\Delta t})}{\partial(\boldsymbol{x}^{t-\frac{1}{2}\Delta t}, \boldsymbol{u}^{t-\frac{1}{2}\Delta t})}\right| = \det \begin{pmatrix} \dfrac{\partial \boldsymbol{x}^{t+\frac{1}{2}\Delta t}}{\partial \boldsymbol{x}^{t-\frac{1}{2}\Delta t}} & \dfrac{\partial \boldsymbol{x}^{t+\frac{1}{2}\Delta t}}{\partial \boldsymbol{u}^{t-\frac{1}{2}\Delta t}} \\ \dfrac{\partial \boldsymbol{u}^{t+\frac{1}{2}\Delta t}}{\partial \boldsymbol{x}^{t-\frac{1}{2}\Delta t}} & \dfrac{\partial \boldsymbol{u}^{t+\frac{1}{2}\Delta t}}{\partial \boldsymbol{u}^{t-\frac{1}{2}\Delta t}} \end{pmatrix} = 1$$

Stability: Volume preservation

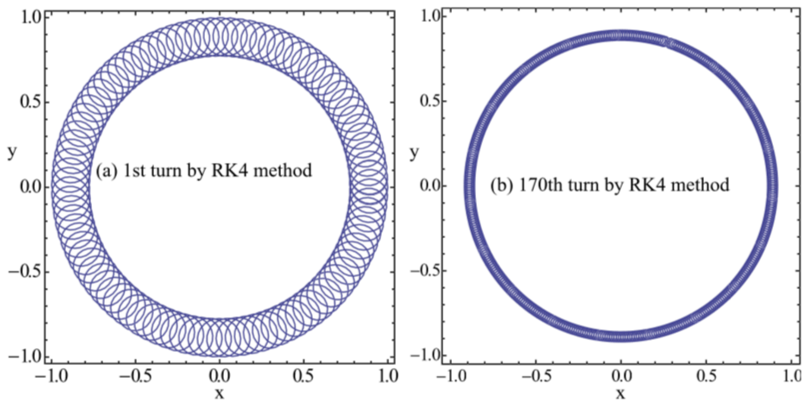
2-step Boris: volume-preserving



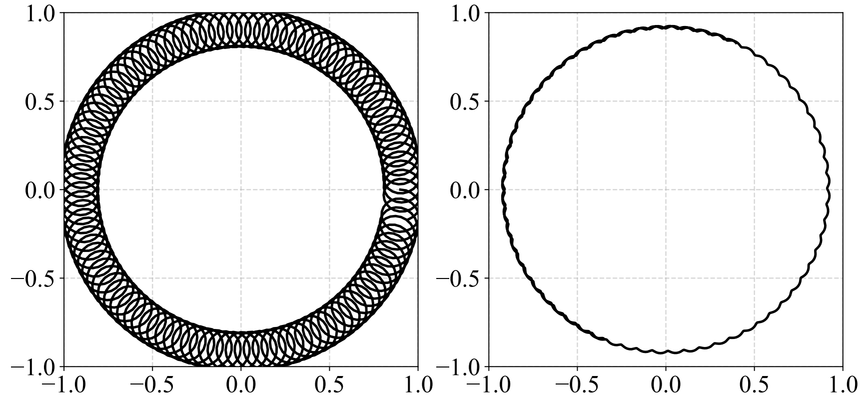
Exact/Zenitani: volume-preserving



RK4



RK4

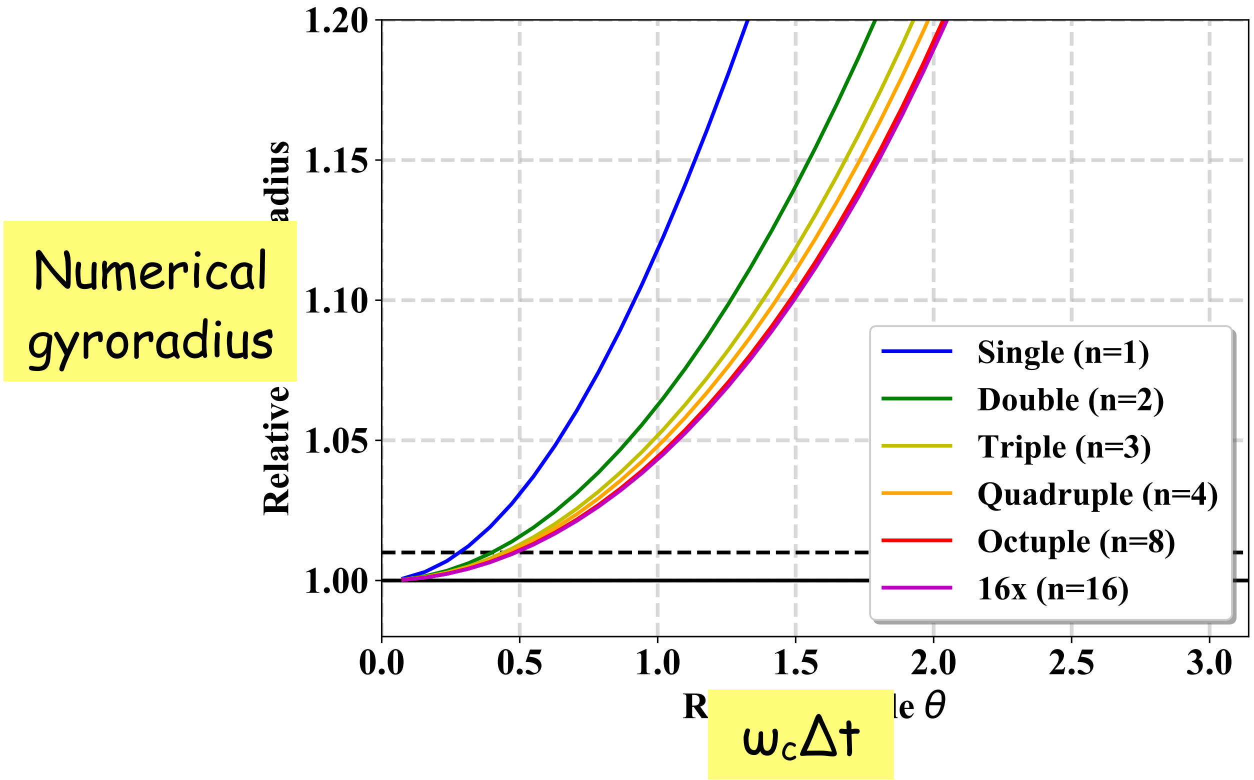


Qin et al. 2013

$\odot$ ***B***

Constraint to the timestep

- Because of a numerical Larmor radius, $\{ n^2/(2+n^2) \}^{0.5}$ times larger Δt is allowed



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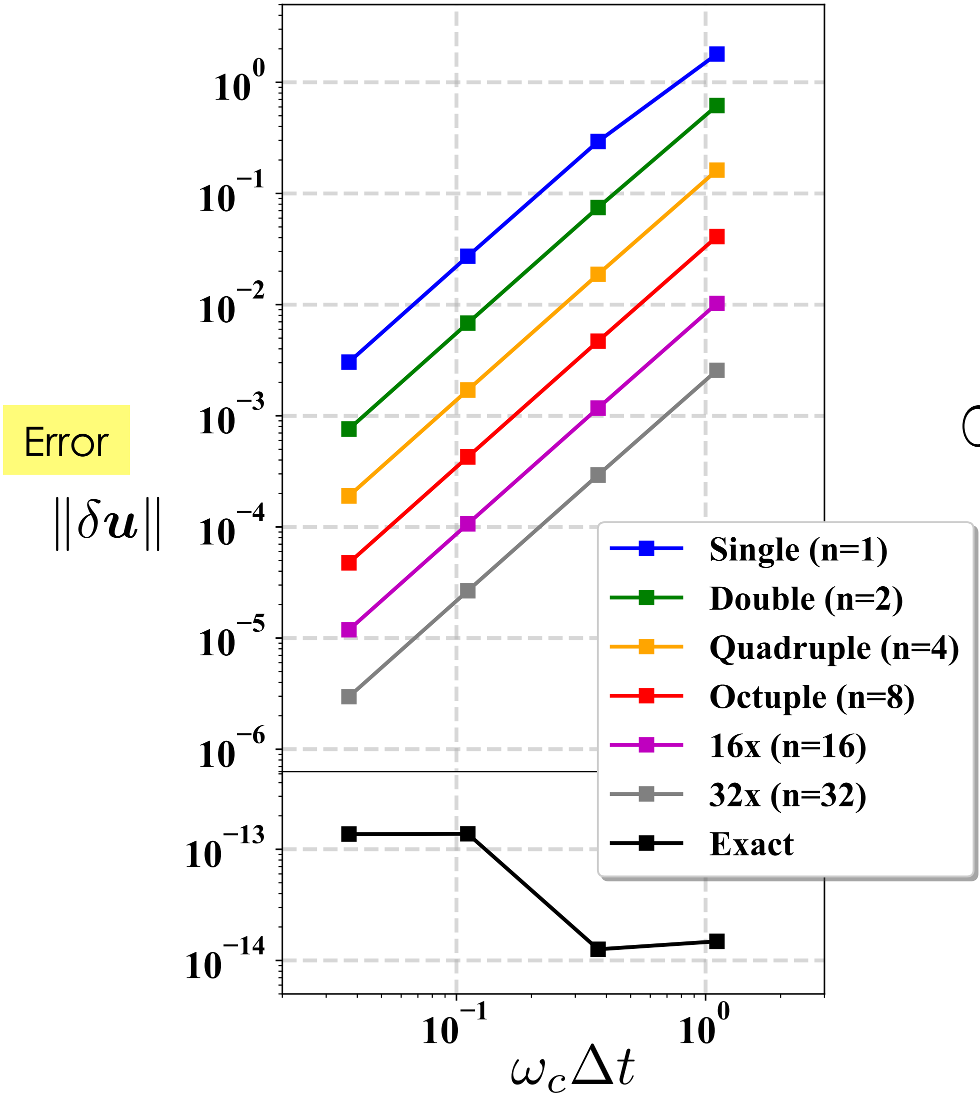
Numerical tests (1): Errors in gyration



$$\propto \left(\frac{\Delta t}{n} \right)^2$$

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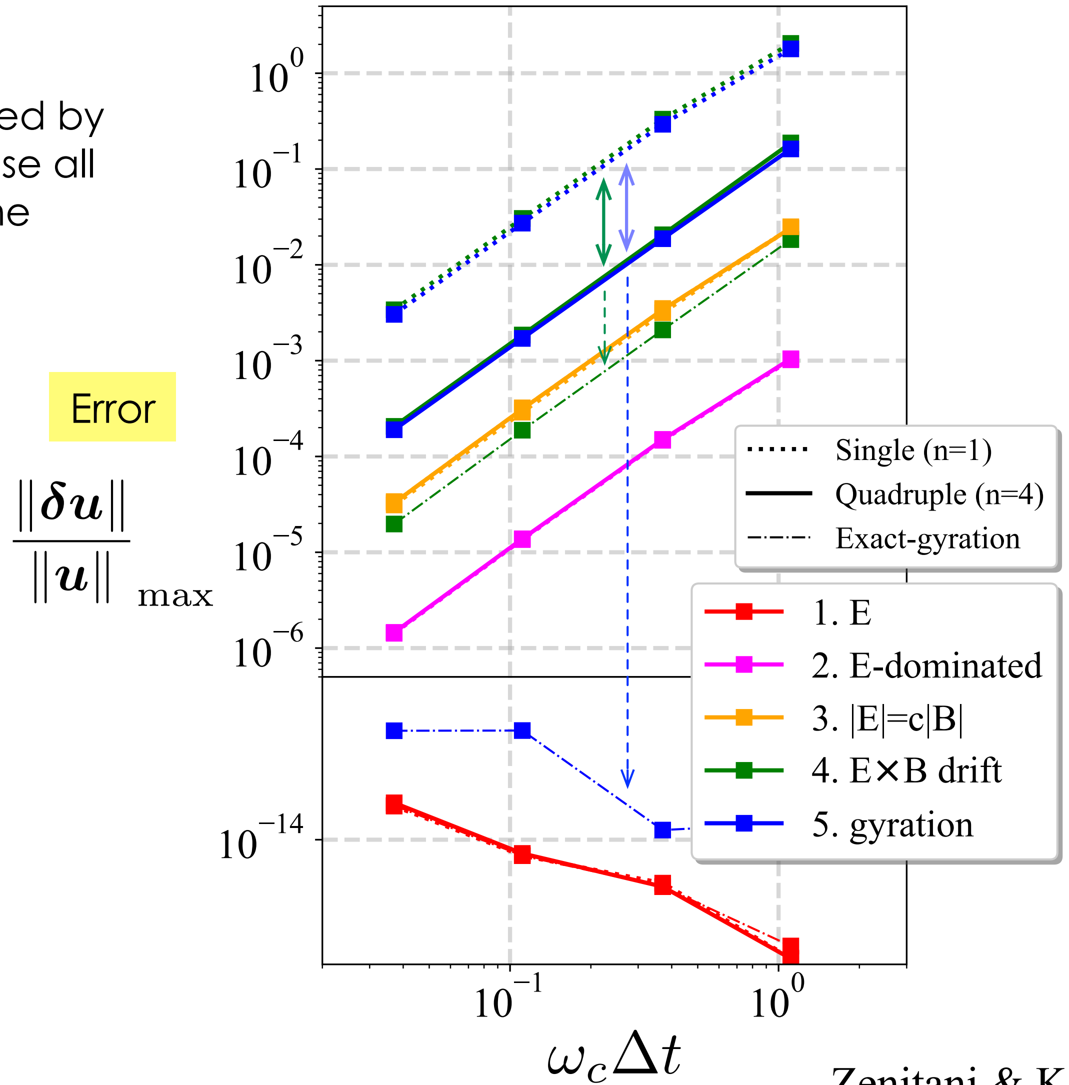
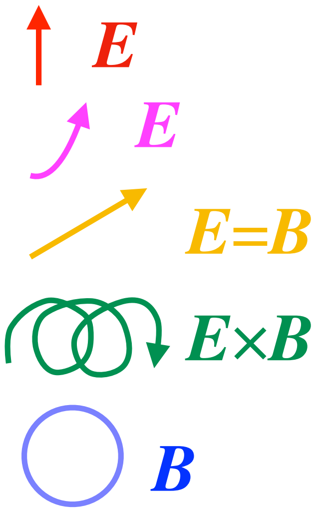
Numerical tests (2): Errors in various field

- Errors are largely controlled by the gyration part, because all the solvers share the same Coulomb-force solver





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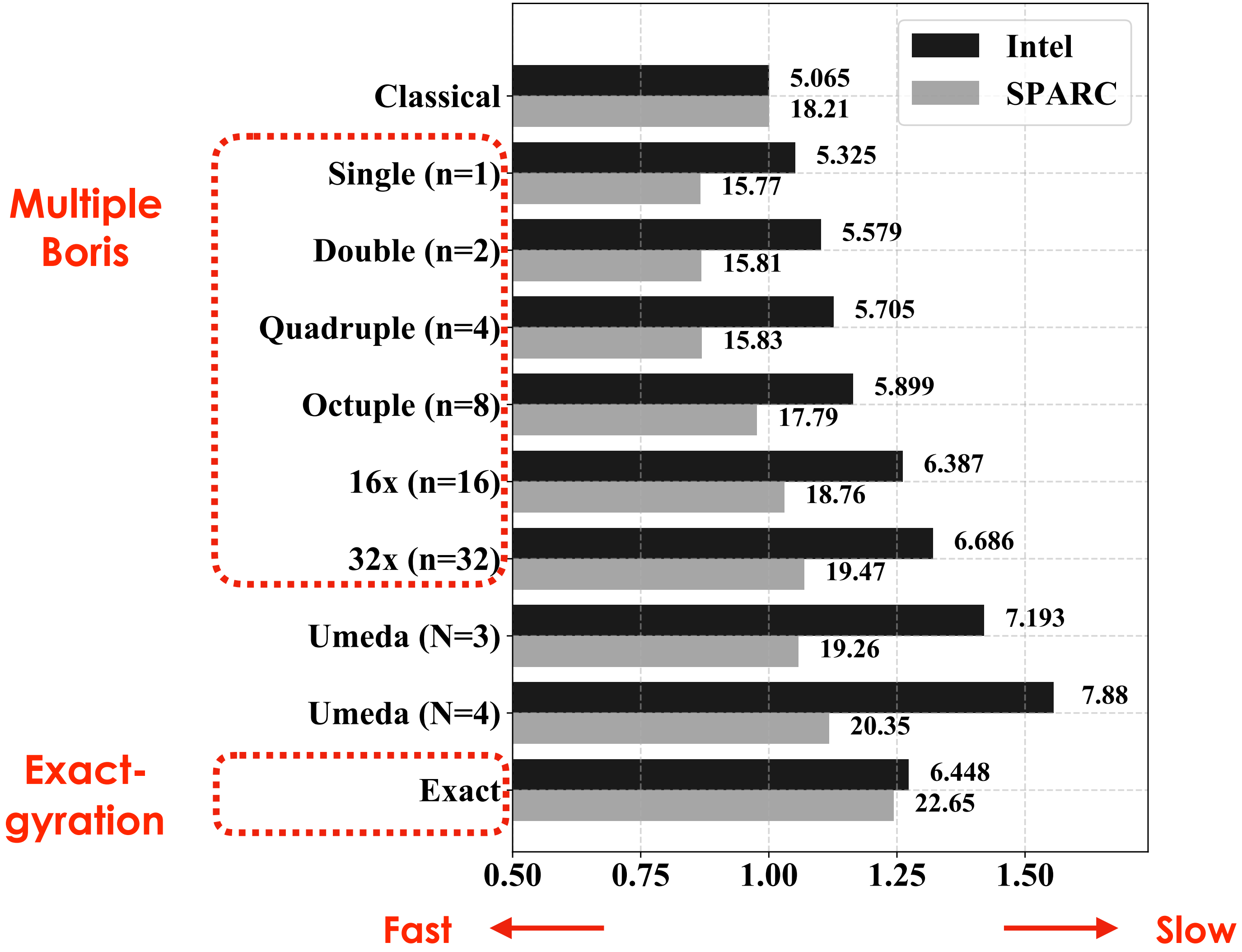
Numerical tests (3): Computation time



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Summary

- Multiple Boris solvers
  - n-times multiplication of the Boris solver
  - Single-step formula with Chebyshev polynomials
  - n^2-times higher accuracy for the gyration part
- Exact-gyration solver
  - Based on the rotation formula
  - Exact accuracy for the gyration part
- Both solvers are computationally affordable

- References:

  - Zenitani & Umeda, *On the Boris solver in particle-in-cell simulation*, Phys. Plasmas. **25**, 112110 (2018)
  - Zenitani & Kato, *Multiple Boris integrators for particle-in-cell simulation*, Comput. Phys. Commun., in press (2019)