New integrator for relativistic equations of motion for charged particles

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Relativistic eq. motion

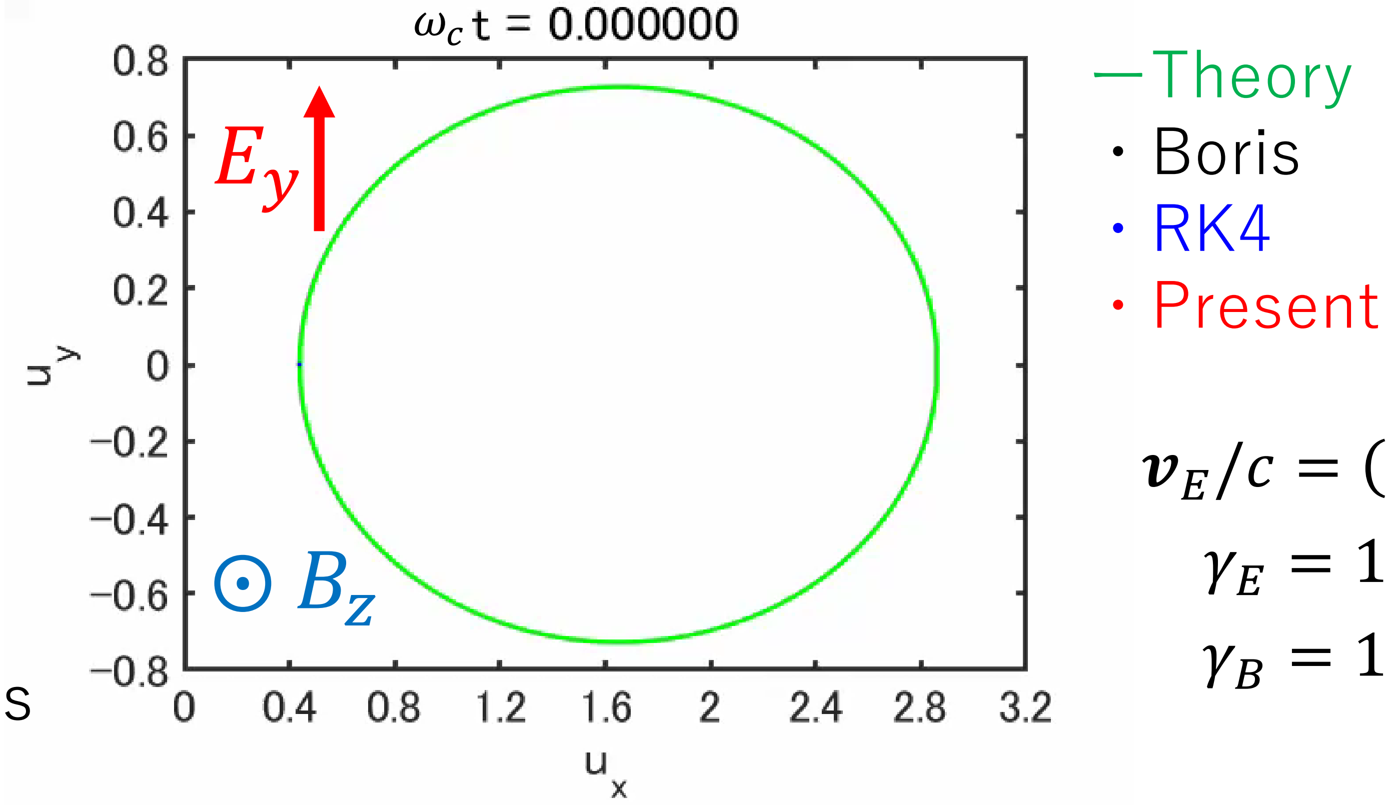
$$\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} = \boldsymbol{v}$$

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = \frac{q}{m}(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B})$$

$$\boldsymbol{u} = \gamma \boldsymbol{v} = \frac{c\boldsymbol{v}}{\sqrt{c^2 - |\boldsymbol{v}|^2}}$$

- Full/hybrid-PIC simulations
- Test-particle calculations

Trajectory in momentum space



$$\boldsymbol{v}_E/c = (0.8,0,0)$$

$$\gamma_E = 1.6666$$

$$\gamma_B = 1.1547$$

Numerical Integrators for Relativistic Charged Particles

- Runge (1895)-Kutta (1901) "RK4"
  - Fourth-order
  - Conservation of nothing
- Boris (1970)
  - Second-order
  - Energy conservation during gyration
- Vay (2008)
- Higuera-Cray (2017)
  - Second-order
  - Modification of Boris
- Implicit methods
  - Iterative convergence, mostly second-order

➢ **Gradually deviates** from the theoretical trajectory.

➢ Good if $|\boldsymbol{v}_E - \boldsymbol{v}_0|$ is large.

➢ Good if $|\boldsymbol{v}_E - \boldsymbol{v}_0|$ is small.

➢ Preserve an elliptical trajectory with a **wrong guiding center**.

Theoretical Solution to Relativistic E-cross-B Motions

[e.g. Friedman & Semon PRE 2005]

- Trajectory of perpendicular momentum vector components:

$$u_x \parallel \boldsymbol{v}_E, u_y \parallel \boldsymbol{E}_\perp, u_z \parallel \boldsymbol{B}$$

$$(u_x - \gamma_B \gamma_E v_E)^2 + \gamma_E^2 u_y^2 = const. \qquad c > |\boldsymbol{v}_E|$$

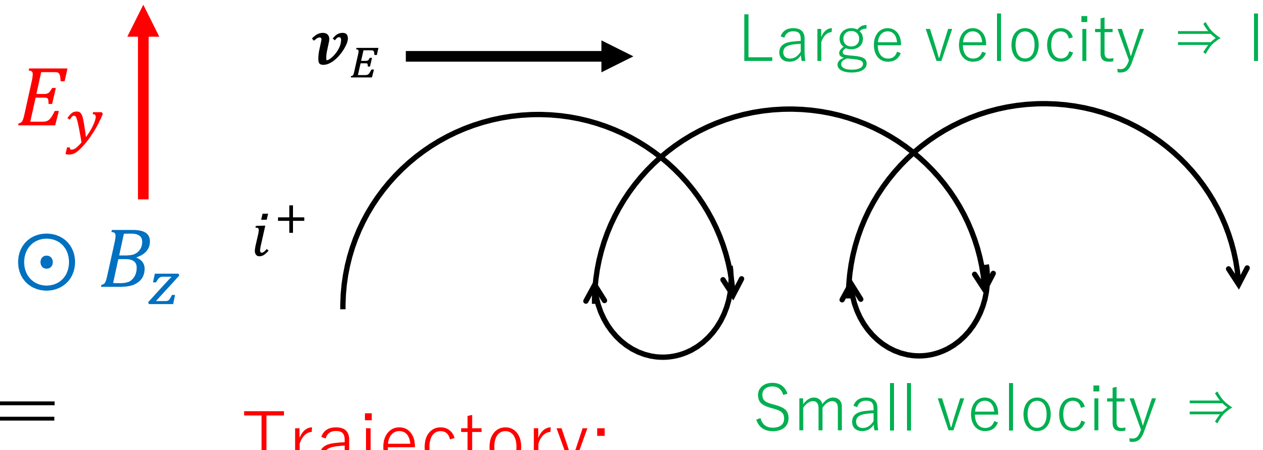
$$\boldsymbol{v}_E = \frac{\boldsymbol{E} \times \boldsymbol{B}}{|\boldsymbol{B}|^2}$$

$$\gamma_E = \frac{c}{\sqrt{c^2 - v_E^2}}$$

$$\gamma_B = \frac{c^2 - v_E v_x}{\sqrt{c^2 - v_E^2}\sqrt{c^2 - v_x^2 - v_y^2 - v_z^2}}$$

$$= \gamma_E \left(\gamma - \frac{\boldsymbol{v}_E \cdot \boldsymbol{v}}{c^2}\right)$$

: "boosted Lorentz factor"



E-cross-B with grad-B (grad-γ)

Trajectory:

- ➢Ellipse $(c > |\boldsymbol{v}_E|,\ \gamma_E^2 > 1)$
- ➢Parabola $(c = |\boldsymbol{v}_E|,\ \gamma_E^2 = \infty)$
- ➢Hyperbola $(c < |\boldsymbol{v}_E|,\ \gamma_E^2 < 0)$

Comparison of Previous Integrators

$$\frac{q\Delta t}{m}|\boldsymbol{B}^t| = \omega_c \Delta t = 1$$

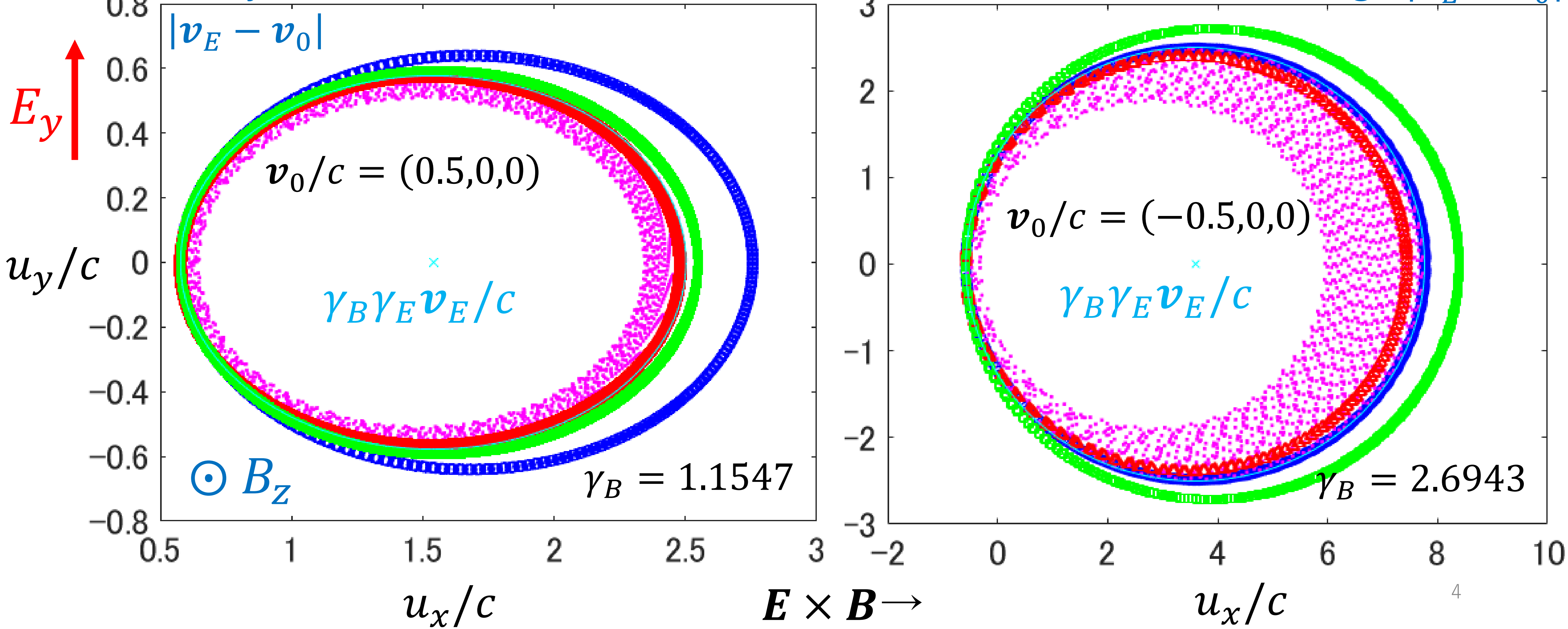
$$\boldsymbol{v}_E/c = (0.8,0,0)$$

$$\gamma_E = 1.6666$$

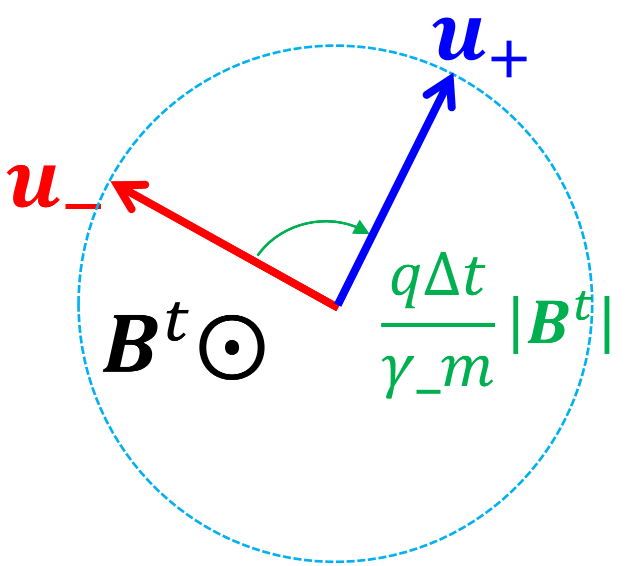
○:Boris □:Vay △:HC ・:RK4

—:$(u_x - \gamma_B \gamma_E v_E)^2 + \gamma_E^2 u_y^2 = const.$

- Vay and HC are better with smaller $|\boldsymbol{v}_E - \boldsymbol{v}_0|$
- Boris is better with large $|\boldsymbol{v}_E - \boldsymbol{v}_0|$



Boris Integrator (1970)



$$\overset{\boldsymbol{u}_+}{\begin{bmatrix} u_x^{t+\frac{\Delta t}{2}} - \frac{q\Delta t}{2m}E_x^t \\ u_y^{t+\frac{\Delta t}{2}} - \frac{q\Delta t}{2m}E_y^t \end{bmatrix}} = \overbrace{\begin{bmatrix} \cos\left(\frac{q\Delta t}{\gamma_- m}|\boldsymbol{B}^t|\right) & -\sin\left(\frac{q\Delta t}{\gamma_- m}|\boldsymbol{B}^t|\right) \\ \sin\left(\frac{q\Delta t}{\gamma_- m}|\boldsymbol{B}^t|\right) & \cos\left(\frac{q\Delta t}{\gamma_- m}|\boldsymbol{B}^t|\right) \end{bmatrix}}^{\text{Circular rotation matrix}} \overset{\boldsymbol{u}_-}{\begin{bmatrix} u_x^{t-\frac{\Delta t}{2}} + \frac{q\Delta t}{2m}E_x^t \\ u_y^{t-\frac{\Delta t}{2}} + \frac{q\Delta t}{2m}E_y^t \end{bmatrix}}$$

$$\cos\theta = \frac{1-\tan^2\frac{\theta}{2}}{1+\tan^2\frac{\theta}{2}}$$

$$\boldsymbol{u}^{t+\frac{\Delta t}{2}} = \boldsymbol{u}^{t-\frac{\Delta t}{2}} + \frac{q}{m}\boldsymbol{E}^t\Delta t + \beta_B\frac{q\Delta t}{\gamma_- m}\left(\boldsymbol{u}^{t-\frac{\Delta t}{2}} \times \boldsymbol{B}^t\right) + 2\beta_B\gamma_-\left(\frac{q\Delta t}{2\gamma_- m}|\boldsymbol{B}^t|\right)^2 \boldsymbol{v}_E^t$$
$$+2\beta_B\left(\frac{q\Delta t}{2\gamma_- m}\right)^2 \underbrace{\left(\boldsymbol{u}^{t-\frac{\Delta t}{2}} \times \boldsymbol{B}^t\right) \times \boldsymbol{B}^t}_{\boldsymbol{u}_\perp^{t-\frac{\Delta t}{2}}} + (1-\beta_B)\frac{q\Delta t}{m}\underbrace{\left(\boldsymbol{v}_E^t \times \boldsymbol{B}^t\right)}_{\boldsymbol{E}_\perp^t}$$

$$\sin\theta = \frac{2\tan\frac{\theta}{2}}{1+\tan^2\frac{\theta}{2}}$$

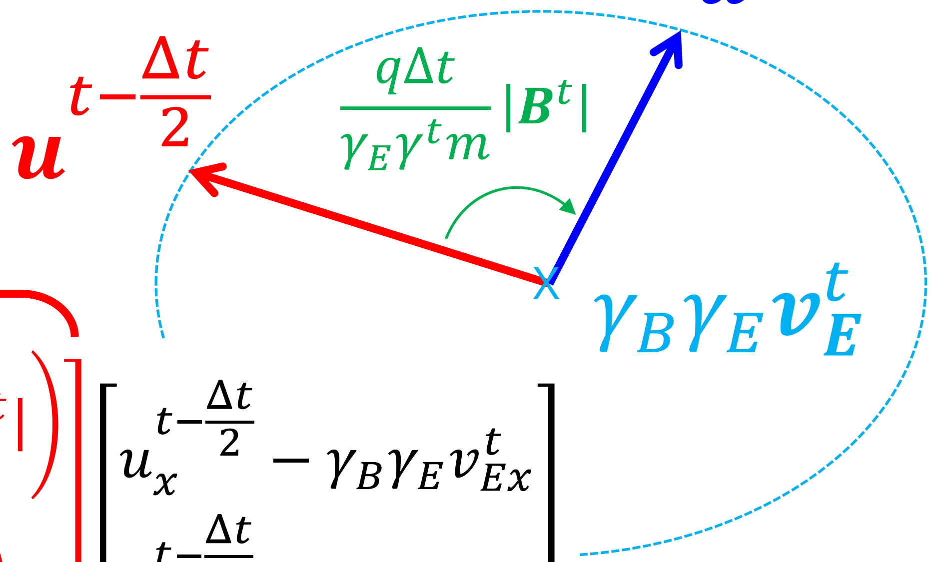
$$\tan\frac{\theta}{2} \approx \frac{\theta}{2} + \frac{\theta^3}{16} + \frac{\theta^5}{240} + \cdots$$

(Zenitani+)

$$\beta_B = \frac{1}{1+\tan^2\left(\frac{q\Delta t}{2\gamma_- m}|\boldsymbol{B}^t|\right)}$$

New Integrator (Umeda JCP 2023)

$$(u_x - \gamma_B \gamma_E v_E)^2 + \gamma_E^2 u_y^2 = const.$$



Elliptical rotation matrix (for $\gamma_E^2 > 1$)

$$\begin{bmatrix} u_x^{t+\frac{\Delta t}{2}} - \gamma_B \gamma_E v_{Ex}^t \\ u_y^{t+\frac{\Delta t}{2}} - \gamma_B \gamma_E v_{Ey}^t \end{bmatrix} = \overbrace{\begin{bmatrix} \cos\left(\frac{q\Delta t}{\gamma_E \gamma^t m}|\boldsymbol{B}^t|\right) & -\gamma_E \sin\left(\frac{q\Delta t}{\gamma_E \gamma^t m}|\boldsymbol{B}^t|\right) \\ \gamma_E \sin\left(\frac{q\Delta t}{\gamma_E \gamma^t m}|\boldsymbol{B}^t|\right) & \cos\left(\frac{q\Delta t}{\gamma_E \gamma^t m}|\boldsymbol{B}^t|\right) \end{bmatrix}}^{\text{Elliptical rotation matrix (for } \gamma_E^2 > 1)} \begin{bmatrix} u_x^{t-\frac{\Delta t}{2}} - \gamma_B \gamma_E v_{Ex}^t \\ u_y^{t-\frac{\Delta t}{2}} - \gamma_B \gamma_E v_{Ey}^t \end{bmatrix}$$

$$\boldsymbol{u}^{t+\frac{\Delta t}{2}} = \boldsymbol{u}^{t-\frac{\Delta t}{2}} + \frac{q}{m}\boldsymbol{E}^t \Delta t + \frac{2}{|\boldsymbol{B}^t|}\frac{\gamma_E \tan\omega_c^*}{1+\tan^2\omega_c^*}\left(\boldsymbol{u}^{t-\frac{\Delta t}{2}} \times \boldsymbol{B}^t\right) + \frac{2\gamma_B}{\gamma_E}\frac{\gamma_E^2 \tan^2\omega_c^*}{1+\tan^2\omega_c^*}\boldsymbol{v}_E^t$$

$$+ \frac{2}{|\boldsymbol{B}^t|^2}\frac{\tan^2\omega_c^*}{1+\tan^2\omega_c^*}\underbrace{\left(\boldsymbol{u}^{t-\frac{\Delta t}{2}} \times \boldsymbol{B}^t\right) \times \boldsymbol{B}^t}_{\boldsymbol{u}_\perp^{t-\frac{\Delta t}{2}}} + \left\{\frac{q\Delta t}{m} - \frac{\gamma^{t-\frac{\Delta t}{2}}}{\gamma^t}\frac{2}{|\boldsymbol{B}^t|}\frac{\gamma_E \tan\omega_c^*}{1+\tan^2\omega_c^*}\right\}\underbrace{\left(\boldsymbol{v}_E^t \times \boldsymbol{B}^t\right)}_{\boldsymbol{E}_\perp^t}$$

$$\omega_c^* \equiv \frac{q\Delta t}{2\gamma_E \gamma^t m}|\boldsymbol{B}^t|$$

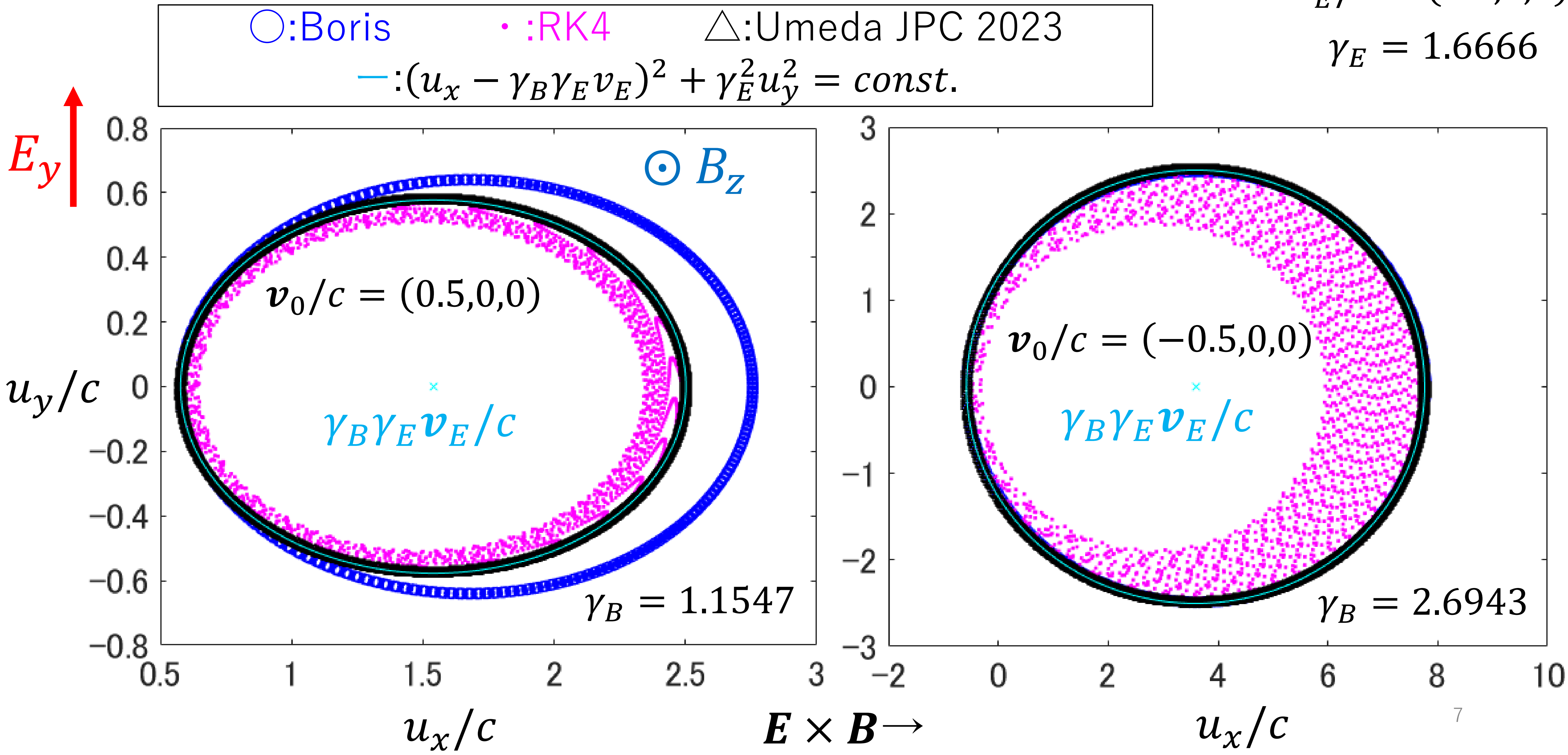
Many choices for γ^t

Comparison of momentum trajectory

$$\frac{q\Delta t}{m}|\boldsymbol{B}^t| = \omega_c \Delta t = 1$$

$$\boldsymbol{v}_E/c = (0.8,0,0)$$

$$\gamma_E = 1.6666$$



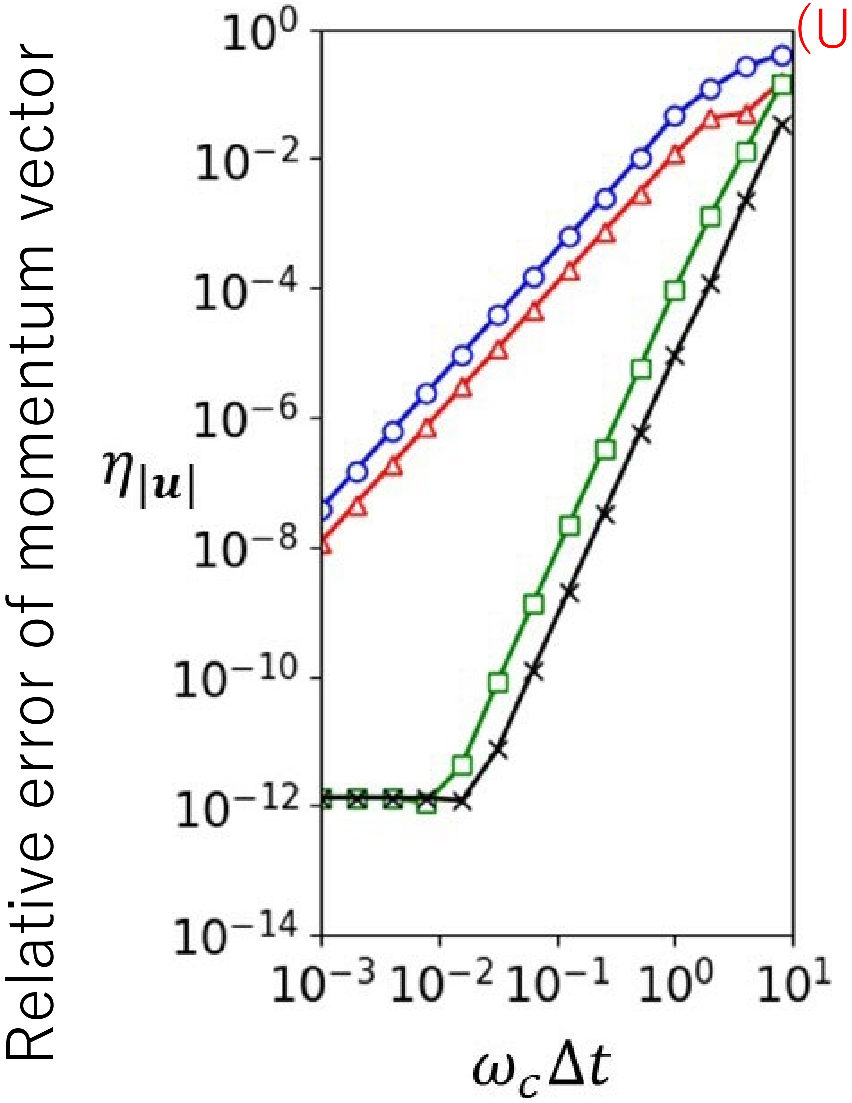
Comparison of numerical accuracy

○:Boris □:RK4 △:Present(2nd) ×:Present(4th)

(Umeda JCP 2023) (Umeda & Ozaki EPS 2023)

$\boldsymbol{v}_0/c = (0.5,0,0)$

$\boldsymbol{v}_E/c = (0.8,0,0)$

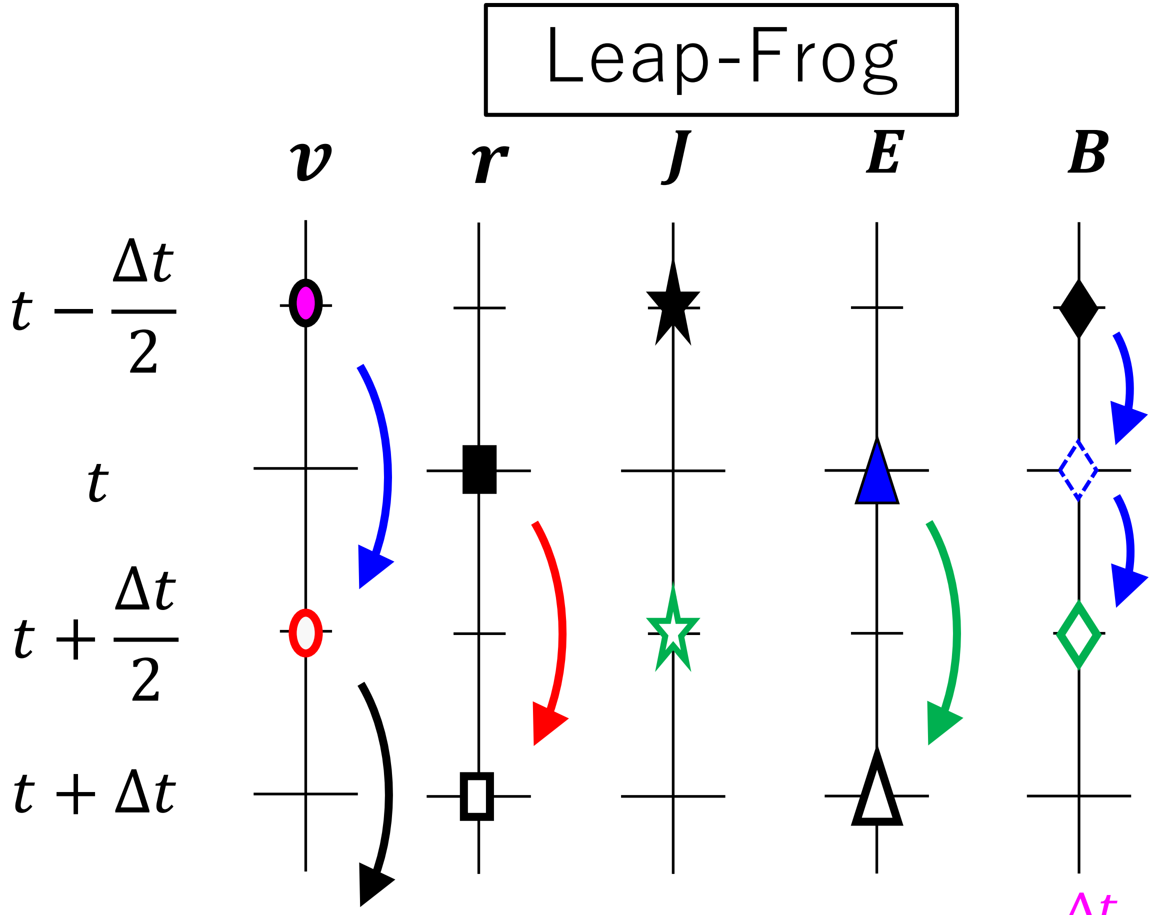


- The new integrator preserves both theoretical trajectory of the momentum vector and boosted Lorentz factor γ_B.
- The fourth-order version of the new integrator is developed by approximating γ^t with RK4.

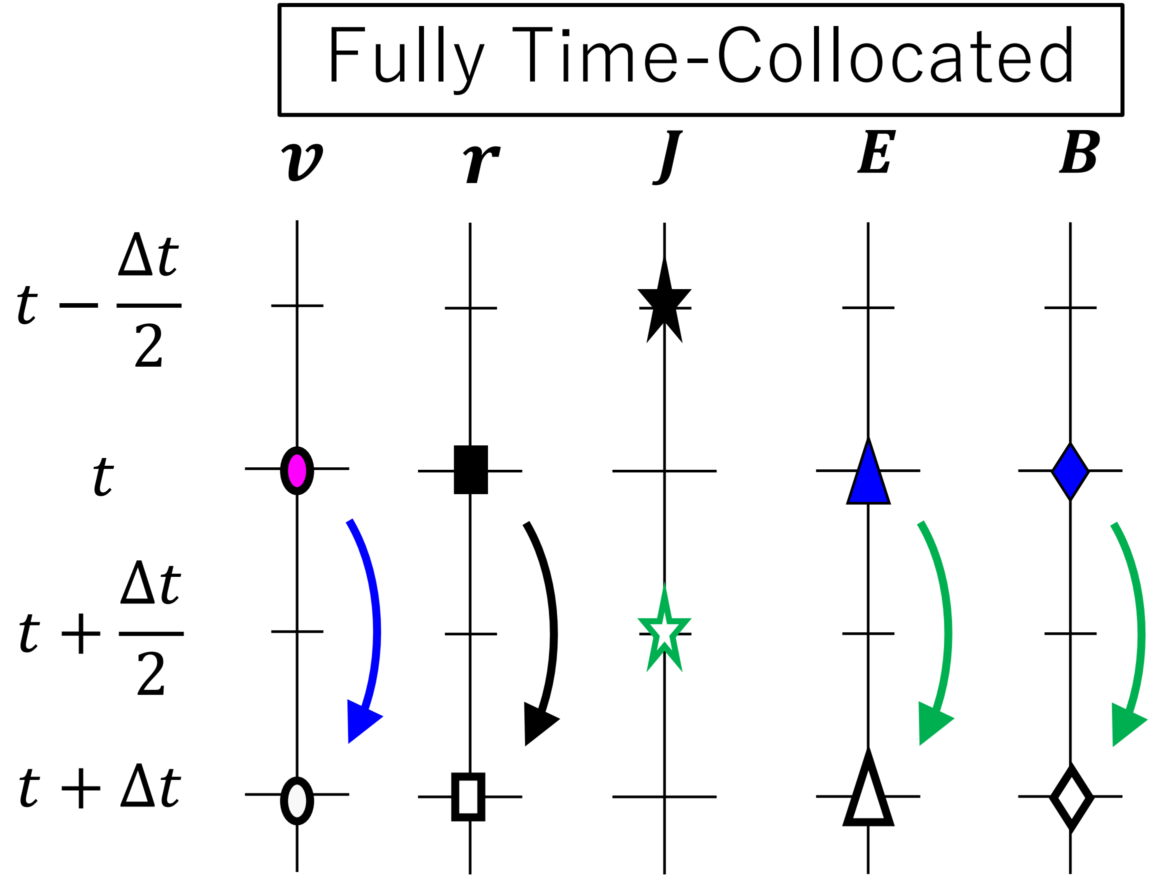
$$\omega_c^* \equiv \frac{q\Delta t}{2\gamma_E \gamma^t m} |\boldsymbol{B}^t|$$

- Numerical errors of the new integrators are one-order lower than the previous ones.

Time-Staggered versus Time-Collocated
(Leap-Frog) (e.g. RK4)



- Use $\boldsymbol{E}^t$ and $\boldsymbol{B}^t$ to update $\boldsymbol{v}^{t-\frac{\Delta t}{2}}$



- Use $\boldsymbol{E}^t$ and $\boldsymbol{B}^t$ to update $\boldsymbol{v}^t$
- $\boldsymbol{J}^{t-\frac{\Delta t}{2}}$ is given after update of $\boldsymbol{r}^t$

Development of fourth-order leap-frog integrator

- Co-located time-stepping is OK for test-particle calculations.
- The leap-frog integrator is necessary to avoid the Euler (first-order) time stepping in PIC.

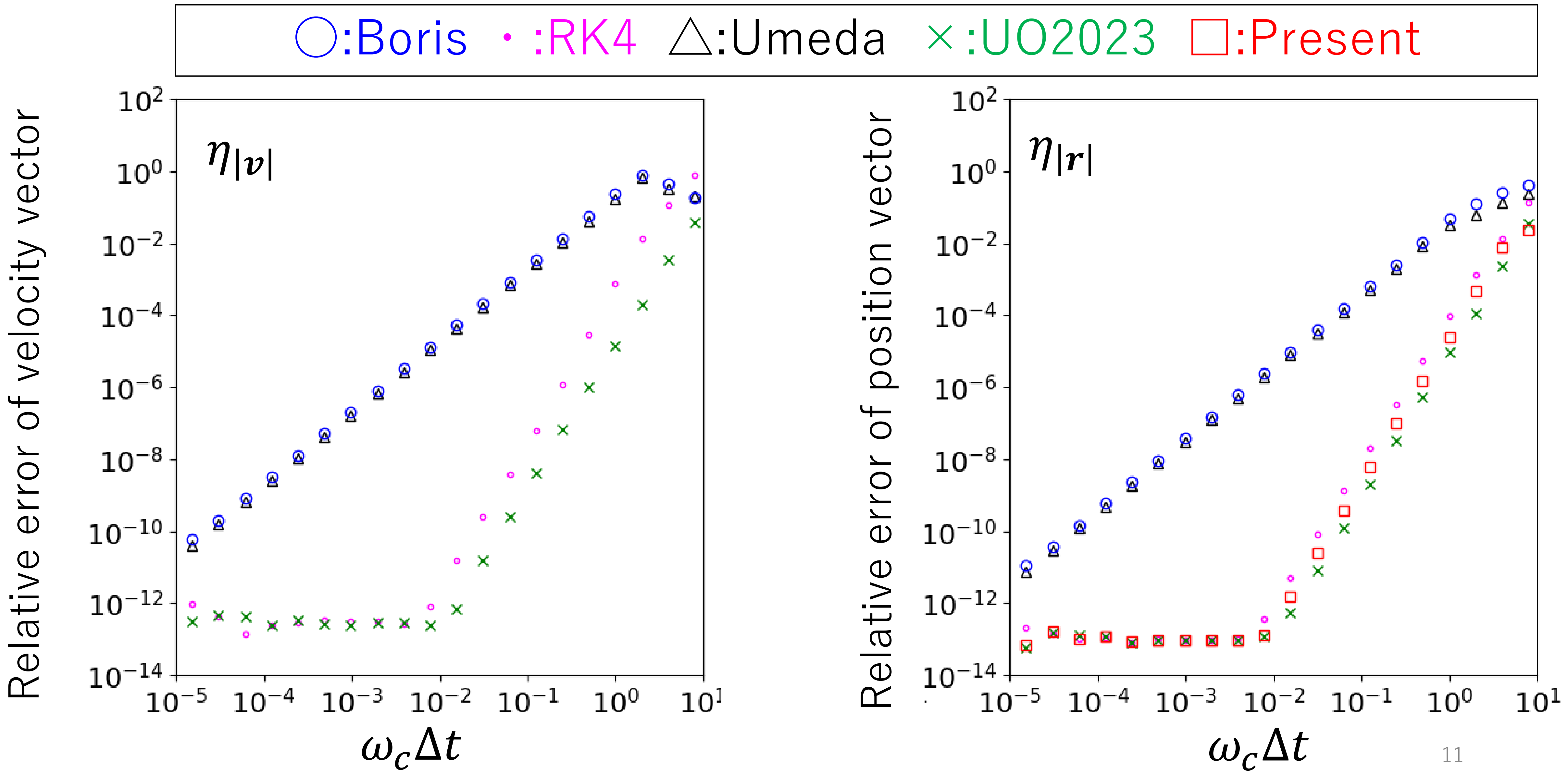
How:

- Multi-stepping based on the Taylor expansion

$$\boldsymbol{r}^{t+\Delta t} = \boldsymbol{r}^{t} + \Delta t \left.\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}\right|^{t+\frac{\Delta t}{2}} + \frac{\Delta t^3}{24}\left.\frac{\mathrm{d}^3\boldsymbol{r}}{\mathrm{d}t^3}\right|^{t+\frac{\Delta t}{2}} + \cdots = \boldsymbol{r}^{t} + \Delta t \boldsymbol{v}^{t+\frac{\Delta t}{2}} + \frac{\Delta t^3}{24}\left.\frac{\mathrm{d}^2\boldsymbol{v}}{\mathrm{d}t^2}\right|^{t+\frac{\Delta t}{2}} + O(\Delta t^5)$$

$$\boldsymbol{r}^{t+\Delta t} = \boldsymbol{r}^{t} + \frac{\Delta t}{2+\alpha}\left(\boldsymbol{v}^{t_+} + \alpha \boldsymbol{v}^{t+\frac{\Delta t}{2}} + \boldsymbol{v}^{t_-}\right) + O(\Delta t^5)$$

Comparison of Numerical Errors



Summary

- Runge (1895)-Kutta (1901) "RK4"
  - Fourth-order
  - Conservation of nothing
- Boris (1970), Vay (2008), Higuera-Cray (2017)
  - Second-order leap frog
  - Preservation of elliptical trajectory but with **wrong** guiding center
  - Energy conservation during gyration
- Present (Umeda 2023; Umeda & Ozaki 2023; in preparation)
  - Preservation of elliptical trajectory with **correct** guiding center
  - Energy conservation during gyration
  - Preservation of boosted Lorentz factor
  - Fourth-order leap frog

Do not use Boris (1970) with large $\omega_c \Delta t$(>0.01) or large γ.

Issues in computational performance:

- Multi-stepping (including) involves loading data (i.e., electromagnetic field on grids) from memory in each step.

⇒ Performance bottleneck in memory bandwidth

- Switching in three cases ($\gamma_E^2 > 1, \gamma_E^2 = \infty, \gamma_E^2 < 0$) is necessary.

$$\lim_{\gamma_E \to \infty} \gamma_E \sin\left(\frac{\omega_c \Delta t}{\gamma_E \gamma^t}\right) = \frac{\omega_c \Delta t}{\gamma^t}$$

$$\mathrm{i}\sqrt{-\gamma_E^2} \sin\left(\frac{\omega_c \Delta t}{\mathrm{i}\sqrt{-\gamma_E^2}\gamma^t}\right) = \sqrt{-\gamma_E^2} \sinh\left(\frac{\omega_c \Delta t}{\sqrt{-\gamma_E^2}\gamma^t}\right)$$

$$\lim_{\gamma_E \to \infty} \gamma_E^2 \left\{1 - \cos\left(\frac{\omega_c \Delta t}{\gamma_E \gamma^t}\right)\right\} = \frac{1}{2}\left(\frac{\omega_c \Delta t}{\gamma^t}\right)^2$$

$$\gamma_E^2 \left\{1 - \cos\left(\frac{\omega_c \Delta t}{\mathrm{i}\sqrt{-\gamma_E^2}\gamma^t}\right)\right\} = \gamma_E^2 \left\{1 - \cosh\left(\frac{\omega_c \Delta t}{\sqrt{-\gamma_E^2}\gamma^t}\right)\right\}$$

⇒An issue in high-performance implementation