1 Full orbit integrator in electromagnetic field

The equation of motion of a particle moving in an electromagnetic field is given by

$$\frac{d\mathbf{v}}{dt}=\frac{q}{m}[\mathbf{E}(\mathbf{x},t)+\mathbf{v}\times\mathbf{B}(\mathbf{x},t)]. \tag{1}$$

and

$$\frac{d\mathbf{x}}{dt}=\mathbf{v}, \tag{2}$$

where $\mathbf{x}$ and $\mathbf{v}$ are particles' location and velocity, respectively. If we desire a centered-difference scheme, then the most obvious choice is given by [1]

$$\frac{\mathbf{v}_{k+1/2}-\mathbf{v}_{k-1/2}}{\Delta t}=\frac{q}{m}\left[\mathbf{E}_k+\frac{\mathbf{v}_{k+1/2}+\mathbf{v}_{k-1/2}}{2}\times\mathbf{B}_k\right]. \tag{3}$$

for particle velocity and

$$\frac{\mathbf{x}_{k+1}-\mathbf{x}_k}{\Delta t}=\mathbf{v}_{k+1/2}, \tag{4}$$

for particle location, where $\mathbf{v}_{k+1/2}=\mathbf{v}(t_{k+1/2})$, $\mathbf{x}_k=\mathbf{x}(t_k)$, $\mathbf{E}_k=\mathbf{E}(\mathbf{x}_k,t_k)$, $\mathbf{B}_k=\mathbf{B}(\mathbf{x}_k,t_k)$, $t_k=k\Delta t$, $t_{k+1/2}=(k+1/2)\Delta t$. Note that we use "staggered" time grids for $\mathbf{v}$ and $\mathbf{x}$, i.e., time grids of $\mathbf{v}$ are at $t=(k+1/2)\Delta t$ while time grids of $\mathbf{x}$ are at $t=k\Delta t$. By using the staggered time grids, all quantities are evolved in a time-centered manner.
Further note that the scheme given in Eq (3) is in an implicit form because the unknown $\mathbf{v}_{k+1/2}$ appears on both sides of the equation. Fortunately, due to the linear dependence on $\mathbf{v}_{k+1/2}$, equation (3) can be analytically solved to give an explicit scheme. Rearrange Eq. (3) as

$$\mathbf{v}_{k+1/2}-\mathbf{v}_{k+1/2}\times\mathbf{B}_k\frac{q\Delta t}{2m}=\mathbf{v}_{k-1/2}+\mathbf{v}_{k-1/2}\times\mathbf{B}_k\frac{q\Delta t}{2m}+\mathbf{E}_k\frac{q\Delta t}{m}, \tag{5}$$

which is a linear 3×3 matrix equation for the three components of $\mathbf{v}_{k+1/2}$. In one version of my codes, I use Cramer's formula to express the explicit solution. [Hope that Cramer's formula is numerically accurate (e.g., no cancellation problem) and numerically efficient for the 3×3 system in question; the results I obtained look as good as that of the Boris algorithm discssed next.] The Boris algorithm is a smart way to obtain the solution, which seems to invlove less numerical computations (need checking) and may be more accurate compared with that given by Cramer's formula. First define $\mathbf{v}^-$ and $\mathbf{v}^+$ by

$$\mathbf{v}_{k-1/2}=\mathbf{v}^- -\frac{q\mathbf{E}_k}{m}\frac{\Delta t}{2}, \tag{6}$$

and

$$\mathbf{v}_{k+1/2}=\mathbf{v}^+ +\frac{q\mathbf{E}_k}{m}\frac{\Delta t}{2}. \tag{7}$$

Substitute the above equation into Eq. (3), we find that $\mathbf{E}_k$ is eliminated, giving

$$\frac{\mathbf{v}^+-\mathbf{v}^-}{\Delta t}=\frac{q}{2m}(\mathbf{v}^++\mathbf{v}^-)\times\mathbf{B}_k. \tag{8}$$

which can be written as

$$\mathbf{v}^+-\mathbf{v}^+\times\mathbf{B}_k\frac{q\Delta t}{2m}=\mathbf{v}^-+\mathbf{v}^-\times\mathbf{B}_k\frac{q\Delta t}{2m}. \tag{9}$$

It is easy to prove that Eq. (8) implies that $|\mathbf{v}^+|=|\mathbf{v}^-|$, i.e., $\mathbf{v}^+$ is a rotation of $\mathbf{v}^-$. Boris' smart way to explictly calculate the rotation to get $\mathbf{v}^+$ is to first calculate $\mathbf{v}'$ via

$$\mathbf{v}'=\mathbf{v}^-+\mathbf{v}^-\times\mathbf{t}, \tag{10}$$

where $\mathbf{t}=q\mathbf{B}_k\Delta t/(2m)$, and then calculate $\mathbf{v}^+$ via

$$\mathbf{v}^+=\mathbf{v}^-+\mathbf{v}'\times\mathbf{s}, \tag{11}$$

where $\mathbf{s}=2\mathbf{t}/(1+t^2)$. Equation (6), (7), (10), and (11) give an explict scheme for evloving $\mathbf{v}$. The steps to compute are: (1) use Eq. (6) to get $\mathbf{v}^-$ from the known $\mathbf{v}_{k-1/2}$, (2) then use Eqs. (10) and 11) to get $\mathbf{v}^+$ from $\mathbf{v}^-$, (3) and finally use Eq. (7) to get $\mathbf{v}_{k+1/2}$ from $\mathbf{v}^+$. This explicit scheme is often called the Boris algorithm.
My comments: An implicit scheme that can be analytically solved, giving an explicit scheme, is usually very powerfull because being implicit in essence makes it more stable/accurate while being explicit in form makes it efficient in computation. Also note that the scheme given in Eq (3) is not implicit in terms of the fields $\mathbf{E}$ and $\mathbf{B}$ since they are evaluated at t_k, which is not at a future time-step. An implicit scheme in terms of the field is often needed in the cases where there exists high-frequency field whose peroid is comparable or even smaller than the time-step used. The powerfulness of Boris' alorithm is not due to the smart way of expressing the explicit solution of the implicit scheme (as mentioned above, I can use the awkward Cramer's rule to get an explicit solution of similar accuracy and with similar computational overhead as Boris's). The powerfulness of Boris' algorithm is due to that it is based on an implicit scheme, which makes it prossess some good properties of an implicit scheme, e.g. conserving volume of the phase-space, as is disccussed in Ref. [8].

1.1 Renormalized equations of motion

Define

$$\bar{\mathbf{B}}=\frac{\mathbf{B}}{B_n},\bar{\mathbf{x}}=\frac{\mathbf{x}}{L_n},\bar{t}=\frac{t}{t_n},\bar{v}=\frac{v}{v_n},\bar{\mathbf{E}}=\frac{\mathbf{E}}{v_nB_n}, \tag{12}$$

where B_n and L_n can be arbitrarily chosen (I usually choose $B_n=1$Tesla and $L_n=1$meter in my code, i.e., use the S.I units for them), and t_n, and v_n are defined by

$$t_n=\frac{2\pi}{\Omega_n},\Omega_n=\frac{B_n|q|}{m},v_n=\frac{L_n}{t_n}. \tag{13}$$

Then the equations of motion are written

$$\frac{d\bar{\mathbf{x}}}{dt}=\bar{\mathbf{v}}, \tag{14}$$

$$\frac{d\bar{\mathbf{v}}}{d\bar{t}}=2\pi\frac{q}{|q|}[\bar{\mathbf{E}}(\mathbf{x})+\bar{\mathbf{v}}\times\bar{\mathbf{B}}(\mathbf{x})]. \tag{15}$$

In the normalized form, there is only one parameter for distinguishing particle species, namely the sign of particle's charge $q/|q|$. The other parameters for particle species enters via $\Omega_n=B_n|q|/m$.

1.2 Full orbit integrator in cylindrical coordinates

It is straightforwad to implement Boris algorithm in Cartesian coordinates. Cartesian coordinates are special in that its basis vectors are constant over the space. In cylindrical coordinates, the basis vectors are not constant over the space, of which we need to take care.
To implement Borsi algorithm in cylindrical coordinates, for each step from $t_{k-1/2}$ to $t_{k+1/2}$, we choose a static Cartesian coordinates with its origin identical to that of the cylindrical coordinates and with the basis vectors $(\hat{\mathbf{x}},\hat{\mathbf{y}},\hat{\mathbf{z}})$ being along the local basis vectors $(\mathbf{e}_{R,k},\mathbf{e}_{\phi,k},\mathbf{e}_{Z,k})$ of the cylindrical coordinates at the location of the particle at $t=t_k$. In the static Cartesian coordinators system $(\mathbf{e}_{R,k},\mathbf{e}_{\phi,k},\mathbf{e}_{Z,k})$, given $(v_{x,k-1/2},v_{y,k-1/2},v_{z,k-1/2})$, we can obtain $v_{x,k+1/2}$, $v_{y,k+1/2}$, and $v_{z,k+1/2}$ by using the Boris rotation, i.e.,

$$\begin{pmatrix}v_{x,k-1/2}\\v_{y,k-1/2}\\v_{z,k-1/2}\end{pmatrix}\rightarrow\begin{pmatrix}v_{x,k+1/2}\\v_{y,k+1/2}\\v_{z,k+1/2}\end{pmatrix}. \tag{16}$$

Note that here all the velocity components at $t_{k-1/2}$ and $t_{k+1/2}$ are defined with respect to the basis vectors $(\mathbf{e}_{R,k},\mathbf{e}_{\phi,k},\mathbf{e}_{Z,k})$. After obtaining $v_{x,k+1/2}$, $v_{y,k+1/2}$, and $v_{z,k+1/2}$, we compute the x_{k+1}, y_{k+1}, and z_{k+1} via

$$x_{k+1}=r_k+v_{x,k+1/2}\Delta t, \tag{17}$$

$$y_{k+1}=0+v_{y,k+1/2}\Delta t, \tag{18}$$

and

$$z_{k+1}=z_k+v_{z,k+1/2}\Delta t, \tag{19}$$

respectively. Then it is obvious that r_{k+1} is given by

$$r_{k+1}=\sqrt{x_{k+1}^2+y_{k+1}^2}, \tag{20}$$

and ϕ_{k+1} is given by

$$\phi_{k+1}=\phi_k+\alpha \tag{21}$$

where $\alpha=\mathrm{asin}(y_{k+1}/r_{k+1})$. Finally, to provide the information needed by the next Boris pushing, the velocity vector at $t_{k+1/2}$ are projected noto the new cylindrical basis vectors $(\mathbf{e}_{R,k+1},\mathbf{e}_{\phi,k+1},\mathbf{e}_{Z,k+1})$, to get the new componenst, $v_{R,k+1/2}$, $v_{\phi,k+1/2}$, $v_{Z,k+1/2}$, via

$$v_{R,k+1/2}=v_{x,k+1/2}\cos\alpha+v_{y,k+1/2}\sin\alpha. \tag{22}$$

$$v_{\phi,k+1/2}=-v_{x,k+1/2}\sin\alpha+v_{y,k+1/2}\cos\alpha, \tag{23}$$

The enssece of this method is that we work in Cartesian coordinates to advance the velocity and then project the velocity to the new cylindrical basis vectors at each step.

1.2.1 Initial backward half-step

Initial location and velocity of a particle are usually given at the same time $t=0$. For the staggered scheme to get started, we need to advance backward half-step to obtain the velocity at $t_{-1/2}$. All conventional schemes other than the staggered schemes can be used for this purpose. Since the time-step used in the Boris staggered scheme can be much larger than that used in the conventional scheme. Multiply-steps are usually needed in the conventional scheme to finish the backward half-step with a desried accuracy (this is important!).
Note that $v_{x,-1/2}$, $v_{y,-1/2}$, and $v_{Z,-1/2}$ needed in scheme (16) are the projections of the velocity on the basis vectors $(\mathbf{e}_{R,k=0},\mathbf{e}_{\phi,k=0},\mathbf{e}_{Z,k=0})$. Therefore, when backward advancing velcoity components from t_0 to $t_{-1/2}$, we are expected to use constant vector basises $(\mathbf{e}_{R,k=0},\mathbf{e}_{\phi,k=0},\mathbf{e}_{Z,k=0})$ and all the velocity compoents are projections of velocity on these constant basis vectors. Therefore we are actually working in Cartesian coordinates (i.e., constant basis vectors) to advance the velocity components from t_0 to $t_{-1/2}$. An obscure way[3] to express this is to say we should use equations of motion in cylindrical coordinates but with the inertial terms being dropped, namely droping the v_ϕ^2/R and $-v_Rv_\phi/R$ terms in Eqs. (295) and (296) with the obvious corresponce $(v_x,v_y,v_Z)\rightarrow(v_R,v_\phi,v_Z)$.

1.3 Equation of motion in Cylindrical coordinates

It is straightforward to derive the equation of motion in cylindrical coordinates (refer to my notes on analytical classic dynameics):

$$\frac{dR}{dt}=v_R \tag{24}$$

$$\frac{d\phi}{dt}=\frac{v_\phi}{R}. \tag{25}$$

$$\frac{dZ}{dt}=v_Z \tag{26}$$

$$\frac{dv_R}{dt}=\frac{q_\alpha}{m}(E_R+v_\phi B_Z-v_ZB_\phi)+\frac{v_\phi^2}{R} \tag{27}$$

$$\frac{dv_\phi}{dt}=\frac{q_\alpha}{m}(E_\phi+v_ZB_R-v_RB_z)-\frac{v_Rv_\phi}{R} \tag{28}$$

$$\frac{dv_Z}{dt}=\frac{q_\alpha}{m}(E_Z+v_RB_\phi-v_\phi B_R) \tag{29}$$

The last term in Eq. (27) is the centripetal term, and the last term in Eq. (28) is the Coriolis term. If we apply the same ideas as that of Eq. (3) in this system of equations (i.e., the velocity components on the right-hand side are approximated by an average, e.g., $(v_{\phi,k-1/2}+v_{\phi,k+1/2})/2$), the velocity components at $t_{k+1/2}$ can not be easily solved analytically in terms of those at $t_{k-1/2}$ because the dependence of the right-hand side on velocity is nonlinear. Therefore an explicit scheme can not be easily obtained, i.e., a Boris scheme directly in cylindrical coordinates is not ready to obtain.

1.4 Transform guiding-center variables to particle variables

Given guiding-center coordinates $(\mathbf{X},\mu,v_\parallel)$, we are asked to determine the corresponding particle coordinates $(\mathbf{x},\mathbf{v})$ in the cylindrical coordinates, namely $(R,\phi,Z,v_R,v_\phi,v_Z)$. To fully determine these coordinates, the gyro-phase α needs to be specified. Assume that we are asked to determine an arbitary point on the gyro-ring. Then we have the freedom of choosing a gyro-phase that can make the calculation easier. Here I choose the gyro-phase for which $v_R=0$. Then (v_R,v_ϕ,v_Z) satisfy the following three equations:

$$\begin{cases}v_R=0\\v_\phi B_\phi+v_ZB_Z=Bv_\parallel\\v_\phi^2+v_Z^2=\dfrac{2B\mu}{m}+v_\parallel^2\end{cases} \tag{30}$$

The above equilibrium magnetic field is evaluated at the particle position. However, the difference between the equilibrium magnetic field at the guiding-center position and particle position is small and hence can be neglected. Therefore B, B_ϕ, B_Z can be evaluated at the guiding-center location, whose value is known (If we want to be more accurate, we can plug the value of particle position computed later back to these equations, and this can be done once or be iterated for several times). The second equation is written as

$$v_\phi=\frac{Bv_\parallel-v_ZB_Z}{B_\phi}. \tag{31}$$

Plugging this expression into the third equation, we obtain an equation for v_Z:

$$\left(\frac{Bv_\parallel-v_ZB_Z}{B_\phi}\right)^2+v_Z^2=\frac{2B\mu}{m}+v_\parallel^2, \tag{32}$$

$$\Longrightarrow\left[\left(\frac{B_Z}{B_\phi}\right)^2+1\right]v_Z^2-\left(2\frac{BB_Z}{B_\phi^2}v_\parallel\right)v_Z+\left(\frac{Bv_\parallel}{B_\phi}\right)^2-\frac{2B\mu}{m}-v_\parallel^2=0, \tag{33}$$

which is a quadratic equations for v_Z, for which there are two roots. It is ready to verify that one of the root is postive and the other is negative (this is obvious in the limit that $B_R=B_Z=0$ and thus $B=|B_\phi|$). It is also physically obvious that there should be two roots with opposite signs. Choosing any of the two roots works for our purpose. After (v_R,v_ϕ,v_Z) are determined, we can use the following equation

$$\mathbf{x}_{n+1}=\mathbf{X}-\mathbf{v}\times\frac{\mathbf{e}_\parallel(\mathbf{x}_n)}{\Omega(\mathbf{x}_n)}. \tag{34}$$

as an iteration scheme to compute $\mathbf{x}$ with the initial guess chosen as $\mathbf{x}_0=\mathbf{X}$. The iteration can usually be terminated after one iteration, giving enough accurate result. The cross product can be done in local Cartesian coordinates. The resulting displacements in the Cartesian basis are then used to calculat the corresponding displacement in R,ϕ,Z coordinates. Specificly,

$$R=R_g+\Delta x \tag{35}$$

$$Z=Z_g+\Delta z \tag{36}$$

$$\phi=\phi_g+\mathrm{asin}\left(\frac{\Delta y}{R}\right) \tag{37}$$

where, (R_g,ϕ_g,Z_g) are the cylindrical coordinates of the guiding-center, Δx, Δy, and Δz are three Cartesian components of $\left(-\mathbf{v}\times\frac{\mathbf{e}_\parallel(\mathbf{x}_n)}{\Omega(\mathbf{x}_n)}\right)$.

1.5 Transform particle variables to guiding-center variables

$$\mathbf{X}=\mathbf{x}+\mathbf{v}\times\frac{\mathbf{e}_\parallel(\mathbf{x})}{\Omega(\mathbf{x})}, \tag{38}$$

$$\Rightarrow\mathbf{X}=\mathbf{x}+\frac{m}{B^2q}\mathbf{v}\times\mathbf{B}, \tag{39}$$

The $\mathbf{v}\times\mathbf{B}$ term can be written as

$$\mathbf{v}\times\mathbf{B}=\begin{vmatrix}\mathbf{e}_R&\mathbf{e}_\phi&\mathbf{e}_Z\\v_R&v_\phi&v_Z\\B_R&B_\phi&B_z\end{vmatrix}=\mathbf{e}_R(v_\phi B_Z-v_ZB_\phi)+\mathbf{e}_\phi(v_ZB_R-v_RB_Z)+\mathbf{e}_Z(v_RB_\phi-v_\phi B_R). \tag{40}$$

Then the cylindrical coordinates of the guiding-center position, (R_g,ϕ_g,Z_g) is written as

$$R_g=\sqrt{\left[R+\frac{m}{B^2q}(v_\phi B_Z-v_ZB_\phi)\right]^2+\left[\frac{m}{B^2q}(v_ZB_R-v_RB_Z)\right]^2}, \tag{41}$$

$$\phi_g=\phi+\mathrm{asin}\left(\frac{m}{B^2q}(v_ZB_R-v_RB_Z)\frac{1}{R_g}\right), \tag{42}$$

$$Z_g=Z+\frac{m}{B^2q}(v_RB_\phi-v_\phi B_R), \tag{43}$$

where the range of the asin function is $[-\pi/2:\pi/2]$.

1.6 Numerical examples

Figure 44 compares the full orbits calculated by the Boris algorithm and that calculated by the 4th Runge-Kutta scheme. The results indicate that the Boris scheme gives more accurate orbits than the 4th Runge-Kutta.

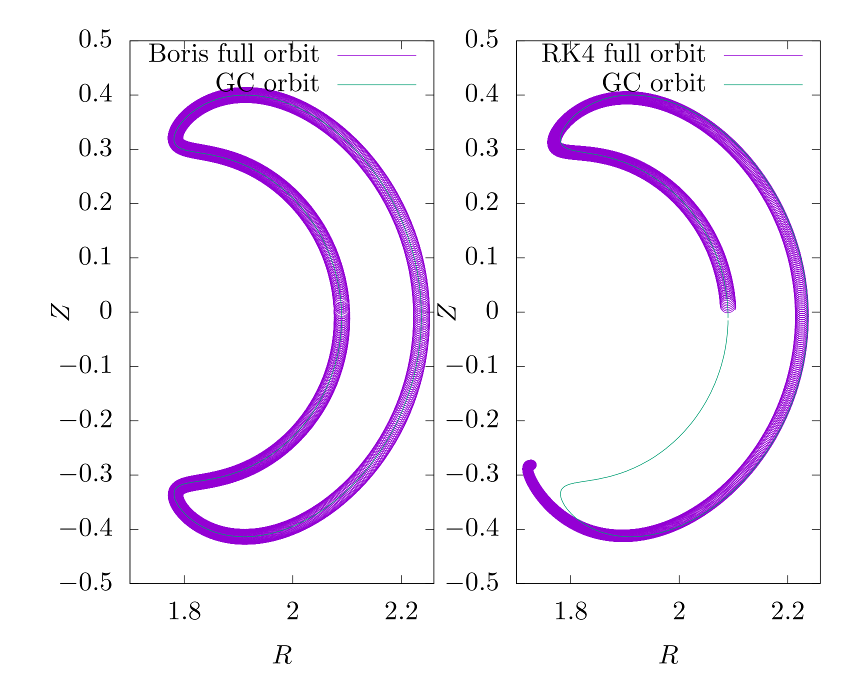

Figure 1. Comparison of the the full orbits calculated by the Boris' algorithm and that calculated by the 4th Runge-Kutta scheme. The time step is chosen as $\Delta t=T/20$, where T is the gyro-period at the initial location. The orbits are advanced by 29000 time-steps, in which Boris' orbit finishes one poloidal banana period. Also plotted on the figure is the guiding-center orbit calculated by directly integrating the guiding-center drift. The results show that the Boris orbit follows the guiding-center orbit while the Runge-Kutta orbit significantly deviates from the guiding-center orbit, which indicates that it is inaccurate. The period given by the 4th Runge-Kutta scheme also significantly deviates from the correct value.
The magnetic configuration is from EAST#59954@3.03s (gfile: g059954.003030 provided by HaoBaoLong). The initial location of the particle (Deuteron) is at ($R=2.1m$, $Z=0m$, $\phi=0$). The initial velocity is given by $v_R=v_Z=1.0\times10^6m/s$, and $v_\phi=5\times10^5m/s$. The initial location of the guiding-center are calculated using the initial conditions of the particle.

As is shown in Fig. 1, the Runge-Kutta method gives less accurate full orbit than Borris scheme. One of the reasons responsible for the inaccuracy is that Runge-Kutta scheme has stronger dissipation than the time-centered Borsis scheme. Figure 45 compares the evolutions of the kinetic energy given by the Runge-Kutta and Boris schemes, which indicates the kinetic energy conservation of Runge-Kutta is not as good as that of Boris.

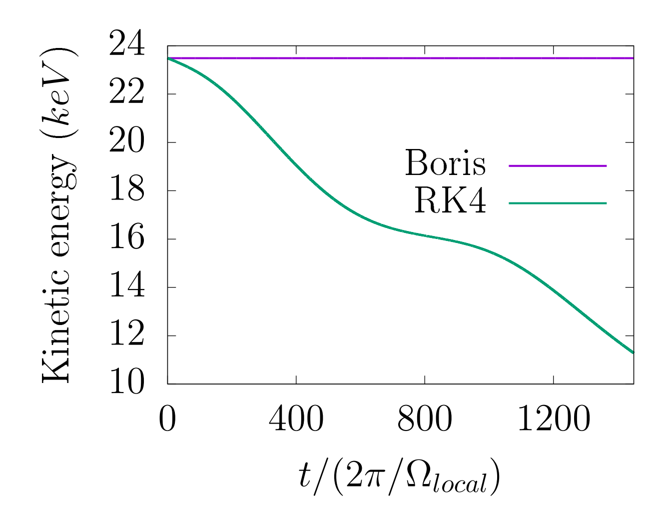

Figure 2. Comparison of the time evolutions of kinetic energy given by the 4th Runge-Kutta and the Boris schemes, where Ω_{local} is the gyro-angular-frequency at the initial particle location. The other parameters are the same as those of Fig. 1. The results show that the Runge-Kutta scheme has stronger dissipation than the Borsis scheme.

The time-centered Boris scheme can reproduce correct drift motion even when using large time-step that is comparable with the gyro-period. Figure 46 shows examples of drift-orbit calculated by the Boris scheme with large time-steps.

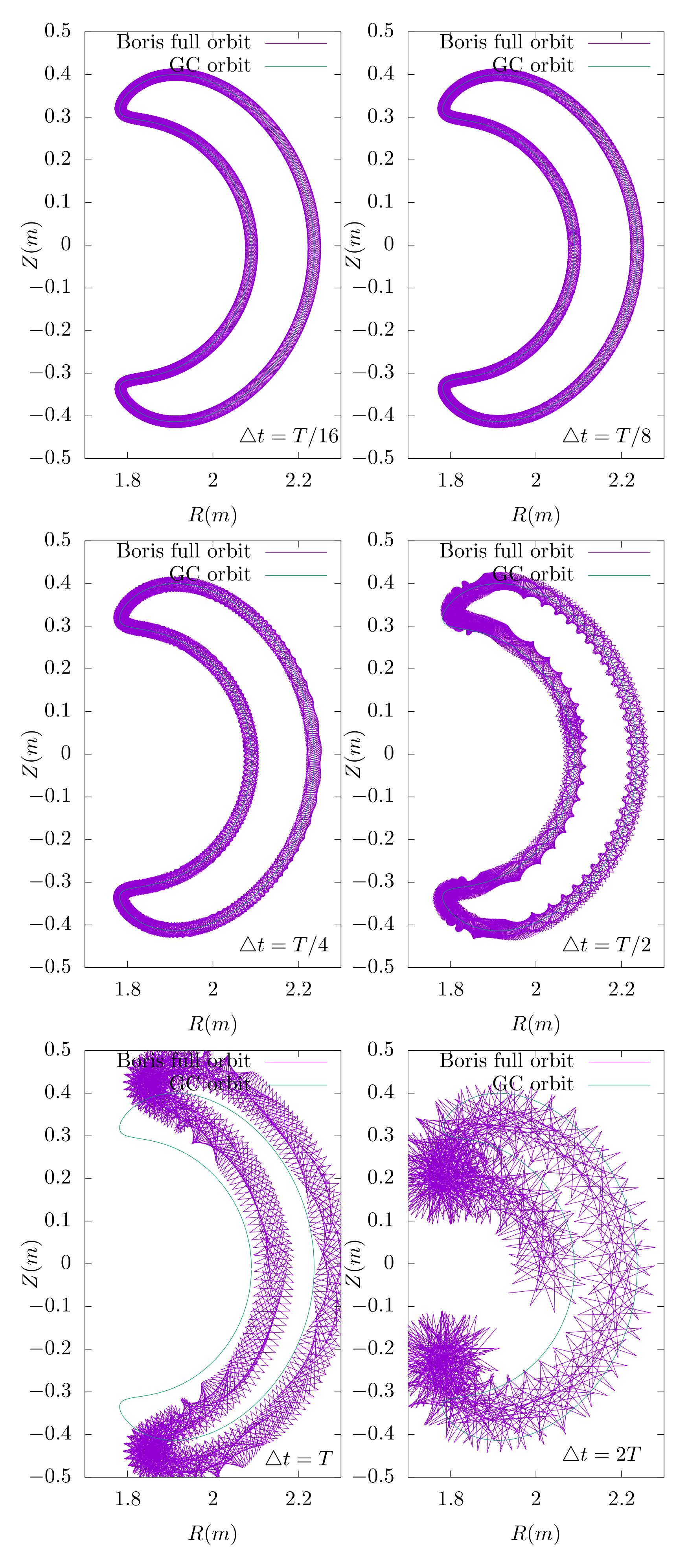

Figure 3. Comparison between the full orbits calculated by Boris' algorithm with differnt time-steps $\Delta t=T/16$, $\Delta t=T/8$, $\Delta t=T/4$, $\Delta t=T/2$, $\Delta t=T$, $\Delta t=2T$, where T is the gyro-period of the particle (Deuteron) at its initial location ($R=2.1m$, $Z=0m$, $\phi=0$). The results show that the full orbits agrees with the guiding-center orbit for the cases with time-step $\Delta t\leqslant T/2$. When Δt is further increased, the full orbits obtained deviate from the guiding-center orbit. Further note that the gyroradius obtained remains nearly the same when the time-step $\Delta t\leqslant T/2$. When Δt is further increased, the gyroradius becomes larger than the correct value. As to the gyrophase, intuitively it seems to be hard to preserve the gyrophase with a time step comparable to the gyro-period.
The magnetic configuration is from EAST#59954@3.03s (EFIT gfile: g059954.003030 provided by HaoBaoLong). The initial velocity is given by $v_R=v_Z=1.0\times10^6m/s$, and $v_\phi=5\times10^5m/s$, which coresponds to a kinetic energy of 23keV. For $\Delta t=T/16$, the orbit is advanced by 23250 time-steps, in which the particle finishes one banana period.

1.7 Double-Boris scheme

The "staggered" time-centered-difference scheme given by Eqs. (3) and (4) is of 2nd order accuracy. Note that this scheme involves only one force evaluation per step while typical 2nd-order-accurate methods (e.g., 2nd Ruger-Kutta scheme) usually involves two force evalutions per step. The reason for this difference is as follows. The 2nd Ruger-Kutta scheme obtain the veloicty and location at both t_k and $t_{k+1/2}$ while the Boris scheme do not obtain the velocity at t_k and location at $t_{k+1/2}$. For the Boris scheme to obtain the lacking information, an additional Boris scheme that begins with $\mathbf{v}_k$ and $\mathbf{r}_{k+1/2}$ can be used, which involves one additional force evaluation, making the total number of force evaluation be also two, the same as the typical 2nd-order-accurate methods. Figure 47 illustrates the combinition of two Boris schemes giving the full information of orbits.

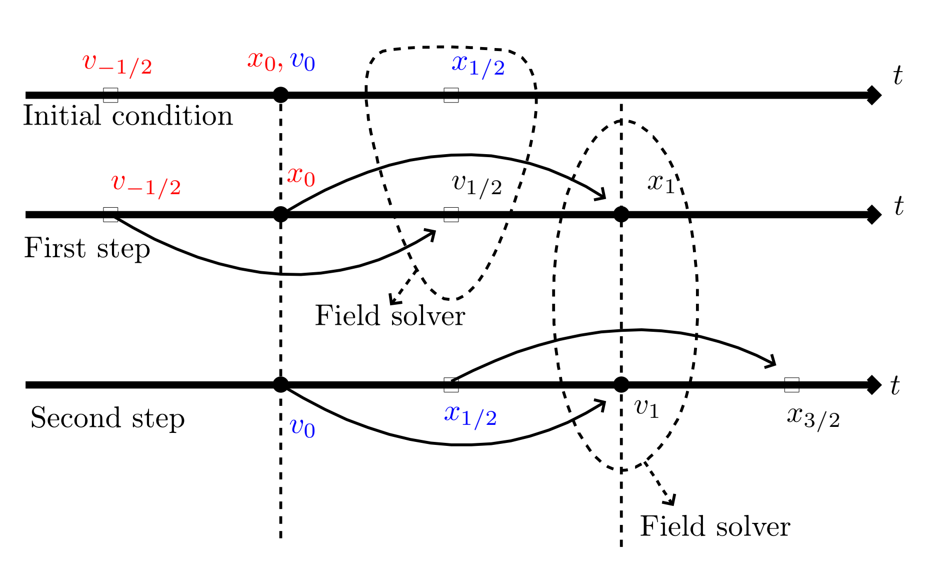

Figure 4. Double-Boris full orbit pusher. Given initial condition (x_0,v_0), the velocity is push backward half-step to get $v_{-1/2}$ and the location is push forward half-step to get $x_{1/2}$ by using a non-staggered scheme. Then the first Boris-pusher uses $(v_{-1/2},x_0)$ as its initial conditions and the second Boris-pusher uses $(v_0,x_{1/2})$ as its initial conditions.

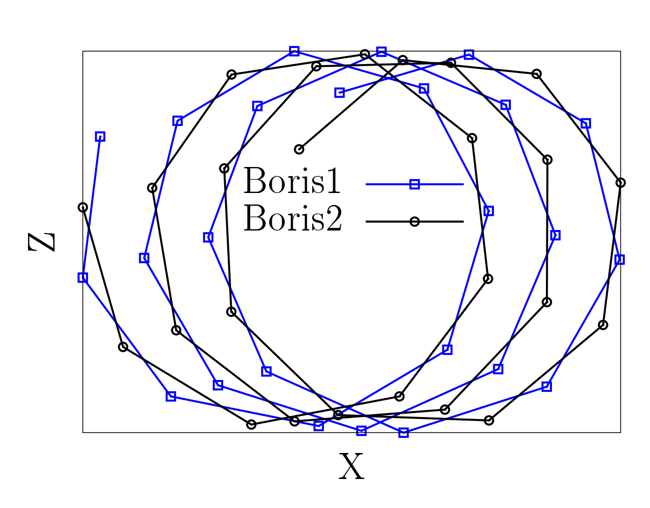

Figure 5. Drift cyclotron motion calculated by two Boris schemes (one is started from $(\mathbf{v}_{-1/2},\mathbf{x}_0)$ and another started from $(\mathbf{v}_0,\mathbf{x}_{1/2})$) with about 8 time-steps per cyclotron-period.