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A GUIDING CENTRE APPROXIMATION APPROACH FOR SIMULATION ELECTRON TRAJECTORIES IN ECR AND MICROWAVE ION SOURCES*

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Abstract

The present work presents a study on the feasibility of the implementation of the guiding centre (GC) approach in electron cyclotron resonance (ECR) ion sources, with the goal of speeding up the electron's orbit integration in certain regimes. The GC algorithm is compared with the Boris method which is commonly used in plasma simulations. It is shown that the GC approximation reproduces accurately the trajectory drifts and periodic behaviour of electrons in a minimum-B field with magnetic field gradients as high as 40 T/m. A typical confined electron orbit far enough from the source's axis is well reproduced for 1 μs of propagation time, with the GC time-step constrained below 100 ps, providing one order of magnitude gain in computation time with respect to the Boris method. For a confined electron orbit close to the axis a coming out of phase of the electron's trajectory is observed, but the spatial envelope is conserved. A comparative study analyses non-confined electron trajectories in a flatter B-field, that in a microwave discharge ion source, where this method's drawbacks may be avoided given a smaller magnetic field gradient and a shorter electron lifetime in the plasma chamber. In this regime electron trajectories were very well reproduced by the GC approximation. The time-step was constrained below 10 ns, providing up to 30 times faster integration compared to Boris.

INTRODUCTION

The numerical simulation of charged particle trajectories is of interest to model the plasma features of ion sources. The explicit Boris algorithm has become the standard for particle trajectory integration in a magnetic field. The high frequency electron cyclotron motion, in the GHz range, common in ion sources, constrains the time-step below 10 ps, which yields to a longer computation time when such small steps in time are required.

A guiding centre approach neglects the detailed particle's cyclotron motion, describing its trajectory through free motion of the centre of mass along the magnetic field lines and corresponding drifts. This approach is more computationally expensive per step than direct trajectory integration (Boris), a shorter overall computation time may be expected by using a larger time-step (~100 ps).

In this study we investigate the feasibility of using the guiding centre approximation for propagating electrons in ion sources. This was done by developing two otherwise identical algorithms in order to compare the resulting electron mean paths given by the guiding centre approximation and the Boris algorithm.

TRAJECTORY INTEGRATION

Two methods for trajectory integration are investigated, namely the Boris algorithm, as a control, and a guiding centre approximation, whose applicability is the focus of this study.

The Boris Algorithm

The Boris method [1] for particle push is an explicit second order scheme and is the standard used for magnetised plasma simulation. That makes it very stable for long term simulations, property usually associated with symplectic algorithms which is the preservation of the phase space volume. This results on an upper bound to the error in the energy and other dynamic properties of the system. Another reason why the Boris algorithm is so widely used is that it conserves the energy indefinitely in the absence of an electric field or collisions.

The Guiding Centre Approximation

One can divide the motion of the charged particle into the cyclotron motion around the magnetic field lines and the motion of the centre of gyration, the guiding centre (GC). [2] The motion can be described by a guiding centre approximation under the condition that the magnetic field gradient varies in a much larger length-scale compared to the Larmor radius, $\rho \ll B/|\nabla B|$, or written differently:

$$\frac{B}{\rho|\nabla B|} \gg 1 \tag{1}$$

This rends the magnetic moment (μ) an adiabatic invariant. [3] From the covariant equation of motion for the GC, neglecting higher order terms and temporal derivatives, under the assumption that the fields vary slowly with time when compared to the variation due to the particle's movement, one can write the following equations for the GC dynamics: [4]

$$\begin{aligned}\frac{d\mathbf{R}}{dt} = v_{\parallel}\hat{\mathbf{b}} - \frac{\hat{\mathbf{b}}\times\mathbf{E}}{B} + \frac{\hat{\mathbf{b}}}{B\left(1-\frac{E_{\perp}^2}{B^2}\right)} \\ \times\left\{\frac{m\gamma}{q}\left(v_{\parallel}^2(\hat{\mathbf{b}}\cdot\nabla)\hat{\mathbf{b}} + v_{\parallel}(\mathbf{u}\cdot\nabla)\hat{\mathbf{b}}\right.\right. \\ + v_{\parallel}(\hat{\mathbf{b}}\cdot\nabla)\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}) \\ \left.\left. + \frac{\mu}{\gamma q}\nabla\left[B\left(1-\frac{E_{\perp}^2}{B^2}\right)^{1/2}\right] + \frac{v_{\parallel}E_{\parallel}}{c^2}\mathbf{u}\right\}\end{aligned} \tag{2}$$

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$$\frac{d(\gamma v_\parallel)}{dt} = \gamma \boldsymbol{u} \cdot \left(v_\parallel (\hat{\boldsymbol{b}} \cdot \nabla)\hat{\boldsymbol{b}} + (\boldsymbol{u} \cdot \nabla)\hat{\boldsymbol{b}}\right) + \frac{q}{m} E_\parallel \quad (3)$$
$$- \frac{\mu}{\gamma m} \hat{b} \cdot \nabla \left[B \left(1 - \frac{E_\perp^2}{B^2} \right)^{1/2} \right]$$

$$\frac{d\left(m\gamma^{*2} v_\perp^{*2}/(2B^*)\right)}{dt} = \frac{d\mu^*}{dt} = 0 \quad (4)$$

$$\boldsymbol{u} = \boldsymbol{E} \times \frac{\hat{\boldsymbol{b}}}{B} \quad (5)$$

An asterisk (*) as upper index in the above equations denotes the quantities in the reference frame moving at the cross fields drift velocity (u), eq. (5).

Equations 2 and 3 were integrated using a fixed time-step (dt) RK4 method. [5] All numerical derivatives were computed at fourth order. The magnetic field gradient was mapped beforehand, in order to avoid having to compute it at each step, thus speeding up the simulation.

ION SOURCES

Two different kinds of ion sources were studied, an ECR ion source, such as PHOENIX V2, and a microwave discharge model, exemplified by the SILHI@GANIL ion source. These ion source designs vary considerably in terms of magnetic field topology and typical electron energy distributions of their corresponding plasmas.

The PHOENIX V2 Ion Source

This compact ECRIS was developed at LPSC and commissioned for the SPIRAL 2 accelerator at GANIL. It operates at 18 GHz microwave frequency and has a cylindrical plasma chamber with a volume of 0.6 L (204 mm long, 63 mm diameter). [6]

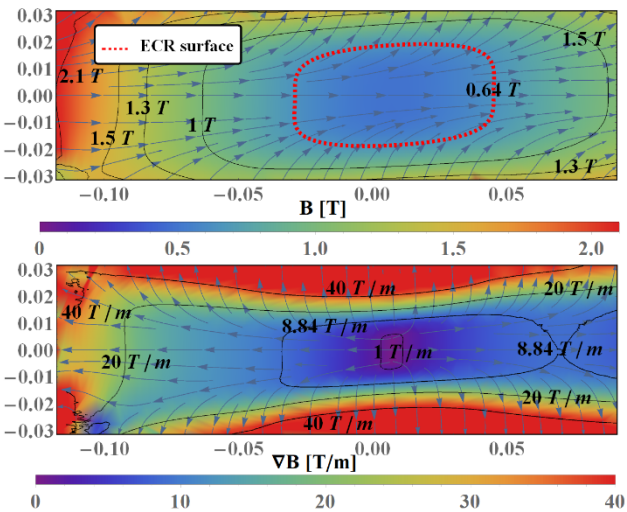

Figure 1: Magnetic field (top) and its gradient (bottom) in a longitudinal cut of PHOENIX V2's plasma chamber. The 18 GHz ECR zone is indicated with a dashed red line.

The magnetic field of PHOENIX V2 (Fig. 1) has 2.1 T at the injection wall, 1.3 T at extraction and a radially confining field strength of 1.35 T. The associated magnetic field gradient is as high as 40 T/m. We also see that for this field geometry the relationship between the field and its gradient is mostly direct, relevant for the validity condition for the GC approximation.

The SILHI@GANIL Ion Source

This Microwave Discharge Ion Source was developed at CEA-Saclay and designed to output a constant high intensity beam of protons or deuteron. As it's typical of this kind of ion sources, it operates with a 2.45 GHz microwave frequency. Its plasma chamber volume is of 0.64 L (100 mm long, 90 mm diameter). [7]

SILHI's magnetic field is produced by three permanent magnet rings located around the plasma chamber (Fig. 2). The maximum field strength is ~0.1 T, which can provide a magnetic mirror for electrons moving towards the extraction wall from the resonance surface. In the absence of other interactions, which are not considered in the present study, electrons undergo at maximum one bounce.

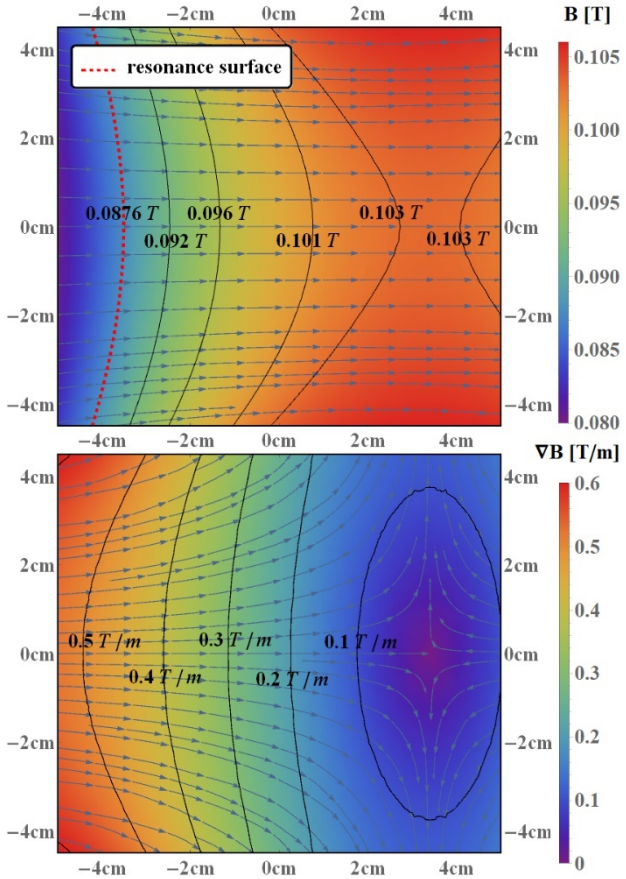

Figure 2: Magnetic field (top) and its gradient (bottom) in a longitudinal cut of SILHI's plasma chamber.

Comparing the magnitude of the field's gradient (Figs. 1 and 2), the one of SILHI is considerably smaller, (0.5 T/m with respect to 40 T/m for PHOENIX V2), pointing to a greater validity of the GC approximation. With this geometry the gradient and field magnitude are inversely related.

Table 1 further suggests that the assumptions made for the GC approximation (see eq. 1) are fulfilled better in the regime given by a microwave resonance ion source, with a typical energy of the order of a few eV and a flatter magnetic field. It also suggests that we would expect the GC

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approximation to be useful for electron energies smaller than 10 keV for either source. The Appendix shows the typical evolutions of the validity ratio (eq.1) *vs* time.

Table 1: GC Approximation Validity Ratio, $(B/|\nabla B|)/\rho$, for PHOENIX V2 (near ECR region) and SILHI (near plasma chamber centre) Ion Sources by Electron Kinetic Energy

$E_{kinetic}$	PHOENIX V2	SILHI@GANIL
1 eV	7792	17813
10 eV	2464	5633
100 eV	779	1781
1 keV	246	563
10 keV	78	177
100 keV	24	54
1 MeV	6	13

RESULTS

ECRIS – PHOENIX V2

One kind of typical orbit in an ECRIS is that of confined electrons reasonably Far From the plasma chamber Axis (FFA). This kind of trajectories present bouncing along the longitudinal direction and a precession around the axis.

The electron's energy is physically conserved as no heating is considered in this study. Using a time-step (*dt*) of 1, 10 and 100 ps for the GC algorithm we see that for 1 µs of propagation, this is roughly the case, the overall energy variation is less than 0.1% from the initial value (Fig. 3).

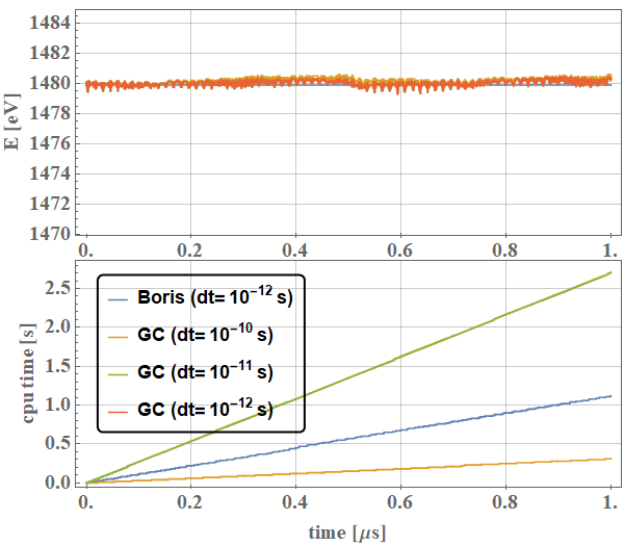

Figure 3: Electron energy (top) and computation time *vs* propagation time for a typical FFA orbit with varied dt.

In terms of computation time, GC was found to be around 20 times more expensive as for Boris' method. A time gain can then be achieved by using a *dt* two orders of magnitude larger (Fig. 3). This gain comes without a noticeable loss of accuracy for this propagation time (Figs. 4 and 5). The simulated GC trajectories agree with Boris' for the valid *dt*. At a *dt* of 1000 ps the GC approximation breaks, shown by diverging residuals (Fig. 5).

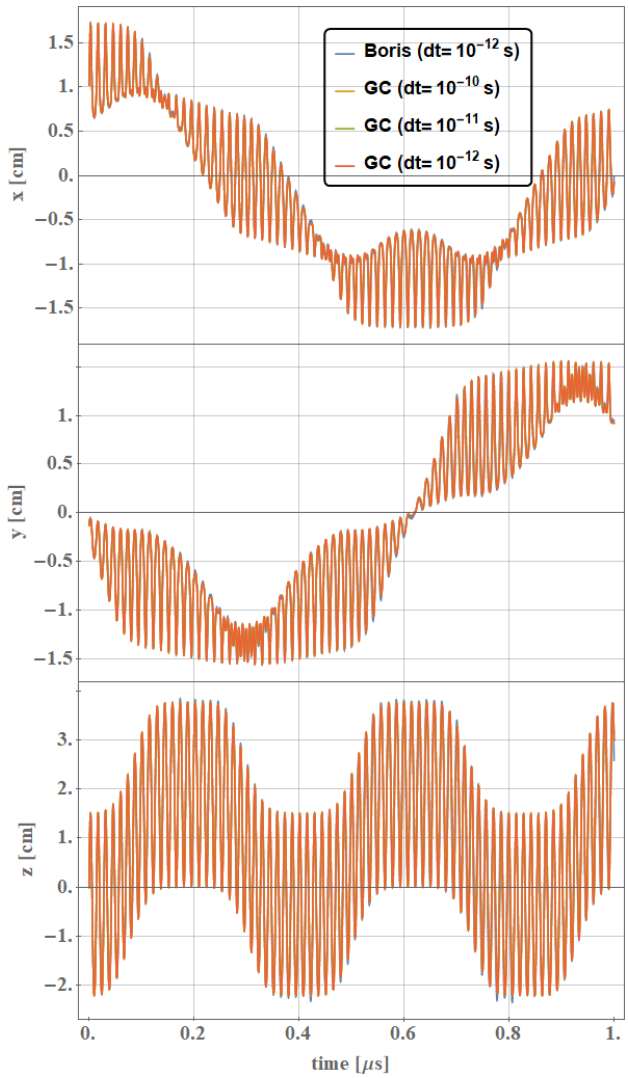

Figure 4: Typical FFA trajectory coordinates. Transversal coordinates x and y and longitudinal coordinate z.

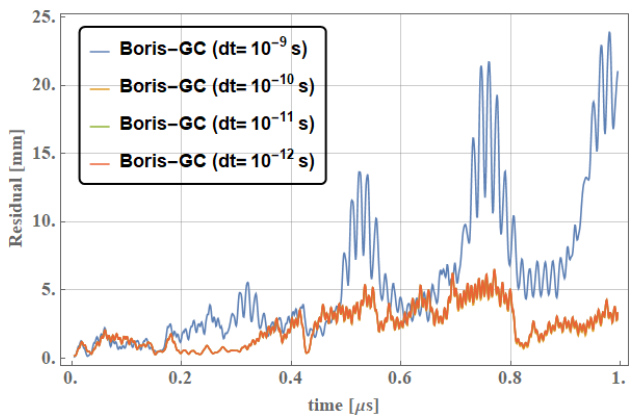

Figure 5: FFA, absolute difference (residual) between simultaneous points during propagation of Boris' and GC.

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Another case to consider is that of confined electron Close To the chamber's Axis (CTA). Here we see that the GC and Boris' orbits fall out of phase, but the spatial envelopes remain consistent (Figs. 4 and 6). The residuals (Fig. 7) confirm this observation, but show that the confined trajectories periodically come to agreement, ~1 mm distance. The electron's energy remains practically constant during propagation (Fig. 8). Given that the proposed use case for this algorithm involves a large number of test particles, for very few collisions (very low pressure), this inaccuracy could be averaged out.

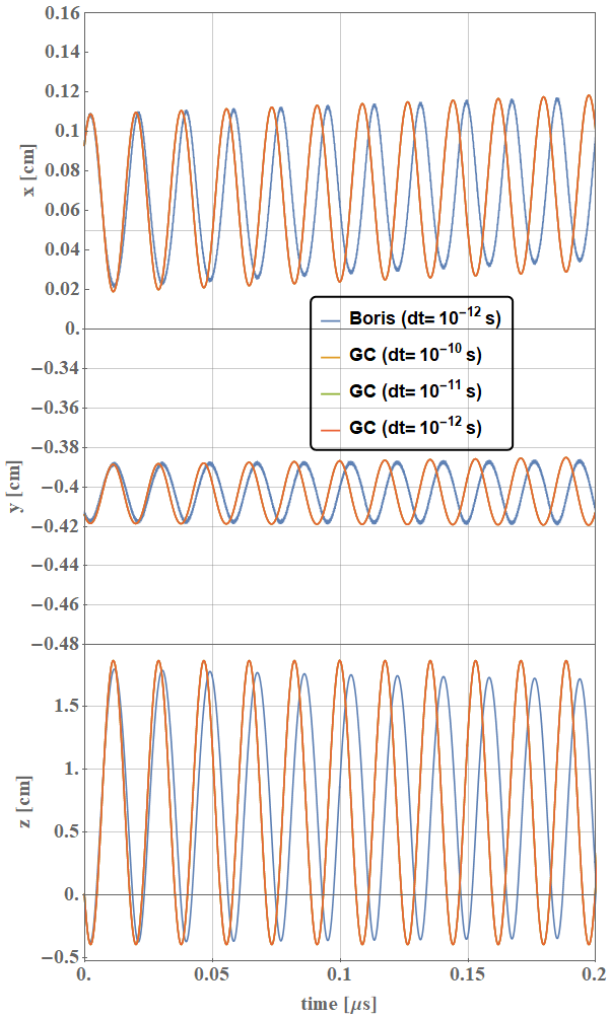

Figure 6: Typical CTA coordinates, for 0.2 µs.

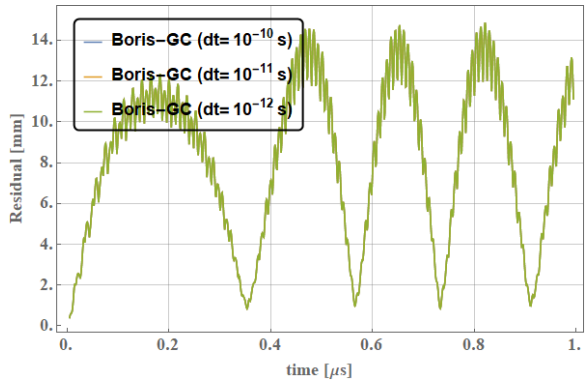

Figure 7: CTA, absolute difference between simultaneous points during propagation of Boris and GC electrons.

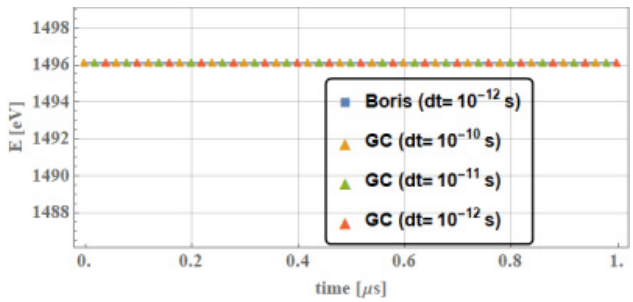

Figure 8: Electron energy *vs* propagation time for a typical CTA orbit with varied *dt*.

Microwave Discharge Ion Source – SILHI

A selected orbit with one bounce in the SILHI ion source shows great coincidence between Boris and GC propagated electrons (Fig. 9). This kind of trajectory was chosen as it represents the most challenging case, excluding higher energy (~100 eV) electrons. A *dt* value of up to 1000 times that of Boris' method still provides good agreement between Boris' and GC orbits.

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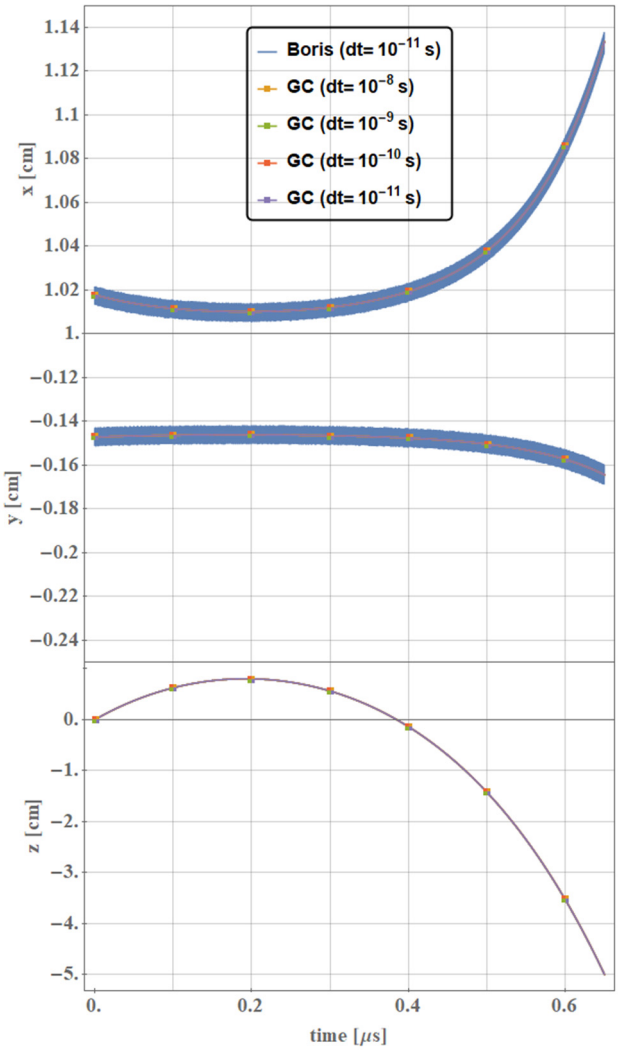

Figure 9: Typical SILHI one bounce electron trajectory coordinates as function of time.

In this case the energy is conserved in the relevant scale for all propagation algorithms, which indicates that the GC approximation's assumption is completely valid in this regime (Fig. 10). With this source's characteristics the GC algorithm was also found to be around 25 times as expensive as Boris, with a time gain obtained from 100 times the *dt* used for Boris: 10 ps (Fig. 11). Using a 10 ns *dt* for the GC provides an almost instantaneous computation, ~30 times faster compared to Boris, and good orbit agreement; however, using such a large *dt* would limit time resolution, therefore its viability depends on the use case.

The residuals show that in this regime (~1eV, SILHI) the GC algorithm breaks at a *dt* = 100 ns, providing an upper usability limit. Good agreement obtained for all smaller *dt* considered (Fig.12).

CONCLUSIONS

The GC algorithm can accurately reproduce electron trajectories in the domain of both studied ion sources and regimes: (i) for the PHOENIX V2 ECRIS being a ~1 T magnetic field and around ~1 keV of electron kinetic energy, and (ii) for the SILHI ion source a lower 0.1 T magnetic field and ~1 eV electron kinetic energy.

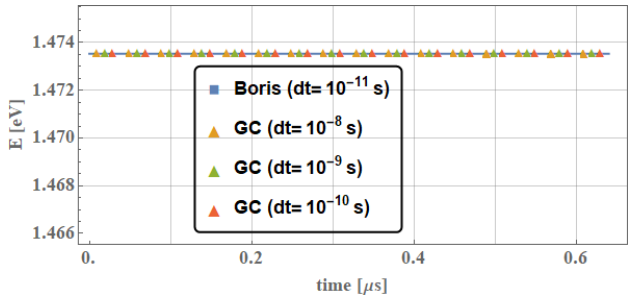

Figure 10: Electron energy *vs* propagation time for a one bounce orbit with varied *dt*.

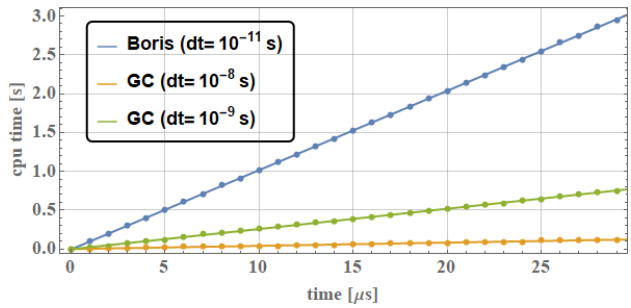

Figure 11: Computation time *vs* propagation time for a 100 sequentially integrated trajectories with varied *dt*.

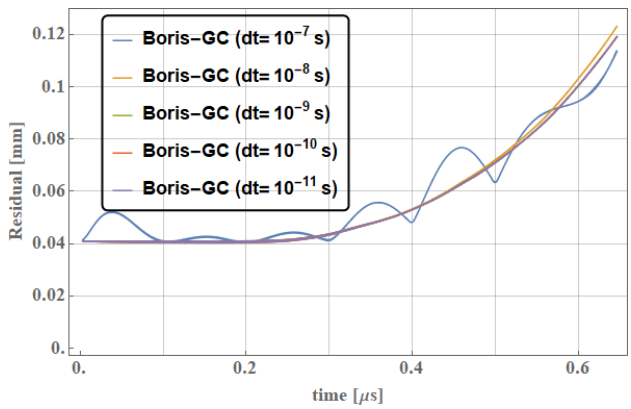

Figure 12: SILHI, absolute difference between simultaneous points during propagation of Boris and GC electrons.

The GC algorithm can provide an advantage in terms of computation time for particle plasma simulations. This advantage is greater for the conditions tested for SILHI, a flatter B-field relative to that of PHOENIX V2. In this regime the time step can be increased by a factor of 10^2 with a computation time ~30 times smaller with respect to Boris' using a 10ps time-step, without considerable loss in accuracy, the time-resolution being the principal limitation.

For the PHOENIX V2 ECRIS the gains are more modest, allowing for a time-step increase of factor of 10^2

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providing around one order of magnitude gain in required computation time. In certain cases, a disphasement between Boris' and GC orbits is evident for 1 µs propagation time, however this seems to preserve the spatial orbit envelope. This effect could be neglected in use cases involving many simulated particles and furthermore, the introduction of plasma interactions allows to re-initialize the electron, thus reducing the impact of this effect.

In terms of prospects to follow this study, a smart switcher for orbit integration could be implemented, where the GC approximation is used with a large time-step when valid and a high time resolution isn't required.

APPENDIX

To support the observed greater validity of the GC approximation in SILHI's regime, below its validity ratio is plotted along representative PHOENIX V2 and SILHI trajectories (Fig. 13).

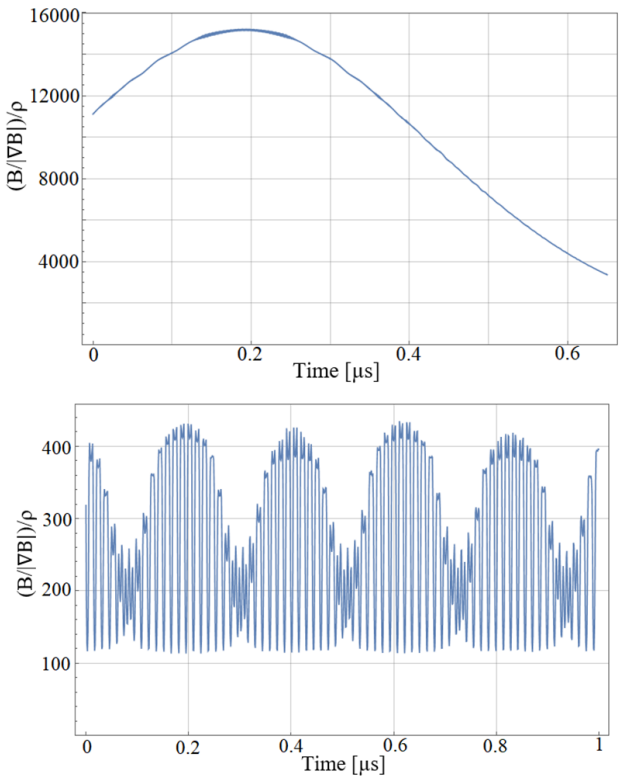

Figure 13: GC approximation validity test ratio along a typical SILHI (top) and PHOENIX V2 (bottom) trajectories.

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