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Guiding Center Equations of High Accuracy

R. B. White,[1] G. Spizzo,[2] and M. Gobbin[2]

[1]*Plasma Physics Laboratory, Princeton University,*

P.O.Box 451, Princeton, New Jersey 08543

[2]*Consorzio RFX, Euratom-ENEA Association,*

Corso Stati Uniti, 4 35127 Padova - Italy

Abstract

Guiding center simulations are an important means of predicting the effect of resistive and ideal magnetohydrodynamic instabilities on particle distributions in toroidal magnetically confined thermonuclear fusion research devices. Because saturated instabilities typically have amplitudes of $\delta B/B$ of a few times 10^{-4} numerical accuracy is of concern in discovering the effect of mode particle resonances. We develop a means of following guiding center orbits which is greatly superior to the methods currently in use. In the presence of ripple or time dependent magnetic perturbations both energy and canonical momentum are conserved to better than one part in 10^{14}, and the relation between changes in canonical momentum and energy is also conserved to very high order.

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I. INTRODUCTION

Guiding center codes are routinely used to simulate the modification of particle distributions in fusion devices caused by a spectrum of unstable modes, including resistive tearing modes, toroidal Alfvén eigenmodes and other kinetic instabilities excited by a high energy particle population such as an injected beam used for heating or thermonuclearly produced alpha particles[1–3].

The equilibrium field in a toroidal axisymmetric equilibrium has covariant and contravariant representations, given by $\vec{B} = \nabla\zeta \times \nabla\psi_p + q\nabla\psi_p \times \nabla\theta = g\nabla\zeta + I\nabla\theta + \delta\nabla\psi_p$ with $q(\psi_p)$ the field line helicity, ψ_p the poloidal flux, θ and ζ poloidal and toroidal coordinates and ψ_p, θ, and ζ forming a right handed coordinate system with Jacobian $1/\mathcal{J}_p = \nabla\psi_p \cdot (\nabla\theta \times \nabla\zeta)$. The toroidal flux is ψ with $d\psi = q(\psi_p)d\psi_p$. The function g is a flux function, and we use Boozer coordinates[4] with $I = I(\psi_p)$. A magnetohydrodynamic (MHD) instability is given by the plasma displacement $\vec{\xi}$, producing a modification of the magnetic field, with linear representations $\delta\vec{B} = \nabla \times (\vec{\xi} \times \vec{B})$ and $\delta\vec{B} = \nabla \times \alpha\vec{B}$. The particle position is given by ψ_p, θ and ζ, and the parallel velocity $\vec{v} \cdot \vec{B}/B$ completes the description of the particle state. Typically these four variables are advanced in time using a Runge–Kutta algorithm[5]. This leads to some numerical diffusion of the particle energy and canonical momentum, and blurs an important relation between them in the case of a time dependent perturbation. In this paper we introduce a means of treating the energy and canonical momentum as primary variables, greatly improving the accuracy of the time step algorithm. In a previous work[6] we have shown the equivalence of the two representations using $\vec{\xi}$ and α for ideal perturbations, but α is more general in that it can also be used to describe resistive modes, and we confine our attention to the use of α in this work. In section II we derive the guiding center equations using the conventional variables. In section III we use these equations to find a simplified means for stepping the energy and the canonical momentum, and devise a much more accurate means of stepping the orbit equations. In section IV are the conclusions.

II. GUIDING CENTER EQUATIONS

We use units of time given by ω_0^{-1}, where $\omega_0 = eB/(mc)$ is the on-axis gyro frequency, e the charge and m the particle mass, and units of distance given by the major radius R. The

basic unit of energy becomes $m\omega_0^2 R^2$, which can also be written as $(mv^2/2)(2R^2/\rho^2)$, the gyro radius is $\rho = v/B \ll 1$, and the magnetic moment $\mu = v_\perp^2/(2B)$ is of order ρ^2. Particle motion both along and across the field lines is of order ρ but to leading order the cross field motion is the cyclotron motion, and cross field drift is of order ρ^2[5].

Introduce a magnetic field perturbation of the form $\delta\vec{B} = \nabla \times \alpha\vec{B}$. Write the guiding center Lagrangian for a charged particle at position $\vec{x}$ in a magnetic field[5, 7]

$$L = (\vec{A} + \rho_\parallel \vec{B}) \cdot \dot{\vec{x}} - H \tag{1}$$

with $\rho_\parallel = v_\parallel/B$, $\vec{A}$ the vector potential, $\vec{v} = \dot{\vec{x}}$ the particle velocity, and H the Hamiltonian

$$H = \frac{\rho_\parallel^2 B^2}{2} + \mu B + \Phi, \tag{2}$$

with μ the magnetic moment and Φ the electric potential. The equilibrium vector potential is $\vec{A} = \psi\nabla\theta - \psi_p\nabla\zeta$ and the perturbation $\delta\vec{A} = \alpha\vec{B}$. The Lagrangian becomes

$$L = (\psi + \rho_\parallel I + \alpha I)\dot{\theta} + (\rho_\parallel g - \psi_p + \alpha g)\dot{\zeta} - H \tag{3}$$

where we have dropped δ, not modifying the particle trajectory in the poloidal plane and giving rise only to small periodic oscillations not changing the toroidal precession rate.

Lagrange's equations are

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q} \tag{4}$$

giving

$$\begin{pmatrix} 0 & -A & -C & 0 \\ A & 0 & -F & I \\ C & F & 0 & g \\ 0 & -I & -g & 0 \end{pmatrix} \begin{pmatrix} \dot{\psi}_p \\ \dot{\theta} \\ \dot{\zeta} \\ \dot{\rho}_\parallel \end{pmatrix} = \begin{pmatrix} -\partial_{\psi_p} H \\ -\partial_\theta H - I\partial_t\alpha \\ -\partial_\zeta H - g\partial_t\alpha \\ -\partial_{\rho_\parallel} H \end{pmatrix} \tag{5}$$

with

$$\begin{aligned} A &= q + \rho_\parallel I' + \alpha I' + I\alpha'_{\psi_p}, \\ C &= \rho_\parallel g' - 1 + \alpha g' + g\alpha'_{\psi_p}, \\ F &= g\alpha'_\theta - I\alpha'_\zeta, \end{aligned} \tag{6}$$

and $\alpha'_\beta = \partial\alpha/\partial\beta$. Invert Eq. 5 to find

$$\begin{pmatrix} \dot{\psi}_p \\ \dot{\theta} \\ \dot{\zeta} \\ \dot{\rho}_\| \end{pmatrix} = \frac{1}{Ag - IC} \begin{pmatrix} 0 & g & -I & -F \\ -g & 0 & 0 & C \\ I & 0 & 0 & -A \\ F & -C & A & 0 \end{pmatrix} \begin{pmatrix} -\partial_{\psi_p} H \\ -\partial_\theta H - I\partial_t \alpha \\ -\partial_\zeta H - g\partial_t \alpha \\ -\partial_{\rho_\|} H \end{pmatrix}. \tag{7}$$

These equations are advanced using a fourth order Runge Kutta algorithm to produce particle trajectories in toroidal geometry. The magnetic moment μ is a constant of the motion. They have been used for many years by a number of authors for the investigation of mode-particle interactions in toroidal plasma confinement devices. For typical simulations with time independent perturbations such as toroidal field ripple, energy conservation per time step is normally kept to one part in 10^8, and for time dependent perturbations such as resistive or ideal MHD modes, the energy is stepped with an accuracy of one part in 10^6.

III. IMPROVING THE STEPPING EQUATIONS

The antisymmetry of the matrix giving the time derivatives, Eq. 7, guarantees energy conservation in the absense of explicit time dependence. From

$$\frac{dH}{dt} = \partial_{\psi_p} H\dot{\psi}_p + \partial_\theta H\dot{\theta} + \partial_\zeta H\dot{\zeta} + \partial_{\rho_\|} H\dot{\rho}_\| + \partial_t H \tag{8}$$

we note that terms cancel one another due to this antisymmetry.

Significant tests of a numerical code for following particle trajectories in a toroidal confinement device consist of Poincaré plots and the observation of energy and momentum conservation. Poincaré plots using very low energy particles with zero magnetic moment and time independent perturbations show detailed structure of the magnetic field, very sensitive to numerical errors. Kinetic Poincaré plots, made following higher energy particle orbits in the presence of a perturbation with a single toroidal mode number and frequency, and recording points whenever $n\zeta - \omega t = 2\pi k$ with k integer, indicate mode-particle resonances and the island structure of these resonances is also very sensitive to numerical error. Location of mode-particle resonances is also a very delicate process requiring high accuracy[8, 9]. If the perturbations are time independent, then energy conservation is a very sensitive test of the numeral integration scheme and if high energy particles are used energy conservation tests also the correctness of the second order drift terms. If the perturbations

are axisymmetric the conservation of canonical momentum is an important test. Another test is the fact that in the presence of a single mode, with α and the Hamiltonian functions of $n\zeta - \omega t$ we have

$$\omega \dot{P}_\zeta = n\dot{H}. \tag{9}$$

This condition restricts the motion of particles in the P_ζ, E plane due to the action of a mode, defining the possible diffusion in this plane for a single mode, and numerical error in this relation produces incorrect particle diffusion.

It is worth confirming this relation. We have

$$H = \frac{\rho_\parallel^2 B^2}{2} + \mu B + \Phi, \qquad \dot{H} = \partial_{\psi_p} H \dot{\psi}_p + \partial_\theta H \dot{\theta} + \partial_{\rho_\parallel} H \dot{\rho}_\parallel + \partial_t H \tag{10}$$

and from the Lagrangian we find

$$\begin{aligned} P_\zeta &= g\rho_\parallel - \psi_p + g\sum_{mn} \alpha_{mn}(\psi_p) sinQ_{mn}, \\ \dot{P}_\zeta &= (g'\rho_\parallel - 1)\dot{\psi}_p + g\dot{\rho}_\parallel + \sum_{mn} \alpha'_{mn} sinQ_{mn}\dot{\psi}_p + \sum_{mn} [n\alpha_{mn}\dot{\zeta} - m\alpha_{mn}\dot{\theta} - \omega\alpha_{mn}] cosQ_{mn} \end{aligned} \tag{11}$$

with $\alpha = \sum_{mn} \alpha_{mn}(\psi_p) sinQ_{mn}$ and $Q_{mn} = n\zeta - m\theta - \omega t$.

We find after some algebra

$$\dot{H} = -\partial_{\rho_\parallel} H \partial_t \alpha + \partial_t H, \qquad \dot{P}_\zeta = \partial_{\rho_\parallel} H \alpha'_\zeta - \partial_\zeta H \tag{12}$$

and we then confirm Eq. 9 for the case of a single n value provided both α and the Hamiltonian are functions of the combination $n\zeta - \omega t$. Note that the changes in energy and in P_ζ are proportional to $\rho_\parallel B^2 \alpha$, whereas the equations for stepping the variables of Eq. 7, in particular that for $\rho_\parallel$, include terms of order $\rho_\parallel B^2$, typically four orders of magnitude larger than this. Thus using Eqs. 7 the accuracy of the time evolution of E and P_ζ is compromised by the necessary cancellation of large terms in the Runge–Kutta process and we find that Eq. 9 is satisfied typically only within about one percent. This is the expected result with stepping equations of accuracy of one part in 10^6, and the evolution of E and P_ζ being smaller by a factor of 10^4.

Thus we wish to make E and P_ζ primary variables, stepping them directly, producing a much more accurate time step than obtained by stepping the variables of Eq. 7. The problem remains as to how to advance ψ_p, θ, and ζ, without compromising accuracy, since they are stepped using terms of order $\rho_\parallel B^2$. A satisfactory solution is the following:

1. Advance the variables E, P_ζ, ψ_p, θ, and ζ using Eqs. 12 and 7 to $t + \Delta t$.

2. Use the new values of ψ_p, θ, and ζ as initial guesses for a Newton iteration search *along the orbit* for values that give E and P_ζ correctly.

To perform step 2, we vary ψ_p, θ, and ζ along the orbit by introducing a subsidary time variable T small compared to the Runge–Kutta step Δt employed, and use the values of $\dot{\psi}_p$, $\dot{\theta}$, and $\dot{\zeta}$ to give

$$\begin{aligned} \psi_p &= \psi_{p0} + \dot{\psi}_p T, \\ \theta &= \theta_0 + \dot{\theta} T, \\ \zeta &= \zeta_0 + \dot{\zeta} T \end{aligned} \tag{13}$$

where ψ_{p0}, θ_0, and ζ_0 and $\dot{\psi}_p$, $\dot{\theta}$, and $\dot{\zeta}$ are the values given by the Runge–Kutta step and T is the variable for Newton's method, used to give the correct stepped values of E and P_ζ. This is accomplished by finding the zero of

$$f(T) = \frac{\rho_\parallel^2 B^2/2 + \mu B + \Phi - E}{E} \tag{14}$$

through iterations of Newton's method while using

$$\rho_\parallel = \frac{P_\zeta + \psi_p - g\alpha}{g} \tag{15}$$

so as to give the stepped value of P_ζ, where all these variables are evaluated at the new coordinates and the time $t + \Delta t$. This Newton iteration begins with the two values $T = \pm 0.05\Delta t$, and typically makes $f(T)$ zero to less than one part in 10^{14}. It can fail near a banana turning point, where $\dot{\psi}_p$, $\dot{\theta}$ and $\dot{\zeta}$ change sign. But if it fails to converge after a few iterations one simply uses the values of ψ_p, θ, and ζ given by the Runge–Kutta step, which already solve $f(T) = 0$ typically to better than one part in 10^6 for $T = 0$. Even in this case, although the values of ψ_p, θ, and ζ are only of the accuracy given by the Runge–Kutta step, the energy and the canonical momenta are stepped only using Eq. 12. Since α is of order 10^{-4} and the relative errors in ψ_p, θ, and ζ are of order 10^{-6} this produces a change in energy and momentum of order 10^{-10}. As soon as the turning point has been passed, the values of ψ_p, θ, and ζ will again become precise, there is very little diffusion in energy or momentum caused by this failure.

Note that T is not a modification of the time step for the orbit. It is a correction to the erroneous Runge–Kutta values for ψ_p, θ, and ζ to bring them into alignment with the more exact values of E and P_ζ at the new time $t + \Delta t$.

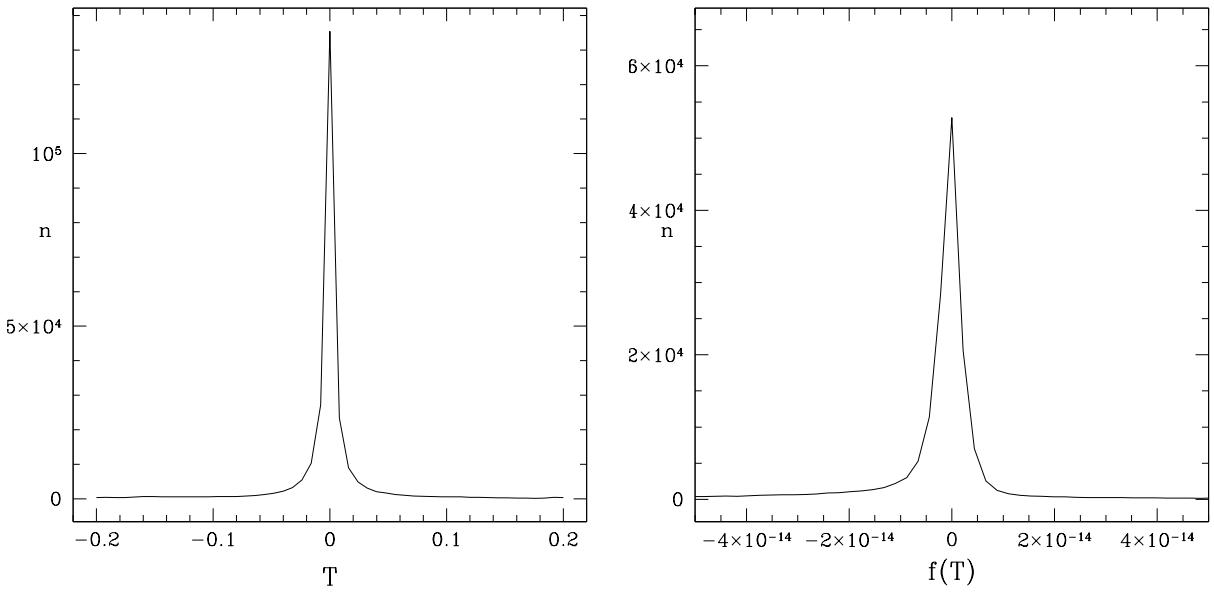

FIG. 1: Values of T obtained by the Newton iteration, normalized to the Runge–Kutta time step dt, and values of $f(T)$, the relative error in stepping the particle energy. The rms value of $f(T)$ is approximately 2×10^{-15}.

To develop and test the method, we used a single mode with amplitude $\alpha = 2 \times 10^{-4} R$, $m = 4$, $n = 3$, and a frequency of 60 kHz. The equilibrium used was a numerical equilibrium with B on axis of 40 kG and a major radius of 100 cm, and the orbit was that of a deuterium ion with an energy of 20 keV. The time step was set to give 50 steps per toroidal transit.

In Fig. 1 are shown histograms of the value of T obtained by the Newton iteration, normalized to the Runge–Kutta time step, and the value of the error in the energy, $f(T)$ for a typical orbit. The subsidary time variable is reliably short compared to the Runge–Kutta step, and is symmetric around zero. The discrepancy in the energy given by $\rho_\|$, ψ_p, θ, and ζ compared to E is also seen to be symmetric about zero, with a rms value of about 2×10^{-15}. The Newton iteration is successful in about 85 % of the time steps in a typical simulation, requiring about 5 iterations to produce an error below the required accuracy set at 10^{-12}. More than 10 iterations was regarded as failure.

The inclusion of a collision operator in between time steps will of course produce additional modifications of energy and momentum, but this does not interfere with the stepping algorithm.

A general search for values of ψ_p, θ, and ζ satisfying Eq. 14 without relating them through

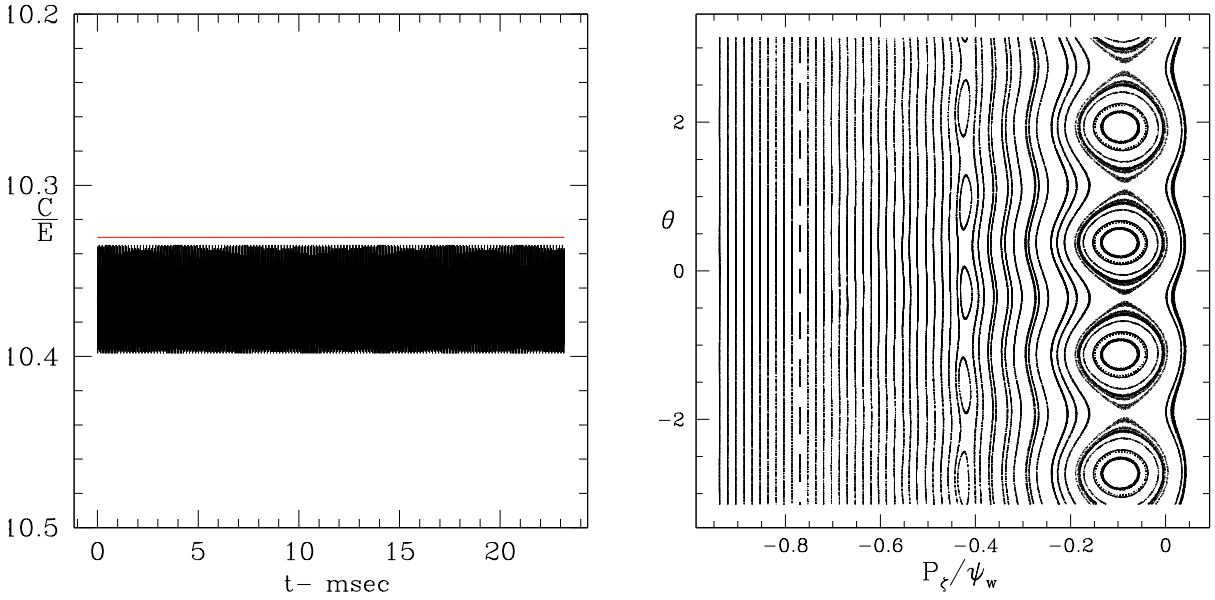

FIG. 2: Variation of $C = \omega P_\zeta - nE$, normalized to the initial particle energy, for a perturbation with amplitude 2×10^{-4}, $m = 4$, $n = 3$, $f = 60kHz$, by the straightforward Runge–Kutta advancement of Eqs. 7 (black) and by stepping E, P_ζ and using the Newton iteration (red) to find ψ_p, θ, and ζ. The error using the Newton iteration, less than 10^{-14}, cannot be seen on this plot. Also shown is a kinetic Poincaré plot showing the clarity of resonances observed with this mode.

Eq. 13 is incorrect, since there exist a multitude of solutions nearby caused by the presence of the perturbation α. Such a search produces an incorrect diffusion in the flux coordinate ψ_p, and is also very time consuming. By restricting the search to the instantaneously projected orbit given by the Runge–Kutta algorithm the search is fairly simple and the initial values for the search are guaranteed to be reasonably correct.

In Fig. 2 is an example of the function $C = \omega P_\zeta - nE$ with C normalized to the initial particle energy, using Eq. 7 and a Runge–Kutta algorithm and also using the new Newton iteration. Also shown is a kinetic Poincaré section of a resonance using the new method. The error in C, about one percent with Runge-Kutta, is typically one part in 10^{14} and not observable on this scale and the Poincaré plot has exceptional clarity.

In an axisymmetric equilibrium with no ζ dependence, P_ζ is conserved to machine accuracy for a simulation of indefinite length. If the perturbation of the equilibrium is time independent the particle energy is conserved to machine accuracy. Occasionally during a simulation the values of ψ_p, θ, and ζ will be slightly incorrect for a short period (typically

near a banana tip), but these errors are only weakly cumulative through Eq. 12, and the values will revert to be very accurately associated with P_ζ and E again as the orbit moves away from the banana tip. Note that the time step must still be sufficiently small to resolve the variation of α in Eq. 12, but it probably can be relaxed compared to that used for Eqs. 7. The present simulations used the same time step for both methods, time step variation will be explored in a future publication. The Newton iteration adds about 30 % to the computing time for a typical simulation.

Paradoxically, in an axisymmetric equilibrium with no perturbation present the Newton iteration will not converge, because there is no toroidal variation along the orbit, all points on the orbit have the same values of P_ζ and E. Thus in this case the values given by the Runge–Kutta procedure are maintained for ψ_p, θ, and ζ, while P_ζ and E are constant in time, possibly leading to a divergence in the values of $\rho_\parallel^2 B^2/2 + \mu B$ with respect to E. The value of $\rho_\parallel g - \psi_p$ will continue to equal P_ζ because this is how $\rho_\parallel$ is defined. The energy conservation will be better than with the original guiding center equations because of this improved advancement of $\rho_\parallel$, conserving P_ζ. To obtain an additional increase in the accuracy of the code it is necessary to at least add toroidal field ripple so that the Newton iteration is sensitive to toroidal location. In any case a realistic problem always involves some kind of field perturbation.

At least one orbit for this particular case is seen to be significantly different in the poloidal plane using these two methods. Shown in Fig. 3 is the time evolution of an orbit over 20 *msec* using Eq. 7 and by advancing E, P_ζ along with the Newton procedure. It is seen that a more exact calculation of the changes in E, P_ζ results in an energy increase producing a transition from a poloidally trapped orbit to a passing orbit, whereas no transition occurs because of random errors in the stepping equations when Eqs. 7 are used. The present method is thus seen to produce a much more reliable treatment of delicate mode-particle resonances.

IV. CONCLUSION

Modified stepping equations for guiding center motion have been developed which have much higher accuracy than those used previously, by directly stepping the energy and canonical momentum. For the case of typical MHD perturbations the changes in energy and

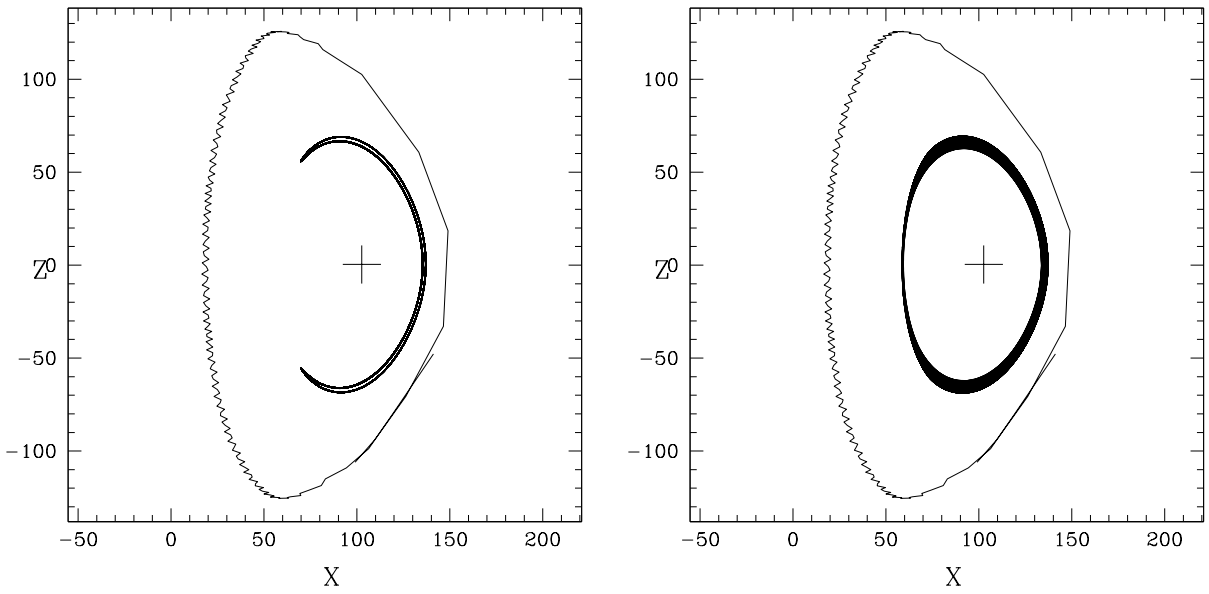

FIG. 3: Trajectory for a perturbation with amplitude 2×10^{-4}, $m = 4$, $n = 3$, $f = 60kHz$ and a time of 20 *msec*. Resonant transition from a poloidally trapped orbit to a passing orbit is seen with the new stepping algorithm (right), whereas no transition occurs using Eqs. 7 (left).

canonical momentum are accurate to better than one part in 10^{14} in one time step, where the previously used Runge–Kutta method gave accuracy of typically one part in 10^6. The new method gives a much more exact description of the effect of field perturbations on particle distributions.

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Information Services
Princeton Plasma Physics Laboratory
P.O. Box 451
Princeton, NJ 08543

Phone: 609-243-2245
Fax: 609-243-2751
e-mail: pppl_info@pppl.gov
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