Simulations of particle dynamics in a global toroidal geometry

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The gyrokinetic toroidal code (GTC) has been upgraded for global simulations by coupling the core and scrape-off layer (SOL) regions across the separatrix with field-aligned particle-grid interpolations. A fully kinetic particle pusher for high frequency waves (ion cyclotron frequency and beyond) and a guiding center pusher for low frequency waves have been implemented using cylindrical coordinates in a global toroidal geometry. The two integrators correctly capture the particle orbits and agree well with each other, conserving energy and canonical angular momentum. As a verification and application of this new capability, ion guiding center simulations have been carried out to study ion orbit losses at the edge of the DIII-D tokamak for single null magnetic separatrix discharges. The ion loss conditions are examined as a function of the pitch angle for cases without and with an electric field. The simulations show good agreement with past theoretical results and with many experimentally observed features. A measure of the ion direct orbit loss fraction shows that the loss fraction increases with the ion energy for DIII-D in the initial velocity space.

I. INTRODUCTION

One of the important challenges in getting to a viable operating regime for ITER and future fusion reactors is associated with the nonlinear turbulent dynamics of the plasma in the scrape-off layer (SOL)1. The plasma characteristics in SOL can greatly affect the overall confinement properties of the device and also regulate the heat load to the tokamak wall. It can also influence the level of fusion ash, the impurity dynamics, sheath physics and plasma shaping effects. Furthermore, the SOL dynamics can degrade the current drive performance of radio frequency (RF) waves through its impact on the density threshold conditions for the onset of parametric decay instabilities2. An indepth understanding of the mechanisms determining the width of the SOL layer remains an outstanding open problem. A study of the SOL plasma dynamics is challenging due to multiple spatial and temporal scales associated with different energy sources (instabilities) in that region. Fluid simulation transport codes such as UEDGE3, SOLPS4 are normally used to simulate the SOL dynamics. These fluid codes use a set of fluid transport equations that are based on the Braginskii equations5. However, the results show a number of discrepancies between experimental findings and fluid simulations including in the characteristics of the radial electric field, parallel ion flow, impurity radiation, etc.6–8. It is believed that kinetic effects could be a significant contributor in the SOL to processes like ion orbit losses9, X point losses10, nonlocal turbulent transport11, plasma sheath dynamics12, parametric decay instabilities2,13–15, etc. To correctly model many of these effects requires a kinetic approach that covers the closed, and open field line regions across the separatrix, and includes realistic SOL physics and tokamak geometry. Due to the difficulty of accessibility of diagnostics in the SOL region such global kinetic simulations can help in developing useful insights for predicting the plasma dynamics in that region for present and future reactors such as ITER and DEMO. A laudable effort in this directions has been the development of the massively parallel kinetic simulation code XGC-116 that takes a first-principles approach and has emerged as an efficient method for describing the complex physics of turbulent transport. Another widely used and successful tool, the gyrokinetic toroidal code (GTC) has also undergone continuous development for the last two decades and has been applied in the study of plasma transport in the core region17. GTC is a well-benchmarked, first principles code which has been extensively applied to study neoclassical transport18,19, microturbulence20–25, mesoscale Alfvén eigenmodes26–27 excited by energetic particles, macroscopic MHD modes28–30 (kink and tearing modes) and radio frequency (RF) waves31–37 in the core region. However, the assumptions used in studying turbulence in the core region may not be valid in the SOL region. GTC normally uses conventional magnetic flux coordinates, in which the equations of motion encounter a mathematical singularity of metric on the magnetic separatrix surface. Recently, the GTC was extended to separately study instabilities in the SOL and core regions of a field reversed configuration (FRC) using Boozer coordinates. However, the code still did not have the capability to couple these two regions21,38. The difficulty lay in the discontinuity of the poloidal angle in Boozer coor-

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ordinates across the separatrix. This limitation restricted the code’s usage to electrostatic simulations either in the core or the SOL region with no cross-separatrix coupling.

In our present work we report a significant enhancement of the GTC through development of a new global nonlinear particle simulation model that couples the core and SOL regions. The code also provides a realistic treatment of the separatrix region through Equilibrium Fitting (EFIT)\textsuperscript{39,40} of equilibrium data files generated by experimental discharges. A particular feature of the upgraded GTC is the use of a cylindrical coordinate system for the advancement of the particle dynamics, which allows particle motion in arbitrary shaped flux surfaces including the magnetic separatrix and the magnetic X-point.

As a first step in developing this nonlinear particle simulation model, we have constructed a field aligned computational mesh to take advantage of the smallest number of grid points in the direction of the magnetic field with high resolution in any given poloidal plane using more fundamental cylindrical coordinates rather than the flux coordinates. Field aligned coordinate approaches have been used in the past in turbulence simulation codes such as GTC\textsuperscript{24}, XGC\textsuperscript{41}, FENICA\textsuperscript{42}, GEM\textsuperscript{43}, etc. The gain in computational efficiency by using appropriate coordinates and computational mesh help to optimize turbulence simulations of large devices like ITER and DEMO. We have also developed a fully kinetic (FK) particle pusher to capture the effect of high frequency waves (ion cyclotron frequency and beyond) and a guiding center (GC) pusher to describe the particle dynamics associated with low frequency waves (much smaller than the ion cyclotron frequency).

To test the effectiveness of these enhancements and appropriately benchmark the code we have carried out ion guiding center simulations to study ion orbit losses at the edge of the DIII-D tokamak for single null magnetic separatrix discharges. Using model calculations some analytic expressions of such losses have been presented by Miyamoto\textsuperscript{44} and have been used in the past to estimate the loss region in velocity space for JET, JT-60 and ITER magnetic geometries. Stacey has introduced the effect of ion orbit loss and X point loss in his fluid calculations for the interpretation of fluid transport in the edge region\textsuperscript{8,45}. Our extended simulation model is meant to benchmark GTC against some of these past results. We have examined the ion orbit losses as a function of the pitch angle both in the presence and absence of an electric field. The simulations show good agreement with past theoretical results and with many experimentally observed features. A measure of the ion direct orbit loss fraction shows that the loss fraction increases with the ion energy for DIII-D in the initial velocity space.

The paper is organized as follows: The next section II contains a detailed description of the coordinate system and the representation of the equilibrium and fluctuating field quantities in the code. Section III describes the computational mesh used in the simulations. The physics model explained the dynamics of the particles is described in section IV followed by our simulation results for the ion orbit losses in section V. Section VI provides a brief summary and some concluding discussions.

II. REPRESENTATION OF EQUILIBRIUM AND COORDINATE SYSTEM

In describing the collective dynamics of a tokamak plasma, it is convenient to represent the physical variables in terms of equilibrium and fluctuating quantities. The equilibrium is described by the Grad-Shafranov equation, while the fluctuations representing wave activity contribute to plasma transport. The input equilibrium magnetic field configuration for GTC can be generated in any of the equilibrium solvers EFIT, VMEC, or M3D-C1 and is normally expressed as a function of the magnetic flux function. In the MHD approximation (ignoring guiding center orbit effects) the plasma profiles of temperature, density, current etc. are also functions of the flux function. In the upgraded GTC version we use a cylindrical set of coordinates ($R, \zeta, Z$) where $R$ is the distance from the geometry axis, $\zeta$ is the toroidal angle and $Z$ is the direction of the torus symmetry axis. The representation of the magnetic field for an axisymmetric system is then given by,

$$\vec{B} = \nabla \psi(R, Z) \times \nabla \zeta + \frac{F(\psi)}{R} \vec{\zeta},$$  \hspace{1cm} (1)

where $\psi(R, Z)$ is the poloidal flux function that labels the magnetic surfaces for both closed and open field lines [cf. Fig 1(b)] and $F(\psi)$ is the poloidal current function [cf. Fig 1(a)], which provides the components of magnetic field in cylindrical coordinates as:

$$B_R = -\frac{1}{R} \frac{\partial \psi}{\partial Z}, \quad B_Z = \frac{1}{R} \frac{\partial \psi}{\partial R}, \quad B_\zeta = \frac{F(\psi)}{R},$$ \hspace{1cm} (2)

The Jacobian for this system can be written as

$$J^{-1} = \nabla R \cdot (\nabla \zeta \times \nabla Z).$$  \hspace{1cm} (3)

The cylindrical toroidal coordinate system is related to the standard Cartesian system as follows

$$x = R \cos \zeta, \quad y = R \sin \zeta, \quad z = Z.$$ \hspace{1cm} (4)

By defining contravariant basis vectors $\vec{e}^R = \nabla R$, $\vec{e}^\zeta = \nabla \zeta$, $\vec{e}^Z = \nabla Z$ the velocity and the electric field can be written as

$$\vec{v} = v^R \vec{e}^R + v^\zeta \vec{e}^\zeta + v^Z \vec{e}^Z,$$ \hspace{1cm} (5)
FIG. 1. (a) Poloidal current function $F(\psi)$ in m-T on uniform flux grid, and (b) poloidal flux function in web/rad on rectangular (R,Z) grid points for DIII-D shot #158103 at 3050 ms. The magnitude of the flux function is indicated by color. Last closed flux surface and limiter points are represented by magenta and red line, respectively.

FIG. 2. Components of magnetic field (a) $B_Z$, (b) $B_R$ and (c) $B_\zeta$ for DIII-D shot #158103 at 3050 ms. The magnitude of the magnetic field components are indicated by color. Last closed flux surface and limiter points are represented by magenta and red line, respectively.
\[ \mathbf{E} = -\nabla \phi = - \left[ \frac{\partial \phi}{\partial R} \nabla R + \frac{\partial \phi}{\partial \zeta} \nabla \zeta + \frac{\partial \phi}{\partial Z} \nabla Z \right]. \] (6)

where
\[ v^R = \dot{R}, \quad v^\zeta = \dot{\zeta}, \quad v^Z = \dot{Z}, \]
\[ \dot{e}^R = \cos \zeta \dot{\zeta} + \sin \zeta \dot{\gamma}, \]
\[ \dot{e}^\zeta = -R \sin \zeta \dot{x} + R \cos \zeta \dot{y}, \]
\[ \dot{e}^Z = \dot{z}. \] (7)

The equilibrium inputs from EFIT only provide equilibrium quantities on a coarse mesh, which usually contains a few tens of grid points in the \( R \) and \( Z \) directions. However, the micro-scale turbulence demands much denser grid points in \( R \) and \( Z \) directions. Therefore, it is necessary to map the equilibrium mesh to a dense computational mesh to achieve sufficient numerical accuracy. For a 1D function \( f(\psi) \), such as the poloidal current function \( F(\psi) \) we can use the following B-spline representation:

\[ f(\psi) = f(1, i) + f(2, i) \Delta \psi + f(3, i) \Delta \psi^2, \] (8)

where \( f(2, i) \) and \( f(3, i) \) are coefficients related to the first and second order differential in \( \psi \) direction, which are calculated using finite difference method on a spline mesh. In our simulations we have calculated the grid size in \( \psi \) using the following three steps:

\[ \Delta \psi = \frac{\psi_{Lim}}{N_\psi - 1} \Rightarrow N_{sep} = \text{integer} \left[ \frac{\psi_{sep}}{\Delta \psi} \right] \Rightarrow \Delta \psi = \frac{\psi_{sep}}{N_{sep}}. \] (9)

where \( \psi_{Lim} \) is the poloidal flux function at the limiter point, \( N_\psi \) is the number of grid points in \( \psi \), \( N_{sep} \) is the grid point number at the separatrix, and \( \psi_{sep} \) is the poloidal flux function at the separatrix. This calculation will provide accurate value of \( \psi \) at the separatrix in the simulation, however will give some minor difference in calculating the \( \psi \) at the limiter points.

A 2D function \( f(R, Z) = \sum_n F_n(R) G_n(Z) \) can be expressed as

\[ f(R, Z) = f(1, i, j) + f(2, i, j) \Delta R + f(3, i, j) \Delta R^2 + f(4, i, j) \Delta Z + f(5, i, j) \Delta R \Delta Z + f(6, i, j) \Delta Z \Delta R^2 + f(7, i, j) \Delta Z^2 + f(8, i, j) \Delta R \Delta Z^2 + f(9, i, j) \Delta R^2 \Delta Z^2, \] (10)

where \( \Delta R = R_{i+1} - R_i, \ i = 0, 1, 2, \cdots, nR, \) and \( \Delta Z = Z_{j+1} - Z_j, \ j = 0, 1, 2, \cdots, nZ. \) Eq. (10) is derived by using the 1D B-spline functions of \( F_n(R) = F_n(1, i) + F_n(2, i) \Delta R + F_n(3, i) \Delta R^2 \) and \( G_n(Z) = G_n(1, j) + G_n(2, j) \Delta Z + G_n(3, j) \Delta Z^2. \) The spline coefficients \( f(1 : 9, i, j) \) are calculated from the spline coefficients \( F_n(1 : 3, i) \) and \( G_n(1 : 3, j). \) Fig. 1(a) and Fig. 1(b) represent the equilibrium poloidal current function on uniform flux grid and poloidal flux function on rectangular \( R-Z \) grid for DIII-D shot #158103 at 3050 ms, respectively. In GTC we use these two functions in Eq.(2) to calculate the magnetic field components for DIII-D [cf. Fig. 2]. In particle pusher we interpolate these field quantities at the particle position using 2D spline function, as described in Eq. (10).

III. FIELD ALIGNED MESH FOR FLUCTUATING QUANTITIES

The field aligned mesh has maximum numerical efficiency and accuracy to address the nonlinear physics of drift wave turbulence. Because the particle moves much faster in the direction parallel to the magnetic field than the drifts across the magnetic field, the parallel wave vector is usually much smaller than the perpendicular wave vector for the drift wave instabilities. Thus, it only requires a small number of grid points to resolve the parallel wave length, which greatly saves the computational costs and suppresses the numerical high \( k_i \) modes efficiently. Furthermore, it helps to simplify the implementation of the field solver, since the field aligned mesh can exactly decouple the parallel and perpendicular directions.

A. Radial grid:

GTC code has in the past utilized the field aligned mesh in Boozer coordinates and successfully applied it for gyrokinetic simulations of drift waves in the core region of toroidal plasmas. In this work, we extend the original GTC field aligned mesh from Boozer coordinates in the core region to cylindrical coordinates in the whole domain across the separatrix. In order to create the field aligned mesh for the whole tokamak domain, we apply an equally spaced radial grid (spacing of size \( \Delta r \)) on the outer midplane for each field line, which can be calculated as:

\[ \Delta r = \frac{1}{N_{SOL} - 1} \left\{ R_{LF}(\psi = \psi_1, Z = 0) - R_{LF}(\psi = \psi_{sep}, Z = 0) \right\}, \] (11)

where \( R_{LF} \) is the radial position as a function of poloidal flux and \( Z \) on the low field side, and \( N_{SOL} \) is the number of field line in the SOL region. \( \psi_1 \) is the maximum value of the poloidal flux on the limiter points (plasma facing components). GTC also has the capability to use a nonuniform grid with grid size in the perpendicular direction correlated with the local gyro-radius. The poloidal flux of each field line for the simulation mesh in the SOL region is:

\[ \psi_{SOL}(i_{SOL}) = \psi \left( R_{LF}(\psi = \psi_{sep}, Z = 0) + (i_{SOL} - 1) \times \Delta r, Z = 0 \right). \] (12)
where $i_{\text{SOL}} \in [1, N_{\text{SOL}}]$.

Then the field line number in the core region $N_{\text{core}}$ can be calculated as:

$$N_{\text{core}} = \text{integer}\left[\frac{R_{LF}(\psi = \psi_{\text{sep}}, Z = 0) - R_0}{\Delta r}\right]$$ (13)

where $R_0$ is the major radius. The poloidal flux of the innermost grids in the core region $\psi_0$ can be determined as:

$$\psi_0 = \psi\left(R_{LF}(\psi = \psi_{\text{sep}}, Z = 0) - (N_{\text{core}} - 1) \times \Delta r, Z = 0\right)$$ (14)

where $\psi_0$ is not necessarily equal to the poloidal flux value at the magnetic axis. The poloidal flux of each field line for the simulation mesh in the core region is:

$$\psi_{\text{core}}(i_{\text{core}}) = \psi\left(R_{LF}(\psi = \psi_0, Z = 0) + (i_{\text{core}} - 1) \times \Delta r, Z = 0\right),$$ (15)

where $i_{\text{core}} \in [1, N_{\text{core}}]$.

Similarly, the field line number in the private region $N_{\text{private}}$ is calculated as:

$$N_{\text{private}} = \text{Integer}\left[\frac{R_{LF}(\psi = \psi_{\text{sep}}, Z = Z_0) - R_{LF}(\psi = \psi_{\text{pmax}}, Z = Z_0)}{\Delta r}\right]$$ (16)

where $\psi_{\text{pmax}}$ is the poloidal flux of the innermost flux surface in the private region, and $Z_0$ is the minimum value in $Z$ direction. The poloidal flux of the innermost grids in the private region $\psi_{p0}$ can be determined as:

$$\psi_{p0} = \psi\left(R_{LF}(\psi = \psi_{\text{sep}}, Z = 0) - (N_{\text{private}} - 1) \times \Delta r, Z = Z_0\right),$$ (17)

where $\psi_{p0}$ is not necessarily equal to $\psi_{\text{pmax}}$. The poloidal flux of each field line for the simulation mesh in the private region is:

$$\psi_{\text{private}}(i_{\text{private}}) = \psi\left(R_{LF}(\psi = \psi_{p0}, Z = Z_0) + (i_{\text{private}} - 1) \times \Delta r, Z = Z_0\right).$$ (18)

where $i_{\text{private}} \in [1, N_{\text{private}}]$.

### B. Poloidal grid:

Next we trace each field line along the poloidal direction and calculate the length of the poloidal projection for each field line by using the unit magnetic vector as:

$$\frac{dR}{dS} = b_R,$$ (19)

and

$$\frac{dZ}{dS} = b_Z,$$ (20)

where $b_R = -(1/B_p)(\partial \psi/\partial R)$, $b_Z = (1/B_p)(\partial \psi/\partial R)$ and $B_p$ is the poloidal magnetic field. The starting points for tracing the field lines are on the low field side of outlet plane with $Z = 0$ for the core region and on the low field side of $Z = Z_0$ plane for the SOL and private regions. The step $\Delta S_i$ for tracing each field line is at least $10^{-5}$ smaller than the order of magnitude of poloidal projected field line length, and we correct the new position for each tracing step to ensure that it lies on the same flux surface by using Newton’s method with the error of the order of floating precision. All the advanced positions during tracing poloidal field line are recorded as tracing grids. The outmost simulation boundary is determined by the limiter as shown by the brown line, so the tracing grids outside the limiter in the SOL and private region are removed by using ray casting algorithm. In the closed field line region, we calculate the length of the poloidal projection of the field line for each flux surface. However, in the open field line regions, we set the intersection points formed by field lines and limiter as the simulation boundary points and calculate the length of the poloidal projection of the field line between each two intersection points on one single continuous field line.

The simulation grid number for each continuous poloidal field line is calculated as:

$$N_i = \text{integer}\left(\frac{l_i}{\Delta S_{i0}}\right),$$ (21)

where $l_i$ and $N_i$ are the poloidal length and the poloidal grid number for $i$-th field line, respectively, and $\Delta S_{i0}$ is the given approximate grid size along the poloidal direction. The exact poloidal grid size $\Delta S_i$ is then determined by $l_i$ and $N_i$ as:

$$\Delta S_i = \frac{l_i}{N_i - 1}.$$ (22)

The position of the field aligned grid along poloidal direction can be derived from poloidal grid size $\Delta S_i$, the much smaller tracing step $\Delta S_i$, and the positions of the dense tracing grids.

In the cylindrical coordinate representation, we only apply the field aligned mesh in the poloidal direction, and the meshes on different poloidal plane are identical as shown by Fig. 3 (axisymmetric). In order to decouple the exact parallel and perpendicular directions and use a small number of poloidal planes, the particle-grid gathering and scattering are along the exact parallel direction by interpolating the value on the identical field line.
IV. PHYSICS MODEL FOR PARTICLE DYNAMICS

The efficiency of particle simulation strongly depends on advancement of dynamical quantities. In the upgraded GTC we have developed particle pushers for both fully kinetic particles and guiding center particles using cylindrical coordinate \((R, \zeta, Z)\) in a global toroidal geometry. The physics model for the fully kinetic dynamics, guiding center dynamics and the numerical methods associated with the time advancement of the physical quantities (particle position and guiding center) are described in the following sections.

A. Fully kinetic particle dynamics

Fully kinetic particle dynamics is described by the six dimensional Vlasov equation

\[
\left[ \frac{\partial}{\partial t} + \vec{v} \cdot \nabla + \frac{q_c}{m} (\vec{E} + \vec{v} \times \vec{B}) \cdot \frac{\partial}{\partial \vec{v}} \right] f_{FK} = 0, \tag{23}
\]

where \(f_{FK}\) is the fully kinetic particle distribution function, \(q_c\) is the particle charge, and \(m\) is the particle mass.

The evolution of the particle distribution function \(f_{FK}\) can be described by the Newtonian equation of motion in the presence of self-consistent electromagnetic field as follows:

\[
\frac{d}{dt} \vec{r} = \vec{v}, \quad \frac{d}{dt} \vec{v} = \frac{q_c}{m} \left( \vec{E} + \vec{v} \times \vec{B} \right). \tag{24}
\]

In our simulation we compute the marker particle trajectory Eq. (24) by the time centered Boris push method\(^{31,33,48–51}\) as discussed in section 4.2. The Lagrangian for the single particle motion in the cylindrical coordinates is written as

\[
\mathcal{L} = \frac{m}{2} \left[ \dot{R}^2 + R^2 \dot{\zeta}^2 + \dot{Z}^2 \right] + q_c \left[ \dot{R} A_R + R \dot{\zeta} A_\zeta + \dot{Z} A_Z \right] - q_c \phi, \tag{25}
\]

where \(\dot{A}\) is the magnetic vector potential. Now the components of generalized momenta are

\[
p_R = \frac{\partial \mathcal{L}}{\partial \dot{R}} = m \dot{R} + q_c A_R, \quad p_\zeta = \frac{\partial \mathcal{L}}{\partial \dot{\zeta}} = m R^2 \dot{\zeta} + q_c R A_\zeta, \quad p_Z = \frac{\partial \mathcal{L}}{\partial \dot{Z}} = m \dot{Z} + q_c A_Z. \tag{26}
\]

In our simulation we use the poloidal flux function \(\psi\), rather than the vector potential \(\dot{A}\) to represent the equilibrium magnetic field components for calculating the toroidal canonical angular momentum. Two constants of motion for fully kinetic dynamics in cylindrical coordinates are defined by\(^{33}\):

- Toroidal angular momentum from Eq. (26) and Eq. (1)

\[
p_\zeta = m R^2 \dot{\zeta} + q_c \psi,
\]

since \(RA_\zeta = \psi\)

B. Boris push for fully kinetic particle dynamics

Boris scheme is the most widely used orbit integrator in explicit particle-in-cell (PIC) simulation of plasmas. In this paper we have extended our Boris push scheme in GTC from Boozer coordinates\(^{33}\) to cylindrical coordinates. This scheme offers second order accuracy while requiring only one force (or field) evaluation per step. The interplay between the PIC cycle and the Boris scheme is schematically represented in Fig.2 of Ref.\(^{33}\). At the beginning of each cycle the position of the particles and their time centered velocity \(\vec{\nu}(t-1/2)\) as well as the grid based electromagnetic fields \(\vec{E}(t), \vec{B}(t)\) are given.

At the first step, we add the first half of the electric field to update the velocity from \((t-1/2)\) to \(t\) as follows:

\[
\vec{\nu}(t) = \vec{\nu}(t-1/2) + \frac{q_c}{m} \frac{\Delta t}{2} \vec{E}(t)
\]

One may write the components of velocity at particle position at \(t\) as

\[
u^\alpha(t) = \sum_{\beta=R,\zeta,Z} \nu^\beta(t-1/2) \epsilon_{\beta \alpha}(t-1/2) \cdot \nabla \alpha(t) + \frac{q_c}{m} \frac{\Delta t}{2} \vec{E}(t) \cdot \nabla \alpha(t), \tag{28}
\]

where \(\alpha = R, \zeta, Z\). For an orthogonal cylindrical system the above Eq. (28) can be rewritten as follows:

\[
u^R(t) = A_1 v^R(t-1/2) + B_1 R(t-1/2) + \frac{q_c}{m} \frac{\Delta t}{2} \vec{E}(t) \cdot \nabla R(t),
\]

\[
u^\zeta(t) = R(2) \left[ A_1 R(1) v^\zeta(t-1/2) - B_1 \frac{\Delta t}{g(\zeta)} \right] v^R(t-1/2) + \frac{q_c}{m} \frac{\Delta t}{2} \vec{E}(t) \cdot \nabla \zeta(t),
\]

\[
u^Z(t) = v^Z(t-1/2) + \frac{q_c}{m} \frac{\Delta t}{2} \vec{E}(t) \cdot \nabla Z(t), \tag{29}
\]

where \(A_1 = \cos(\zeta_2 - \zeta_1), B_1 = \cos(\zeta_1 \sin(\zeta_2 - \sin(\zeta_1 \cos \zeta_2), \zeta_1 = \zeta(t-1/2), \zeta_2 = \zeta(t), R(1) = R(t-1/2)\) and \(R(2) = R(t)\).

In the second step we consider the rotation of the velocity at time \(t\). Rotated vector can be written as

\[
\vec{\nu}^+(t) = \vec{\nu}^-(t) + \vec{s}(t),
\]

\[
\vec{s}(t) = \left[ \vec{\nu}^-(t) \times \vec{T}(t) \right] \times \vec{s}(t), \tag{30}
\]
FIG. 3. GTC computational grids on a poloidal plane coupling core and SOL. Field aligned mesh at the core, separatrix, SOL, and private regions are represented by red, black, magenta, and green, respectively. Fully kinetic (blue and green) and guiding center (magenta and yellow) calculations of trapped particle orbits in the core (51.66keV) and cross separatrix (59.42keV) for DIII-D shot #158103 at 3050 ms. Limiter points are represented by dark brown line.
where \(\vec{T} = (q_c \vec{B} / m)(\Delta t / 2)\) and \(\vec{s} = 2\vec{T} / (1 + T^2)\). The components of rotated vector become

\[
\begin{align*}
\vec{u}^{R+}(t) &= \left[1 - PQ\left(B_R^2 + B_Z^2\right)\right] \vec{u}^{R-}(t) \\
&\quad + \left[PQB_B B_\zeta R + PB_Z \frac{\zeta \zeta}{J}\right] \vec{u}^{-}(t) \\
&\quad + \left[PQB_B B_Z - PB_R \zeta 1 \right] \vec{u}^{-}(t), \\
\end{align*}
\]

(31)

\[
\begin{align*}
\vec{u}^{\zeta+}(t) &= \left[1 - PQ\left(B_R + B_Z\right)\right] \vec{u}^{\zeta-}(t) \\
&\quad + \left[PQB_B B_\zeta R - PB_R \zeta 1 \right] \vec{u}^{-}(t) \\
&\quad + \left[PQB_B B_Z + PB_R \zeta 1 \right] \vec{u}^{-}(t), \\
\end{align*}
\]

(32)

\[
\begin{align*}
\vec{u}^{Z+}(t) &= \left[1 - PQ\left(B_R + B_\zeta\right)\right] \vec{u}^{Z-}(t) \\
&\quad + \left[PQB_B B_\zeta R - PB_Z \zeta 1 \right] \vec{u}^{-}(t) \\
&\quad + \left[PQB_B B_Z + PB_R \zeta 1 \right] \vec{u}^{-}(t), \\
\end{align*}
\]

(33)

where \(Q = (q_c/m)(\Delta t/2), P = 2/(1 + T^2)(q_c/m)(\Delta t/2), g_{\zeta} = R^2,\) and \(J^2 = \det(g_{\zeta\zeta}) = R^2\). In the third step, we add the other half electric acceleration to the rotated vectors to obtain the velocity at time \((t + 1/2)\)

\[
\vec{u}^{\alpha}(t + 1/2) = \vec{u}^{\alpha+}(t) + \frac{q_c}{m} \frac{\Delta t}{2} \mathcal{E}(t) \cdot \nabla \alpha(t). \\
\]

(34)

To update the particle position we need to recover \(\vec{v}(t+1/2),\) which can be done through the following transformation (cf. Fig. 2 of Ref.\textsuperscript{33} dark purple arrow)

\[
\vec{v}(t+1/2) = \sum_{\alpha=R,\zeta,Z} \vec{v}^{\alpha}(t+1/2) \mathcal{E}_\alpha(t) \cdot \nabla \gamma(t+1/2), \\
\]

(35)

where \(\gamma = R, \zeta, Z.\) However, the basis vector \(\nabla \gamma(t + 1/2)\) is still unknown, since \(\gamma(t + 1/2)\) does not exist in standard leap-frog scheme. Here we use a prediction for \(\gamma(t + 1/2)\) as

\[
\gamma(t + 1/2) = \gamma(t) + \gamma(t + 1/2) \Delta t / 2. \\
\]

(36)

After we find the velocity at time \((t+1/2),\) we can update the particle position using the leap-frog scheme as

\[
\gamma(t + 1) = \gamma(t) + \gamma(t + 1/2) \Delta t. \\
\]

(37)

In Eq. (35) we have the dot-product of two basis vectors at different time steps. We have calculated this equation in the similar fashion as discussed in Eqs. (28)-(29).

In this section, we have described the time advancement of the dynamical quantities such as velocity and position of the particle using time centered approach. However, the self-consistent simulation requires update of particle weight (representing perturbed distribution function), guiding center and electric field. In our future simulations, we will use the second order Runge-Kutta (RK) method, to advance these quantities\textsuperscript{33,34}.

### C. Guiding center dynamics

Guiding center particle dynamics is described by the five-dimensional phase space

\[
\left[ \frac{\partial}{\partial t} + \mathbf{\dot{X}} \cdot \nabla + \mathbf{\dot{v}_R} \frac{\partial}{\partial v_R} \right] f_{GC} = 0, \\
\]

(38)

where \(f_{GC}\) is the guiding center distribution function, \(\mathbf{\dot{X}}\) is the guiding center position and \(\mathbf{\dot{v}_R}\) is the parallel velocity. The evolution of the guiding center distribution function can be described by the following equations of guiding center motion\textsuperscript{32}:

\[
\begin{align*}
\mathbf{\dot{X}} &= v_R \mathbf{\hat{b}} + v_\zeta \mathbf{\hat{c}} + v_c + \mathbf{\hat{g}}, \\
\mathbf{\dot{v}_R} &= -\frac{1}{m} \frac{\vec{B}^*}{B} \cdot (\mu \nabla B + q_c \nabla \phi), \\
\end{align*}
\]

(39)

where \(\vec{B}^* = \vec{B} + B_{||}/\omega_c \nabla \times \vec{b},\) and \(\mu = m v_c^2 / 2B.\) The \(\vec{B} \times \vec{B}\) drift velocity \(\vec{v}_B,\) the grad-B drift velocity \(\vec{v}_g,\) and curvature drift velocity \(\vec{v}_c,\) are given by

\[
\begin{align*}
\vec{v}_B &= \mathbf{\hat{c}} \frac{\nabla \phi}{\mathbf{\hat{b}}}, \\
\vec{v}_g &= \frac{\mu}{m \omega_c} \mathbf{\hat{b}} \times \nabla B, \\
\vec{v}_c &= \frac{v_c^2}{\omega_c} \mathbf{\hat{b}} \times \nabla \mathbf{\hat{b}}. \\
\end{align*}
\]

(40)

In GC description following order is adopted:

\[
\frac{\omega_c}{\omega_e} \sim \frac{k_{||}}{k_\perp} \sim \frac{q_c \phi}{T_c} \sim O(\epsilon), \\
\]

where \(\omega_c\) is the frequency of the mode of interest, \(k_{||}\) and \(k_\perp\) are the wave vectors in the parallel and perpendicular direction, respectively. Two constants of motion for guiding center dynamics are defined by:

- **Kinetic Energy**

  \[
  E = (m/2)v_c^2 + \mu B, \\
  \]

- **Toroidal angular momentum**

  \[
  p_\zeta = mRv_c(B_\zeta + q_c \psi). \\
  \]

For an axisymmetric system, Eq. (39) can be rewritten in cylindrical coordinate \((R,\zeta,Z)\) as follows:

\[
\begin{align*}
v_R &= \frac{B_R}{B} + \frac{c}{B} \frac{B_\zeta}{B} \frac{\partial \phi}{\partial Z} - \frac{v_c^2}{\omega_c} \frac{\partial}{\partial Z} \left( \frac{B_\zeta}{B} \right) + \frac{\mu}{m \omega_c} \frac{B_\zeta}{B} \frac{\partial B}{\partial Z}, \\
\end{align*}
\]

(41)
FIG. 4. Time step convergence of fully kinetic Boris integrator. Fig.(a), Fig.(c) represent the relative energy error (in the range of floating point cutoff error) and panel.(b), Fig.(d) show relative canonical angular momentum error for DIII-D geometry core and cross-separatrix region, respectively.

\[
v^c = v^\parallel \frac{B_c}{B} + \frac{c}{BJ} \left[ \frac{B_Z \partial \phi}{B} \frac{\partial}{\partial R} - \frac{B_R \partial \phi}{B} \frac{\partial}{\partial Z} \right] + \frac{v^\parallel}{\omega_c} \left[ \frac{1}{J} \left( \frac{\partial}{\partial Z} \left( \frac{B_R}{B} \right) - \frac{\partial}{\partial R} \left( \frac{B_Z}{B} \right) \right) - \frac{\mu}{m \omega_c J} \left( \frac{B_R \partial B}{B} \frac{\partial}{\partial R} - \frac{B_Z \partial B}{B} \frac{\partial}{\partial Z} \right) \right],
\]

\[
\dot{v}^\parallel = -\frac{\mu}{m} \left( \frac{B_R}{B} \frac{\partial B}{\partial R} + \frac{B_Z}{B} \frac{\partial B}{\partial Z} \right) - \frac{q_c}{m} \left( \frac{B_R}{B} \frac{\partial \phi}{\partial R} + \frac{B_Z}{B} \frac{\partial \phi}{\partial Z} \right) - \frac{\mu v^\parallel}{m \omega_c J} \left[ \frac{1}{J} \left( \frac{\partial}{\partial R} \left( \frac{B_R \partial B}{B} \right) - \frac{\partial}{\partial Z} \left( \frac{B_Z \partial B}{B} \right) \right) - \frac{v^\parallel q_c}{m \omega_c J} \left( \frac{\partial}{\partial R} \left( \frac{B_R \partial \phi}{B} \right) - \frac{\partial}{\partial Z} \left( \frac{B_Z \partial \phi}{B} \right) \right) \right].
\]

For guiding center particle dynamics GTC normally uses second order Runge Kutta (RK) method (cf. Fig.2 of Ref.33).

To test our integration schemes (FK and GC), we consider the collisionless single particle motion of the trapped one in the core and cross-separatrix regions using the initial conditions from Table I and Table II for DIII-D geometry, respectively. The projection of the FK and GC trapped particle orbit on R-Z plane in the core
FIG. 5. Time step convergence of guiding center second order Runge Kutta integrator. Panel (a), Fig. (c) represent the relative energy error and panel (b), Fig. (d) show relative canonical angular momentum error for DIII-D geometry core and cross-separatrix region, respectively.

TABLE I. Initial conditions for FK integrator

| Parameter      | Core  | Cross-Separatrix |
|----------------|-------|------------------|
| $R/R_0$        | 1.154 | 1.289            |
| $Z/R_0$        | 0.0   | 0.0              |
| $\zeta$        | 1.570 | 1.570            |
| $v_R/\omega_c R_0$ | $3.371 \times 10^{-3}$ | $3.371 \times 10^{-3}$ |
| $v_Z/\omega_c R_0$ | $5.371 \times 10^{-3}$ | $5.371 \times 10^{-3}$ |
| $v_\parallel/\omega_c R_0$ | $1.271 \times 10^{-3}$ | $1.271 \times 10^{-3}$ |

$R_0$ is the $R$ at magnetic axis

TABLE II. Initial conditions for GC integrator

| Parameter      | Core  | Cross-Separatrix |
|----------------|-------|------------------|
| $R/R_0$        | 1.147 | 1.281            |
| $Z/R_0$        | 0.0   | 0.0              |
| $\zeta$        | 1.570 | 1.570            |
| $v_\parallel/\omega_c R_0$ | $2.547 \times 10^{-3}$ | $3.017 \times 10^{-3}$ |
| $v_\perp/\omega_c R_0$ | $4.545 \times 10^{-3}$ | $4.642 \times 10^{-3}$ |
| $\sqrt{\mu B_0/\omega_c R_0}$ | $4.545 \times 10^{-3}$ | $4.642 \times 10^{-3}$ |

$B_0$ is the $B$ at magnetic axis

and cross-separatrix regions are shown in Fig. 3. Both integrators correctly capture the trapped particle orbit and agree well with each other. The conservation properties of our integrators are tested with two exact constant of motion, viz., kinetic energy $E$ and toroidal angular momentum $p_\zeta$.

In numerical simulation the dynamical quantities accumulate error with time. In our integrators the magnitude of the velocity provides better accuracy than the individual components of velocity. As a result the energy conservation is better than the toroidal angular momentum. The toroidal angular momentum is conserved due to the symmetry of the magnetic field along the toroidal direc-
tion. Fig. 4 shows the relative variation of E and \( p_k \) for FK Boris integrator over a time of 15000 cyclotron period for different time step sizes in core and cross-separatrix regions. Boris algorithm maintains adequate accuracy with 20 time steps per cyclotron period (\( \omega_b \Delta t = 0.292 \)). The relative energy error arises mostly due to floating point cutoff (floating precision). Whereas, the GC second order RK demonstrate that E and \( p_k \) can converge with 240 time steps per bounce period (\( \omega_b \Delta t = 0.027 \)) in core and cross-separatrix regions, where \( \omega_b \) is the bounce frequency of the particle [cf. Fig. (5)]. From these convergence studies, it is found that the FK Boris integrator provides better energy convergence than the second order Runge Kutta GC integrator. If there are high frequency electromagnetic perturbations, the condition of \( v_{per} \Delta t < 1 \) will set an upper bound for the time step size. In the present simulations, the particles orbit are studied without electric and perturbed magnetic field. However, previously Wei et al.\(^{31} \) have demonstrated the effect of electric field on trapped particle orbit (Ware pinch) in the core region of tokamak using Boozer coordinates.

V. ION ORBIT LOSS NEAR PLASMA EDGE

In a tokamak plasma, ions have drift motions due to the gradient-B and curvature drift. As a result, ion orbits are shifted from a magnetic surface. Due to this shift of ion orbit from magnetic surface, the hot ions that exist close to the separatrix, can pass near the X point region. In this region, the poloidal magnetic field is very weak and the ions have a very small poloidal displacement in time. These ions experience vertical curvature and gradient-B drifts and move towards the divertor, resulting in ion orbit loss\(^{4,44,45} \). In an axisymmetric configuration, the drift orbit of ion is obtained by solving the following three equations as described in Sec 4.3. These are the conservation of kinetic energy, magnetic moment and canonical angular momentum.

\[
\frac{1}{2} m (v_{\perp}^2 + v_{\parallel}^2) + q_e \phi = \text{constant} = \frac{1}{2} m (v_{\perp a}^2 + v_{\parallel a}^2) + q_e \phi a, \\
\frac{m v_{\parallel a}^2}{2B} = \text{constant} = \frac{m v_{\perp a}^2}{2B a},
\]

\[
mR v_{\parallel a} (B_c/B) + q_e \psi = \text{constant} = mR_a v_{\parallel a} (B_{\perp a}/B_a) + q_e \psi a. \tag{47}
\]

The subscript ‘a’ means the value at the starting point of the ions. The conservation of above quantities with \( B_c \approx B \) gives the drift orbit surface as follows\(^{44} \):

\[
\frac{q_e \psi}{m v_a} + \frac{R v_{\parallel a}}{v_a} = \frac{q_e \psi a}{m v_a} + R_a v_{\parallel a}/v_a, \tag{48}
\]

\[
\frac{v_{\parallel}}{v_a} = \pm \left[ 1 - (1 - \xi_0^2) \frac{R_a}{R} + \frac{q_e}{m v_a^2} (\phi_a - \phi) \right]^{1/2}, \tag{49}
\]

where \( \xi_0 = (v_{\parallel}/v_a) \) is the initial pitch angle. In the above equation, we assume that \( B_c > 0 \), and use the approximation \( B_c \propto (1/R) \). A minus sign must be used instead of a plus sign in Eq. (47) when \( B_c < 0 \). We also consider that the poloidal magnetic field is directed clockwise and the ion toroidal drift (\( \tilde{v}_j \)) is away from the X point. The coordinates of the X point are \( (R_X, Z_X) \) and the poloidal magnetic flux function of X point satisfies \( (\partial \psi / \partial R)_{X} = 0 \) and \( (\partial \psi / \partial Z)_{X} = 0 \). When the initial position \( R_a \) of a test ion is at the outer midplane, that is \( R_a > R_X \) there are following two cases for orbit ion loss\(^{44} \):

- **Case-I**: Trapped ion loss (\( v_{\parallel} \) changes its sign before escape). The necessary conditions for escape are
  1. \( \xi_0 < 0, \quad v_{\parallel} > 0 \),
  2. \( 1 - (1 - \xi_0^2) (R_a/R_{in}) - (\xi_0/\alpha_{cr}) \tilde{\phi}/V_a \leq 0 \),
  3. \( 1 - (1 - \xi_0^2) (R_a/R_{XD}) + \tilde{\phi}/V_a^2 \geq 0 \),
  4. \( (q_e/mv_a R_a) (\psi_a - \psi_{XD}) < -\xi_0 + (R_{XD}/R_a) V_X \)

where \( R_{in} \) is the radial coordinate of the innermost point along the separatrix, \( X_D(R_{XD}, Z_{XD}) \) is the null point of the separatrix for the drift surface, and

\[
\tilde{\phi} = \frac{q_e (\phi_a - \phi_{XD})}{m \omega_c^2 R_{in}^2/2}, \quad V_X = \left[ 1 - (1 - \xi_0^2) \frac{R_a}{R_{XD}} + \frac{\tilde{\phi}}{V_a^2} \right]^{1/2},
\]

(50)

This case is represented in Fig. 6(a). In this case a test ion starting from the outer midplane initial position (green square) \( (R_a > R_X) \) with initial pitch angle \( \xi_0 = -0.623 \) is reflected at M, changes the sign of \( v_{\parallel} \) and escapes near the \( X_D \) point to the outside divertor plate. Case-I(2) is the condition for the mirror reflection of test ion at \( R > R_{in} \) and Case-I(3) is the condition for that ion to escape through the region near \( X_D \) point to the outer divertor plate.

- **Case-II**: Passing ion loss (\( v_{\parallel} \) does not change its sign before escape). The necessary conditions for escape are
  1. \( \xi_0 < 0, \quad v_{\parallel} < 0 \),
  2. \( 1 - (1 - \xi_0^2) (R_a/R_{in}) - (\xi_0/\alpha_{cr}) \tilde{\phi}/V_a \geq 0 \),
  3. \( (q_e/mv_a R_a) (\psi_a - \psi_{XD}) < -\xi_0 - (R_{XD}/R_a) V_X \)

This case is shown in Fig. 6(b). In this case a test ion starting from the outer midplane initial position (green square) \( (R_a > R_X) \) with initial pitch angle \( \xi_0 = -0.752 \) escapes without mirror reflection near the \( X_D \) point to the inside divertor plate as described by the condition Case-II(2).
FIG. 6. Ion drift orbits (solid red line) of DIII-D with a single null divertor. The ion toroidal grad-B drift is away from the X point ($B_\zeta > 0$). Initial position of the test ion is represented by green square. (a) An ion starting from the outer midplane ($R_a > R_X$) is reflected at M, changes the sign of $v_\parallel$ and escapes near the X point to the outside divertor plate [case-I]. (b) An ion starting from the outer midplane escapes without mirror reflection to the inside divertor plate [case-II]. (c) An ion starting from the inner midplane ($R_a < R_X$) escapes near the X point to the outside divertor plate [case-III]. Last close surface and limiter points are represented by dotted dark brown and magenta line, respectively.

| TABLE III. Parameters for ion orbit loss region |
|-----------------------------------------------|
| Parameter | Case-I | Case-II |
|-----------|--------|--------|
| $(R_a/R_0, Z_a/R_0)$ | (1.2748, 0.0) | (1.2748, 0.0) |
| $(R_{in}/R_0, Z_{in}/R_0)$ | (0.6134, 0.0) | (0.6134, 0.0) |
| $(R_{XD}/R_0, Z_{XD}/R_0)$ | (0.8442, -0.6680) | (0.6253, -0.6680) |
| $(\psi_{XD}/B_0 R_0^2, \psi_a/B_0 R_0^2)$ | $(5.253 \times 10^{-2}, 4.688 \times 10^{-2})$ | $(5.138 \times 10^{-2}, 4.688 \times 10^{-2})$ |

When $\xi_0 > 0$ and $R_a > R_X$, the relative position of magnetic surface and drift orbit surface [cf. Eq. (48)], clearly indicates that direct ion orbit loss is not possible. However, when the initial position of the test ion is selected as $R_a < R_X$ the following Case-III is possible for ion orbit loss.

- Case-III: Passing ion loss. The necessary conditions for escape are
  1. $\xi_0 > 0$, $v_\parallel > 0$,
  2. $1 - (1 - \xi_0^2)(R_a/R_{in}) - (\xi_0/\alpha_{cr}) \tilde{\phi}/V_a \geq 0$,
  3. $(q_e/m v_a R_a)(\psi_a - \psi_{XD}) < -\xi_0 + (R_{XD}/R_a) V_X$

This case is described in Fig. 6(c). In this case a test ion starting from the inner midplane initial position (green square) ($R_a < R_X$) with initial pitch angle $\xi_0 = 0.872$ escapes without mirror reflection near the X point to the outside divertor plate.

In the above GTC simulations (cf. Fig. 6) we did not include the radial electric field on ion orbit loss. However, one must mention here that in a tokamak scenario the radial electric field shifts the velocity space boundaries separating trapped and passing orbits. Also the ion orbit loss contributes to the generation of radial electric field, which affects the ion orbit loss. Therefore, the ion orbit loss and the radial electric field should be considered self-consistently for more accurate calculation. Similarly, it is important to study the effect of ion orbit loss and X point loss for understanding the plasma transport, particle distribution, plasma rotation, etc. Simulation related to these effects will be reported in a future work. To see how the electric field affects the velocity space boundaries, we have calculated the minimum velocity of...
FIG. 7. Ion orbit loss region for DIII-D$^{46}$ in the initial velocity space for the same parameters of Fig.6. (a) The minimum energy for which the orbits of ions launched from $R_a > R_X$ will be lost. (b) Pitch angle dependent ion orbit loss fraction for $T_i=40$ keV. Parts AB (A'B'), BC (B'C') and CD (C'D') of the curve ABCD (A'B'C'D') correspond to the conditions Case-II, Case-I(ii) and Case-I(iii) without $\phi$ (with $\tilde{\phi}$), respectively. (c) Cumulative ion orbit loss fraction as a function of ion energy ($T_i$).
the ion and particle loss fractions for DIII-D in the following paragraph.

In order to find the minimum initial ion speed $v_0$ that is required for the ion to reach the final location (near X point) we combine Eq. (48) and Eq. (49). The minimum loss speed of ion is

$$v_0 = \left[ \frac{R_a^2 \xi_0^2}{R_{XD}^2} - \frac{R_{X}^2}{R_{XD}} \left\{ 1 - (1 - \frac{\xi_0^2}{R_{XD}^2}) \frac{R_a}{R_{XD}} \right\} \right]^{-1} \times \frac{\Psi R_a \xi_0}{\sqrt{\Phi^2 R_a^2 \xi_0^2 - \left[ \Phi^2 - R_{XD}^2 \phi \right] \left\{ R_a^2 \xi_0^2 - R_{XD}^2 \left\{ 1 - (1 - \frac{\xi_0^2}{R_{XD}^2}) \frac{R_a}{R_{XD}} \right\} \right\}}$$

where $\Psi = (q_e/m)(\psi_a - \psi_{XD})$. For passing ion orbit loss the sign of the second term of the numerator in Eq. (51) is positive and for the trapped ion orbit loss it is negative, respectively. We solve Eq. (51) to find the ion orbit loss region for DIII-D model parameters as described in Table III. Here, we examine the loss of ion for which $-1 \leq \xi_0 \leq 0$. The loss region in the initial velocity space of an ion starting from outer midplane point $R_a$ is described by the solid curves in Fig. 7(a). Case-I and Case-II represent boundary curves CD (C′D′) and AB (A′B′) of the loss region without $\phi$ (with $\phi$), respectively. Boundary curves BC (B′C′) i.e the condition for mirror reflection of the test ion without $\phi$ (with $\phi$) is given by Case-I(ii), where $\phi > 0$ and $\phi < 0$ correspond to the outward and inward radial electric field, respectively. The value of minimum energy ($mv_0^2/2$) is obtained from Eq. (51) [cf. Fig. 7(a)] without $\phi$ demonstrate good agreements with the simulation results of Fig. 6(a) and Fig. 6(b).

After the minimum loss energy is determined, particle loss fraction due to direct ion orbit loss is calculated. The ion loss rate is determined by the rate of supply of ions to the loss regions. The corresponding cumulative particle loss fraction of ions, which follow distribution function $g$ in velocity space is defined as:

$$f_L = \int_{-1}^{1} \int_{v_0}^{\infty} \frac{v^2 g(v) dv}{\sqrt{\Psi^2 R_a^2 \xi_0^2 - \left[ \Psi^2 - R_{XD}^2 \phi \right] \left\{ R_a^2 \xi_0^2 - R_{XD}^2 \left\{ 1 - (1 - \frac{\xi_0^2}{R_{XD}^2}) \frac{R_a}{R_{XD}} \right\} \right\}}} d\xi_0$$

For a Maxwellian distribution function the above equation turns out to be, $f_L = f_L^{T_i} \Gamma(3/2, \epsilon_{min}(\xi_0)) d\xi_0/2 \Gamma(3/2)$, where $\epsilon_{min}(\xi_0) = mv_0^2(\xi_0)/2T_i$ is the energy corresponding to the minimum velocity for which ion orbit loss is possible [cf. Eq. (51)], $T_i$ is the ion temperature, and $\Gamma(3/2, \epsilon_{min}(\xi_0))$ is the upper incomplete gamma function of order 3/2. The $\xi_0$ dependent cumulative particle loss fraction $f_L$ starting from $R_a > R_X$ without $\phi$ (ABCD) and with $\phi$ (A′B′C′D′) are shown in Fig. 7(b). These results clearly demonstrate that radial electric field shifts the velocity space boundaries of loss regions for trapped and passing particles. Fig. 7(c) represents the cumulative ion loss fraction for different ion energy ($T_i$).

VI. SUMMARY AND CONCLUSIONS

As a first step in developing the self-consistent global simulation model to couple SOL and core region by incorporating the separatrix, we have developed the particle dynamics for FK and GC particles using cylindrical coordinates. To get the maximum numerical efficiency, field aligned mesh in the cylindrical coordinates is developed for the whole device from magnetic axis to the material wall (plasma facing components). This field aligned mesh in cylindrical coordinates helps to avoid the difficulty associated with the X point on the poloidal plane without nonsingular metric. Finally, we have extended this particle orbit simulation techniques to study the ion orbit loss near the X-point of DIII-D single null divertor. Based on three constants of motion, the minimum loss speed and ion orbit loss fraction at the edge of the tokamak are calculated. However, these particles need proper boundary conditions near the divertor wall. Presently GTC does not have the capability of handling the plasma particle loss to the material wall (plasma facing components), recycling the neutral particles, and calculating the Monte-Carlo neutral particle transport with a charge exchange and ionization interaction with the plasma.

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